



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 05:43 PM BST

PDB ID : 4CTG  
EMDB ID: : EMD-2390  
Title : The limits of structural plasticity in a picornavirus capsid revealed by a massively expanded equine rhinitis A virus particle  
Authors : Bakker, S.E.; Groppelli, E.; Pearson, A.R.; Stockley, P.G.; Rowlands, D.J.; Ranson, N.A.  
Deposited on : 2014-05-21  
Resolution : 17.00 Å(reported)  
Based on PDB ID : 2WFF

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

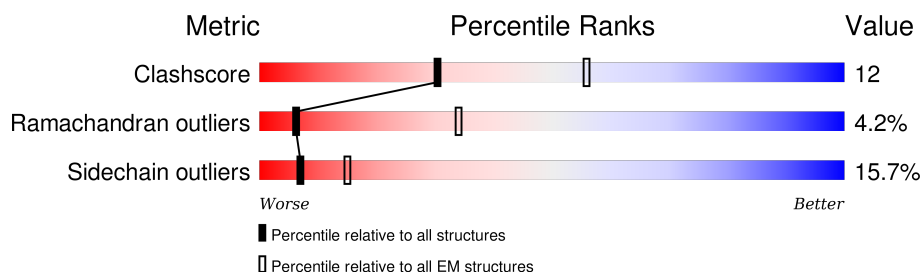
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 17.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
















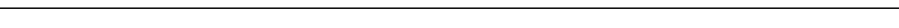











| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 114402                      | 924                         |
| Ramachandran outliers | 111179                      | 726                         |
| Sidechain outliers    | 111093                      | 686                         |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A0    | 246    |                  |
| 1   | A1    | 246    |                  |
| 1   | A2    | 246    |                  |
| 1   | A3    | 246    |                  |
| 1   | A4    | 246    |                  |
| 1   | A5    | 246    |                  |
| 1   | A6    | 246    |                  |
| 1   | A7    | 246    |                  |
| 1   | A8    | 246    |                  |


























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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | A9    | 246    |  60% 28% 10% •   |
| 1   | AA    | 246    |  61% 27% 10% •   |
| 1   | AB    | 246    |  61% 27% 10% •   |
| 1   | AC    | 246    |  61% 27% 10% •   |
| 1   | AD    | 246    |  60% 28% 10% •   |
| 1   | AE    | 246    |  60% 28% 10% •   |
| 1   | AF    | 246    |  60% 28% 10% •   |
| 1   | AG    | 246    |  60% 28% 9% •    |
| 1   | AH    | 246    |  60% 28% 10% •   |
| 1   | AI    | 246    |  61% 27% 10% •   |
| 1   | AJ    | 246    |  60% 28% 9% •    |
| 1   | AK    | 246    |  60% 28% 10% •   |
| 1   | AL    | 246    |  59% 28% 10% • |
| 1   | AM    | 246    |  61% 27% 10% • |
| 1   | AN    | 246    |  60% 28% 10% • |
| 1   | AO    | 246    |  60% 28% 10% • |
| 1   | AP    | 246    |  60% 28% 10% • |
| 1   | AQ    | 246    |  61% 28% 9% •  |
| 1   | AR    | 246    |  60% 28% 10% • |
| 1   | AS    | 246    |  61% 28% 9% •  |
| 1   | AT    | 246    |  61% 27% 10% • |
| 1   | AU    | 246    |  61% 27% 10% • |
| 1   | AV    | 246    |  61% 28% 9% •  |
| 1   | AW    | 246    |  60% 28% 10% • |
| 1   | AX    | 246    |  60% 28% 10% • |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | AY    | 246    |  60% 28% 10% •   |
| 1   | AZ    | 246    |  61% 27% 10% •   |
| 1   | Aa    | 246    |  82% 15% •       |
| 1   | Ab    | 246    |  82% 15% •       |
| 1   | Ac    | 246    |  82% 15% ••      |
| 1   | Ad    | 246    |  82% 15% •       |
| 1   | Ae    | 246    |  81% 15% •       |
| 1   | Af    | 246    |  82% 15% •       |
| 1   | Ag    | 246    |  82% 15% •       |
| 1   | Ah    | 246    |  82% 15% ••      |
| 1   | Ai    | 246    |  82% 15% ••      |
| 1   | Aj    | 246    |  82% 15% •       |
| 1   | Ak    | 246    |  82% 15% •     |
| 1   | Al    | 246    |  82% 15% •     |
| 1   | Am    | 246    |  82% 15% •     |
| 1   | An    | 246    |  82% 15% •     |
| 1   | Ao    | 246    |  82% 15% •     |
| 1   | DC    | 246    |  61% 27% 10% • |
| 1   | DD    | 246    |  61% 27% 10% • |
| 1   | DE    | 246    |  61% 27% 9% •  |
| 1   | DF    | 246    |  61% 28% 9% •  |
| 1   | DG    | 246    |  60% 28% 10% • |
| 1   | DH    | 246    |  60% 28% 10% • |
| 1   | DI    | 246    |  61% 27% 10% • |
| 1   | DJ    | 246    |  61% 28% 9% •  |

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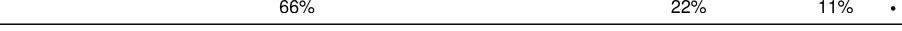







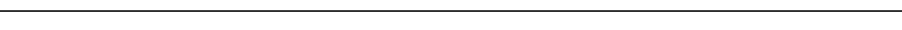

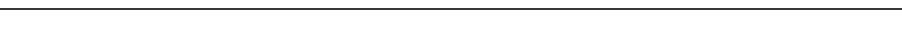
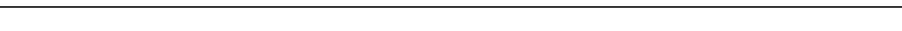




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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | DK    | 246    |  60% 28% 10% .   |
| 2   | B0    | 200    |  66% 23% 11% .   |
| 2   | B1    | 200    |  66% 22% 11% .   |
| 2   | B2    | 200    |  66% 22% 11% .   |
| 2   | B3    | 200    |  65% 23% 11% .   |
| 2   | B4    | 200    |  64% 23% 12% .   |
| 2   | B5    | 200    |  67% 21% 11% .   |
| 2   | B6    | 200    |  66% 21% 12% .   |
| 2   | B7    | 200    |  67% 21% 11% .   |
| 2   | B8    | 200    |  65% 23% 11% .   |
| 2   | B9    | 200    |  67% 22% 11% .   |
| 2   | BA    | 200    |  65% 23% 11% .   |
| 2   | BB    | 200    |  66% 22% 12% . |
| 2   | BC    | 200    |  66% 22% 11% . |
| 2   | BD    | 200    |  66% 21% 12% . |
| 2   | BE    | 200    |  65% 23% 12% . |
| 2   | BF    | 200    |  65% 22% 12% . |
| 2   | BG    | 200    |  65% 23% 11% . |
| 2   | BH    | 200    |  65% 23% 11% . |
| 2   | BI    | 200    |  65% 22% 12% . |
| 2   | BJ    | 200    |  67% 21% 12% . |
| 2   | BK    | 200    |  66% 22% 11% . |
| 2   | BL    | 200    |  66% 23% 11% . |
| 2   | BM    | 200    |  66% 22% 11% . |
| 2   | BN    | 200    |  65% 23% 12% . |














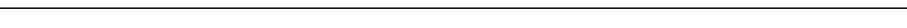











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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 2   | BO    | 200    |  64% 24% 11% .  |
| 2   | BP    | 200    |  66% 22% 11% .  |
| 2   | BQ    | 200    |  66% 22% 12% .  |
| 2   | BR    | 200    |  65% 23% 11% .  |
| 2   | BS    | 200    |  66% 22% 11% .  |
| 2   | BT    | 200    |  66% 21% 12% .  |
| 2   | BU    | 200    |  66% 22% 11% .  |
| 2   | BV    | 200    |  66% 22% 11% .  |
| 2   | BW    | 200    |  66% 23% 11% .  |
| 2   | BX    | 200    |  66% 22% 11% .  |
| 2   | BY    | 200    |  67% 21% 11% .  |
| 2   | BZ    | 200    |  66% 22% 11% . |
| 2   | Ba    | 200    |  81% 17% ..   |
| 2   | Bb    | 200    |  81% 17% ..   |
| 2   | Bc    | 200    |  81% 17% ..   |
| 2   | Bd    | 200    |  81% 17% ..   |
| 2   | Be    | 200    |  81% 17% ..   |
| 2   | Bf    | 200    |  81% 17% ..   |
| 2   | Bg    | 200    |  81% 17% ..   |
| 2   | Bh    | 200    |  81% 17% ..   |
| 2   | Bi    | 200    |  81% 17% ..   |
| 2   | Bj    | 200    |  81% 17% ..   |
| 2   | Bk    | 200    |  81% 17% ..   |
| 2   | Bl    | 200    |  81% 17% ..   |
| 2   | Bm    | 200    |  81% 17% ..   |














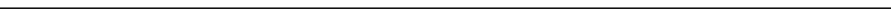











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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 2   | Bn    | 200    |  81% 17% ..     |
| 2   | Bo    | 200    |  81% 17% ..     |
| 2   | Bp    | 200    |  81% 17% ..     |
| 2   | Bq    | 200    |  81% 17% ..     |
| 2   | Br    | 200    |  81% 17% ..     |
| 2   | Bs    | 200    |  81% 17% ..     |
| 2   | Bt    | 200    |  81% 17% ..     |
| 2   | Bu    | 200    |  81% 17% ..     |
| 2   | Bv    | 200    |  81% 17% ..     |
| 2   | Bw    | 200    |  81% 17% ..     |
| 2   | Bx    | 200    |  81% 17% ..     |
| 3   | C0    | 226    |  64% 26% 9% .   |
| 3   | C1    | 226    |  62% 28% 8% . |
| 3   | C2    | 226    |  62% 28% 9% . |
| 3   | C3    | 226    |  64% 26% 9% . |
| 3   | C4    | 226    |  62% 28% 8% . |
| 3   | C5    | 226    |  62% 28% 9% . |
| 3   | C6    | 226    |  63% 27% 9% . |
| 3   | C7    | 226    |  63% 27% 9% . |
| 3   | C8    | 226    |  62% 28% 9% . |
| 3   | C9    | 226    |  62% 28% 8% . |
| 3   | CA    | 226    |  62% 28% 8% . |
| 3   | CB    | 226    |  62% 27% 9% . |
| 3   | CC    | 226    |  62% 28% 9% . |
| 3   | CD    | 226    |  62% 28% 9% . |













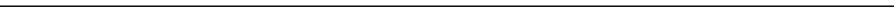
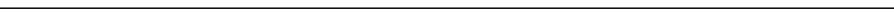







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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 3   | CE    | 226    |  62% 27% 9% .   |
| 3   | CF    | 226    |  62% 28% 8% .   |
| 3   | CG    | 226    |  62% 29% 8% .   |
| 3   | CH    | 226    |  62% 28% 8% .   |
| 3   | CI    | 226    |  62% 27% 9% .   |
| 3   | CJ    | 226    |  62% 28% 8% .   |
| 3   | CK    | 226    |  62% 27% 9% .   |
| 3   | CL    | 226    |  62% 27% 9% .   |
| 3   | CM    | 226    |  62% 27% 9% .   |
| 3   | CN    | 226    |  62% 28% 8% .   |
| 3   | CO    | 226    |  62% 28% 8% .   |
| 3   | CP    | 226    |  62% 28% 9% .  |
| 3   | CQ    | 226    |  62% 28% 9% . |
| 3   | CR    | 226    |  62% 28% 8% . |
| 3   | CS    | 226    |  62% 27% 9% . |
| 3   | CT    | 226    |  62% 28% 9% . |
| 3   | CU    | 226    |  62% 28% 8% . |
| 3   | CV    | 226    |  62% 28% 9% . |
| 3   | CW    | 226    |  62% 27% 9% . |
| 3   | CX    | 226    |  62% 27% 9% . |
| 3   | CY    | 226    |  62% 28% 9% . |
| 3   | CZ    | 226    |  64% 27% 9% . |
| 3   | Cc    | 226    |  80% 16% .    |
| 3   | Cd    | 226    |  80% 16% .    |
| 3   | Ce    | 226    |  80% 16% .    |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 3   | Cf    | 226    |  80% 16% .      |
| 3   | Cg    | 226    |  80% 16% .      |
| 3   | Ch    | 226    |  80% 16% .      |
| 3   | Ci    | 226    |  80% 16% .      |
| 3   | Cj    | 226    |  80% 16% .      |
| 3   | Ck    | 226    |  80% 16% .      |
| 3   | Cl    | 226    |  80% 16% .      |
| 3   | Cm    | 226    |  80% 16% .      |
| 3   | Cn    | 226    |  80% 16% .      |
| 3   | Co    | 226    |  80% 16% .      |
| 3   | Cp    | 226    |  80% 16% .      |
| 3   | Cq    | 226    |  80% 16% .      |
| 3   | Cr    | 226    |  80% 16% .    |
| 3   | Cs    | 226    |  80% 16% .    |
| 3   | Ct    | 226    |  80% 16% .    |
| 3   | Cu    | 226    |  80% 16% .    |
| 3   | Cv    | 226    |  80% 16% .    |
| 3   | Cw    | 226    |  80% 16% .    |
| 3   | Cx    | 226    |  80% 16% .    |
| 3   | DA    | 226    |  63% 27% 8% . |
| 3   | DB    | 226    |  62% 28% 9% . |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 311940 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called P1.

| Mol | Chain | Residues | Atoms         |           |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 1   | AA    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | AB    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | AC    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | AD    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | AE    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | AF    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | AG    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | AH    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | AI    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | AJ    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | AK    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | AL    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | AM    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | AN    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | AO    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | AP    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | AQ    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 1   | AR    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | AS    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | AT    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | AU    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | AV    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | AW    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | AX    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | AY    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | AZ    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | A0    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | A1    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | A2    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | A3    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | A4    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | A5    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | A6    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | A7    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | A8    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | A9    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | Aa    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | Ab    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |

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| Mol | Chain | Residues | Atoms         |           |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 1   | Ac    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | Ad    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | Ae    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | Af    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | Ag    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | Ah    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | Ai    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | Aj    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | Ak    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | Al    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | Am    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | An    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | Ao    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | DC    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | DD    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | DE    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | DF    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | DG    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | DH    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | DI    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |
| 1   | DJ    | 246      | Total<br>1928 | C<br>1240 | N<br>329 | O<br>351 | S<br>8 | 0       | 0     |

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| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | DK    | 246      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1928  | 1240 | 329 | 351 | 8 |         |       |

- Molecule 2 is a protein called P1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | BA    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | BB    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | BC    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | BD    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | BE    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | BF    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | BG    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | BH    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | BI    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | BJ    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | BK    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | BL    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | BM    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | BN    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | BR    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | BO    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | BS    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | BP    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | BQ    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | BT    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | BU    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | BV    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | BW    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | BX    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | BY    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | BZ    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | B0    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | B1    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | B2    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | B3    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | B4    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | B5    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | B6    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | B7    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | B8    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | B9    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | Ba    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | Bb    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | Bc    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | Bd    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | Be    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | Bf    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | Bg    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | Bh    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | Bi    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | Bj    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | Bk    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | Bl    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | Bm    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | Bn    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | Bo    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | Bp    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | Bq    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | Br    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | Bs    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | Bt    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | Bu    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | Bv    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | Bw    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |
| 2   | Bx    | 200      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1553  | 997 | 266 | 283 | 7 |         |       |

There are 60 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| B0    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| B1    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| B2    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| B3    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| B4    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| B5    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| B6    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| B7    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| B8    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| B9    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| BA    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| BB    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| BC    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| BD    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| BE    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| BF    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| BG    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| BH    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| BI    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| BJ    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| BK    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| BL    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| BM    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| BN    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| BO    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| BP    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| BQ    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| BR    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| BS    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| BT    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| BU    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| BV    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| BW    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| BX    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| BY    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| BZ    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| Ba    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| Bb    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| Bc    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| Bd    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| Be    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| Bf    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| Bg    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| Bh    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| Bi    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| Bj    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| Bk    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| Bl    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| Bm    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| Bn    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| Bo    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| Bp    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| Bq    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| Br    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| Bs    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| Bt    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| Bu    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| Bv    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| Bw    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |
| Bx    | 85      | SER      | GLY    | CONFLICT | UNP Q91B42 |

- Molecule 3 is a protein called P1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | CA    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | CB    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | CC    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | CD    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | CE    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | CF    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | CG    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | CH    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | CI    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | CJ    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | CK    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | CL    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | CM    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | CN    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | CO    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | CP    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | CQ    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | CR    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | CS    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | CT    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | CU    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | CV    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | CW    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | CX    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | CY    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | CZ    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | C0    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | C1    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | C2    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | C3    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | C4    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | C5    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | C6    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | C7    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | C8    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | C9    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | Cc    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | Cd    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | Ce    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | Cf    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | Cg    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | Ch    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | Ci    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | Cj    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | Ck    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | Cl    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | Cm    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | Cn    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | Co    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | Cp    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | Cq    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | Cr    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |

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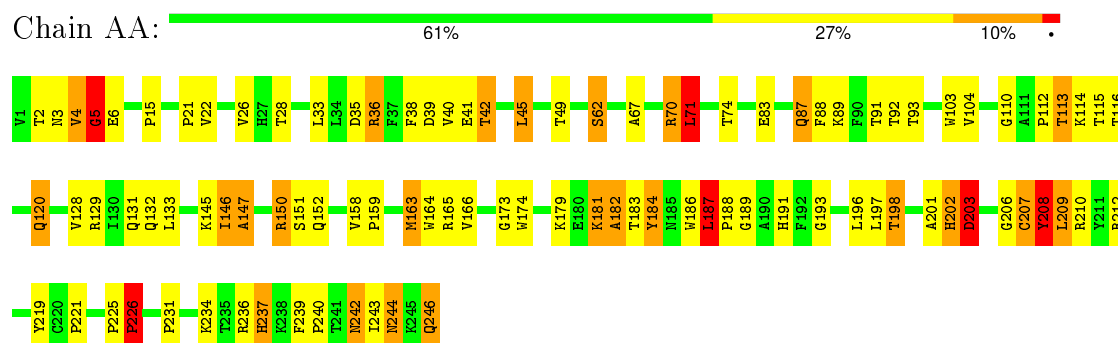
| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | Cs    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | Ct    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | Cu    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | Cv    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | Cw    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | Cx    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | DA    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |
| 3   | DB    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1718  | 1107 | 280 | 325 | 6 |         |       |



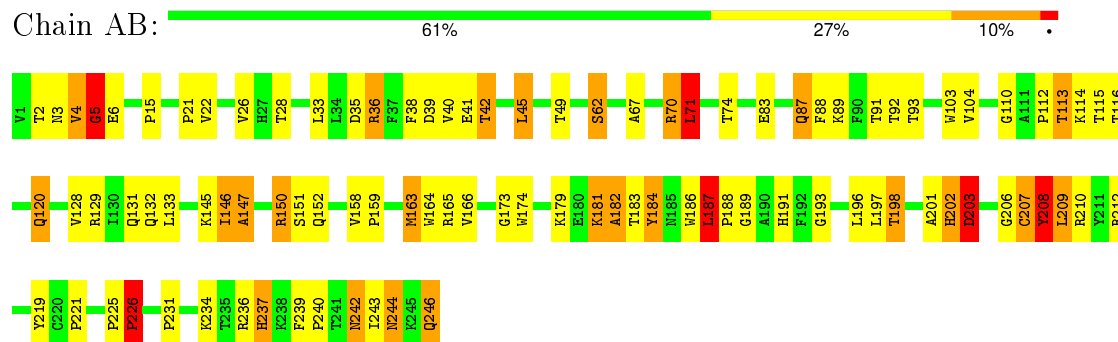
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

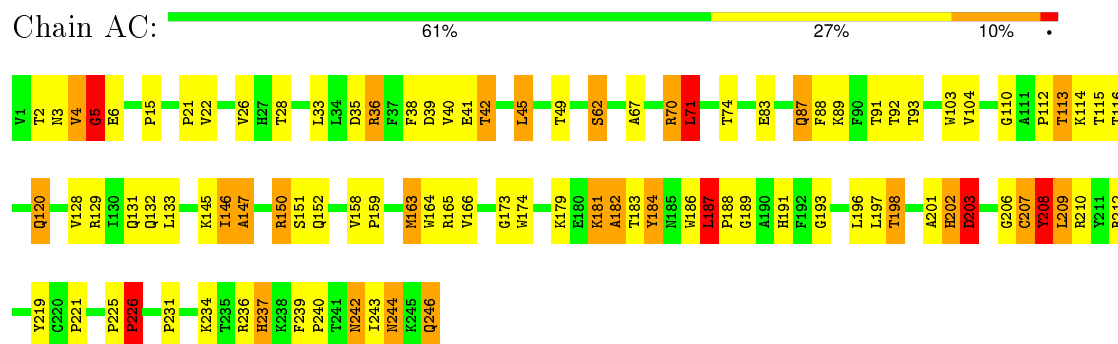
- Molecule 1: P1



- Molecule 1: P1



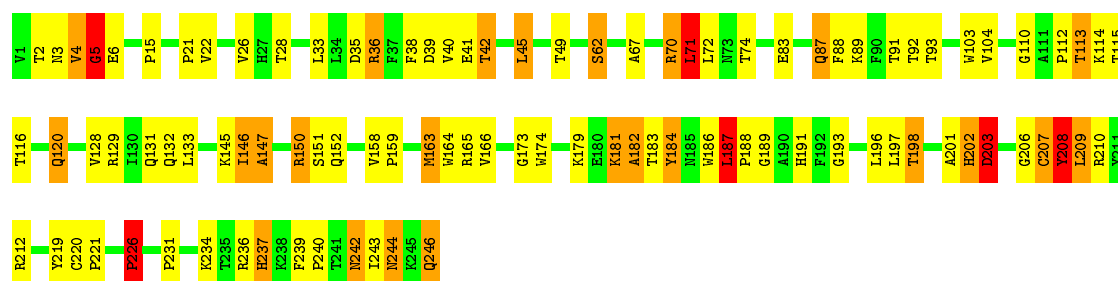
- Molecule 1: P1



- Molecule 1: P1

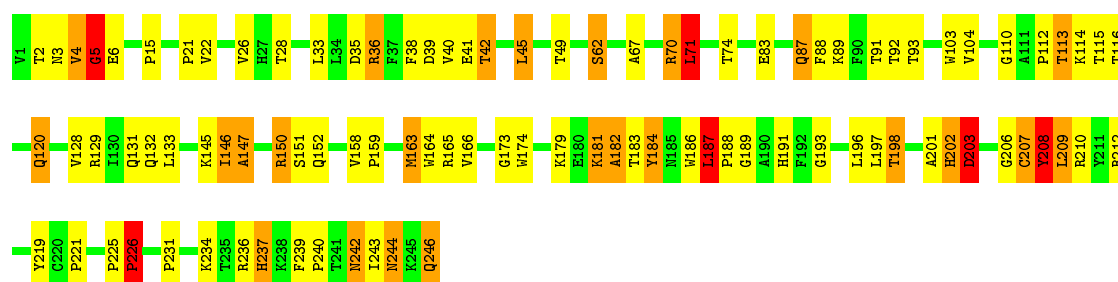


Chain AH: 



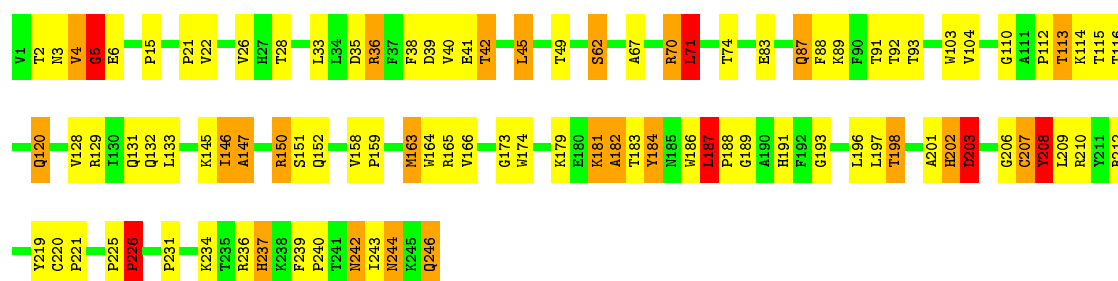
- Molecule 1: P1

Chain AI:  61% 27% 10% 2%



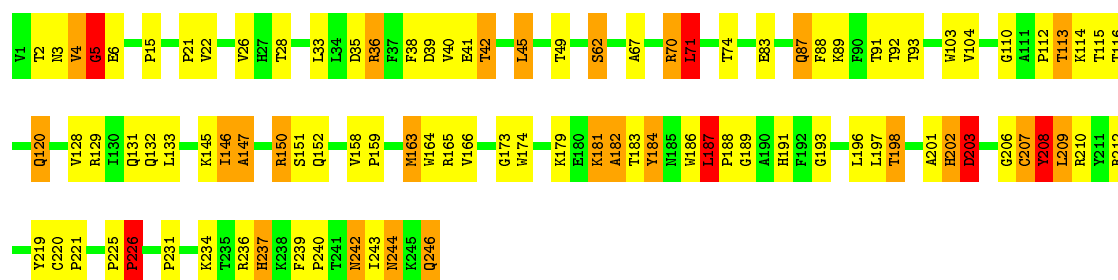
- Molecule 1: P1

Chain AJ:  60% 28% 9% 3%



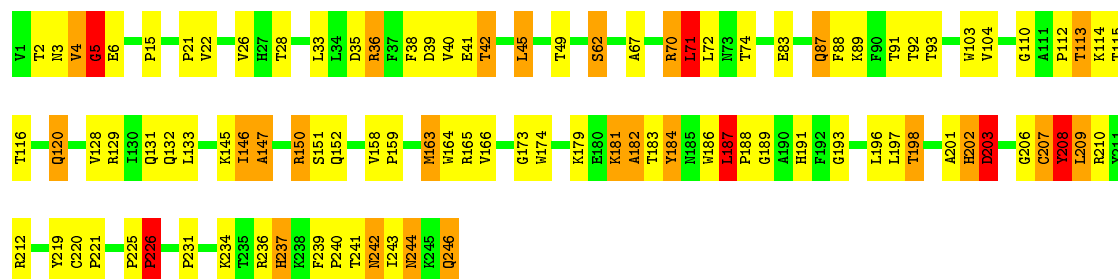
- Molecule 1: P1

Chain AK: 



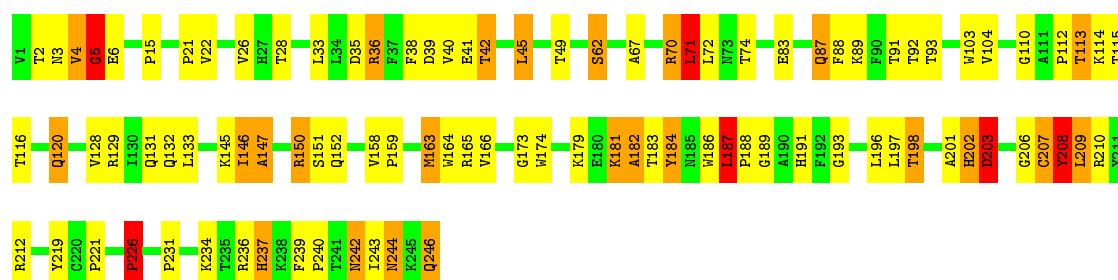
- Molecule 1: P1

Chain AL:



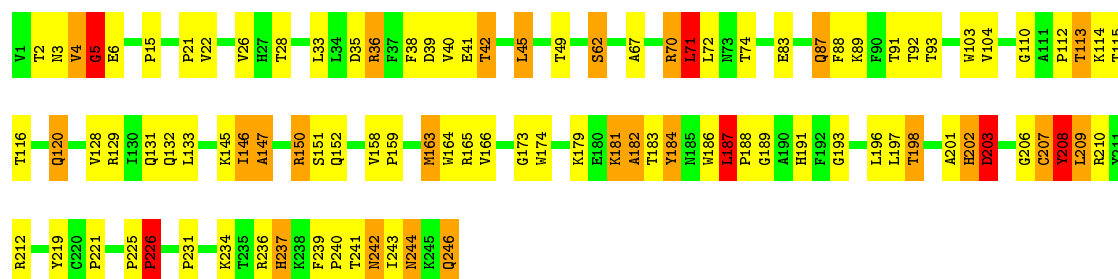
- Molecule 1: P1

Chain AM:



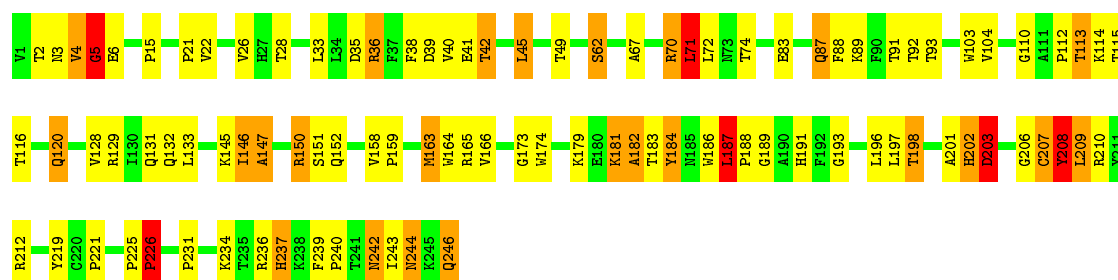
- Molecule 1: P1

Chain AN:



- Molecule 1: P1

Chain AO:



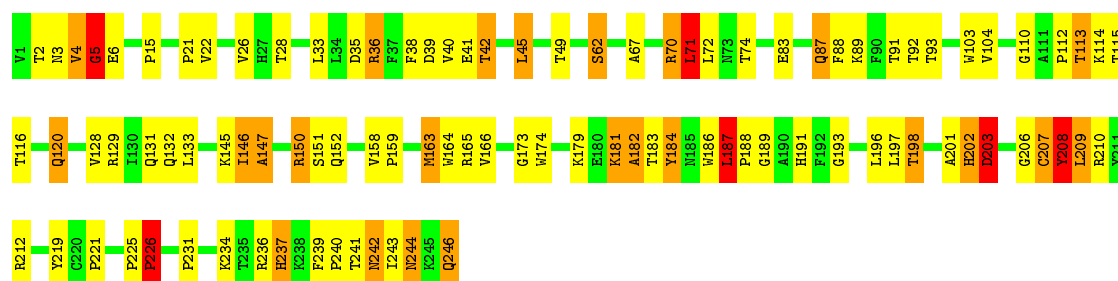
- Molecule 1: P1



- Molecule 1: P1

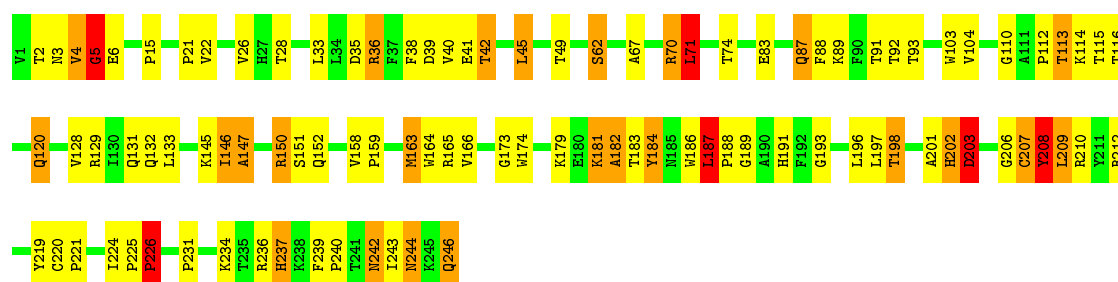


Chain A1:



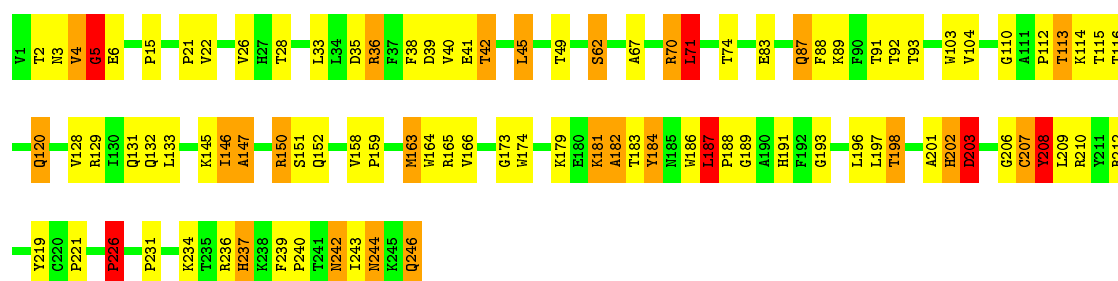
- Molecule 1: P1

Chain A2:



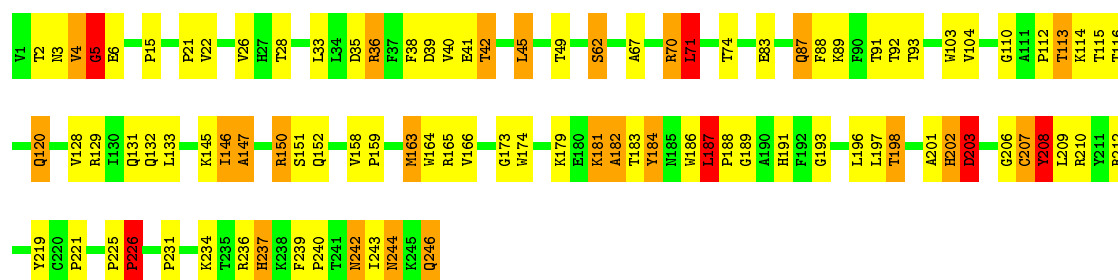
- Molecule 1: P1

Chain A3:



- Molecule 1: P1

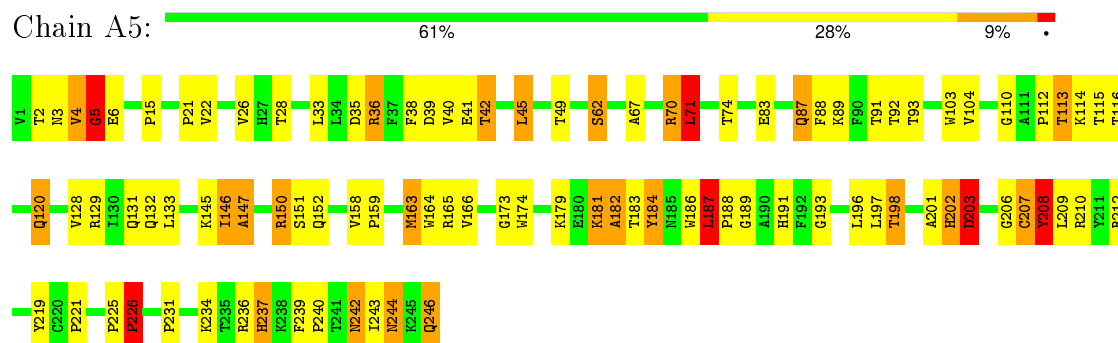
Chain A4:



- Molecule 1: P1

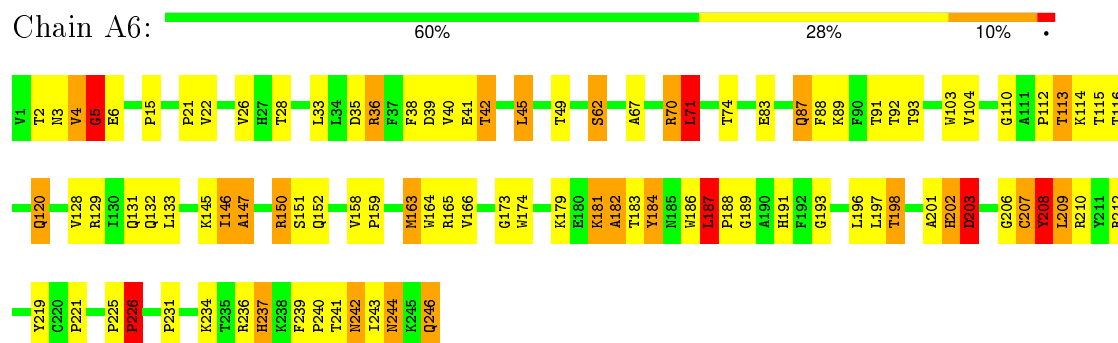


Chain A5:



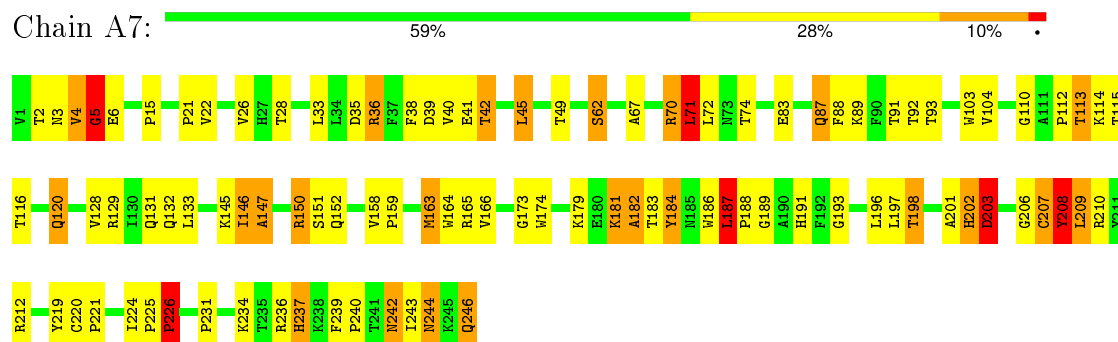
- Molecule 1: P1

Chain A6:



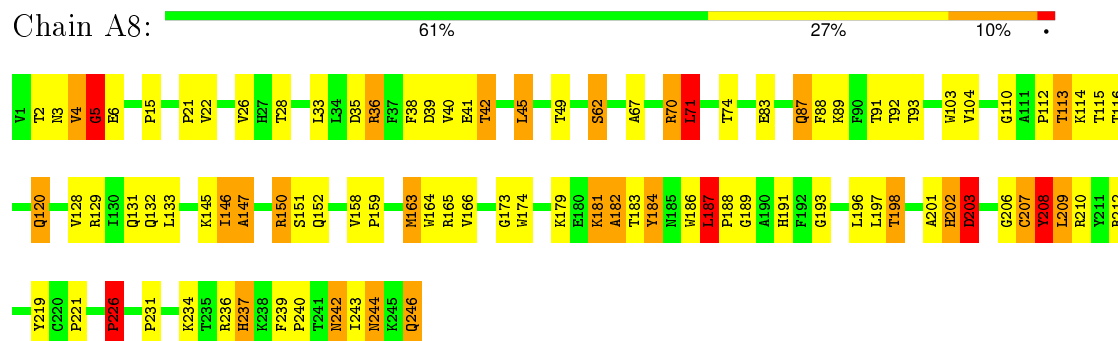
- Molecule 1: P1

Chain A7:

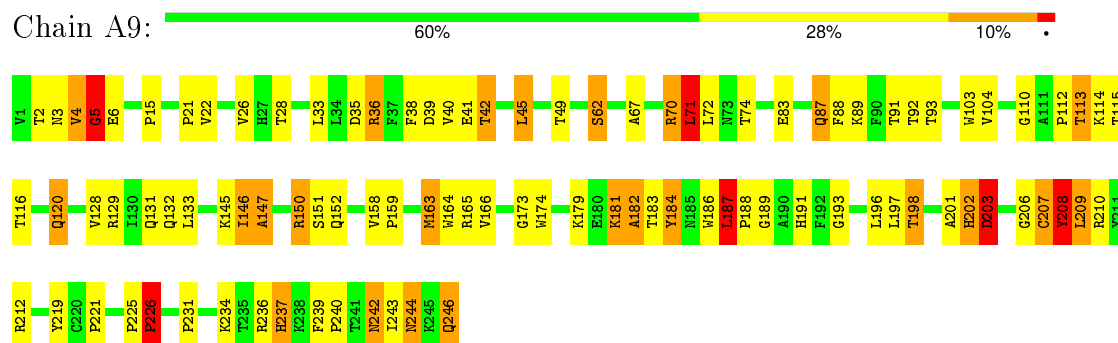


- Molecule 1: P1

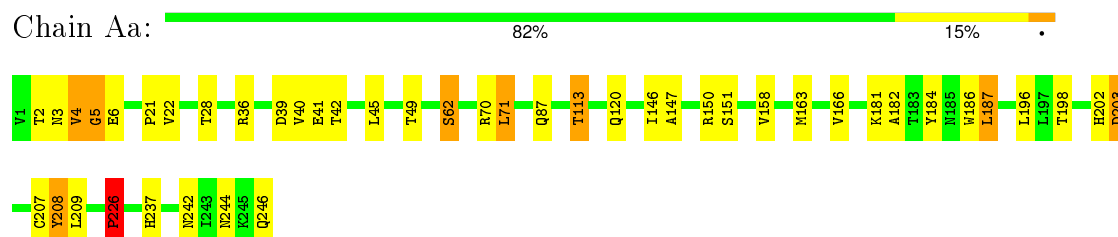
Chain A8:



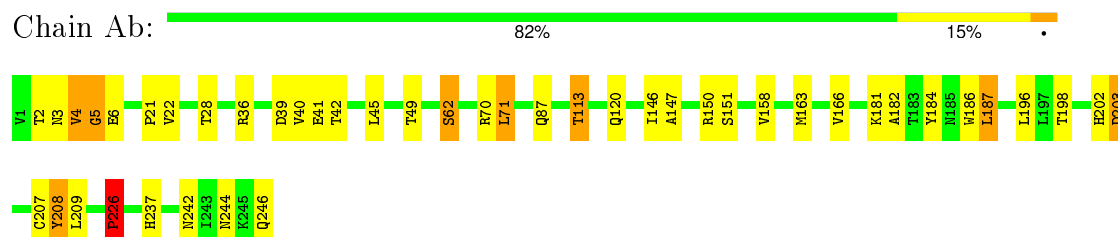
- Molecule 1: P1



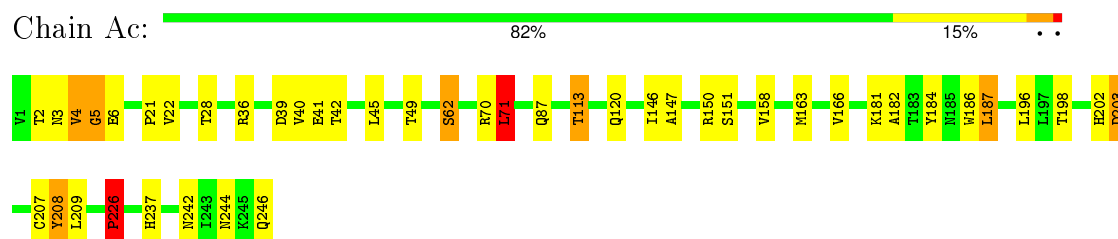
- Molecule 1: P1



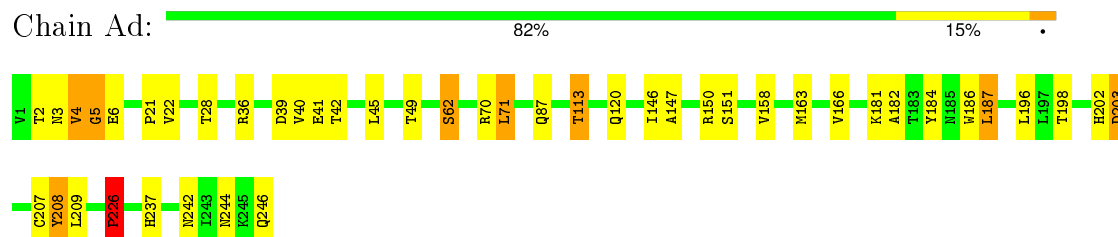
- Molecule 1: P1



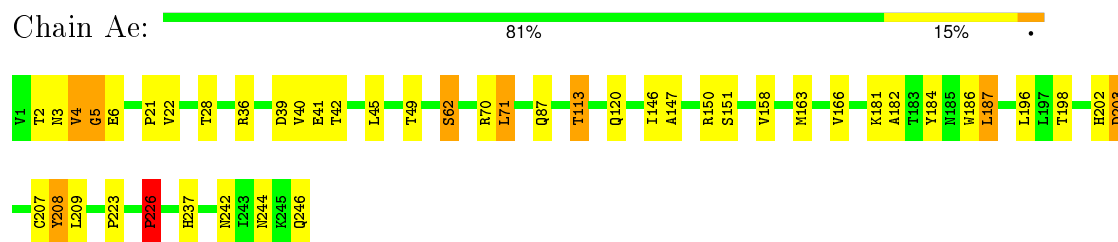
- Molecule 1: P1



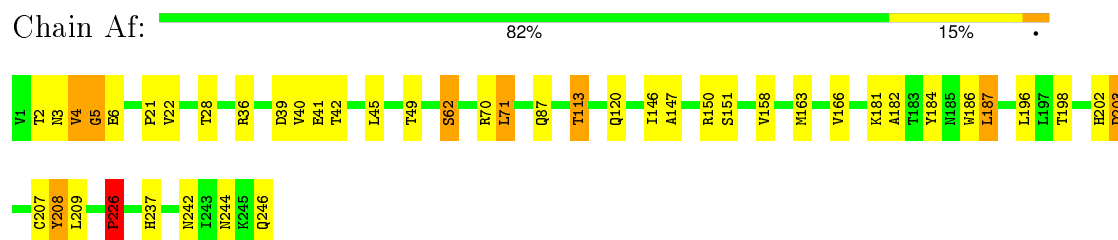
- Molecule 1: P1



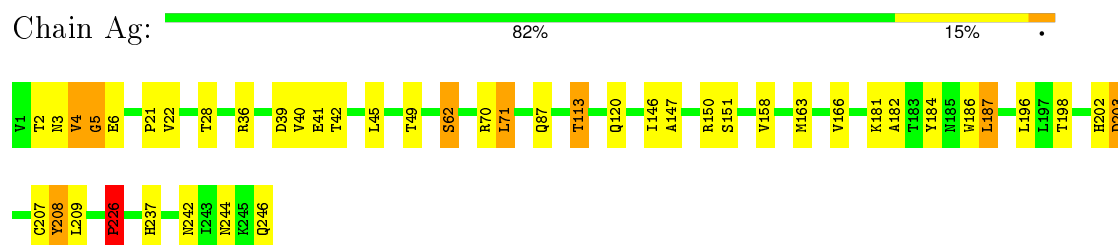
- Molecule 1: P1



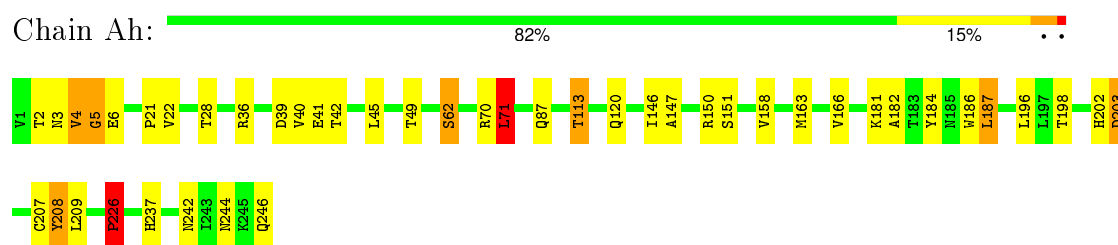
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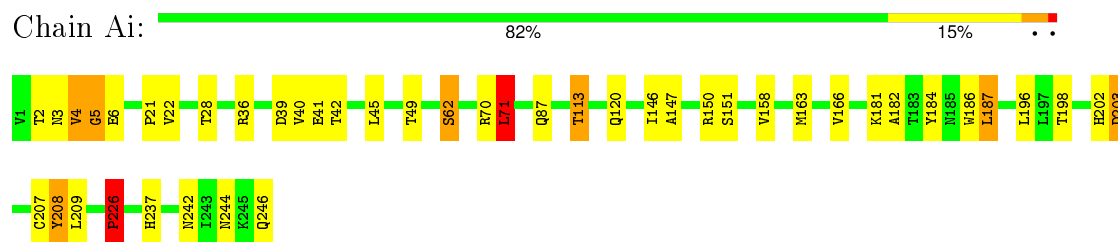
- Molecule 1: P1



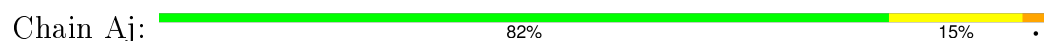
- Molecule 1: P1

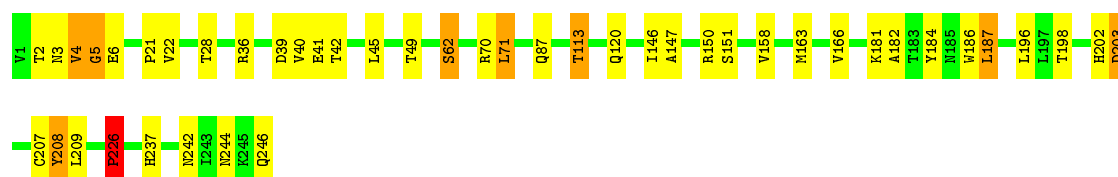


- Molecule 1: P1



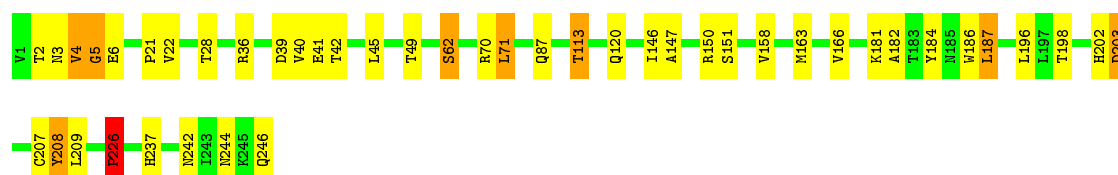
- Molecule 1: P1





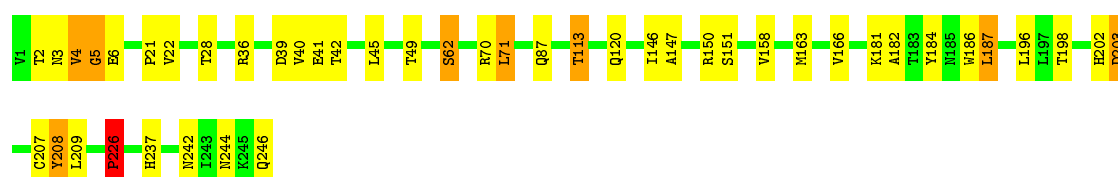
- Molecule 1: P1

Chain Ak: 82% 15% •



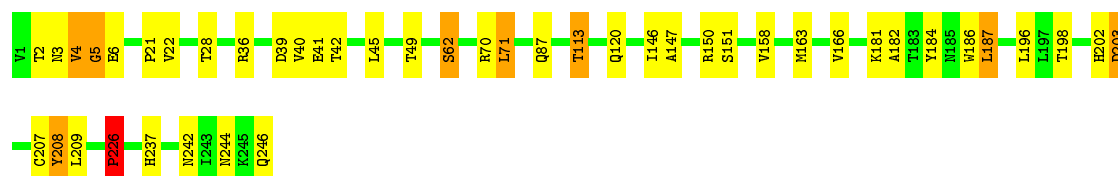
- Molecule 1: P1

Chain Al: 82% 15% •



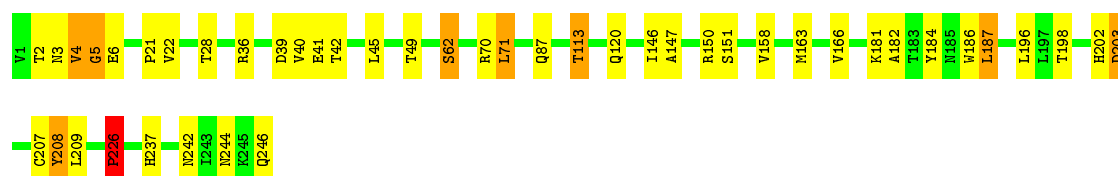
- Molecule 1: P1

Chain Am: 82% 15% •



- Molecule 1: P1

Chain An: 82% 15% •



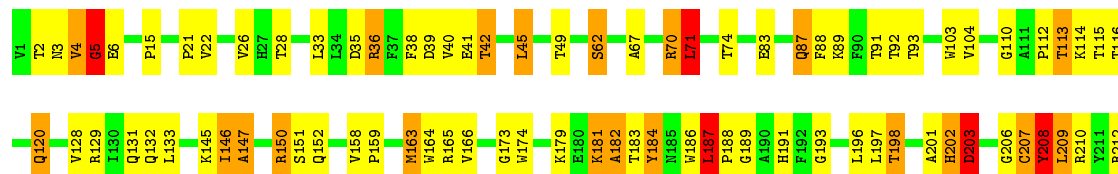
- Molecule 1: P1

Chain Ao: 82% 15% •

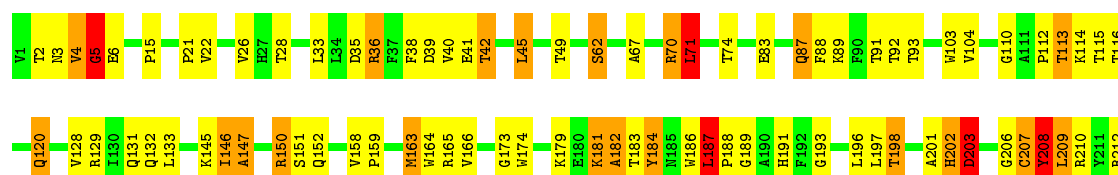




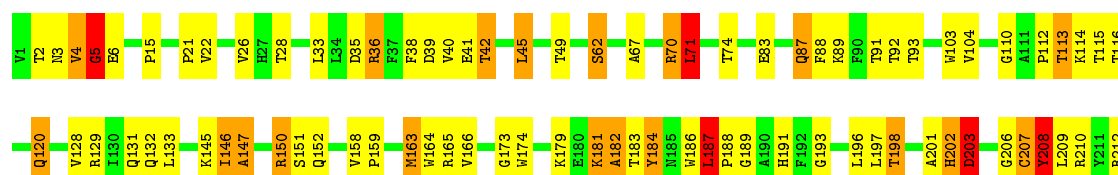
- Molecule 1: P1



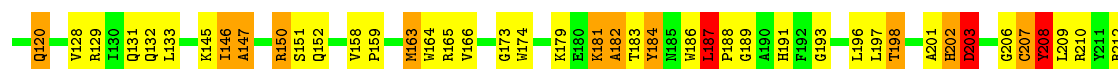
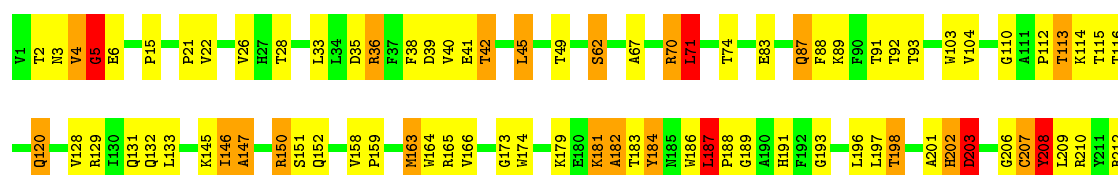
- Molecule 1: P1

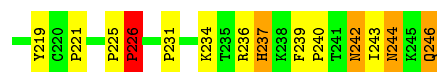


- Molecule 1: P1



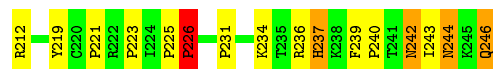
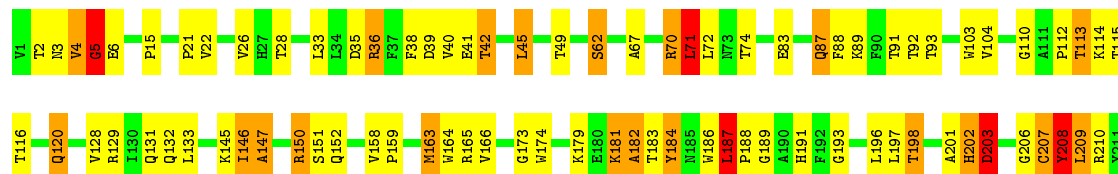
- Molecule 1: P1





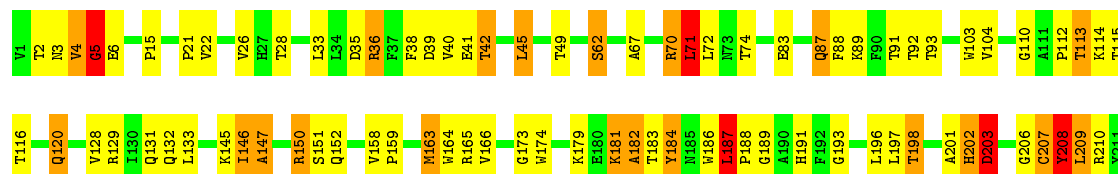
• Molecule 1: P1

Chain DG: 60% 28% 10% •



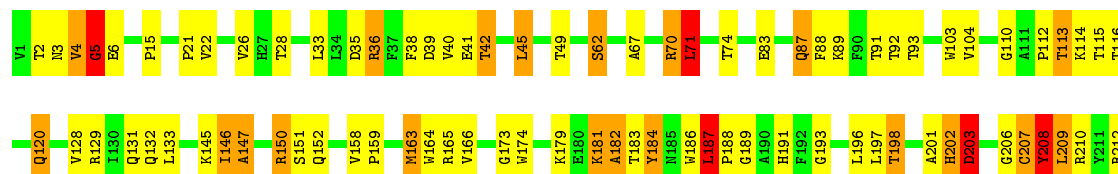
• Molecule 1: P1

Chain DH: 60% 28% 10% •



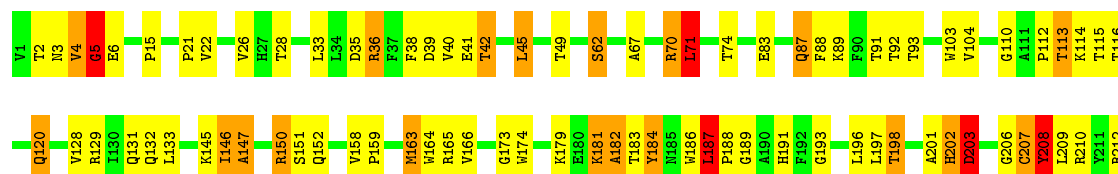
• Molecule 1: P1

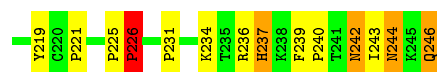
Chain DI: 61% 27% 10% •



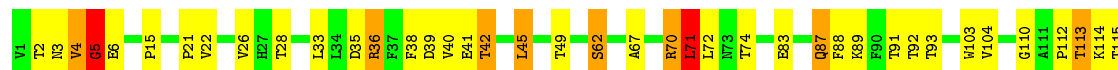
• Molecule 1: P1

Chain DJ: 61% 28% 9% •

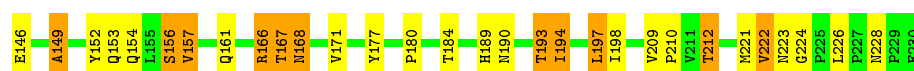




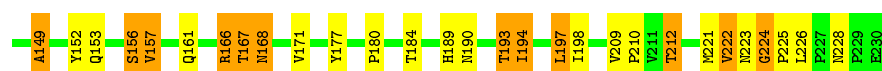
- Molecule 1: P1



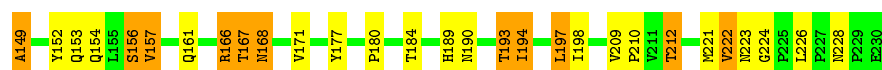
- Molecule 2: P1



- Molecule 2: P1



- Molecule 2: P1



- Molecule 2: P1





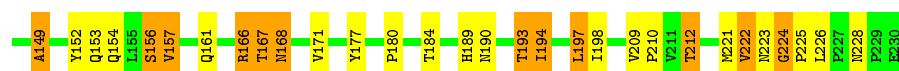
- Molecule 2: P1



- Molecule 2: P1



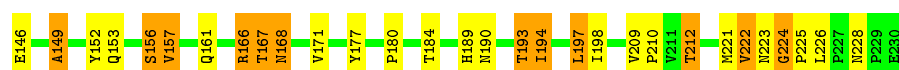
- Molecule 2: P1



- Molecule 2: P1

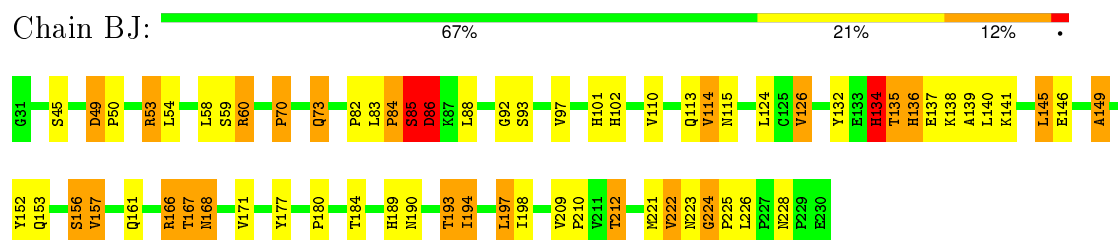


- Molecule 2: P1

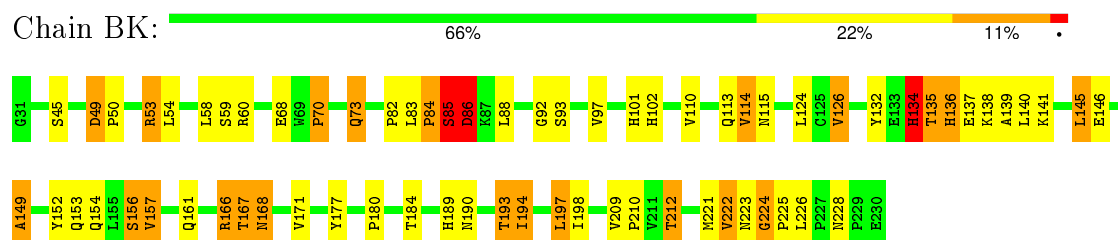




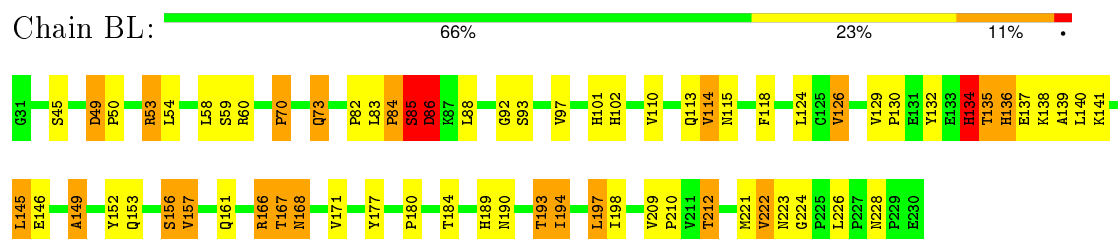
- Molecule 2: P1



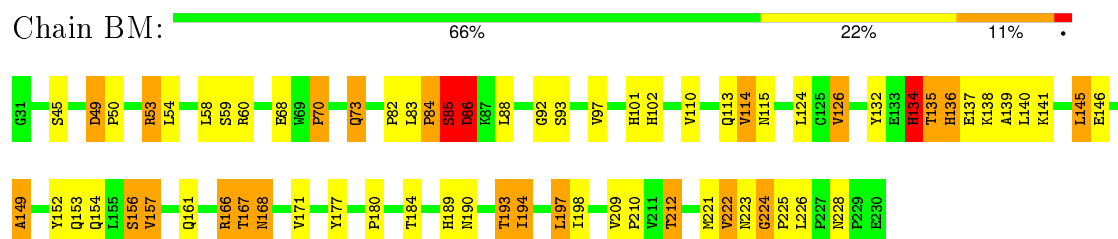
- Molecule 2: P1



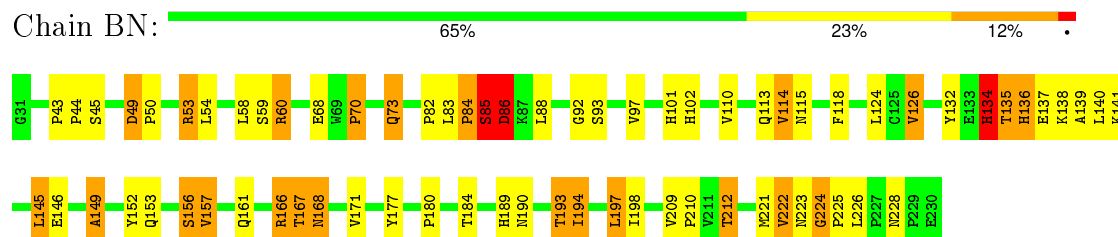
- Molecule 2: P1



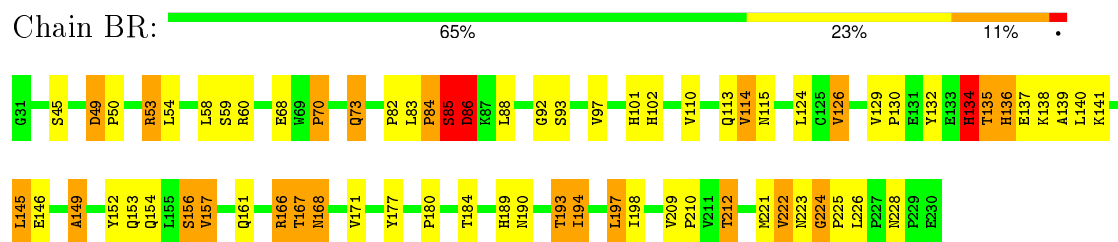
- Molecule 2: P1



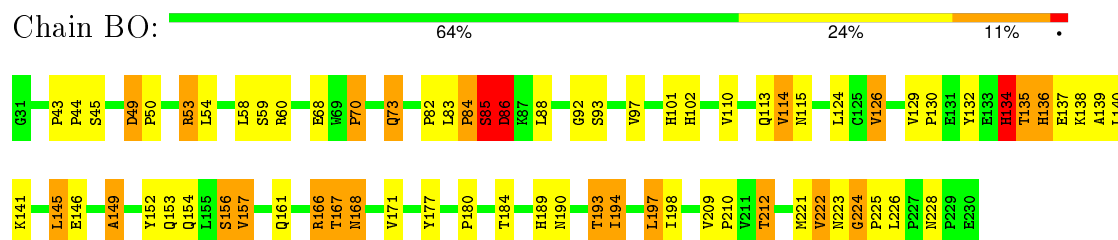
- Molecule 2: P1



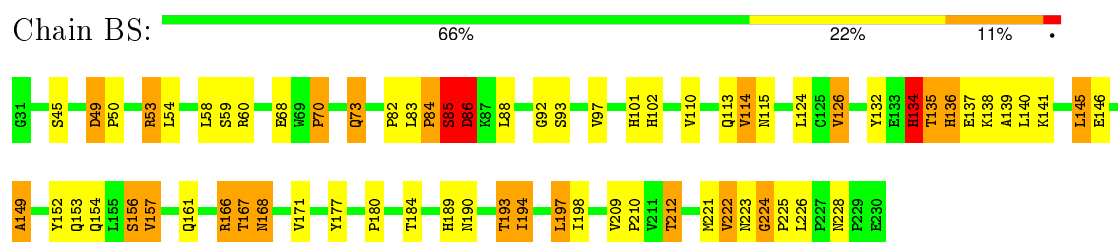
- Molecule 2: P1



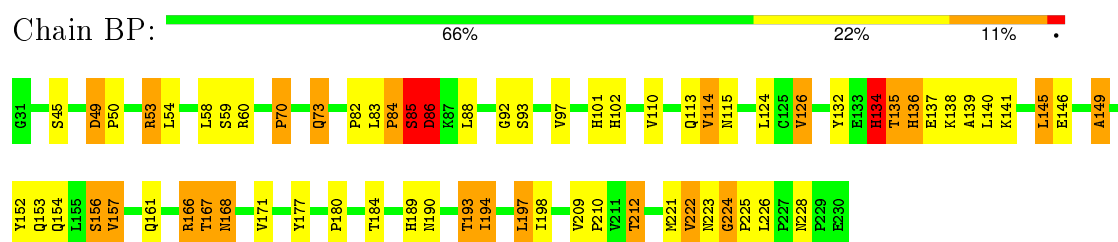
- Molecule 2: P1



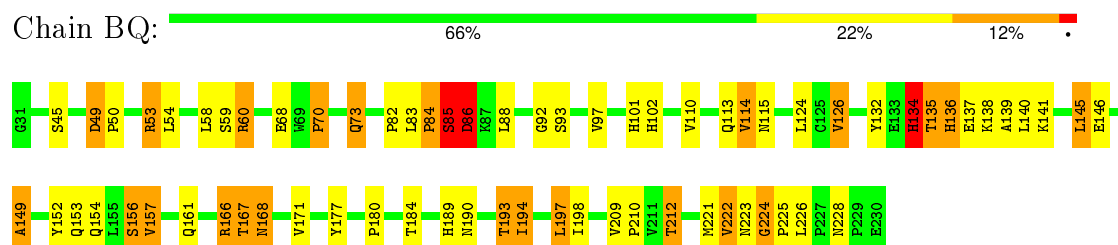
- Molecule 2: P1



- Molecule 2: P1

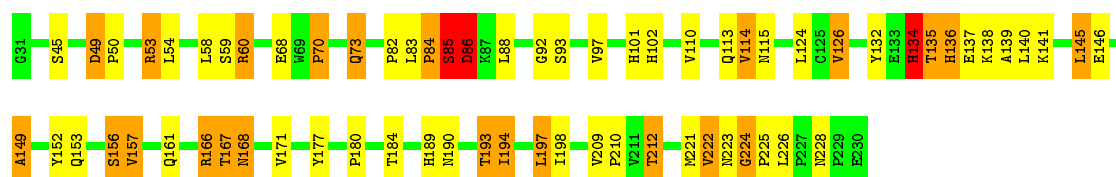


- Molecule 2: P1

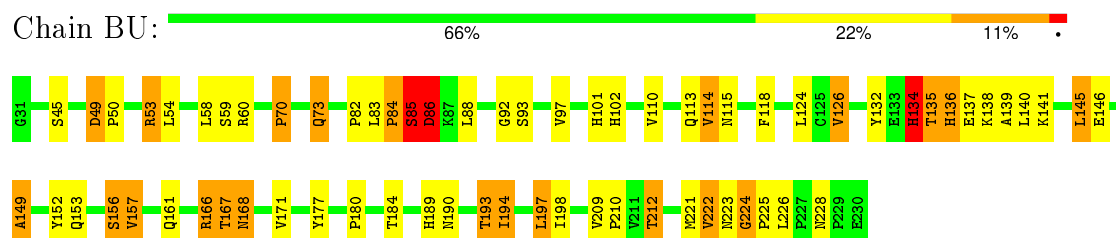


- Molecule 2: P1

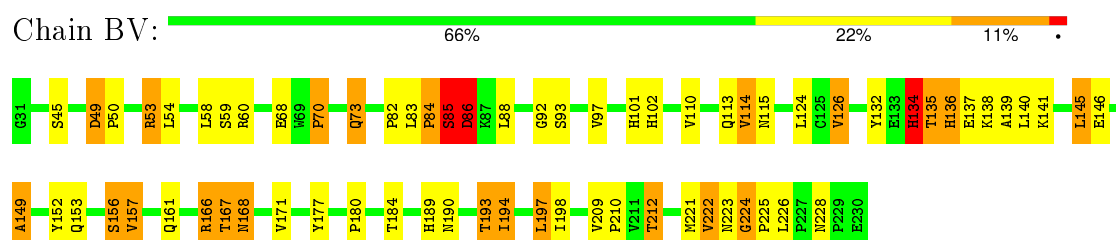




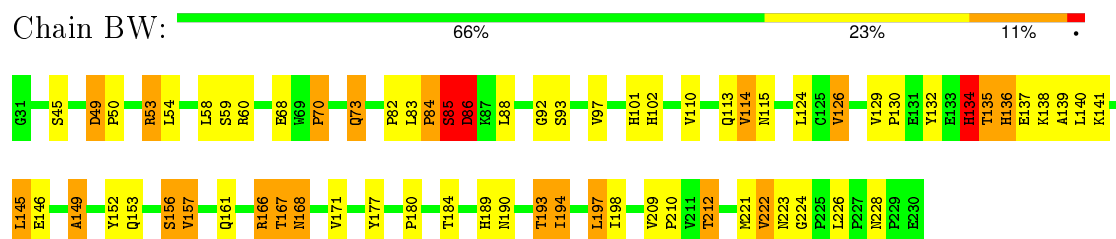
- Molecule 2: P1



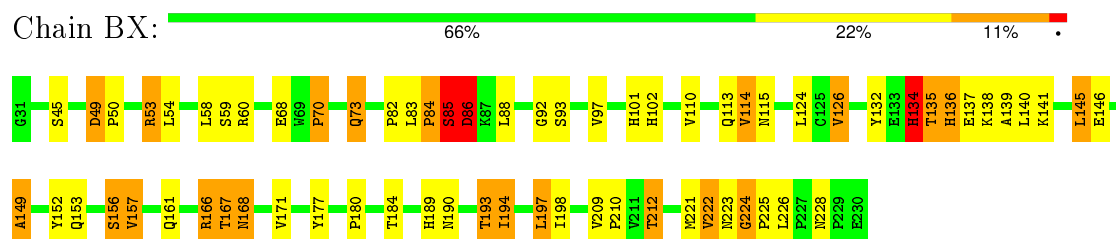
- Molecule 2: P1



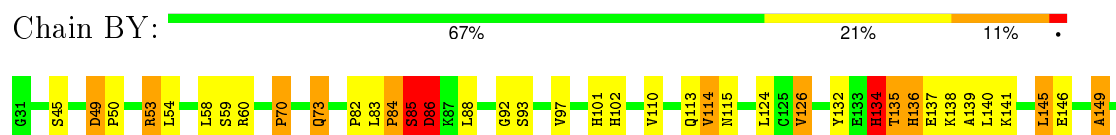
- Molecule 2: P1

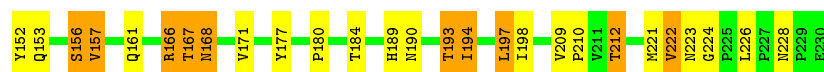


- Molecule 2: P1

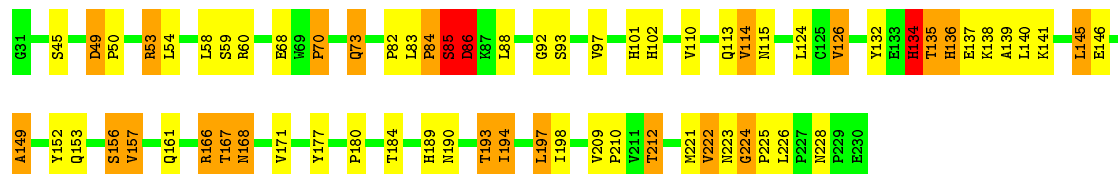


- Molecule 2: P1

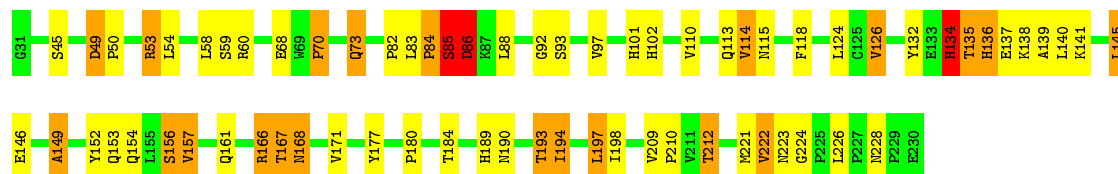




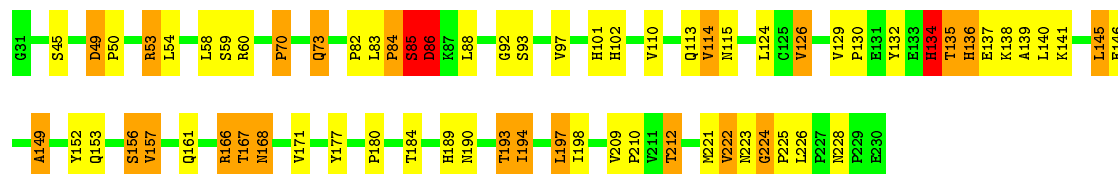
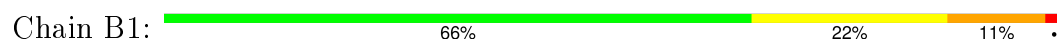
• Molecule 2: P1



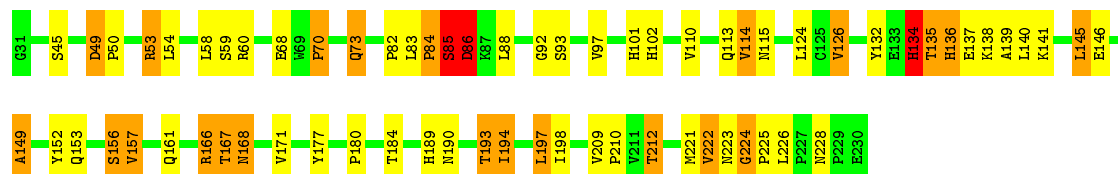
• Molecule 2: P1



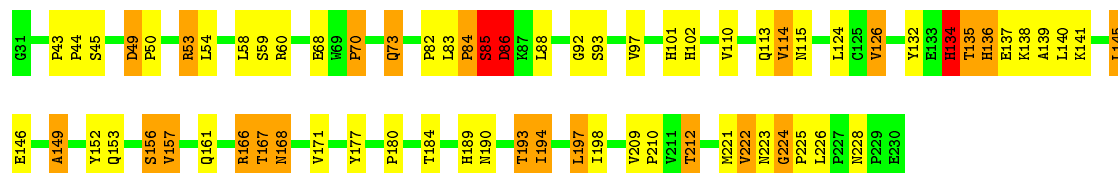
• Molecule 2: P1



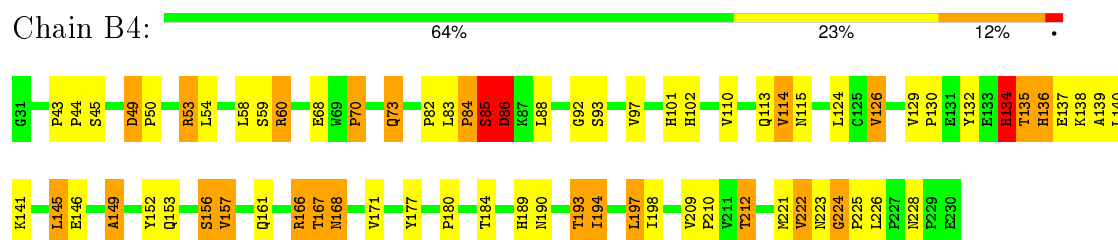
• Molecule 2: P1



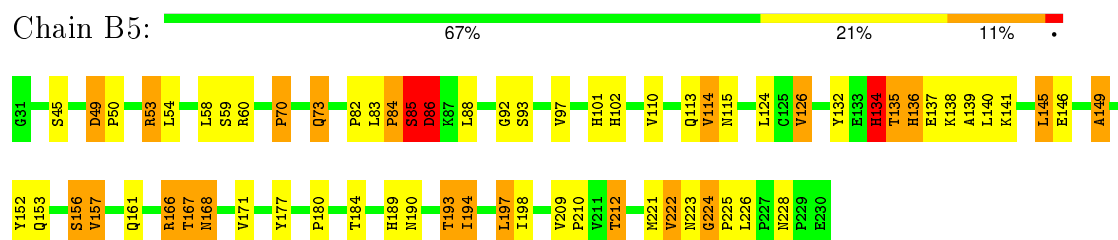
• Molecule 2: P1



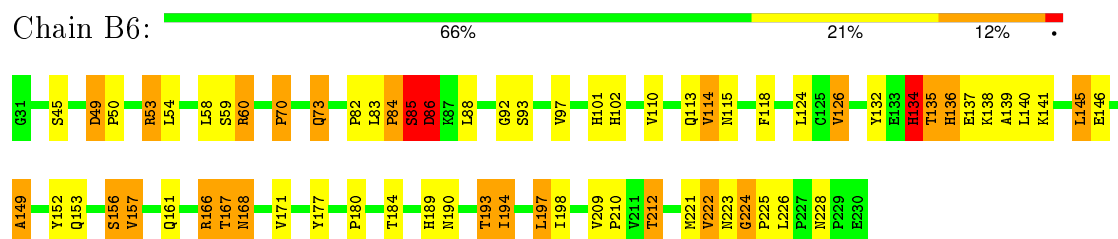
- Molecule 2: P1



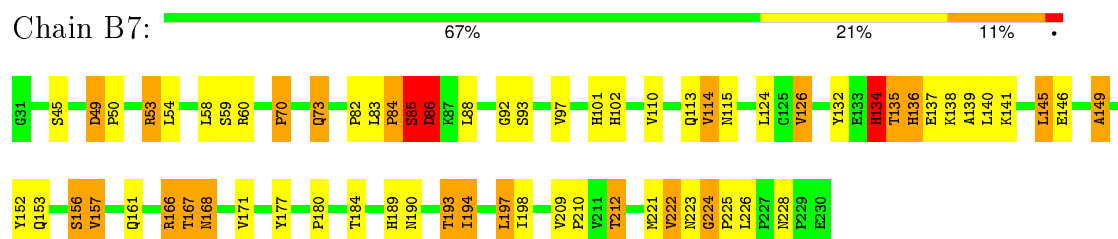
- Molecule 2: P1



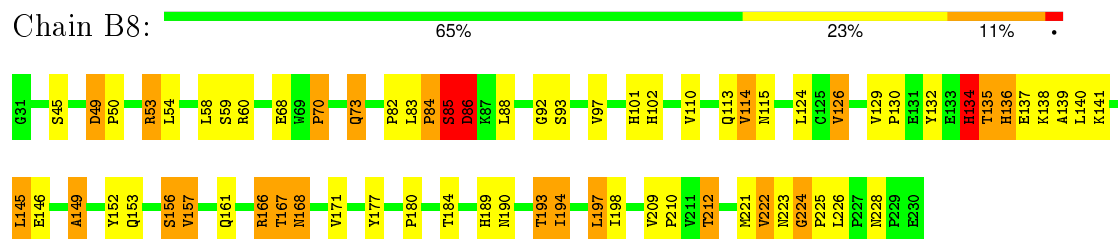
- Molecule 2: P1



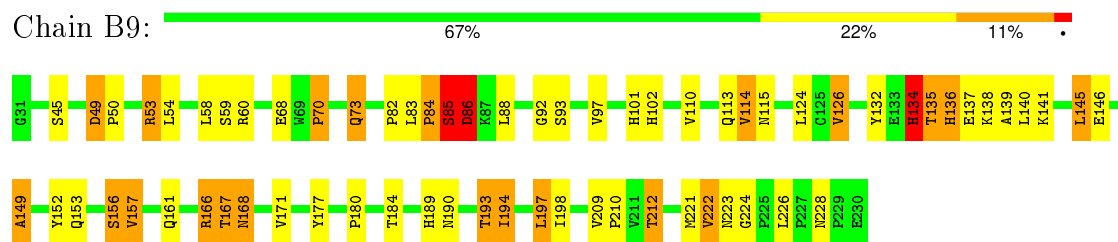
- Molecule 2: P1



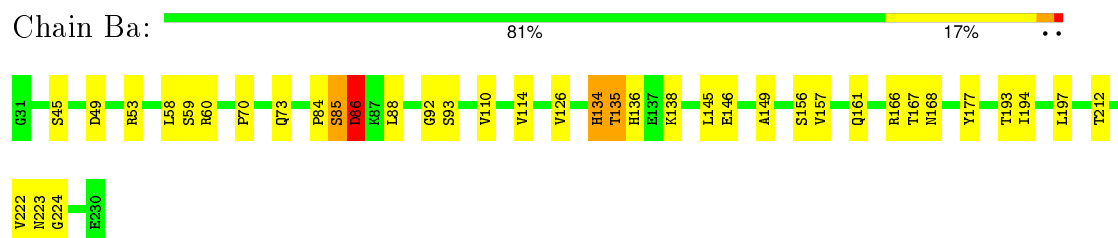
- Molecule 2: P1



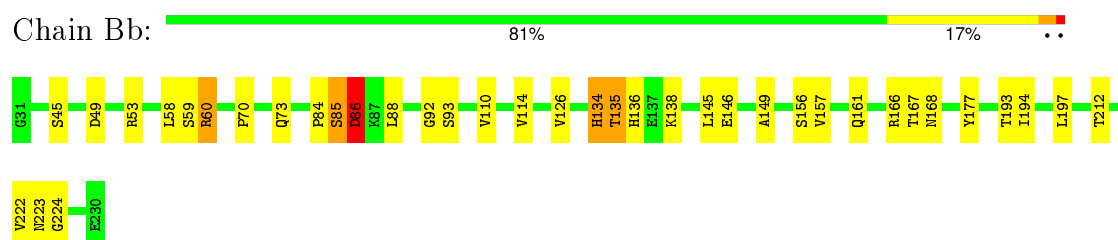
- Molecule 2: P1



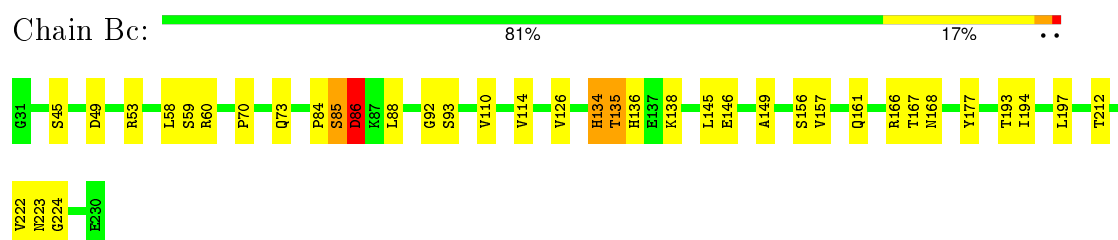
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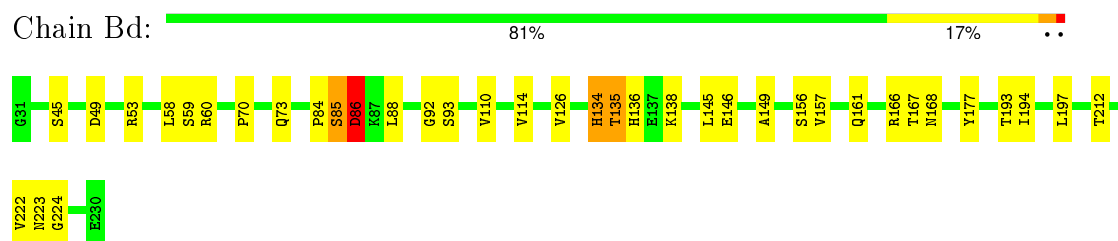
• Molecule 2: P1



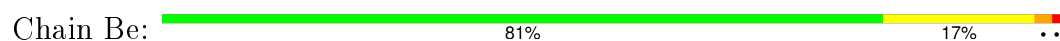
• Molecule 2: P1

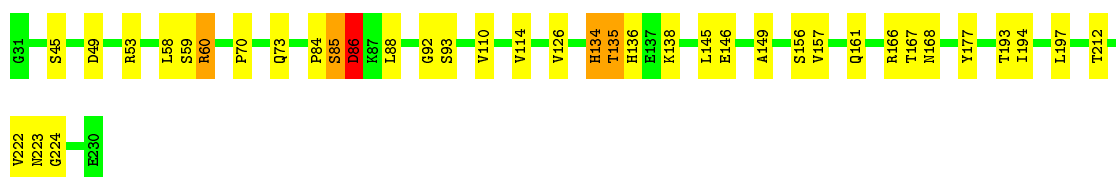


• Molecule 2: P1



• Molecule 2: P1





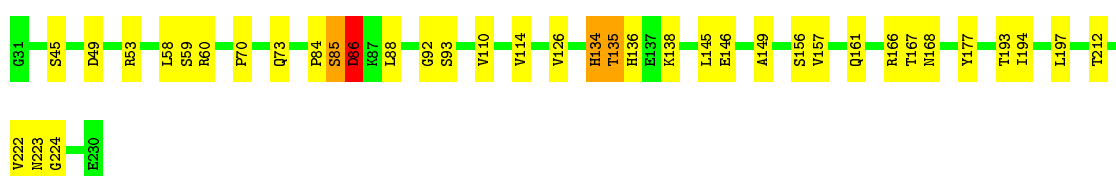
- Molecule 2: P1

Chain Bf: 81% 17% ..



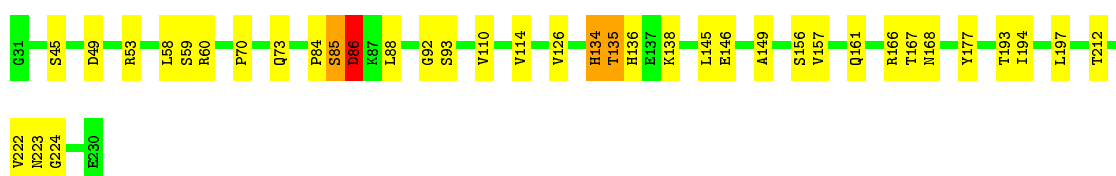
- Molecule 2: P1

Chain Bg: 81% 17% ..



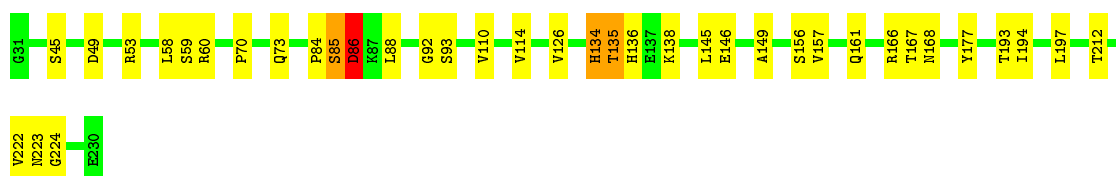
- Molecule 2: P1

Chain Bh: 81% 17% ..



- Molecule 2: P1

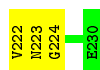
Chain Bi: 81% 17% ..



- Molecule 2: P1

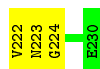
Chain Bj: 81% 17% ..





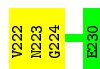
## ● Molecule 2: P1

Chain Bk: 81% 17% ..



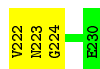
## ● Molecule 2: P1

Chain Bl: 81% 17% ..



## ● Molecule 2: P1

Chain Bm: 81% 17% ..



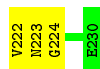
## ● Molecule 2: P1

Chain Bn: 81% 17% ..



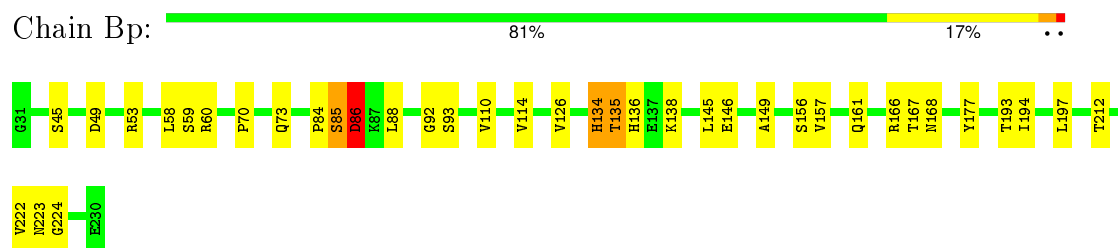
## ● Molecule 2: P1

Chain Bo: 81% 17% ..

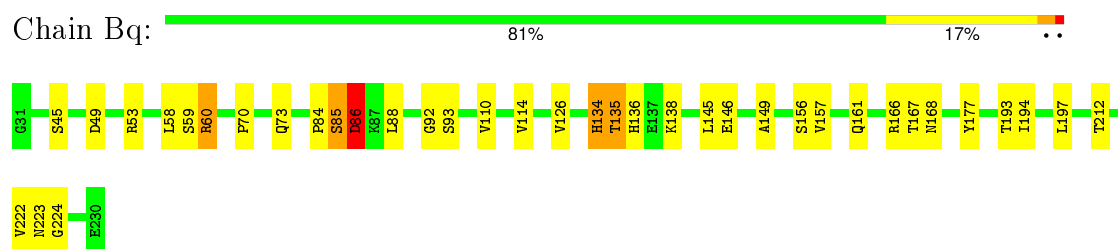




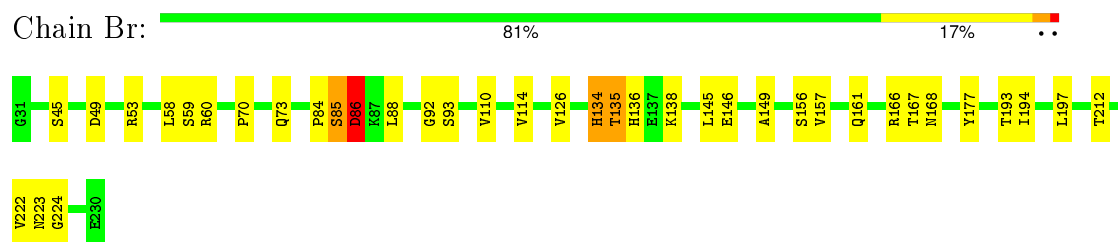
## ● Molecule 2: P1



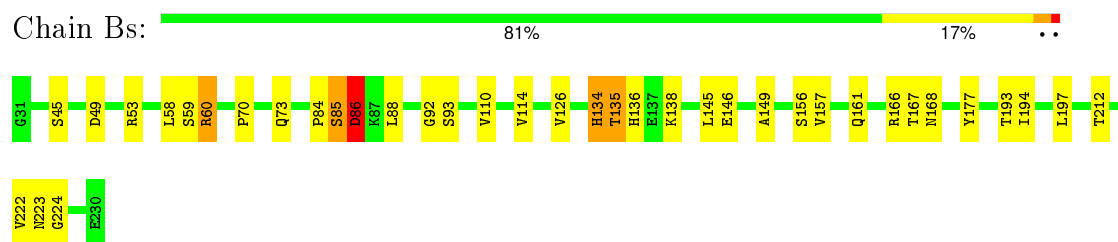
## ● Molecule 2: P1



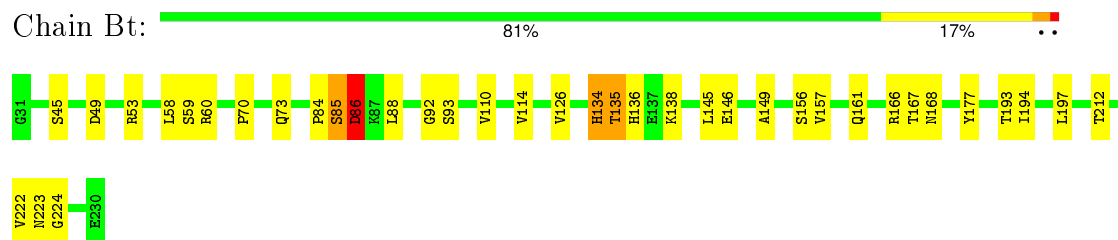
## ● Molecule 2: P1



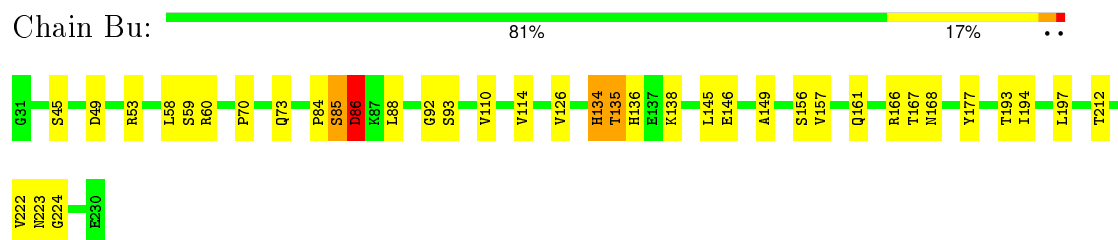
## ● Molecule 2: P1



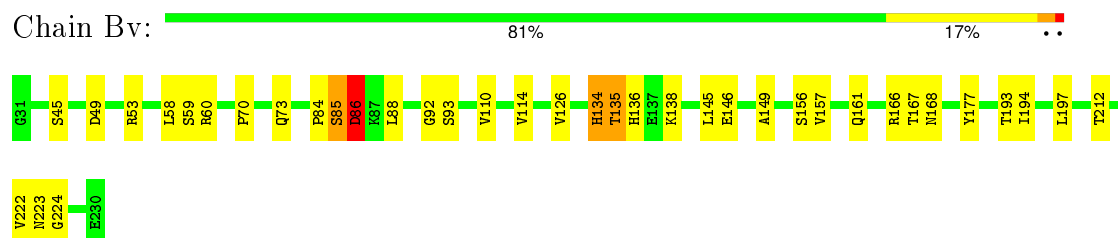
## ● Molecule 2: P1



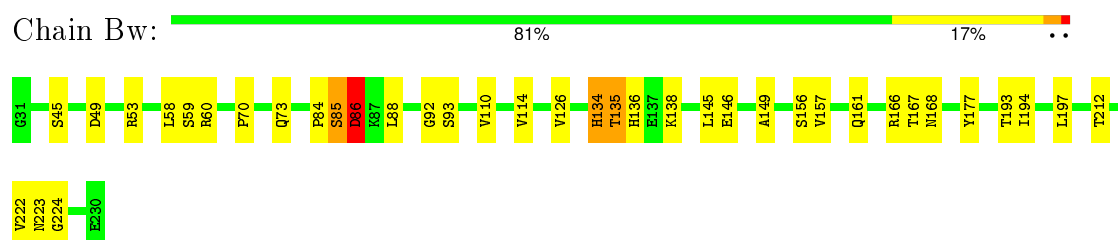
## ● Molecule 2: P1



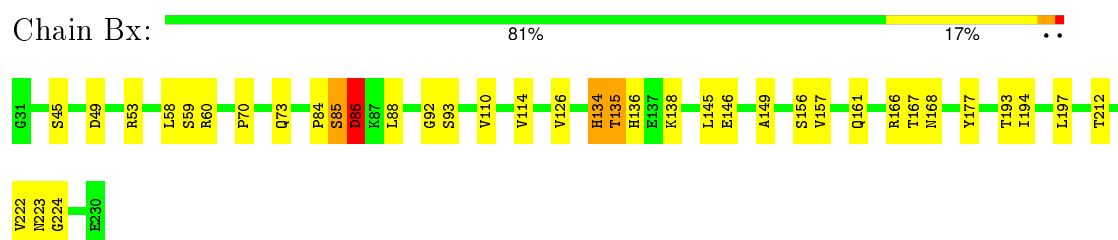
- Molecule 2: P1



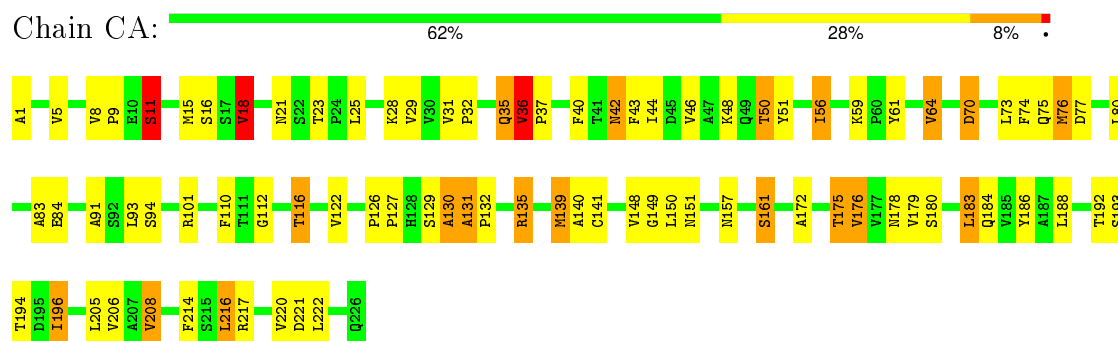
- Molecule 2: P1



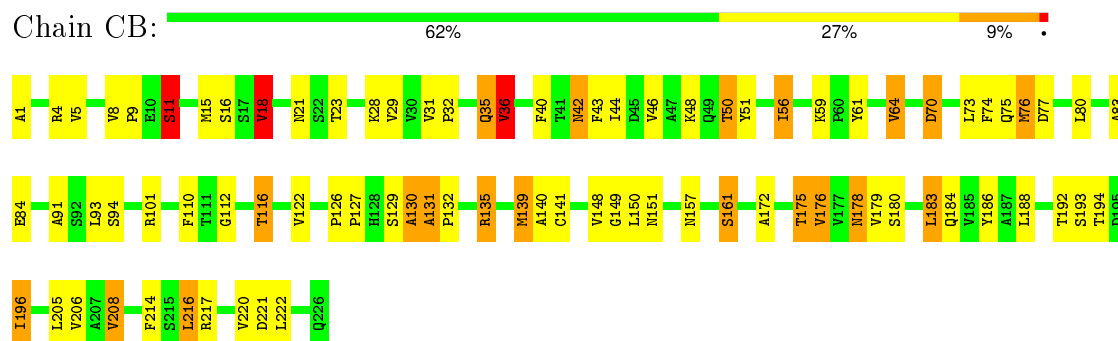
- Molecule 2: P1



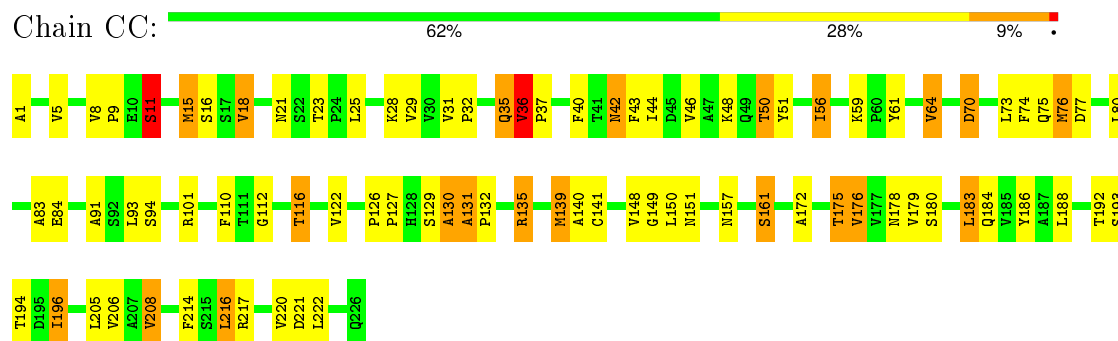
- Molecule 3: P1



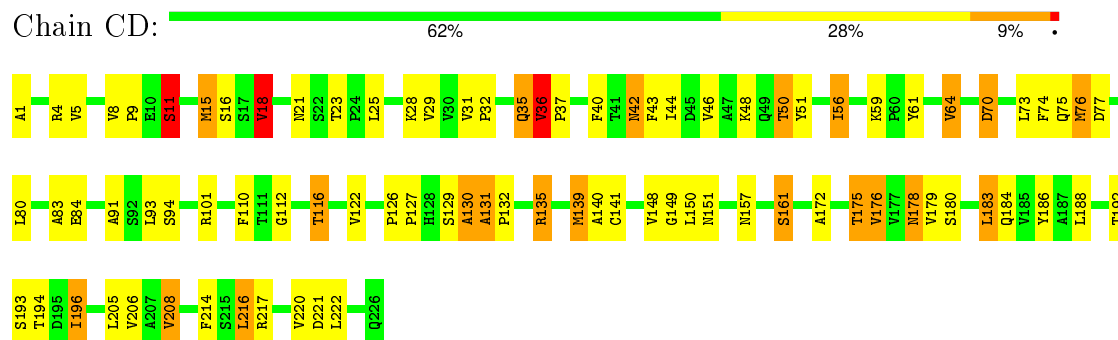
- Molecule 3: P1



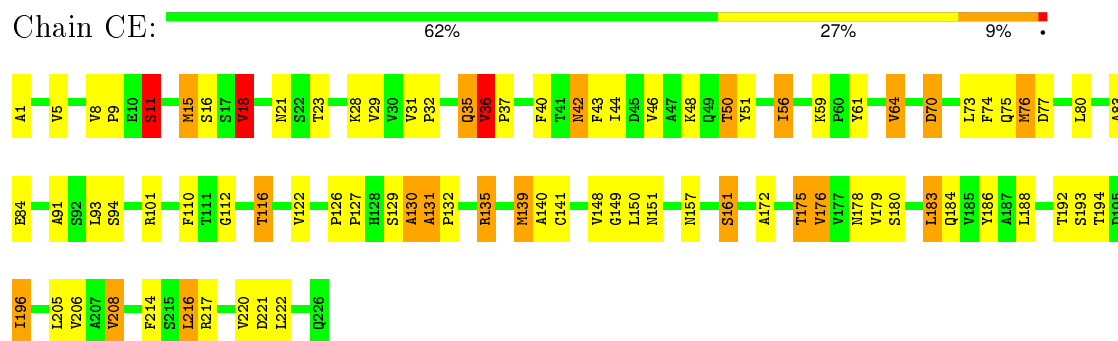
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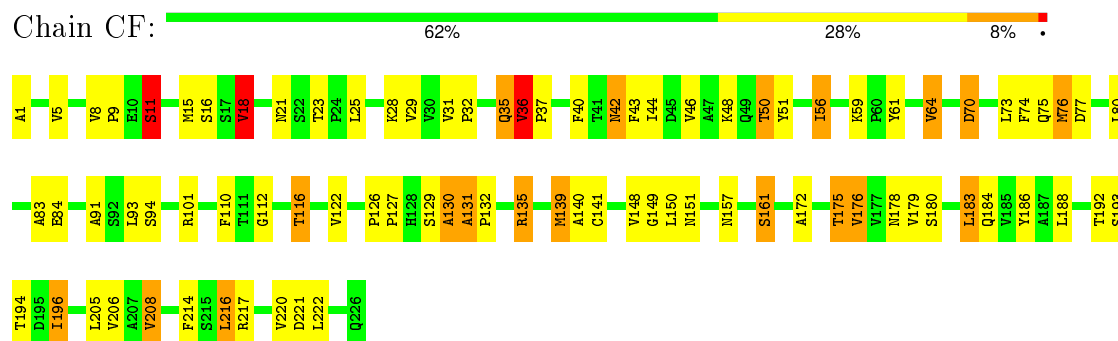
- Molecule 3: P1



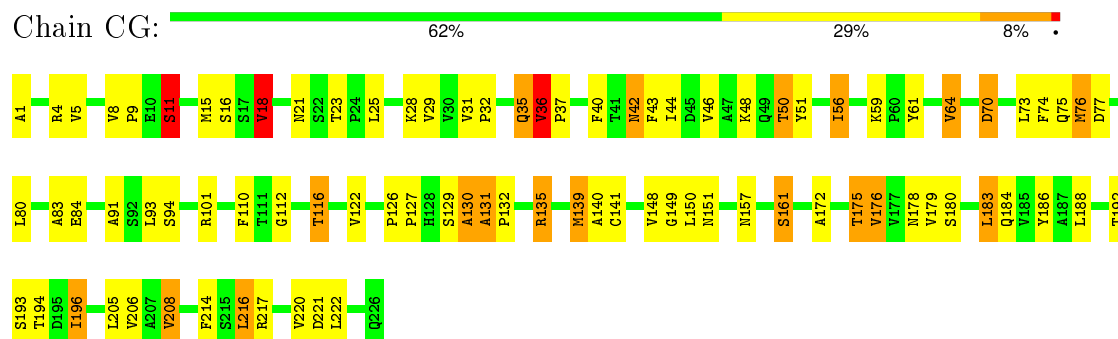
- Molecule 3: P1



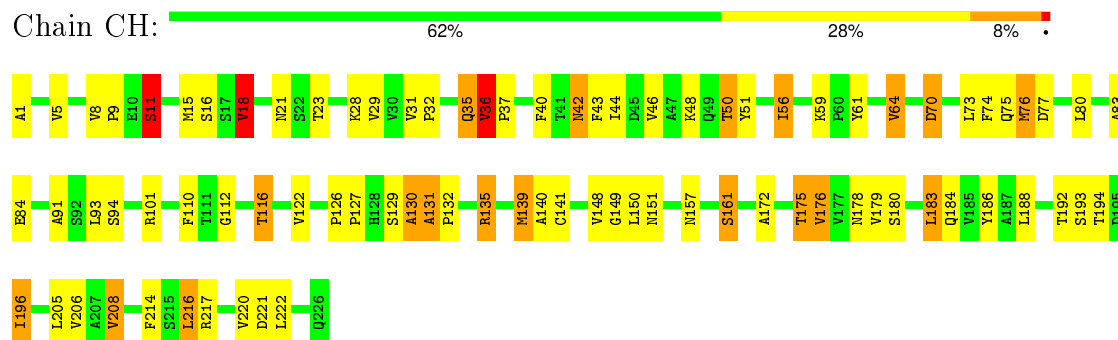
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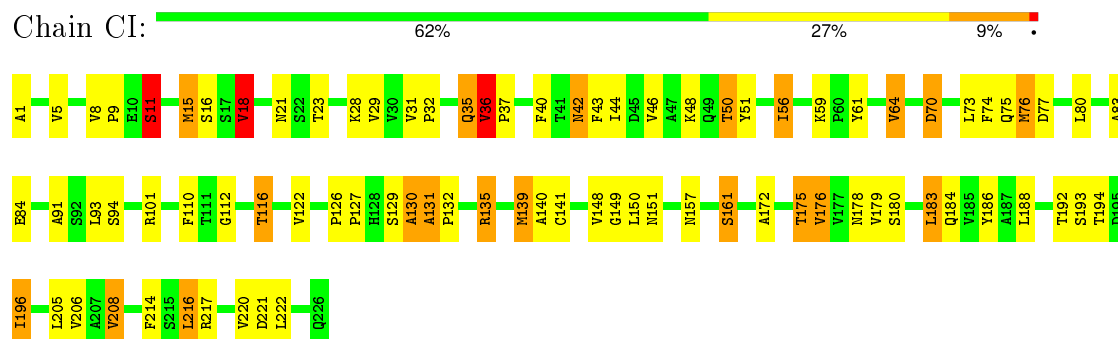
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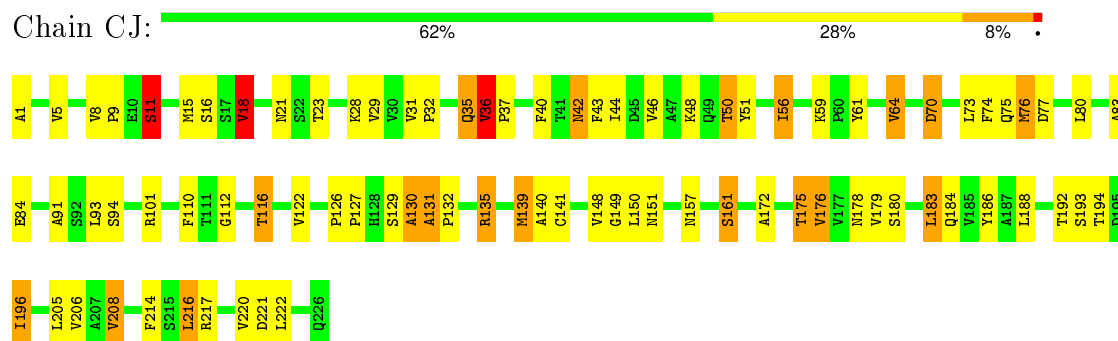
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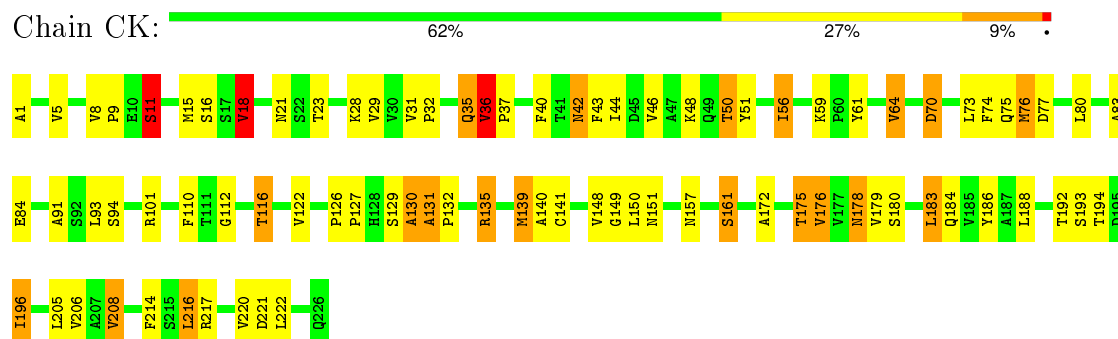
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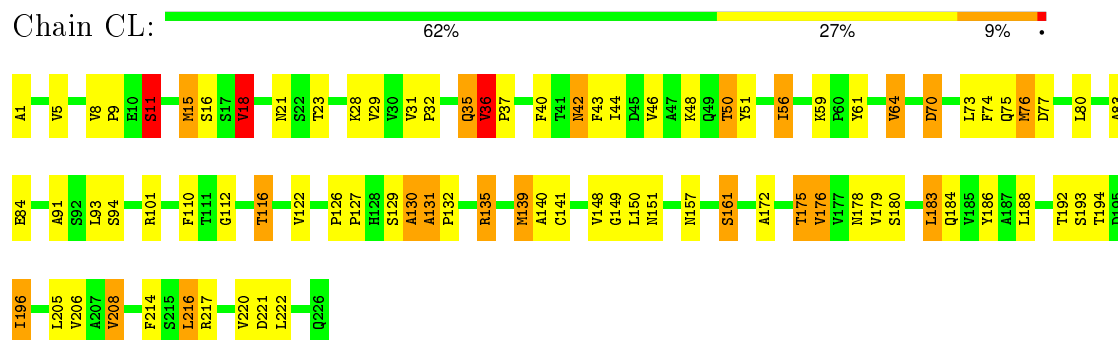
- Molecule 3: P1



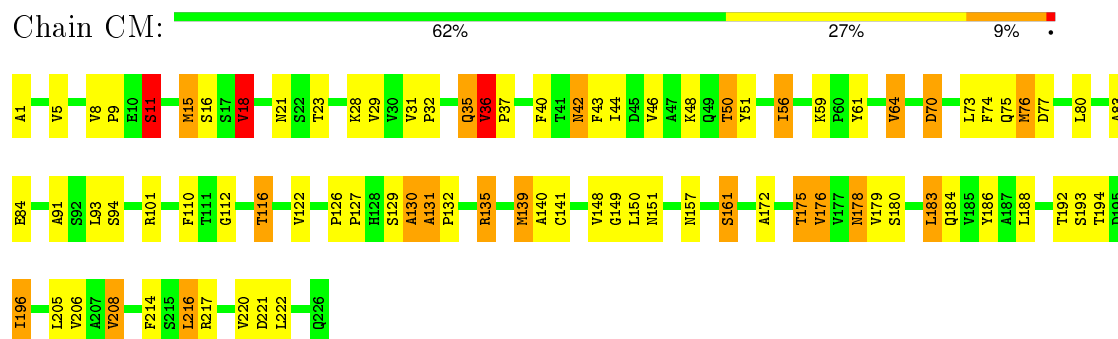
- Molecule 3: P1



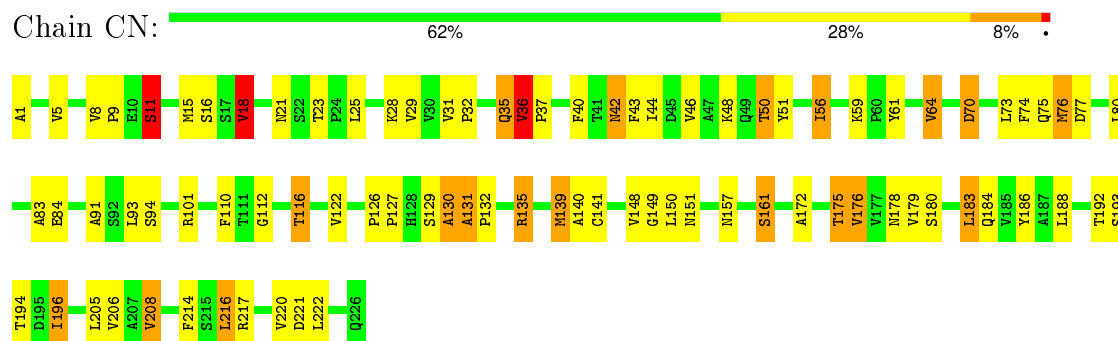
- Molecule 3: P1



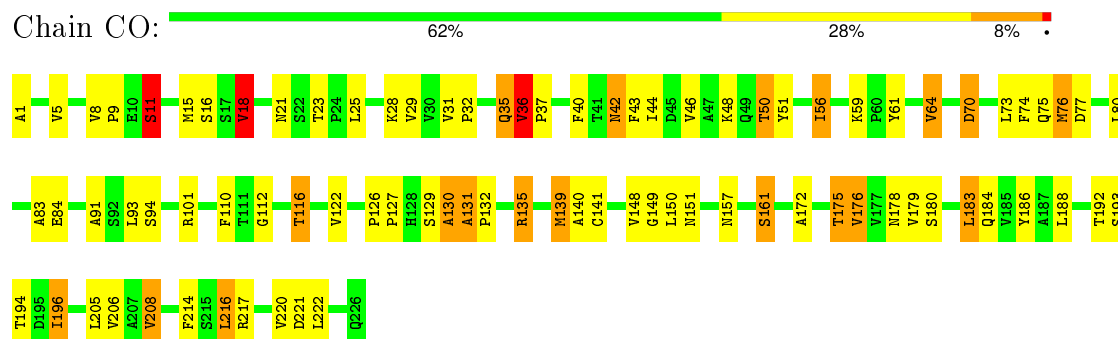
- Molecule 3: P1



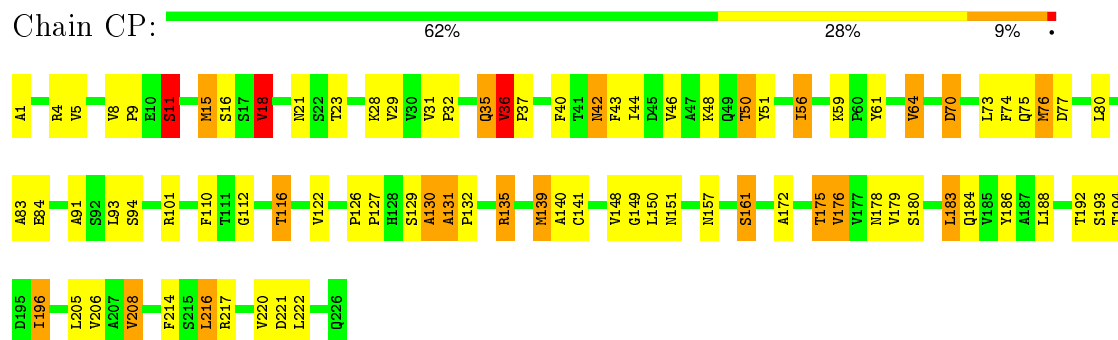
- Molecule 3: P1



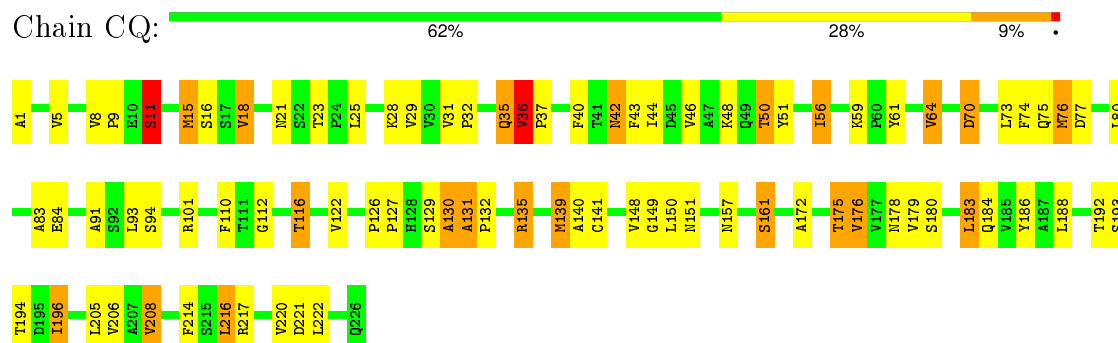
- Molecule 3: P1



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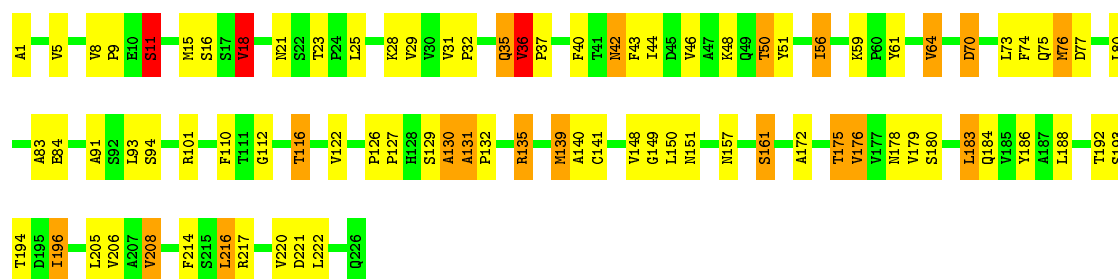


- Molecule 3: P1



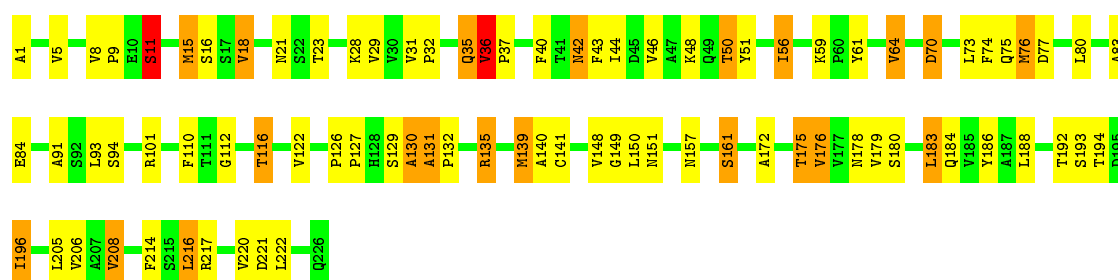
- Molecule 3: P1

Chain CR:  62% 28% 8%



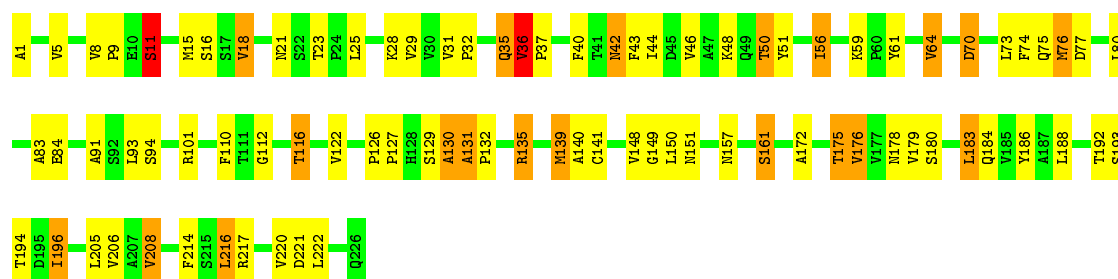
• Molecule 3: P1

Chain CS:  62% 27% 9%



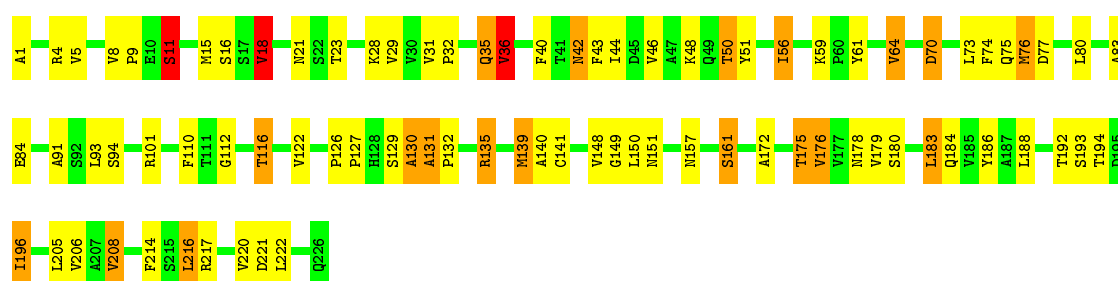
• Molecule 3: P1

Chain CT:  62% 28% 9%

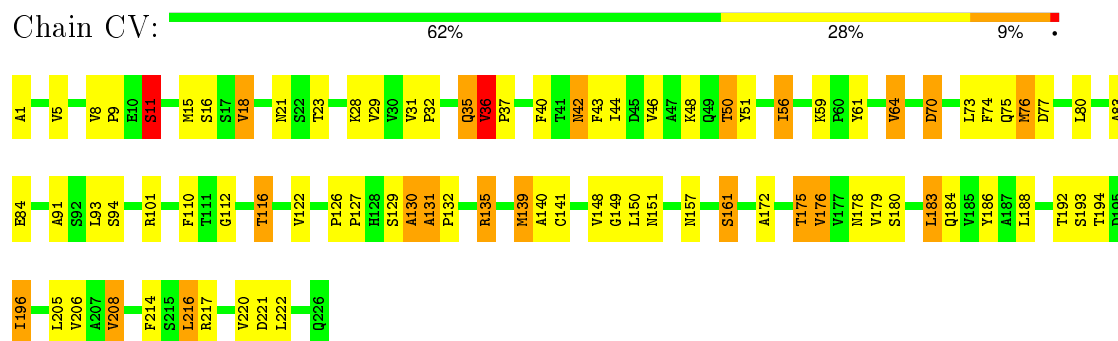


• Molecule 3: P1

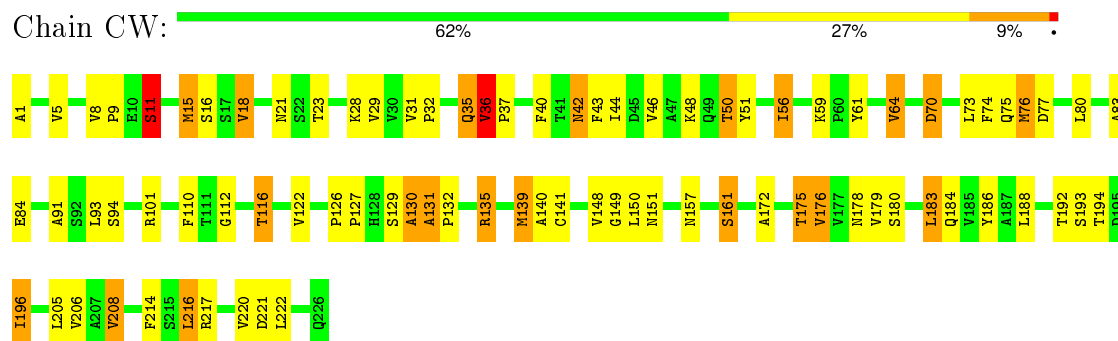
Chain CU:  62% 28% 8%



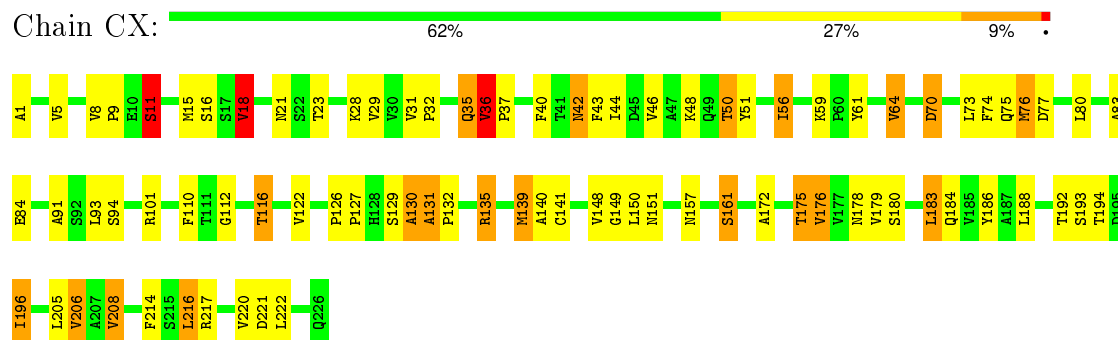
• Molecule 3: P1



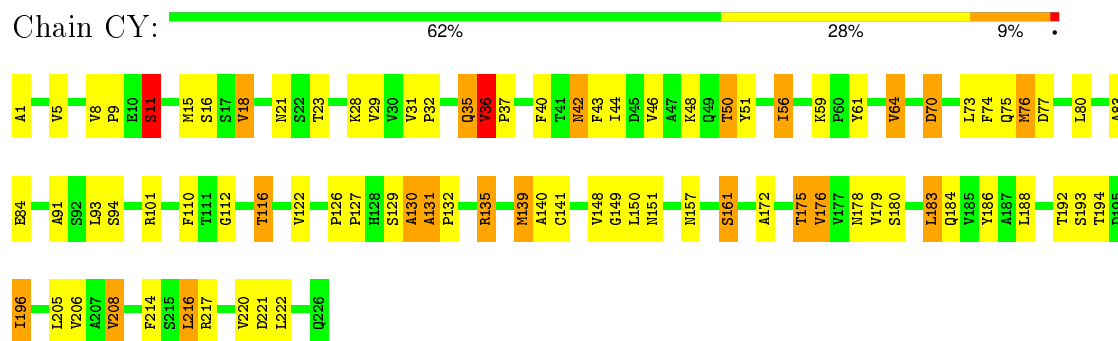
- Molecule 3: P1



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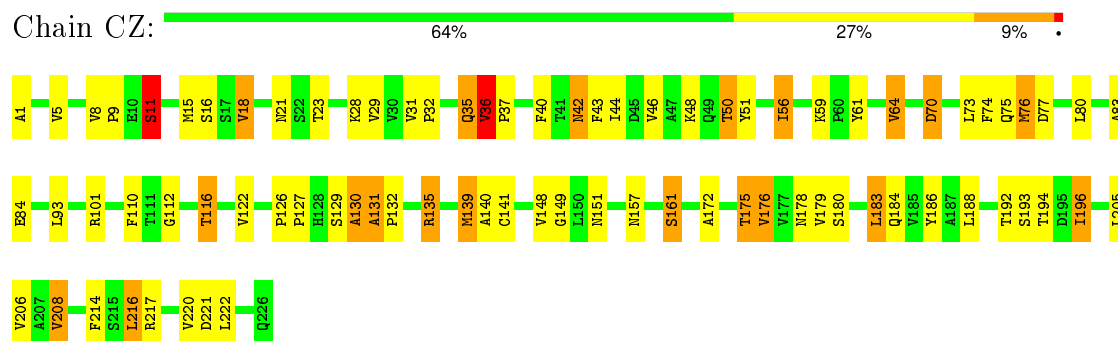


- Molecule 3: P1

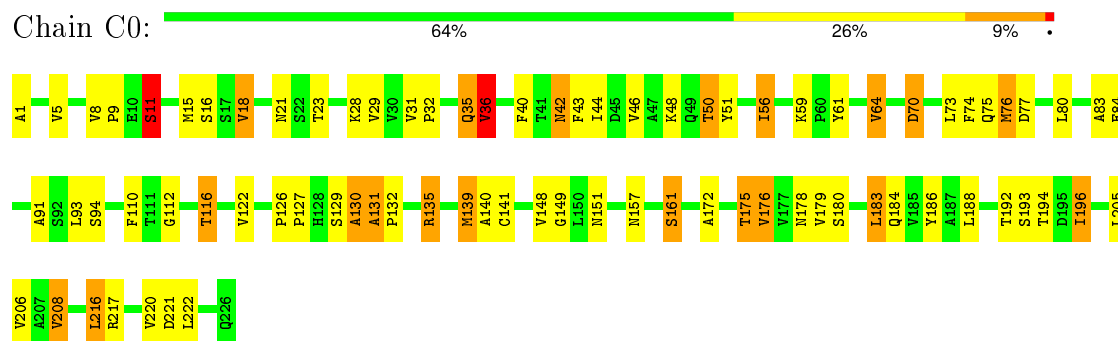


- Molecule 3: P1

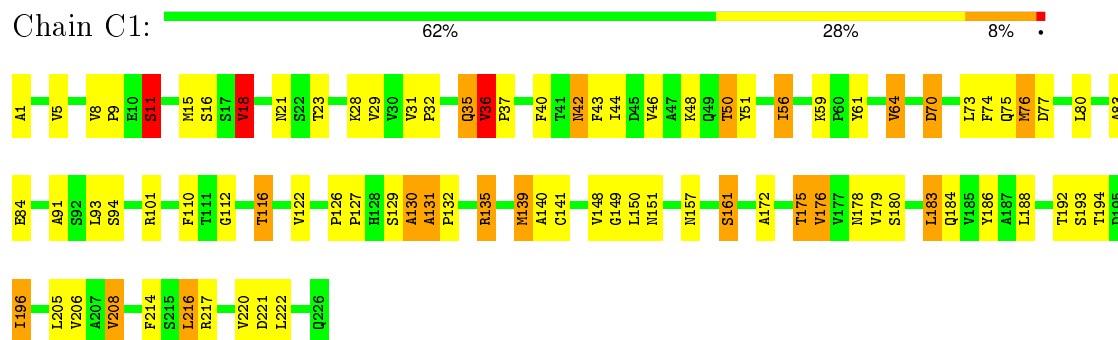




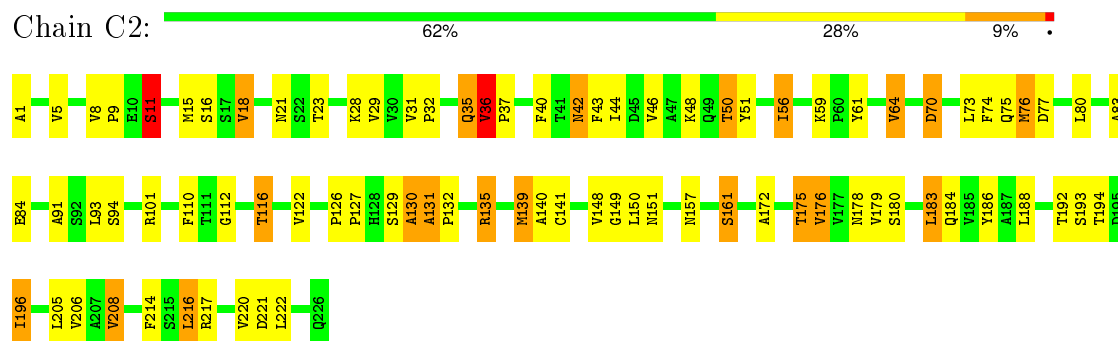
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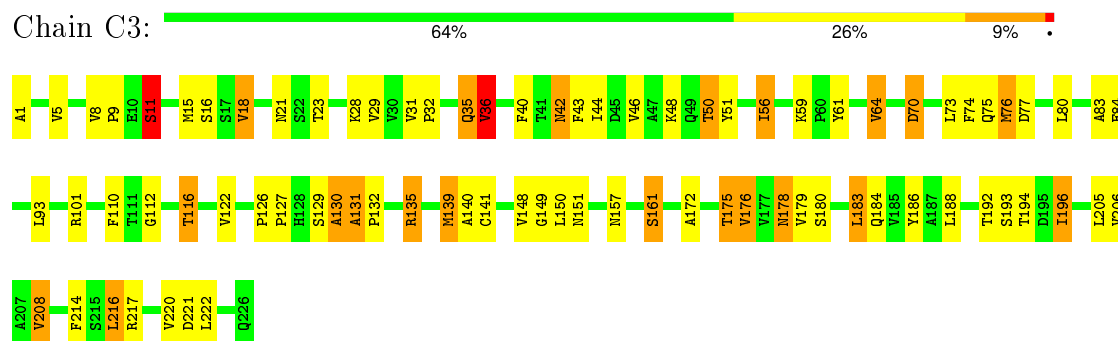
- Molecule 3: P1



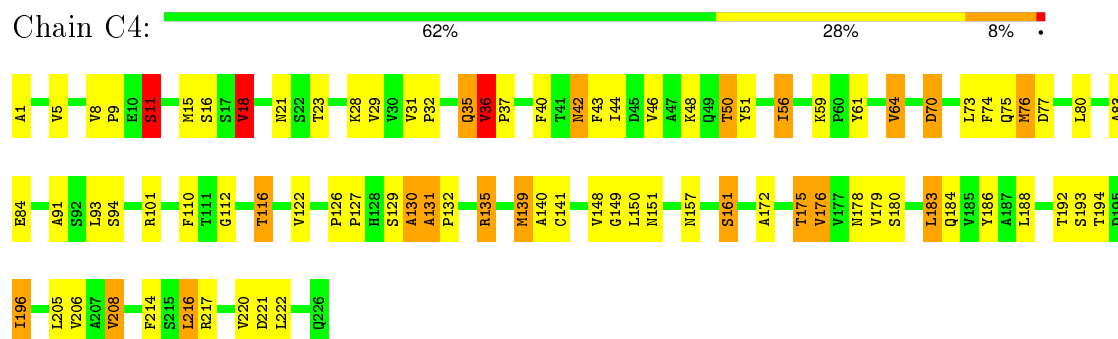
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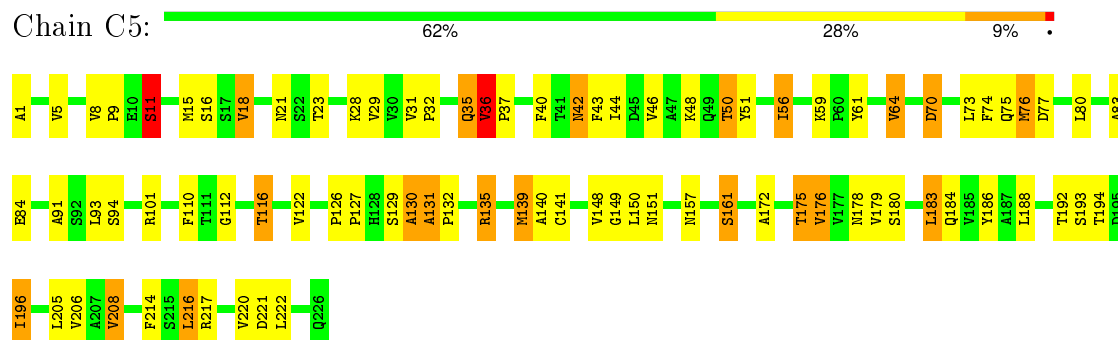
- Molecule 3: P1



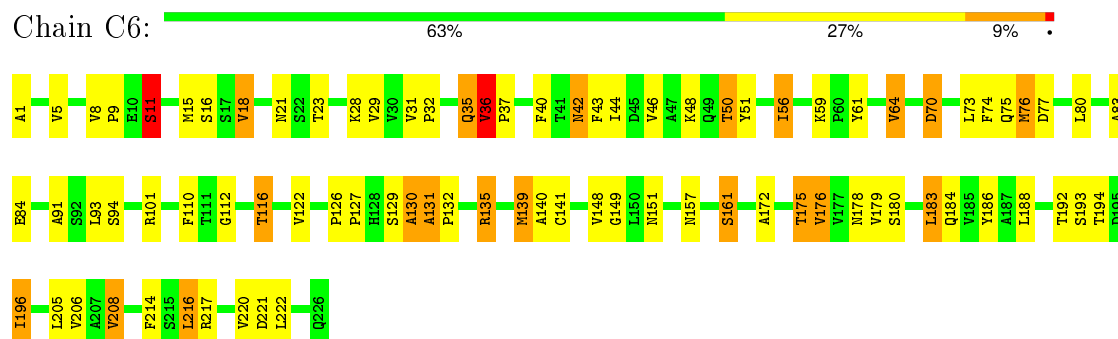
- Molecule 3: P1



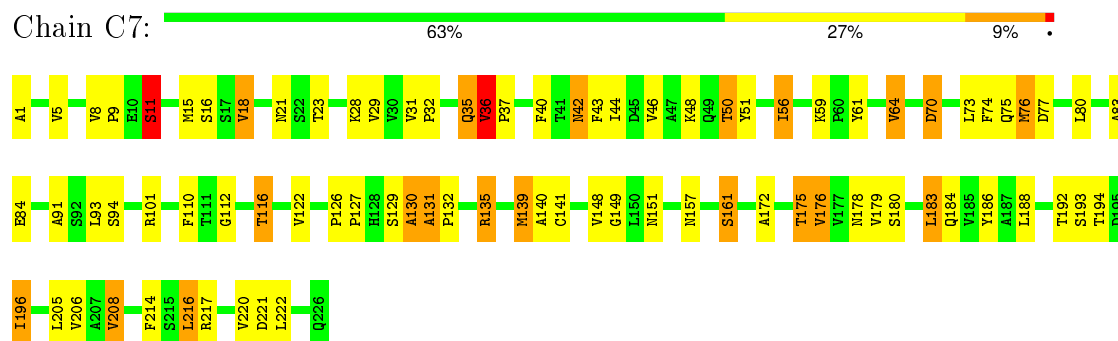
- Molecule 3: P1



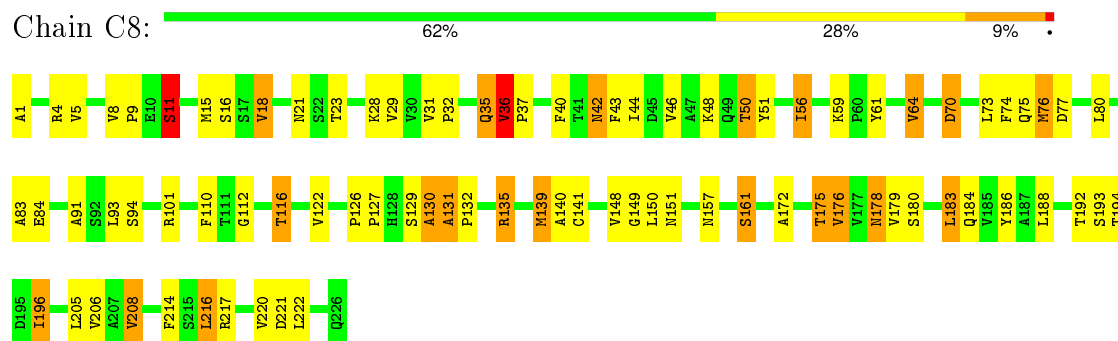
- Molecule 3: P1



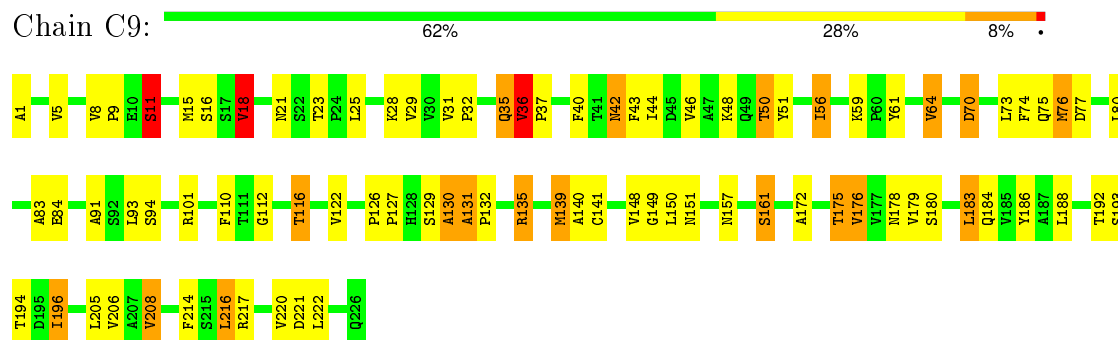
- Molecule 3: P1



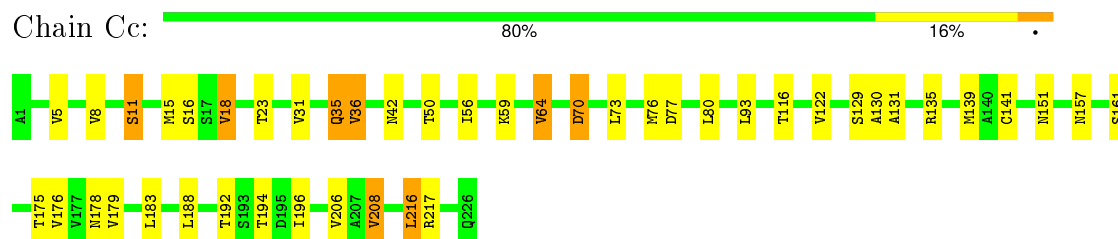
- Molecule 3: P1



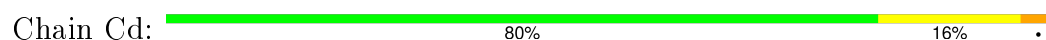
- Molecule 3: P1

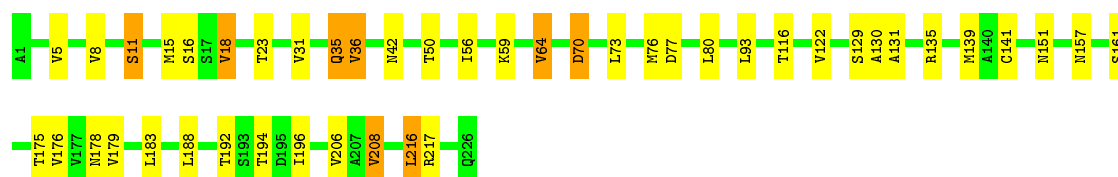


- Molecule 3: P1



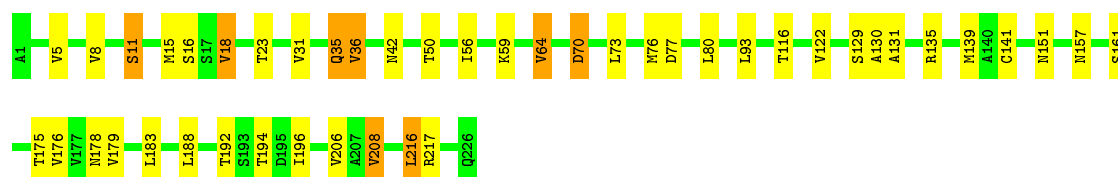
- Molecule 3: P1





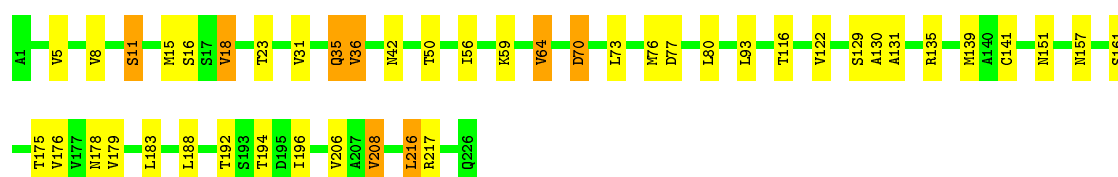
- Molecule 3: P1

Chain Ce: 80% 16%



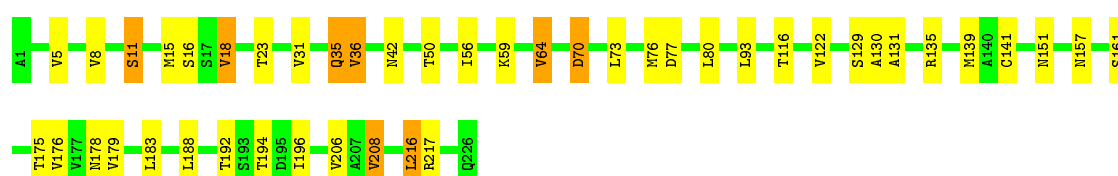
- Molecule 3: P1

Chain Cf: 80% 16%



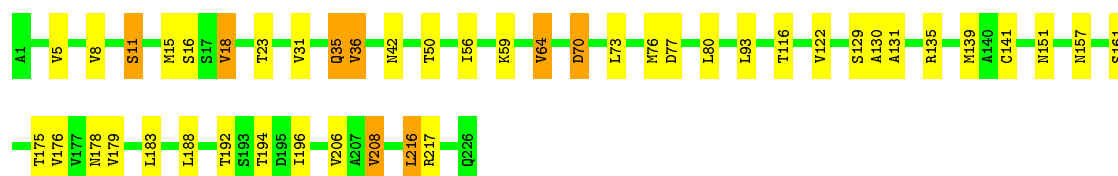
- Molecule 3: P1

Chain Cg: 80% 16%



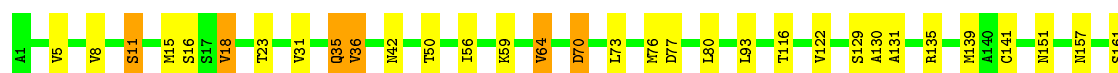
- Molecule 3: P1

Chain Ch: 80% 16%



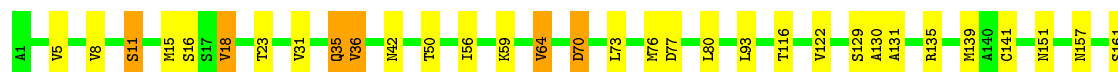
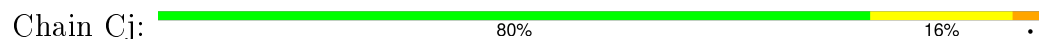
- Molecule 3: P1

Chain Ci: 80% 16%

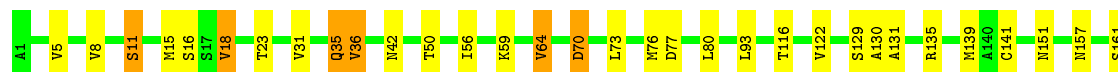
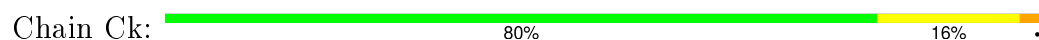




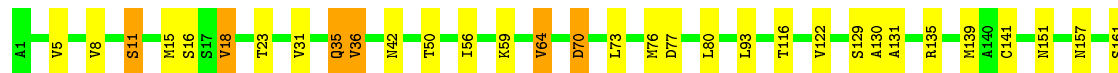
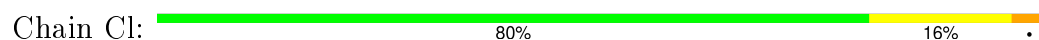
- Molecule 3: P1



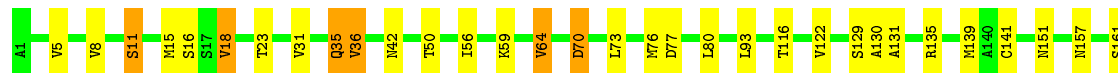
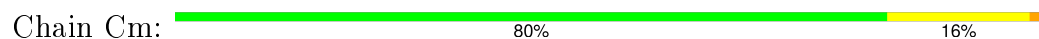
- Molecule 3: P1



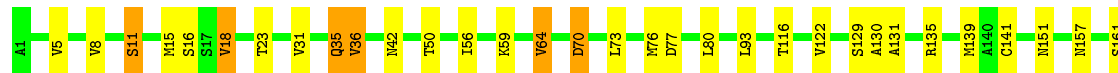
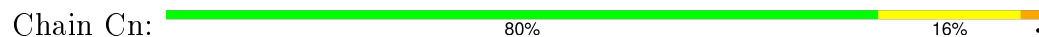
- Molecule 3: P1



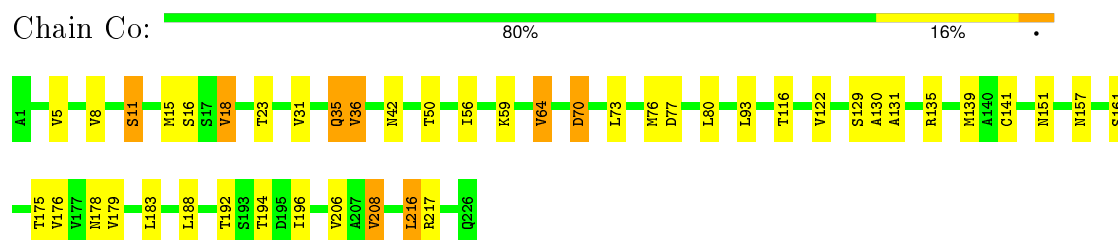
- Molecule 3: P1



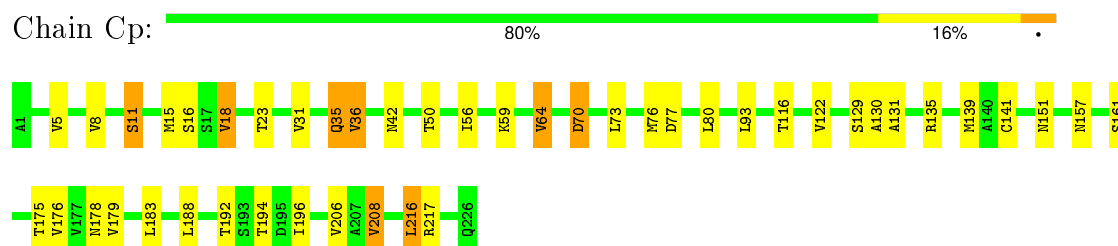
- Molecule 3: P1



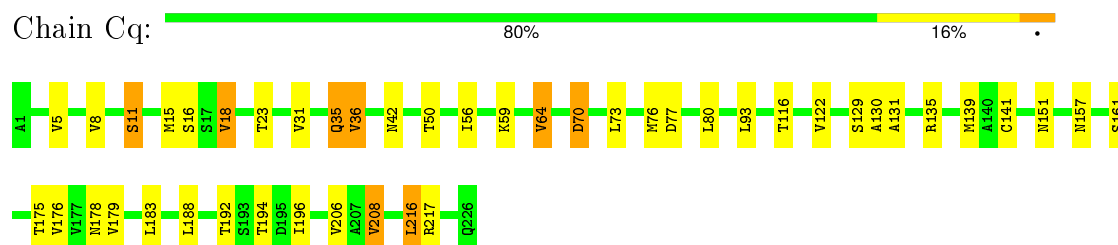
- Molecule 3: P1



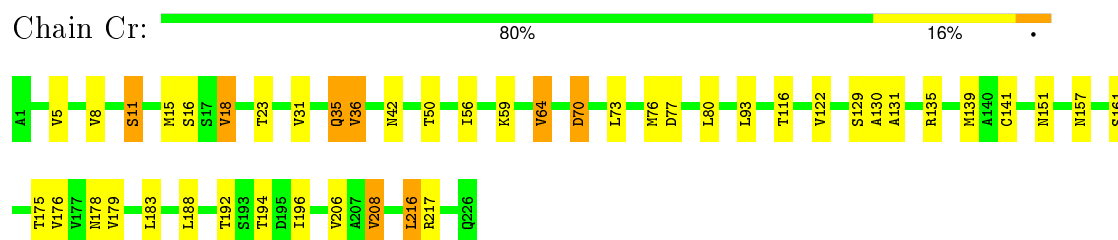
- Molecule 3: P1



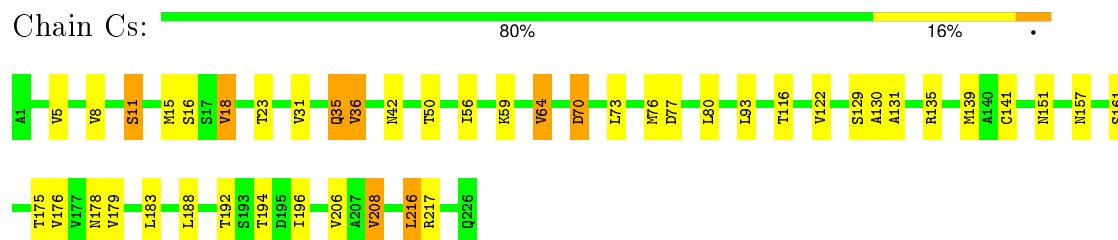
- Molecule 3: P1



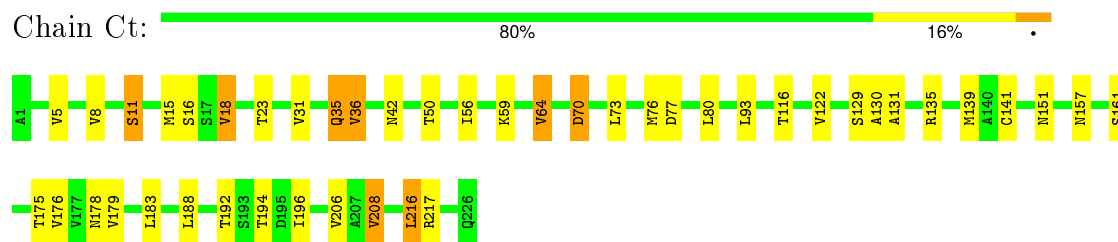
- Molecule 3: P1



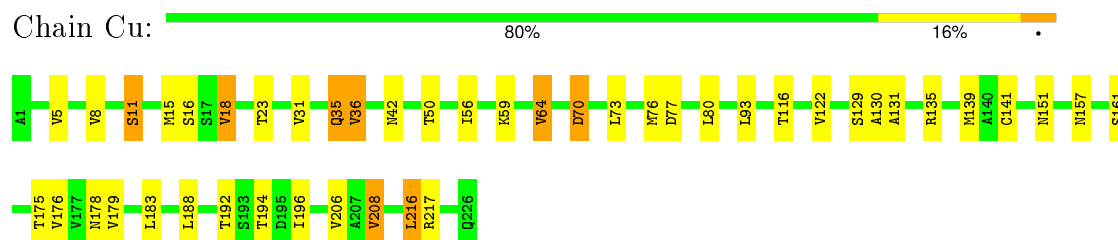
- Molecule 3: P1



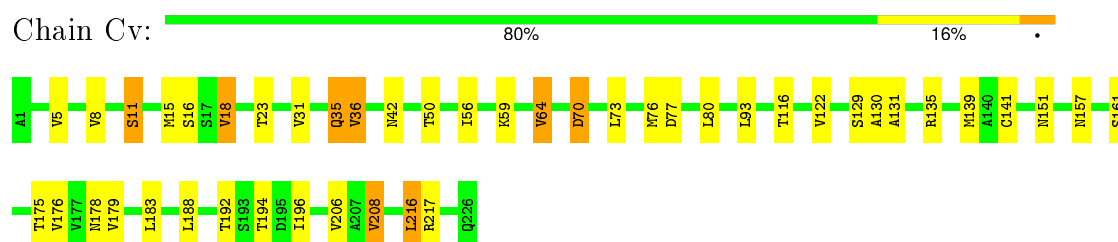
- Molecule 3: P1



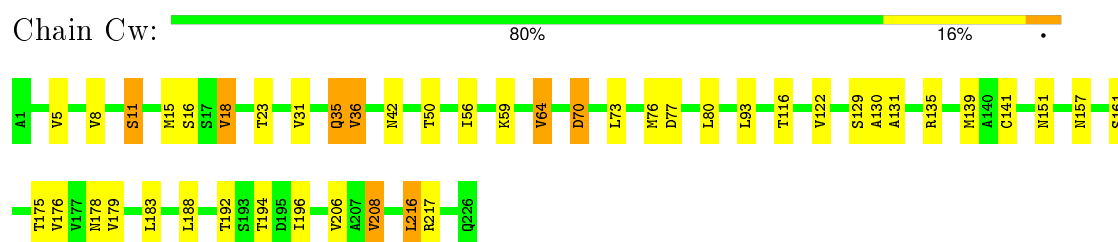
- Molecule 3: P1



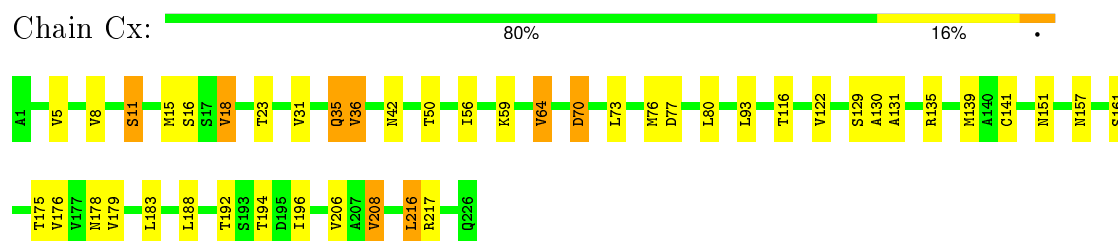
- Molecule 3: P1



- Molecule 3: P1

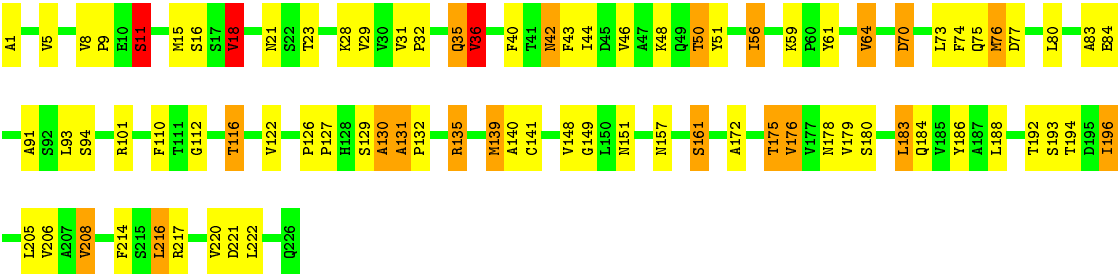


- Molecule 3: P1

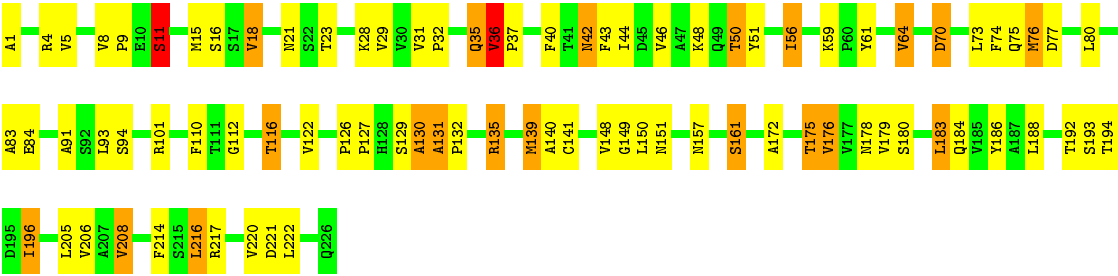


- Molecule 3: P1





● Molecule 3: P1





## 4 Experimental information

| Property                             | Value                         | Source    |
|--------------------------------------|-------------------------------|-----------|
| Reconstruction method                | SINGLE PARTICLE               | Depositor |
| Imposed symmetry                     | POINT, Not provided           | Depositor |
| Number of images                     | Not provided                  | Depositor |
| Resolution determination method      | Not provided                  | Depositor |
| CTF correction method                | PHASE FLIPPING, EACH PARTICLE | Depositor |
| Microscope                           | FEI TECNAI F20                | Depositor |
| Voltage (kV)                         | 200                           | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 15                            | Depositor |
| Minimum defocus (nm)                 | Not provided                  | Depositor |
| Maximum defocus (nm)                 | Not provided                  | Depositor |
| Magnification                        | Not provided                  | Depositor |
| Image detector                       | GATAN US4000SP                | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |             | Bond angles |                |
|-----|-------|--------------|-------------|-------------|----------------|
|     |       | RMSZ         | $\# Z  > 2$ | RMSZ        | $\# Z  > 2$    |
| 1   | A0    | 0.77         | 0/1992      | 1.12        | 17/2721 (0.6%) |
| 1   | A1    | 0.76         | 0/1992      | 1.12        | 17/2721 (0.6%) |
| 1   | A2    | 0.76         | 0/1992      | 1.13        | 17/2721 (0.6%) |
| 1   | A3    | 0.76         | 0/1992      | 1.12        | 17/2721 (0.6%) |
| 1   | A4    | 0.76         | 0/1992      | 1.12        | 17/2721 (0.6%) |
| 1   | A5    | 0.76         | 0/1992      | 1.13        | 17/2721 (0.6%) |
| 1   | A6    | 0.77         | 0/1992      | 1.12        | 17/2721 (0.6%) |
| 1   | A7    | 0.76         | 0/1992      | 1.12        | 18/2721 (0.7%) |
| 1   | A8    | 0.76         | 0/1992      | 1.13        | 17/2721 (0.6%) |
| 1   | A9    | 0.76         | 0/1992      | 1.12        | 17/2721 (0.6%) |
| 1   | AA    | 0.76         | 0/1992      | 1.12        | 17/2721 (0.6%) |
| 1   | AB    | 0.76         | 0/1992      | 1.12        | 17/2721 (0.6%) |
| 1   | AC    | 0.76         | 0/1992      | 1.12        | 17/2721 (0.6%) |
| 1   | AD    | 0.76         | 0/1992      | 1.12        | 17/2721 (0.6%) |
| 1   | AE    | 0.76         | 0/1992      | 1.12        | 18/2721 (0.7%) |
| 1   | AF    | 0.76         | 0/1992      | 1.12        | 18/2721 (0.7%) |
| 1   | AG    | 0.76         | 0/1992      | 1.12        | 17/2721 (0.6%) |
| 1   | AH    | 0.76         | 0/1992      | 1.12        | 17/2721 (0.6%) |
| 1   | AI    | 0.76         | 0/1992      | 1.12        | 17/2721 (0.6%) |
| 1   | AJ    | 0.76         | 0/1992      | 1.12        | 17/2721 (0.6%) |
| 1   | AK    | 0.76         | 0/1992      | 1.12        | 18/2721 (0.7%) |
| 1   | AL    | 0.76         | 0/1992      | 1.12        | 17/2721 (0.6%) |
| 1   | AM    | 0.76         | 0/1992      | 1.12        | 17/2721 (0.6%) |
| 1   | AN    | 0.77         | 0/1992      | 1.12        | 17/2721 (0.6%) |
| 1   | AO    | 0.76         | 0/1992      | 1.12        | 18/2721 (0.7%) |
| 1   | AP    | 0.76         | 0/1992      | 1.12        | 17/2721 (0.6%) |
| 1   | AQ    | 0.77         | 0/1992      | 1.12        | 17/2721 (0.6%) |
| 1   | AR    | 0.76         | 0/1992      | 1.12        | 17/2721 (0.6%) |
| 1   | AS    | 0.76         | 0/1992      | 1.12        | 18/2721 (0.7%) |
| 1   | AT    | 0.76         | 0/1992      | 1.12        | 17/2721 (0.6%) |
| 1   | AU    | 0.76         | 0/1992      | 1.12        | 17/2721 (0.6%) |
| 1   | AV    | 0.76         | 0/1992      | 1.12        | 17/2721 (0.6%) |
| 1   | AW    | 0.76         | 0/1992      | 1.12        | 17/2721 (0.6%) |
| 1   | AX    | 0.76         | 0/1992      | 1.12        | 18/2721 (0.7%) |

| Mol | Chain | Bond lengths |               | Bond angles |                |
|-----|-------|--------------|---------------|-------------|----------------|
|     |       | RMSZ         | # Z  >2       | RMSZ        | # Z  >2        |
| 1   | AY    | 0.76         | 0/1992        | 1.12        | 17/2721 (0.6%) |
| 1   | AZ    | 0.77         | 0/1992        | 1.12        | 17/2721 (0.6%) |
| 1   | Aa    | 0.76         | 0/1992        | 1.12        | 17/2721 (0.6%) |
| 1   | Ab    | 0.76         | 0/1992        | 1.12        | 17/2721 (0.6%) |
| 1   | Ac    | 0.77         | 0/1992        | 1.12        | 18/2721 (0.7%) |
| 1   | Ad    | 0.76         | 0/1992        | 1.12        | 17/2721 (0.6%) |
| 1   | Ae    | 0.76         | 0/1992        | 1.12        | 17/2721 (0.6%) |
| 1   | Af    | 0.76         | 0/1992        | 1.12        | 17/2721 (0.6%) |
| 1   | Ag    | 0.76         | 0/1992        | 1.12        | 17/2721 (0.6%) |
| 1   | Ah    | 0.76         | 0/1992        | 1.12        | 18/2721 (0.7%) |
| 1   | Ai    | 0.76         | 0/1992        | 1.12        | 18/2721 (0.7%) |
| 1   | Aj    | 0.76         | 0/1992        | 1.12        | 17/2721 (0.6%) |
| 1   | Ak    | 0.76         | 0/1992        | 1.12        | 17/2721 (0.6%) |
| 1   | Al    | 0.76         | 0/1992        | 1.12        | 17/2721 (0.6%) |
| 1   | Am    | 0.76         | 0/1992        | 1.12        | 17/2721 (0.6%) |
| 1   | An    | 0.76         | 0/1992        | 1.12        | 17/2721 (0.6%) |
| 1   | Ao    | 0.76         | 0/1992        | 1.12        | 17/2721 (0.6%) |
| 1   | DC    | 0.76         | 0/1992        | 1.12        | 17/2721 (0.6%) |
| 1   | DD    | 0.76         | 0/1992        | 1.12        | 17/2721 (0.6%) |
| 1   | DE    | 0.76         | 0/1992        | 1.12        | 17/2721 (0.6%) |
| 1   | DF    | 0.76         | 0/1992        | 1.12        | 17/2721 (0.6%) |
| 1   | DG    | 0.76         | 0/1992        | 1.12        | 17/2721 (0.6%) |
| 1   | DH    | 0.76         | 0/1992        | 1.12        | 17/2721 (0.6%) |
| 1   | DI    | 0.76         | 0/1992        | 1.12        | 17/2721 (0.6%) |
| 1   | DJ    | 0.76         | 0/1992        | 1.12        | 17/2721 (0.6%) |
| 1   | DK    | 0.76         | 0/1992        | 1.12        | 17/2721 (0.6%) |
| 2   | B0    | 0.77         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%)  |
| 2   | B1    | 0.78         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%)  |
| 2   | B2    | 0.78         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%)  |
| 2   | B3    | 0.78         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%)  |
| 2   | B4    | 0.77         | 1/1607 (0.1%) | 0.99        | 7/2208 (0.3%)  |
| 2   | B5    | 0.78         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%)  |
| 2   | B6    | 0.77         | 1/1607 (0.1%) | 0.99        | 7/2208 (0.3%)  |
| 2   | B7    | 0.78         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%)  |
| 2   | B8    | 0.77         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%)  |
| 2   | B9    | 0.77         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%)  |
| 2   | BA    | 0.77         | 1/1607 (0.1%) | 0.99        | 7/2208 (0.3%)  |
| 2   | BB    | 0.77         | 1/1607 (0.1%) | 0.99        | 7/2208 (0.3%)  |
| 2   | BC    | 0.77         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%)  |
| 2   | BD    | 0.78         | 1/1607 (0.1%) | 0.99        | 7/2208 (0.3%)  |
| 2   | BE    | 0.77         | 1/1607 (0.1%) | 0.99        | 7/2208 (0.3%)  |
| 2   | BF    | 0.77         | 1/1607 (0.1%) | 0.99        | 7/2208 (0.3%)  |
| 2   | BG    | 0.77         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%)  |

| Mol | Chain | Bond lengths |               | Bond angles |               |
|-----|-------|--------------|---------------|-------------|---------------|
|     |       | RMSZ         | # Z  >2       | RMSZ        | # Z  >2       |
| 2   | BH    | 0.78         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |
| 2   | BI    | 0.78         | 1/1607 (0.1%) | 0.99        | 7/2208 (0.3%) |
| 2   | BJ    | 0.77         | 1/1607 (0.1%) | 0.99        | 7/2208 (0.3%) |
| 2   | BK    | 0.77         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |
| 2   | BL    | 0.78         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |
| 2   | BM    | 0.78         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |
| 2   | BN    | 0.78         | 1/1607 (0.1%) | 0.99        | 7/2208 (0.3%) |
| 2   | BO    | 0.78         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |
| 2   | BP    | 0.78         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |
| 2   | BQ    | 0.77         | 1/1607 (0.1%) | 0.99        | 7/2208 (0.3%) |
| 2   | BR    | 0.77         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |
| 2   | BS    | 0.77         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |
| 2   | BT    | 0.77         | 1/1607 (0.1%) | 0.99        | 7/2208 (0.3%) |
| 2   | BU    | 0.78         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |
| 2   | BV    | 0.77         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |
| 2   | BW    | 0.78         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |
| 2   | BX    | 0.78         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |
| 2   | BY    | 0.78         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |
| 2   | BZ    | 0.77         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |
| 2   | Ba    | 0.78         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |
| 2   | Bb    | 0.77         | 1/1607 (0.1%) | 0.99        | 7/2208 (0.3%) |
| 2   | Bc    | 0.77         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |
| 2   | Bd    | 0.77         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |
| 2   | Be    | 0.78         | 1/1607 (0.1%) | 0.99        | 7/2208 (0.3%) |
| 2   | Bf    | 0.77         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |
| 2   | Bg    | 0.78         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |
| 2   | Bh    | 0.77         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |
| 2   | Bi    | 0.78         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |
| 2   | Bj    | 0.77         | 1/1607 (0.1%) | 0.99        | 7/2208 (0.3%) |
| 2   | Bk    | 0.78         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |
| 2   | Bl    | 0.77         | 1/1607 (0.1%) | 0.99        | 8/2208 (0.4%) |
| 2   | Bm    | 0.77         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |
| 2   | Bn    | 0.78         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |
| 2   | Bo    | 0.77         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |
| 2   | Bp    | 0.78         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |
| 2   | Bq    | 0.77         | 1/1607 (0.1%) | 0.99        | 8/2208 (0.4%) |
| 2   | Br    | 0.77         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |
| 2   | Bs    | 0.78         | 1/1607 (0.1%) | 0.99        | 7/2208 (0.3%) |
| 2   | Bt    | 0.78         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |
| 2   | Bu    | 0.78         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |
| 2   | Bv    | 0.77         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |
| 2   | Bw    | 0.77         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |
| 2   | Bx    | 0.77         | 1/1607 (0.1%) | 0.99        | 6/2208 (0.3%) |

| Mol | Chain | Bond lengths |               | Bond angles |               |
|-----|-------|--------------|---------------|-------------|---------------|
|     |       | RMSZ         | # Z  >2       | RMSZ        | # Z  >2       |
| 3   | C0    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | C1    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | C2    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | C3    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | C4    | 0.82         | 1/1768 (0.1%) | 1.04        | 6/2420 (0.2%) |
| 3   | C5    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | C6    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | C7    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | C8    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | C9    | 0.82         | 1/1768 (0.1%) | 1.04        | 6/2420 (0.2%) |
| 3   | CA    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | CB    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | CC    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | CD    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | CE    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | CF    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | CG    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | CH    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | CI    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | CJ    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | CK    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | CL    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | CM    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | CN    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | CO    | 0.82         | 1/1768 (0.1%) | 1.04        | 6/2420 (0.2%) |
| 3   | CP    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | CQ    | 0.82         | 1/1768 (0.1%) | 1.04        | 6/2420 (0.2%) |
| 3   | CR    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | CS    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | CT    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | CU    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | CV    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | CW    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | CX    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | CY    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | CZ    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | Cc    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | Cd    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | Ce    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | Cf    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | Cg    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | Ch    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |
| 3   | Ci    | 0.82         | 1/1768 (0.1%) | 1.03        | 6/2420 (0.2%) |

| Mol | Chain | Bond lengths |                   | Bond angles |                    |
|-----|-------|--------------|-------------------|-------------|--------------------|
|     |       | RMSZ         | # Z  >2           | RMSZ        | # Z  >2            |
| 3   | Cj    | 0.82         | 1/1768 (0.1%)     | 1.04        | 6/2420 (0.2%)      |
| 3   | Ck    | 0.82         | 1/1768 (0.1%)     | 1.03        | 7/2420 (0.3%)      |
| 3   | Cl    | 0.82         | 1/1768 (0.1%)     | 1.03        | 6/2420 (0.2%)      |
| 3   | Cm    | 0.82         | 1/1768 (0.1%)     | 1.03        | 6/2420 (0.2%)      |
| 3   | Cn    | 0.82         | 1/1768 (0.1%)     | 1.03        | 6/2420 (0.2%)      |
| 3   | Co    | 0.82         | 1/1768 (0.1%)     | 1.03        | 6/2420 (0.2%)      |
| 3   | Cp    | 0.82         | 1/1768 (0.1%)     | 1.03        | 6/2420 (0.2%)      |
| 3   | Cq    | 0.82         | 1/1768 (0.1%)     | 1.03        | 6/2420 (0.2%)      |
| 3   | Cr    | 0.82         | 1/1768 (0.1%)     | 1.03        | 6/2420 (0.2%)      |
| 3   | Cs    | 0.82         | 1/1768 (0.1%)     | 1.03        | 6/2420 (0.2%)      |
| 3   | Ct    | 0.82         | 1/1768 (0.1%)     | 1.03        | 6/2420 (0.2%)      |
| 3   | Cu    | 0.82         | 1/1768 (0.1%)     | 1.03        | 6/2420 (0.2%)      |
| 3   | Cv    | 0.82         | 1/1768 (0.1%)     | 1.03        | 6/2420 (0.2%)      |
| 3   | Cw    | 0.82         | 1/1768 (0.1%)     | 1.03        | 6/2420 (0.2%)      |
| 3   | Cx    | 0.82         | 1/1768 (0.1%)     | 1.03        | 6/2420 (0.2%)      |
| 3   | DA    | 0.82         | 1/1768 (0.1%)     | 1.03        | 6/2420 (0.2%)      |
| 3   | DB    | 0.82         | 1/1768 (0.1%)     | 1.03        | 6/2420 (0.2%)      |
| All | All   | 0.79         | 120/322020 (0.0%) | 1.06        | 1771/440940 (0.4%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A0    | 0                   | 1                   |
| 1   | A1    | 0                   | 1                   |
| 1   | A2    | 0                   | 1                   |
| 1   | A3    | 0                   | 1                   |
| 1   | A4    | 0                   | 1                   |
| 1   | A5    | 0                   | 1                   |
| 1   | A6    | 0                   | 1                   |
| 1   | A7    | 0                   | 1                   |
| 1   | A8    | 0                   | 1                   |
| 1   | A9    | 0                   | 1                   |
| 1   | AA    | 0                   | 1                   |
| 1   | AB    | 0                   | 1                   |
| 1   | AC    | 0                   | 1                   |
| 1   | AD    | 0                   | 1                   |
| 1   | AE    | 0                   | 1                   |
| 1   | AF    | 0                   | 1                   |
| 1   | AG    | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | AH    | 0                   | 1                   |
| 1   | AI    | 0                   | 1                   |
| 1   | AJ    | 0                   | 1                   |
| 1   | AK    | 0                   | 1                   |
| 1   | AL    | 0                   | 1                   |
| 1   | AM    | 0                   | 1                   |
| 1   | AN    | 0                   | 1                   |
| 1   | AO    | 0                   | 1                   |
| 1   | AP    | 0                   | 1                   |
| 1   | AQ    | 0                   | 1                   |
| 1   | AR    | 0                   | 1                   |
| 1   | AS    | 0                   | 1                   |
| 1   | AT    | 0                   | 1                   |
| 1   | AU    | 0                   | 1                   |
| 1   | AV    | 0                   | 1                   |
| 1   | AW    | 0                   | 1                   |
| 1   | AX    | 0                   | 1                   |
| 1   | AY    | 0                   | 1                   |
| 1   | AZ    | 0                   | 1                   |
| 1   | Aa    | 0                   | 1                   |
| 1   | Ab    | 0                   | 1                   |
| 1   | Ac    | 0                   | 1                   |
| 1   | Ad    | 0                   | 1                   |
| 1   | Ae    | 0                   | 1                   |
| 1   | Af    | 0                   | 1                   |
| 1   | Ag    | 0                   | 1                   |
| 1   | Ah    | 0                   | 1                   |
| 1   | Ai    | 0                   | 1                   |
| 1   | Aj    | 0                   | 1                   |
| 1   | Ak    | 0                   | 1                   |
| 1   | Al    | 0                   | 1                   |
| 1   | Am    | 0                   | 1                   |
| 1   | An    | 0                   | 1                   |
| 1   | Ao    | 0                   | 1                   |
| 1   | DC    | 0                   | 1                   |
| 1   | DD    | 0                   | 1                   |
| 1   | DE    | 0                   | 1                   |
| 1   | DF    | 0                   | 1                   |
| 1   | DG    | 0                   | 1                   |
| 1   | DH    | 0                   | 1                   |
| 1   | DI    | 0                   | 1                   |
| 1   | DJ    | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | DK    | 0                   | 1                   |
| 2   | B0    | 0                   | 2                   |
| 2   | B1    | 0                   | 2                   |
| 2   | B2    | 0                   | 2                   |
| 2   | B3    | 0                   | 2                   |
| 2   | B4    | 0                   | 2                   |
| 2   | B5    | 0                   | 2                   |
| 2   | B6    | 0                   | 2                   |
| 2   | B7    | 0                   | 2                   |
| 2   | B8    | 0                   | 2                   |
| 2   | B9    | 0                   | 2                   |
| 2   | BA    | 0                   | 2                   |
| 2   | BB    | 0                   | 2                   |
| 2   | BC    | 0                   | 2                   |
| 2   | BD    | 0                   | 2                   |
| 2   | BE    | 0                   | 2                   |
| 2   | BF    | 0                   | 2                   |
| 2   | BG    | 0                   | 2                   |
| 2   | BH    | 0                   | 2                   |
| 2   | BI    | 0                   | 2                   |
| 2   | BJ    | 0                   | 2                   |
| 2   | BK    | 0                   | 2                   |
| 2   | BL    | 0                   | 2                   |
| 2   | BM    | 0                   | 2                   |
| 2   | BN    | 0                   | 2                   |
| 2   | BO    | 0                   | 2                   |
| 2   | BP    | 0                   | 2                   |
| 2   | BQ    | 0                   | 2                   |
| 2   | BR    | 0                   | 2                   |
| 2   | BS    | 0                   | 2                   |
| 2   | BT    | 0                   | 2                   |
| 2   | BU    | 0                   | 2                   |
| 2   | BV    | 0                   | 2                   |
| 2   | BW    | 0                   | 2                   |
| 2   | BX    | 0                   | 2                   |
| 2   | BY    | 0                   | 2                   |
| 2   | BZ    | 0                   | 2                   |
| 2   | Ba    | 0                   | 2                   |
| 2   | Bb    | 0                   | 2                   |
| 2   | Bc    | 0                   | 2                   |
| 2   | Bd    | 0                   | 2                   |
| 2   | Be    | 0                   | 2                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | Bf    | 0                   | 2                   |
| 2   | Bg    | 0                   | 2                   |
| 2   | Bh    | 0                   | 2                   |
| 2   | Bi    | 0                   | 2                   |
| 2   | Bj    | 0                   | 2                   |
| 2   | Bk    | 0                   | 2                   |
| 2   | Bl    | 0                   | 2                   |
| 2   | Bm    | 0                   | 2                   |
| 2   | Bn    | 0                   | 2                   |
| 2   | Bo    | 0                   | 2                   |
| 2   | Bp    | 0                   | 2                   |
| 2   | Bq    | 0                   | 2                   |
| 2   | Br    | 0                   | 2                   |
| 2   | Bs    | 0                   | 2                   |
| 2   | Bt    | 0                   | 2                   |
| 2   | Bu    | 0                   | 2                   |
| 2   | Bv    | 0                   | 2                   |
| 2   | Bw    | 0                   | 2                   |
| 2   | Bx    | 0                   | 2                   |
| All | All   | 0                   | 180                 |

All (120) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | B2    | 222 | VAL  | CB-CG1 | -5.18 | 1.42        | 1.52     |
| 3   | Cc    | 141 | CYS  | CB-SG  | -5.17 | 1.73        | 1.81     |
| 3   | Cg    | 141 | CYS  | CB-SG  | -5.16 | 1.73        | 1.81     |
| 3   | C1    | 141 | CYS  | CB-SG  | -5.15 | 1.73        | 1.81     |
| 3   | Cq    | 141 | CYS  | CB-SG  | -5.15 | 1.73        | 1.81     |
| 3   | CN    | 141 | CYS  | CB-SG  | -5.15 | 1.73        | 1.81     |
| 2   | BK    | 222 | VAL  | CB-CG1 | -5.14 | 1.42        | 1.52     |
| 2   | BO    | 222 | VAL  | CB-CG1 | -5.14 | 1.42        | 1.52     |
| 2   | BU    | 222 | VAL  | CB-CG1 | -5.14 | 1.42        | 1.52     |
| 2   | B4    | 222 | VAL  | CB-CG1 | -5.14 | 1.42        | 1.52     |
| 2   | B6    | 222 | VAL  | CB-CG1 | -5.14 | 1.42        | 1.52     |
| 2   | Bn    | 222 | VAL  | CB-CG1 | -5.14 | 1.42        | 1.52     |
| 2   | B3    | 222 | VAL  | CB-CG1 | -5.14 | 1.42        | 1.52     |
| 2   | BR    | 222 | VAL  | CB-CG1 | -5.13 | 1.42        | 1.52     |
| 2   | BX    | 222 | VAL  | CB-CG1 | -5.13 | 1.42        | 1.52     |
| 3   | C5    | 141 | CYS  | CB-SG  | -5.13 | 1.73        | 1.81     |
| 3   | Cf    | 141 | CYS  | CB-SG  | -5.13 | 1.73        | 1.81     |
| 2   | Bc    | 222 | VAL  | CB-CG1 | -5.13 | 1.42        | 1.52     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | Bg    | 222 | VAL  | CB-CG1 | -5.13 | 1.42        | 1.52     |
| 2   | Bm    | 222 | VAL  | CB-CG1 | -5.13 | 1.42        | 1.52     |
| 3   | CC    | 141 | CYS  | CB-SG  | -5.13 | 1.73        | 1.81     |
| 3   | Cx    | 141 | CYS  | CB-SG  | -5.13 | 1.73        | 1.81     |
| 2   | B8    | 222 | VAL  | CB-CG1 | -5.12 | 1.42        | 1.52     |
| 2   | BE    | 222 | VAL  | CB-CG1 | -5.12 | 1.42        | 1.52     |
| 2   | Bd    | 222 | VAL  | CB-CG1 | -5.12 | 1.42        | 1.52     |
| 2   | Bb    | 222 | VAL  | CB-CG1 | -5.12 | 1.42        | 1.52     |
| 3   | Ch    | 141 | CYS  | CB-SG  | -5.12 | 1.73        | 1.81     |
| 2   | BS    | 222 | VAL  | CB-CG1 | -5.12 | 1.42        | 1.52     |
| 2   | BT    | 222 | VAL  | CB-CG1 | -5.12 | 1.42        | 1.52     |
| 3   | CD    | 141 | CYS  | CB-SG  | -5.12 | 1.73        | 1.81     |
| 3   | Cv    | 141 | CYS  | CB-SG  | -5.12 | 1.73        | 1.81     |
| 2   | Bs    | 222 | VAL  | CB-CG1 | -5.12 | 1.42        | 1.52     |
| 3   | CW    | 141 | CYS  | CB-SG  | -5.12 | 1.73        | 1.81     |
| 2   | BD    | 222 | VAL  | CB-CG1 | -5.12 | 1.42        | 1.52     |
| 2   | Bo    | 222 | VAL  | CB-CG1 | -5.12 | 1.42        | 1.52     |
| 2   | BQ    | 222 | VAL  | CB-CG1 | -5.12 | 1.42        | 1.52     |
| 2   | Bh    | 222 | VAL  | CB-CG1 | -5.12 | 1.42        | 1.52     |
| 3   | C6    | 141 | CYS  | CB-SG  | -5.12 | 1.73        | 1.81     |
| 3   | Cr    | 141 | CYS  | CB-SG  | -5.12 | 1.73        | 1.81     |
| 2   | Bi    | 222 | VAL  | CB-CG1 | -5.11 | 1.42        | 1.52     |
| 2   | Bu    | 222 | VAL  | CB-CG1 | -5.11 | 1.42        | 1.52     |
| 3   | Cm    | 141 | CYS  | CB-SG  | -5.11 | 1.73        | 1.81     |
| 2   | Br    | 222 | VAL  | CB-CG1 | -5.11 | 1.42        | 1.52     |
| 2   | BA    | 222 | VAL  | CB-CG1 | -5.11 | 1.42        | 1.52     |
| 2   | BZ    | 222 | VAL  | CB-CG1 | -5.11 | 1.42        | 1.52     |
| 2   | Bw    | 222 | VAL  | CB-CG1 | -5.11 | 1.42        | 1.52     |
| 3   | CS    | 141 | CYS  | CB-SG  | -5.11 | 1.73        | 1.81     |
| 3   | C8    | 141 | CYS  | CB-SG  | -5.11 | 1.73        | 1.81     |
| 2   | BN    | 222 | VAL  | CB-CG1 | -5.10 | 1.42        | 1.52     |
| 3   | CA    | 141 | CYS  | CB-SG  | -5.10 | 1.73        | 1.81     |
| 3   | Ci    | 141 | CYS  | CB-SG  | -5.10 | 1.73        | 1.81     |
| 2   | Bj    | 222 | VAL  | CB-CG1 | -5.10 | 1.42        | 1.52     |
| 2   | Bv    | 222 | VAL  | CB-CG1 | -5.10 | 1.42        | 1.52     |
| 2   | BJ    | 222 | VAL  | CB-CG1 | -5.10 | 1.42        | 1.52     |
| 2   | B7    | 222 | VAL  | CB-CG1 | -5.10 | 1.42        | 1.52     |
| 2   | Bq    | 222 | VAL  | CB-CG1 | -5.10 | 1.42        | 1.52     |
| 3   | CL    | 141 | CYS  | CB-SG  | -5.10 | 1.73        | 1.81     |
| 3   | CR    | 141 | CYS  | CB-SG  | -5.10 | 1.73        | 1.81     |
| 3   | Cp    | 141 | CYS  | CB-SG  | -5.10 | 1.73        | 1.81     |
| 2   | BI    | 222 | VAL  | CB-CG1 | -5.10 | 1.42        | 1.52     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | CB    | 141 | CYS  | CB-SG  | -5.10 | 1.73        | 1.81     |
| 3   | Cw    | 141 | CYS  | CB-SG  | -5.10 | 1.73        | 1.81     |
| 2   | B0    | 222 | VAL  | CB-CG1 | -5.10 | 1.42        | 1.52     |
| 3   | C7    | 141 | CYS  | CB-SG  | -5.09 | 1.73        | 1.81     |
| 2   | B5    | 222 | VAL  | CB-CG1 | -5.09 | 1.42        | 1.52     |
| 3   | CV    | 141 | CYS  | CB-SG  | -5.09 | 1.73        | 1.81     |
| 2   | Bf    | 222 | VAL  | CB-CG1 | -5.09 | 1.42        | 1.52     |
| 3   | CM    | 141 | CYS  | CB-SG  | -5.09 | 1.73        | 1.81     |
| 3   | DA    | 141 | CYS  | CB-SG  | -5.09 | 1.73        | 1.81     |
| 3   | C2    | 141 | CYS  | CB-SG  | -5.09 | 1.73        | 1.81     |
| 3   | Cu    | 141 | CYS  | CB-SG  | -5.09 | 1.73        | 1.81     |
| 2   | Ba    | 222 | VAL  | CB-CG1 | -5.09 | 1.42        | 1.52     |
| 3   | CY    | 141 | CYS  | CB-SG  | -5.09 | 1.73        | 1.81     |
| 3   | C3    | 141 | CYS  | CB-SG  | -5.09 | 1.73        | 1.81     |
| 3   | CJ    | 141 | CYS  | CB-SG  | -5.08 | 1.73        | 1.81     |
| 2   | BB    | 222 | VAL  | CB-CG1 | -5.08 | 1.42        | 1.52     |
| 2   | BC    | 222 | VAL  | CB-CG1 | -5.08 | 1.42        | 1.52     |
| 2   | Bl    | 222 | VAL  | CB-CG1 | -5.08 | 1.42        | 1.52     |
| 2   | BM    | 222 | VAL  | CB-CG1 | -5.08 | 1.42        | 1.52     |
| 3   | DB    | 141 | CYS  | CB-SG  | -5.08 | 1.73        | 1.81     |
| 2   | BF    | 222 | VAL  | CB-CG1 | -5.08 | 1.42        | 1.52     |
| 2   | BP    | 222 | VAL  | CB-CG1 | -5.08 | 1.42        | 1.52     |
| 2   | Bp    | 222 | VAL  | CB-CG1 | -5.08 | 1.42        | 1.52     |
| 3   | CP    | 141 | CYS  | CB-SG  | -5.08 | 1.73        | 1.81     |
| 2   | BL    | 222 | VAL  | CB-CG1 | -5.07 | 1.42        | 1.52     |
| 2   | B9    | 222 | VAL  | CB-CG1 | -5.07 | 1.42        | 1.52     |
| 3   | CG    | 141 | CYS  | CB-SG  | -5.07 | 1.73        | 1.81     |
| 3   | CH    | 141 | CYS  | CB-SG  | -5.07 | 1.73        | 1.81     |
| 3   | CI    | 141 | CYS  | CB-SG  | -5.07 | 1.73        | 1.81     |
| 3   | CZ    | 141 | CYS  | CB-SG  | -5.07 | 1.73        | 1.81     |
| 2   | BW    | 222 | VAL  | CB-CG1 | -5.07 | 1.42        | 1.52     |
| 2   | B1    | 222 | VAL  | CB-CG1 | -5.07 | 1.42        | 1.52     |
| 3   | Cn    | 141 | CYS  | CB-SG  | -5.07 | 1.73        | 1.81     |
| 2   | Bk    | 222 | VAL  | CB-CG1 | -5.07 | 1.42        | 1.52     |
| 3   | Co    | 141 | CYS  | CB-SG  | -5.07 | 1.73        | 1.81     |
| 3   | Ce    | 141 | CYS  | CB-SG  | -5.06 | 1.73        | 1.81     |
| 3   | Ct    | 141 | CYS  | CB-SG  | -5.06 | 1.73        | 1.81     |
| 2   | BV    | 222 | VAL  | CB-CG1 | -5.06 | 1.42        | 1.52     |
| 3   | CF    | 141 | CYS  | CB-SG  | -5.06 | 1.73        | 1.81     |
| 2   | Bt    | 222 | VAL  | CB-CG1 | -5.06 | 1.42        | 1.52     |
| 3   | C9    | 141 | CYS  | CB-SG  | -5.06 | 1.73        | 1.81     |
| 3   | CU    | 141 | CYS  | CB-SG  | -5.05 | 1.73        | 1.81     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | CX    | 141 | CYS  | CB-SG  | -5.05 | 1.73        | 1.81     |
| 3   | C0    | 141 | CYS  | CB-SG  | -5.05 | 1.73        | 1.81     |
| 3   | Cs    | 141 | CYS  | CB-SG  | -5.05 | 1.73        | 1.81     |
| 3   | CQ    | 141 | CYS  | CB-SG  | -5.05 | 1.73        | 1.81     |
| 3   | Cd    | 141 | CYS  | CB-SG  | -5.05 | 1.73        | 1.81     |
| 2   | Be    | 222 | VAL  | CB-CG1 | -5.05 | 1.42        | 1.52     |
| 3   | Ck    | 141 | CYS  | CB-SG  | -5.04 | 1.73        | 1.81     |
| 3   | CE    | 141 | CYS  | CB-SG  | -5.04 | 1.73        | 1.81     |
| 3   | Cj    | 141 | CYS  | CB-SG  | -5.04 | 1.73        | 1.81     |
| 2   | BH    | 222 | VAL  | CB-CG1 | -5.04 | 1.42        | 1.52     |
| 2   | BY    | 222 | VAL  | CB-CG1 | -5.04 | 1.42        | 1.52     |
| 2   | Bx    | 222 | VAL  | CB-CG1 | -5.04 | 1.42        | 1.52     |
| 3   | CK    | 141 | CYS  | CB-SG  | -5.04 | 1.73        | 1.81     |
| 3   | C4    | 141 | CYS  | CB-SG  | -5.03 | 1.73        | 1.81     |
| 3   | CT    | 141 | CYS  | CB-SG  | -5.02 | 1.73        | 1.81     |
| 3   | Cl    | 141 | CYS  | CB-SG  | -5.02 | 1.73        | 1.81     |
| 3   | CO    | 141 | CYS  | CB-SG  | -5.01 | 1.73        | 1.81     |
| 2   | BG    | 222 | VAL  | CB-CG1 | -5.00 | 1.42        | 1.52     |

All (1771) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | DE    | 5   | GLY  | N-CA-C | 10.76 | 140.00      | 113.10   |
| 1   | Ah    | 5   | GLY  | N-CA-C | 10.76 | 140.00      | 113.10   |
| 1   | A1    | 5   | GLY  | N-CA-C | 10.76 | 139.99      | 113.10   |
| 1   | A2    | 5   | GLY  | N-CA-C | 10.75 | 139.97      | 113.10   |
| 1   | AM    | 5   | GLY  | N-CA-C | 10.75 | 139.97      | 113.10   |
| 1   | A5    | 5   | GLY  | N-CA-C | 10.75 | 139.96      | 113.10   |
| 1   | A7    | 5   | GLY  | N-CA-C | 10.75 | 139.97      | 113.10   |
| 1   | Am    | 5   | GLY  | N-CA-C | 10.74 | 139.96      | 113.10   |
| 1   | DI    | 5   | GLY  | N-CA-C | 10.74 | 139.96      | 113.10   |
| 1   | AV    | 5   | GLY  | N-CA-C | 10.74 | 139.96      | 113.10   |
| 1   | DK    | 5   | GLY  | N-CA-C | 10.74 | 139.96      | 113.10   |
| 1   | Ab    | 5   | GLY  | N-CA-C | 10.74 | 139.95      | 113.10   |
| 1   | AN    | 5   | GLY  | N-CA-C | 10.74 | 139.94      | 113.10   |
| 1   | A6    | 5   | GLY  | N-CA-C | 10.74 | 139.94      | 113.10   |
| 1   | Ai    | 5   | GLY  | N-CA-C | 10.74 | 139.94      | 113.10   |
| 1   | AS    | 5   | GLY  | N-CA-C | 10.73 | 139.94      | 113.10   |
| 1   | Ag    | 5   | GLY  | N-CA-C | 10.73 | 139.93      | 113.10   |
| 1   | AH    | 5   | GLY  | N-CA-C | 10.73 | 139.93      | 113.10   |
| 1   | DJ    | 5   | GLY  | N-CA-C | 10.73 | 139.93      | 113.10   |
| 1   | AC    | 5   | GLY  | N-CA-C | 10.73 | 139.93      | 113.10   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | AE    | 5   | GLY  | N-CA-C | 10.73 | 139.93      | 113.10   |
| 1   | AR    | 5   | GLY  | N-CA-C | 10.73 | 139.93      | 113.10   |
| 1   | AW    | 5   | GLY  | N-CA-C | 10.73 | 139.93      | 113.10   |
| 1   | Ad    | 5   | GLY  | N-CA-C | 10.73 | 139.93      | 113.10   |
| 1   | DD    | 5   | GLY  | N-CA-C | 10.73 | 139.93      | 113.10   |
| 1   | A9    | 5   | GLY  | N-CA-C | 10.73 | 139.92      | 113.10   |
| 1   | AP    | 5   | GLY  | N-CA-C | 10.73 | 139.92      | 113.10   |
| 1   | Aa    | 5   | GLY  | N-CA-C | 10.73 | 139.92      | 113.10   |
| 1   | Ac    | 5   | GLY  | N-CA-C | 10.73 | 139.92      | 113.10   |
| 1   | AX    | 5   | GLY  | N-CA-C | 10.72 | 139.91      | 113.10   |
| 1   | AI    | 5   | GLY  | N-CA-C | 10.72 | 139.90      | 113.10   |
| 1   | AY    | 5   | GLY  | N-CA-C | 10.72 | 139.90      | 113.10   |
| 1   | A4    | 5   | GLY  | N-CA-C | 10.72 | 139.90      | 113.10   |
| 1   | AB    | 5   | GLY  | N-CA-C | 10.72 | 139.90      | 113.10   |
| 1   | A0    | 5   | GLY  | N-CA-C | 10.72 | 139.90      | 113.10   |
| 1   | Ao    | 5   | GLY  | N-CA-C | 10.72 | 139.90      | 113.10   |
| 1   | AD    | 5   | GLY  | N-CA-C | 10.72 | 139.89      | 113.10   |
| 1   | AG    | 5   | GLY  | N-CA-C | 10.72 | 139.89      | 113.10   |
| 1   | AJ    | 5   | GLY  | N-CA-C | 10.71 | 139.88      | 113.10   |
| 1   | AQ    | 5   | GLY  | N-CA-C | 10.71 | 139.89      | 113.10   |
| 1   | AL    | 5   | GLY  | N-CA-C | 10.71 | 139.88      | 113.10   |
| 1   | AO    | 5   | GLY  | N-CA-C | 10.71 | 139.88      | 113.10   |
| 1   | AZ    | 5   | GLY  | N-CA-C | 10.71 | 139.88      | 113.10   |
| 1   | Ae    | 5   | GLY  | N-CA-C | 10.71 | 139.88      | 113.10   |
| 1   | Aj    | 5   | GLY  | N-CA-C | 10.71 | 139.88      | 113.10   |
| 1   | DC    | 5   | GLY  | N-CA-C | 10.71 | 139.88      | 113.10   |
| 1   | AU    | 5   | GLY  | N-CA-C | 10.71 | 139.87      | 113.10   |
| 1   | Af    | 5   | GLY  | N-CA-C | 10.71 | 139.87      | 113.10   |
| 1   | Al    | 5   | GLY  | N-CA-C | 10.71 | 139.87      | 113.10   |
| 1   | DH    | 5   | GLY  | N-CA-C | 10.71 | 139.86      | 113.10   |
| 1   | AA    | 5   | GLY  | N-CA-C | 10.70 | 139.85      | 113.10   |
| 1   | AK    | 5   | GLY  | N-CA-C | 10.70 | 139.85      | 113.10   |
| 1   | AF    | 5   | GLY  | N-CA-C | 10.70 | 139.84      | 113.10   |
| 1   | Ak    | 5   | GLY  | N-CA-C | 10.70 | 139.85      | 113.10   |
| 1   | DG    | 5   | GLY  | N-CA-C | 10.70 | 139.85      | 113.10   |
| 1   | A8    | 5   | GLY  | N-CA-C | 10.70 | 139.84      | 113.10   |
| 1   | AT    | 5   | GLY  | N-CA-C | 10.69 | 139.82      | 113.10   |
| 1   | DF    | 5   | GLY  | N-CA-C | 10.69 | 139.82      | 113.10   |
| 1   | A3    | 5   | GLY  | N-CA-C | 10.68 | 139.81      | 113.10   |
| 1   | An    | 5   | GLY  | N-CA-C | 10.67 | 139.78      | 113.10   |
| 1   | AS    | 207 | CYS  | N-CA-C | 8.43  | 133.77      | 111.00   |
| 1   | AG    | 207 | CYS  | N-CA-C | 8.43  | 133.76      | 111.00   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | AZ    | 207 | CYS  | N-CA-C | 8.43 | 133.76      | 111.00   |
| 1   | AR    | 207 | CYS  | N-CA-C | 8.43 | 133.75      | 111.00   |
| 1   | DH    | 207 | CYS  | N-CA-C | 8.43 | 133.76      | 111.00   |
| 1   | Ag    | 207 | CYS  | N-CA-C | 8.43 | 133.75      | 111.00   |
| 1   | Ao    | 207 | CYS  | N-CA-C | 8.43 | 133.75      | 111.00   |
| 1   | AL    | 207 | CYS  | N-CA-C | 8.42 | 133.74      | 111.00   |
| 1   | Aa    | 207 | CYS  | N-CA-C | 8.42 | 133.74      | 111.00   |
| 1   | AF    | 207 | CYS  | N-CA-C | 8.42 | 133.74      | 111.00   |
| 1   | A5    | 207 | CYS  | N-CA-C | 8.42 | 133.74      | 111.00   |
| 1   | AQ    | 207 | CYS  | N-CA-C | 8.42 | 133.73      | 111.00   |
| 1   | AW    | 207 | CYS  | N-CA-C | 8.42 | 133.72      | 111.00   |
| 1   | A9    | 207 | CYS  | N-CA-C | 8.42 | 133.73      | 111.00   |
| 1   | Ab    | 207 | CYS  | N-CA-C | 8.42 | 133.73      | 111.00   |
| 1   | AY    | 207 | CYS  | N-CA-C | 8.42 | 133.72      | 111.00   |
| 1   | A0    | 207 | CYS  | N-CA-C | 8.42 | 133.72      | 111.00   |
| 1   | Ac    | 207 | CYS  | N-CA-C | 8.42 | 133.73      | 111.00   |
| 1   | Af    | 207 | CYS  | N-CA-C | 8.42 | 133.72      | 111.00   |
| 1   | DG    | 207 | CYS  | N-CA-C | 8.42 | 133.72      | 111.00   |
| 1   | AK    | 207 | CYS  | N-CA-C | 8.41 | 133.72      | 111.00   |
| 1   | Al    | 207 | CYS  | N-CA-C | 8.41 | 133.72      | 111.00   |
| 1   | AC    | 207 | CYS  | N-CA-C | 8.41 | 133.71      | 111.00   |
| 1   | AP    | 207 | CYS  | N-CA-C | 8.41 | 133.71      | 111.00   |
| 1   | Aj    | 207 | CYS  | N-CA-C | 8.41 | 133.71      | 111.00   |
| 1   | DC    | 207 | CYS  | N-CA-C | 8.41 | 133.70      | 111.00   |
| 1   | AB    | 207 | CYS  | N-CA-C | 8.41 | 133.70      | 111.00   |
| 1   | AE    | 207 | CYS  | N-CA-C | 8.41 | 133.70      | 111.00   |
| 1   | AI    | 207 | CYS  | N-CA-C | 8.41 | 133.70      | 111.00   |
| 1   | AU    | 207 | CYS  | N-CA-C | 8.41 | 133.70      | 111.00   |
| 1   | Am    | 207 | CYS  | N-CA-C | 8.40 | 133.69      | 111.00   |
| 1   | An    | 207 | CYS  | N-CA-C | 8.40 | 133.69      | 111.00   |
| 1   | DJ    | 207 | CYS  | N-CA-C | 8.40 | 133.69      | 111.00   |
| 1   | AD    | 207 | CYS  | N-CA-C | 8.40 | 133.68      | 111.00   |
| 1   | AH    | 207 | CYS  | N-CA-C | 8.40 | 133.69      | 111.00   |
| 1   | AM    | 207 | CYS  | N-CA-C | 8.40 | 133.68      | 111.00   |
| 1   | A3    | 207 | CYS  | N-CA-C | 8.40 | 133.68      | 111.00   |
| 1   | Ad    | 207 | CYS  | N-CA-C | 8.40 | 133.68      | 111.00   |
| 1   | DD    | 207 | CYS  | N-CA-C | 8.40 | 133.68      | 111.00   |
| 1   | DE    | 207 | CYS  | N-CA-C | 8.40 | 133.68      | 111.00   |
| 1   | A7    | 207 | CYS  | N-CA-C | 8.40 | 133.68      | 111.00   |
| 1   | AA    | 207 | CYS  | N-CA-C | 8.40 | 133.67      | 111.00   |
| 1   | AJ    | 207 | CYS  | N-CA-C | 8.40 | 133.67      | 111.00   |
| 1   | AO    | 207 | CYS  | N-CA-C | 8.40 | 133.67      | 111.00   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | AT    | 207 | CYS  | N-CA-C | 8.40  | 133.67      | 111.00   |
| 1   | AV    | 207 | CYS  | N-CA-C | 8.40  | 133.67      | 111.00   |
| 1   | Ae    | 207 | CYS  | N-CA-C | 8.40  | 133.67      | 111.00   |
| 1   | A1    | 207 | CYS  | N-CA-C | 8.39  | 133.67      | 111.00   |
| 1   | A4    | 207 | CYS  | N-CA-C | 8.39  | 133.66      | 111.00   |
| 1   | A6    | 207 | CYS  | N-CA-C | 8.39  | 133.67      | 111.00   |
| 1   | A8    | 207 | CYS  | N-CA-C | 8.39  | 133.66      | 111.00   |
| 1   | DI    | 207 | CYS  | N-CA-C | 8.39  | 133.66      | 111.00   |
| 1   | A2    | 207 | CYS  | N-CA-C | 8.39  | 133.65      | 111.00   |
| 1   | Ak    | 207 | CYS  | N-CA-C | 8.39  | 133.65      | 111.00   |
| 1   | DK    | 207 | CYS  | N-CA-C | 8.39  | 133.65      | 111.00   |
| 1   | AX    | 207 | CYS  | N-CA-C | 8.38  | 133.64      | 111.00   |
| 1   | Ai    | 207 | CYS  | N-CA-C | 8.38  | 133.64      | 111.00   |
| 1   | DF    | 207 | CYS  | N-CA-C | 8.38  | 133.61      | 111.00   |
| 1   | Ah    | 207 | CYS  | N-CA-C | 8.37  | 133.60      | 111.00   |
| 1   | AN    | 207 | CYS  | N-CA-C | 8.37  | 133.59      | 111.00   |
| 2   | B8    | 138 | LYS  | N-CA-C | -7.74 | 90.11       | 111.00   |
| 2   | B7    | 138 | LYS  | N-CA-C | -7.73 | 90.14       | 111.00   |
| 2   | Bb    | 138 | LYS  | N-CA-C | -7.72 | 90.14       | 111.00   |
| 2   | BQ    | 138 | LYS  | N-CA-C | -7.72 | 90.15       | 111.00   |
| 2   | BX    | 138 | LYS  | N-CA-C | -7.72 | 90.15       | 111.00   |
| 2   | Bu    | 138 | LYS  | N-CA-C | -7.72 | 90.15       | 111.00   |
| 2   | Bd    | 138 | LYS  | N-CA-C | -7.72 | 90.16       | 111.00   |
| 2   | Bh    | 138 | LYS  | N-CA-C | -7.72 | 90.16       | 111.00   |
| 2   | Bj    | 138 | LYS  | N-CA-C | -7.72 | 90.16       | 111.00   |
| 2   | Bn    | 138 | LYS  | N-CA-C | -7.72 | 90.16       | 111.00   |
| 2   | BD    | 138 | LYS  | N-CA-C | -7.72 | 90.16       | 111.00   |
| 2   | B6    | 138 | LYS  | N-CA-C | -7.72 | 90.16       | 111.00   |
| 2   | BF    | 138 | LYS  | N-CA-C | -7.72 | 90.17       | 111.00   |
| 2   | BI    | 138 | LYS  | N-CA-C | -7.72 | 90.17       | 111.00   |
| 2   | BY    | 138 | LYS  | N-CA-C | -7.72 | 90.17       | 111.00   |
| 2   | Bt    | 138 | LYS  | N-CA-C | -7.72 | 90.17       | 111.00   |
| 2   | BK    | 138 | LYS  | N-CA-C | -7.71 | 90.17       | 111.00   |
| 2   | Bl    | 138 | LYS  | N-CA-C | -7.71 | 90.17       | 111.00   |
| 2   | Bp    | 138 | LYS  | N-CA-C | -7.71 | 90.17       | 111.00   |
| 2   | Bv    | 138 | LYS  | N-CA-C | -7.71 | 90.17       | 111.00   |
| 2   | BN    | 138 | LYS  | N-CA-C | -7.71 | 90.17       | 111.00   |
| 2   | Ba    | 138 | LYS  | N-CA-C | -7.71 | 90.17       | 111.00   |
| 2   | BP    | 138 | LYS  | N-CA-C | -7.71 | 90.18       | 111.00   |
| 2   | Bg    | 138 | LYS  | N-CA-C | -7.71 | 90.18       | 111.00   |
| 2   | Bm    | 138 | LYS  | N-CA-C | -7.71 | 90.18       | 111.00   |
| 2   | Bs    | 138 | LYS  | N-CA-C | -7.71 | 90.18       | 111.00   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | Bx    | 138 | LYS  | N-CA-C | -7.71 | 90.18       | 111.00   |
| 2   | BO    | 138 | LYS  | N-CA-C | -7.71 | 90.18       | 111.00   |
| 2   | BC    | 138 | LYS  | N-CA-C | -7.71 | 90.19       | 111.00   |
| 2   | BJ    | 138 | LYS  | N-CA-C | -7.71 | 90.19       | 111.00   |
| 2   | Be    | 138 | LYS  | N-CA-C | -7.71 | 90.19       | 111.00   |
| 2   | Bw    | 138 | LYS  | N-CA-C | -7.71 | 90.19       | 111.00   |
| 2   | BB    | 138 | LYS  | N-CA-C | -7.71 | 90.19       | 111.00   |
| 2   | B1    | 138 | LYS  | N-CA-C | -7.71 | 90.19       | 111.00   |
| 2   | B2    | 138 | LYS  | N-CA-C | -7.71 | 90.19       | 111.00   |
| 2   | B3    | 138 | LYS  | N-CA-C | -7.71 | 90.19       | 111.00   |
| 2   | B4    | 138 | LYS  | N-CA-C | -7.71 | 90.19       | 111.00   |
| 2   | Bq    | 138 | LYS  | N-CA-C | -7.71 | 90.19       | 111.00   |
| 2   | BE    | 138 | LYS  | N-CA-C | -7.70 | 90.20       | 111.00   |
| 2   | BR    | 138 | LYS  | N-CA-C | -7.70 | 90.20       | 111.00   |
| 2   | B5    | 138 | LYS  | N-CA-C | -7.70 | 90.20       | 111.00   |
| 2   | Bi    | 138 | LYS  | N-CA-C | -7.70 | 90.20       | 111.00   |
| 2   | BA    | 138 | LYS  | N-CA-C | -7.70 | 90.20       | 111.00   |
| 2   | BW    | 138 | LYS  | N-CA-C | -7.70 | 90.20       | 111.00   |
| 2   | Bo    | 138 | LYS  | N-CA-C | -7.70 | 90.20       | 111.00   |
| 2   | BL    | 138 | LYS  | N-CA-C | -7.70 | 90.21       | 111.00   |
| 2   | BZ    | 138 | LYS  | N-CA-C | -7.70 | 90.21       | 111.00   |
| 2   | Bf    | 138 | LYS  | N-CA-C | -7.70 | 90.21       | 111.00   |
| 2   | BM    | 138 | LYS  | N-CA-C | -7.70 | 90.22       | 111.00   |
| 2   | BT    | 138 | LYS  | N-CA-C | -7.70 | 90.22       | 111.00   |
| 2   | BG    | 138 | LYS  | N-CA-C | -7.70 | 90.22       | 111.00   |
| 2   | BU    | 138 | LYS  | N-CA-C | -7.69 | 90.22       | 111.00   |
| 2   | B9    | 138 | LYS  | N-CA-C | -7.69 | 90.23       | 111.00   |
| 2   | BH    | 138 | LYS  | N-CA-C | -7.69 | 90.24       | 111.00   |
| 2   | BS    | 138 | LYS  | N-CA-C | -7.69 | 90.24       | 111.00   |
| 2   | B0    | 138 | LYS  | N-CA-C | -7.69 | 90.23       | 111.00   |
| 2   | Br    | 138 | LYS  | N-CA-C | -7.69 | 90.23       | 111.00   |
| 2   | Bk    | 138 | LYS  | N-CA-C | -7.69 | 90.24       | 111.00   |
| 2   | Bc    | 138 | LYS  | N-CA-C | -7.69 | 90.24       | 111.00   |
| 2   | BV    | 138 | LYS  | N-CA-C | -7.68 | 90.27       | 111.00   |
| 1   | Aa    | 21  | PRO  | N-CA-C | 7.63  | 131.93      | 112.10   |
| 1   | Ah    | 21  | PRO  | N-CA-C | 7.63  | 131.94      | 112.10   |
| 1   | A2    | 21  | PRO  | N-CA-C | 7.63  | 131.93      | 112.10   |
| 1   | DJ    | 21  | PRO  | N-CA-C | 7.63  | 131.93      | 112.10   |
| 1   | Am    | 21  | PRO  | N-CA-C | 7.62  | 131.92      | 112.10   |
| 1   | An    | 21  | PRO  | N-CA-C | 7.62  | 131.92      | 112.10   |
| 1   | DG    | 21  | PRO  | N-CA-C | 7.62  | 131.91      | 112.10   |
| 1   | AE    | 21  | PRO  | N-CA-C | 7.62  | 131.91      | 112.10   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | DC    | 21  | PRO  | N-CA-C | 7.62 | 131.90      | 112.10   |
| 1   | AO    | 21  | PRO  | N-CA-C | 7.62 | 131.90      | 112.10   |
| 1   | AX    | 21  | PRO  | N-CA-C | 7.62 | 131.90      | 112.10   |
| 1   | DF    | 21  | PRO  | N-CA-C | 7.62 | 131.90      | 112.10   |
| 1   | AH    | 21  | PRO  | N-CA-C | 7.61 | 131.89      | 112.10   |
| 1   | DK    | 21  | PRO  | N-CA-C | 7.61 | 131.90      | 112.10   |
| 1   | A7    | 21  | PRO  | N-CA-C | 7.61 | 131.89      | 112.10   |
| 1   | AP    | 21  | PRO  | N-CA-C | 7.61 | 131.89      | 112.10   |
| 1   | Ad    | 21  | PRO  | N-CA-C | 7.61 | 131.89      | 112.10   |
| 1   | Ae    | 21  | PRO  | N-CA-C | 7.61 | 131.89      | 112.10   |
| 1   | AK    | 21  | PRO  | N-CA-C | 7.61 | 131.88      | 112.10   |
| 1   | AJ    | 21  | PRO  | N-CA-C | 7.61 | 131.88      | 112.10   |
| 1   | DE    | 21  | PRO  | N-CA-C | 7.61 | 131.88      | 112.10   |
| 1   | AT    | 21  | PRO  | N-CA-C | 7.61 | 131.87      | 112.10   |
| 1   | AG    | 21  | PRO  | N-CA-C | 7.60 | 131.87      | 112.10   |
| 1   | AQ    | 21  | PRO  | N-CA-C | 7.60 | 131.87      | 112.10   |
| 1   | Ao    | 21  | PRO  | N-CA-C | 7.60 | 131.87      | 112.10   |
| 1   | AA    | 21  | PRO  | N-CA-C | 7.60 | 131.87      | 112.10   |
| 1   | AV    | 21  | PRO  | N-CA-C | 7.60 | 131.86      | 112.10   |
| 1   | AY    | 21  | PRO  | N-CA-C | 7.60 | 131.86      | 112.10   |
| 1   | Af    | 21  | PRO  | N-CA-C | 7.60 | 131.86      | 112.10   |
| 1   | DI    | 21  | PRO  | N-CA-C | 7.60 | 131.86      | 112.10   |
| 1   | AS    | 21  | PRO  | N-CA-C | 7.60 | 131.85      | 112.10   |
| 1   | A4    | 21  | PRO  | N-CA-C | 7.60 | 131.85      | 112.10   |
| 1   | A8    | 21  | PRO  | N-CA-C | 7.60 | 131.85      | 112.10   |
| 1   | Ak    | 21  | PRO  | N-CA-C | 7.60 | 131.85      | 112.10   |
| 1   | AB    | 21  | PRO  | N-CA-C | 7.59 | 131.85      | 112.10   |
| 1   | AM    | 21  | PRO  | N-CA-C | 7.59 | 131.84      | 112.10   |
| 1   | Ac    | 21  | PRO  | N-CA-C | 7.59 | 131.84      | 112.10   |
| 1   | AC    | 21  | PRO  | N-CA-C | 7.59 | 131.84      | 112.10   |
| 1   | Ai    | 21  | PRO  | N-CA-C | 7.59 | 131.83      | 112.10   |
| 1   | AF    | 21  | PRO  | N-CA-C | 7.59 | 131.83      | 112.10   |
| 1   | AL    | 21  | PRO  | N-CA-C | 7.59 | 131.83      | 112.10   |
| 1   | AU    | 21  | PRO  | N-CA-C | 7.59 | 131.82      | 112.10   |
| 1   | Ab    | 21  | PRO  | N-CA-C | 7.59 | 131.82      | 112.10   |
| 1   | AZ    | 21  | PRO  | N-CA-C | 7.58 | 131.82      | 112.10   |
| 1   | A1    | 21  | PRO  | N-CA-C | 7.58 | 131.82      | 112.10   |
| 1   | A9    | 21  | PRO  | N-CA-C | 7.58 | 131.82      | 112.10   |
| 1   | AD    | 21  | PRO  | N-CA-C | 7.58 | 131.81      | 112.10   |
| 1   | A0    | 21  | PRO  | N-CA-C | 7.58 | 131.81      | 112.10   |
| 1   | A5    | 21  | PRO  | N-CA-C | 7.58 | 131.81      | 112.10   |
| 1   | DD    | 21  | PRO  | N-CA-C | 7.58 | 131.81      | 112.10   |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 1   | DH    | 21  | PRO  | N-CA-C  | 7.58 | 131.81      | 112.10   |
| 1   | AR    | 21  | PRO  | N-CA-C  | 7.58 | 131.81      | 112.10   |
| 1   | Aj    | 21  | PRO  | N-CA-C  | 7.58 | 131.80      | 112.10   |
| 1   | A3    | 21  | PRO  | N-CA-C  | 7.58 | 131.80      | 112.10   |
| 1   | Al    | 21  | PRO  | N-CA-C  | 7.57 | 131.79      | 112.10   |
| 1   | AW    | 21  | PRO  | N-CA-C  | 7.57 | 131.79      | 112.10   |
| 1   | AN    | 21  | PRO  | N-CA-C  | 7.57 | 131.78      | 112.10   |
| 1   | AI    | 21  | PRO  | N-CA-C  | 7.56 | 131.76      | 112.10   |
| 1   | Ag    | 21  | PRO  | N-CA-C  | 7.56 | 131.76      | 112.10   |
| 1   | A6    | 21  | PRO  | N-CA-C  | 7.55 | 131.74      | 112.10   |
| 2   | BU    | 86  | ASP  | CB-CA-C | 7.03 | 124.46      | 110.40   |
| 2   | B4    | 86  | ASP  | CB-CA-C | 7.03 | 124.46      | 110.40   |
| 2   | Bd    | 86  | ASP  | CB-CA-C | 7.02 | 124.44      | 110.40   |
| 2   | BA    | 86  | ASP  | CB-CA-C | 7.02 | 124.44      | 110.40   |
| 2   | Bn    | 86  | ASP  | CB-CA-C | 7.02 | 124.43      | 110.40   |
| 2   | BF    | 86  | ASP  | CB-CA-C | 7.01 | 124.43      | 110.40   |
| 2   | B6    | 86  | ASP  | CB-CA-C | 7.01 | 124.43      | 110.40   |
| 2   | BO    | 86  | ASP  | CB-CA-C | 7.01 | 124.42      | 110.40   |
| 2   | BQ    | 86  | ASP  | CB-CA-C | 7.01 | 124.42      | 110.40   |
| 2   | Bs    | 86  | ASP  | CB-CA-C | 7.01 | 124.42      | 110.40   |
| 2   | BI    | 86  | ASP  | CB-CA-C | 7.01 | 124.42      | 110.40   |
| 2   | Bi    | 86  | ASP  | CB-CA-C | 7.01 | 124.42      | 110.40   |
| 2   | Bv    | 86  | ASP  | CB-CA-C | 7.01 | 124.41      | 110.40   |
| 2   | BD    | 86  | ASP  | CB-CA-C | 7.00 | 124.41      | 110.40   |
| 2   | BX    | 86  | ASP  | CB-CA-C | 7.00 | 124.40      | 110.40   |
| 2   | BZ    | 86  | ASP  | CB-CA-C | 7.00 | 124.40      | 110.40   |
| 2   | B3    | 86  | ASP  | CB-CA-C | 7.00 | 124.40      | 110.40   |
| 2   | Bm    | 86  | ASP  | CB-CA-C | 7.00 | 124.40      | 110.40   |
| 2   | BP    | 86  | ASP  | CB-CA-C | 7.00 | 124.39      | 110.40   |
| 2   | BN    | 86  | ASP  | CB-CA-C | 7.00 | 124.39      | 110.40   |
| 2   | BS    | 86  | ASP  | CB-CA-C | 7.00 | 124.39      | 110.40   |
| 2   | B0    | 86  | ASP  | CB-CA-C | 7.00 | 124.39      | 110.40   |
| 2   | Bx    | 86  | ASP  | CB-CA-C | 7.00 | 124.39      | 110.40   |
| 2   | BK    | 86  | ASP  | CB-CA-C | 6.99 | 124.39      | 110.40   |
| 2   | Bb    | 86  | ASP  | CB-CA-C | 6.99 | 124.39      | 110.40   |
| 2   | Bc    | 86  | ASP  | CB-CA-C | 6.99 | 124.39      | 110.40   |
| 2   | Bl    | 86  | ASP  | CB-CA-C | 6.99 | 124.39      | 110.40   |
| 2   | Bt    | 86  | ASP  | CB-CA-C | 6.99 | 124.39      | 110.40   |
| 2   | BC    | 86  | ASP  | CB-CA-C | 6.99 | 124.38      | 110.40   |
| 2   | BV    | 86  | ASP  | CB-CA-C | 6.99 | 124.38      | 110.40   |
| 2   | BB    | 86  | ASP  | CB-CA-C | 6.99 | 124.38      | 110.40   |
| 2   | B8    | 86  | ASP  | CB-CA-C | 6.99 | 124.38      | 110.40   |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2   | Bp    | 86  | ASP  | CB-CA-C | 6.99 | 124.38      | 110.40   |
| 2   | Bo    | 86  | ASP  | CB-CA-C | 6.99 | 124.38      | 110.40   |
| 2   | Bh    | 86  | ASP  | CB-CA-C | 6.99 | 124.37      | 110.40   |
| 2   | BE    | 86  | ASP  | CB-CA-C | 6.99 | 124.37      | 110.40   |
| 2   | B9    | 86  | ASP  | CB-CA-C | 6.99 | 124.37      | 110.40   |
| 2   | BG    | 86  | ASP  | CB-CA-C | 6.98 | 124.37      | 110.40   |
| 2   | BH    | 86  | ASP  | CB-CA-C | 6.98 | 124.37      | 110.40   |
| 2   | Bj    | 86  | ASP  | CB-CA-C | 6.98 | 124.37      | 110.40   |
| 2   | BT    | 86  | ASP  | CB-CA-C | 6.98 | 124.36      | 110.40   |
| 2   | Ba    | 86  | ASP  | CB-CA-C | 6.98 | 124.36      | 110.40   |
| 2   | Br    | 86  | ASP  | CB-CA-C | 6.98 | 124.36      | 110.40   |
| 2   | Bf    | 86  | ASP  | CB-CA-C | 6.98 | 124.36      | 110.40   |
| 2   | BJ    | 86  | ASP  | CB-CA-C | 6.98 | 124.35      | 110.40   |
| 2   | BY    | 86  | ASP  | CB-CA-C | 6.98 | 124.35      | 110.40   |
| 2   | BR    | 86  | ASP  | CB-CA-C | 6.97 | 124.35      | 110.40   |
| 2   | BL    | 86  | ASP  | CB-CA-C | 6.97 | 124.34      | 110.40   |
| 2   | B7    | 86  | ASP  | CB-CA-C | 6.97 | 124.34      | 110.40   |
| 2   | BM    | 86  | ASP  | CB-CA-C | 6.97 | 124.34      | 110.40   |
| 2   | Be    | 86  | ASP  | CB-CA-C | 6.97 | 124.34      | 110.40   |
| 2   | Bu    | 86  | ASP  | CB-CA-C | 6.96 | 124.33      | 110.40   |
| 2   | B5    | 86  | ASP  | CB-CA-C | 6.96 | 124.32      | 110.40   |
| 2   | Bk    | 86  | ASP  | CB-CA-C | 6.96 | 124.32      | 110.40   |
| 2   | Bg    | 86  | ASP  | CB-CA-C | 6.96 | 124.32      | 110.40   |
| 2   | Bq    | 86  | ASP  | CB-CA-C | 6.96 | 124.31      | 110.40   |
| 2   | B1    | 86  | ASP  | CB-CA-C | 6.96 | 124.31      | 110.40   |
| 2   | B2    | 86  | ASP  | CB-CA-C | 6.96 | 124.31      | 110.40   |
| 2   | Bw    | 86  | ASP  | CB-CA-C | 6.95 | 124.31      | 110.40   |
| 2   | BW    | 86  | ASP  | CB-CA-C | 6.94 | 124.28      | 110.40   |
| 3   | Cv    | 130 | ALA  | N-CA-C  | 6.90 | 129.62      | 111.00   |
| 3   | Cx    | 130 | ALA  | N-CA-C  | 6.89 | 129.61      | 111.00   |
| 3   | CE    | 130 | ALA  | N-CA-C  | 6.89 | 129.60      | 111.00   |
| 3   | Cd    | 130 | ALA  | N-CA-C  | 6.89 | 129.60      | 111.00   |
| 3   | Cm    | 130 | ALA  | N-CA-C  | 6.89 | 129.60      | 111.00   |
| 3   | C6    | 130 | ALA  | N-CA-C  | 6.89 | 129.60      | 111.00   |
| 3   | CF    | 130 | ALA  | N-CA-C  | 6.89 | 129.59      | 111.00   |
| 3   | CM    | 130 | ALA  | N-CA-C  | 6.89 | 129.59      | 111.00   |
| 3   | Ci    | 130 | ALA  | N-CA-C  | 6.89 | 129.60      | 111.00   |
| 3   | Cn    | 130 | ALA  | N-CA-C  | 6.89 | 129.59      | 111.00   |
| 3   | CT    | 130 | ALA  | N-CA-C  | 6.88 | 129.59      | 111.00   |
| 3   | C3    | 130 | ALA  | N-CA-C  | 6.88 | 129.59      | 111.00   |
| 3   | Co    | 130 | ALA  | N-CA-C  | 6.88 | 129.59      | 111.00   |
| 3   | CN    | 130 | ALA  | N-CA-C  | 6.88 | 129.58      | 111.00   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 3   | C8    | 130 | ALA  | N-CA-C | 6.88 | 129.58      | 111.00   |
| 3   | CC    | 130 | ALA  | N-CA-C | 6.88 | 129.58      | 111.00   |
| 3   | CO    | 130 | ALA  | N-CA-C | 6.88 | 129.58      | 111.00   |
| 3   | CY    | 130 | ALA  | N-CA-C | 6.88 | 129.58      | 111.00   |
| 3   | C1    | 130 | ALA  | N-CA-C | 6.88 | 129.58      | 111.00   |
| 3   | CR    | 130 | ALA  | N-CA-C | 6.88 | 129.58      | 111.00   |
| 3   | Ct    | 130 | ALA  | N-CA-C | 6.88 | 129.58      | 111.00   |
| 3   | C5    | 130 | ALA  | N-CA-C | 6.88 | 129.57      | 111.00   |
| 3   | C7    | 130 | ALA  | N-CA-C | 6.88 | 129.57      | 111.00   |
| 3   | Cl    | 130 | ALA  | N-CA-C | 6.88 | 129.57      | 111.00   |
| 3   | CW    | 130 | ALA  | N-CA-C | 6.88 | 129.57      | 111.00   |
| 3   | CH    | 130 | ALA  | N-CA-C | 6.88 | 129.56      | 111.00   |
| 3   | CU    | 130 | ALA  | N-CA-C | 6.88 | 129.56      | 111.00   |
| 3   | Cs    | 130 | ALA  | N-CA-C | 6.88 | 129.56      | 111.00   |
| 3   | CA    | 130 | ALA  | N-CA-C | 6.87 | 129.56      | 111.00   |
| 3   | Ce    | 130 | ALA  | N-CA-C | 6.87 | 129.56      | 111.00   |
| 3   | Ch    | 130 | ALA  | N-CA-C | 6.87 | 129.56      | 111.00   |
| 3   | Cw    | 130 | ALA  | N-CA-C | 6.87 | 129.56      | 111.00   |
| 3   | CI    | 130 | ALA  | N-CA-C | 6.87 | 129.56      | 111.00   |
| 3   | C2    | 130 | ALA  | N-CA-C | 6.87 | 129.55      | 111.00   |
| 3   | Cg    | 130 | ALA  | N-CA-C | 6.87 | 129.56      | 111.00   |
| 3   | Cj    | 130 | ALA  | N-CA-C | 6.87 | 129.55      | 111.00   |
| 3   | Cp    | 130 | ALA  | N-CA-C | 6.87 | 129.56      | 111.00   |
| 3   | CQ    | 130 | ALA  | N-CA-C | 6.87 | 129.55      | 111.00   |
| 3   | Ck    | 130 | ALA  | N-CA-C | 6.87 | 129.54      | 111.00   |
| 3   | Cq    | 130 | ALA  | N-CA-C | 6.87 | 129.54      | 111.00   |
| 3   | CV    | 130 | ALA  | N-CA-C | 6.87 | 129.54      | 111.00   |
| 3   | CZ    | 130 | ALA  | N-CA-C | 6.87 | 129.54      | 111.00   |
| 3   | DB    | 130 | ALA  | N-CA-C | 6.87 | 129.54      | 111.00   |
| 3   | CD    | 130 | ALA  | N-CA-C | 6.86 | 129.53      | 111.00   |
| 3   | CK    | 130 | ALA  | N-CA-C | 6.86 | 129.53      | 111.00   |
| 3   | CP    | 130 | ALA  | N-CA-C | 6.86 | 129.53      | 111.00   |
| 3   | C4    | 130 | ALA  | N-CA-C | 6.86 | 129.53      | 111.00   |
| 3   | Cc    | 130 | ALA  | N-CA-C | 6.86 | 129.53      | 111.00   |
| 3   | DA    | 130 | ALA  | N-CA-C | 6.86 | 129.53      | 111.00   |
| 3   | Cu    | 130 | ALA  | N-CA-C | 6.86 | 129.52      | 111.00   |
| 3   | Cf    | 130 | ALA  | N-CA-C | 6.86 | 129.51      | 111.00   |
| 3   | CG    | 130 | ALA  | N-CA-C | 6.86 | 129.51      | 111.00   |
| 3   | CL    | 130 | ALA  | N-CA-C | 6.86 | 129.51      | 111.00   |
| 3   | C0    | 130 | ALA  | N-CA-C | 6.86 | 129.51      | 111.00   |
| 3   | Cr    | 130 | ALA  | N-CA-C | 6.86 | 129.51      | 111.00   |
| 3   | CJ    | 130 | ALA  | N-CA-C | 6.85 | 129.50      | 111.00   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | CB    | 130 | ALA  | N-CA-C  | 6.85  | 129.49      | 111.00   |
| 3   | C9    | 130 | ALA  | N-CA-C  | 6.85  | 129.49      | 111.00   |
| 3   | CX    | 130 | ALA  | N-CA-C  | 6.85  | 129.48      | 111.00   |
| 3   | CS    | 130 | ALA  | N-CA-C  | 6.84  | 129.48      | 111.00   |
| 2   | BV    | 223 | ASN  | CB-CA-C | -6.64 | 97.12       | 110.40   |
| 2   | BG    | 223 | ASN  | CB-CA-C | -6.63 | 97.13       | 110.40   |
| 2   | BI    | 223 | ASN  | CB-CA-C | -6.63 | 97.14       | 110.40   |
| 2   | Bo    | 223 | ASN  | CB-CA-C | -6.62 | 97.15       | 110.40   |
| 2   | Bx    | 223 | ASN  | CB-CA-C | -6.62 | 97.15       | 110.40   |
| 2   | BU    | 223 | ASN  | CB-CA-C | -6.62 | 97.16       | 110.40   |
| 2   | B0    | 223 | ASN  | CB-CA-C | -6.61 | 97.18       | 110.40   |
| 2   | Be    | 223 | ASN  | CB-CA-C | -6.61 | 97.18       | 110.40   |
| 2   | Bl    | 223 | ASN  | CB-CA-C | -6.61 | 97.18       | 110.40   |
| 2   | B9    | 223 | ASN  | CB-CA-C | -6.61 | 97.18       | 110.40   |
| 2   | BN    | 223 | ASN  | CB-CA-C | -6.60 | 97.20       | 110.40   |
| 2   | B2    | 223 | ASN  | CB-CA-C | -6.60 | 97.20       | 110.40   |
| 2   | B6    | 223 | ASN  | CB-CA-C | -6.60 | 97.19       | 110.40   |
| 2   | BB    | 223 | ASN  | CB-CA-C | -6.60 | 97.20       | 110.40   |
| 2   | Bt    | 223 | ASN  | CB-CA-C | -6.60 | 97.20       | 110.40   |
| 2   | Bd    | 223 | ASN  | CB-CA-C | -6.60 | 97.21       | 110.40   |
| 2   | BS    | 223 | ASN  | CB-CA-C | -6.59 | 97.21       | 110.40   |
| 2   | BZ    | 223 | ASN  | CB-CA-C | -6.59 | 97.21       | 110.40   |
| 2   | Bj    | 223 | ASN  | CB-CA-C | -6.59 | 97.21       | 110.40   |
| 2   | BT    | 223 | ASN  | CB-CA-C | -6.59 | 97.22       | 110.40   |
| 2   | BL    | 223 | ASN  | CB-CA-C | -6.59 | 97.22       | 110.40   |
| 1   | Ag    | 87  | GLN  | N-CA-C  | 6.59  | 128.79      | 111.00   |
| 2   | BQ    | 223 | ASN  | CB-CA-C | -6.59 | 97.23       | 110.40   |
| 2   | BK    | 223 | ASN  | CB-CA-C | -6.58 | 97.23       | 110.40   |
| 2   | B8    | 223 | ASN  | CB-CA-C | -6.58 | 97.23       | 110.40   |
| 1   | Ah    | 87  | GLN  | N-CA-C  | 6.58  | 128.77      | 111.00   |
| 2   | BY    | 223 | ASN  | CB-CA-C | -6.58 | 97.24       | 110.40   |
| 2   | Bq    | 223 | ASN  | CB-CA-C | -6.58 | 97.23       | 110.40   |
| 2   | Bv    | 223 | ASN  | CB-CA-C | -6.58 | 97.24       | 110.40   |
| 2   | BD    | 223 | ASN  | CB-CA-C | -6.58 | 97.24       | 110.40   |
| 1   | AR    | 87  | GLN  | N-CA-C  | 6.58  | 128.76      | 111.00   |
| 2   | BH    | 223 | ASN  | CB-CA-C | -6.58 | 97.25       | 110.40   |
| 1   | AO    | 87  | GLN  | N-CA-C  | 6.58  | 128.76      | 111.00   |
| 1   | AW    | 87  | GLN  | N-CA-C  | 6.58  | 128.76      | 111.00   |
| 2   | Bg    | 223 | ASN  | CB-CA-C | -6.58 | 97.25       | 110.40   |
| 2   | Bs    | 223 | ASN  | CB-CA-C | -6.58 | 97.25       | 110.40   |
| 1   | AQ    | 87  | GLN  | N-CA-C  | 6.58  | 128.75      | 111.00   |
| 1   | An    | 87  | GLN  | N-CA-C  | 6.58  | 128.75      | 111.00   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B3    | 223 | ASN  | CB-CA-C | -6.58 | 97.25       | 110.40   |
| 1   | Al    | 87  | GLN  | N-CA-C  | 6.57  | 128.75      | 111.00   |
| 2   | BF    | 223 | ASN  | CB-CA-C | -6.57 | 97.25       | 110.40   |
| 2   | BM    | 223 | ASN  | CB-CA-C | -6.57 | 97.25       | 110.40   |
| 2   | Bu    | 223 | ASN  | CB-CA-C | -6.57 | 97.25       | 110.40   |
| 1   | AM    | 87  | GLN  | N-CA-C  | 6.57  | 128.74      | 111.00   |
| 1   | Aa    | 87  | GLN  | N-CA-C  | 6.57  | 128.74      | 111.00   |
| 2   | BW    | 223 | ASN  | CB-CA-C | -6.57 | 97.26       | 110.40   |
| 2   | B5    | 223 | ASN  | CB-CA-C | -6.57 | 97.26       | 110.40   |
| 2   | Bh    | 223 | ASN  | CB-CA-C | -6.57 | 97.26       | 110.40   |
| 1   | DJ    | 87  | GLN  | N-CA-C  | 6.57  | 128.74      | 111.00   |
| 1   | A5    | 87  | GLN  | N-CA-C  | 6.57  | 128.74      | 111.00   |
| 2   | BX    | 223 | ASN  | CB-CA-C | -6.57 | 97.26       | 110.40   |
| 2   | B4    | 223 | ASN  | CB-CA-C | -6.57 | 97.26       | 110.40   |
| 1   | AL    | 87  | GLN  | N-CA-C  | 6.57  | 128.73      | 111.00   |
| 2   | BJ    | 223 | ASN  | CB-CA-C | -6.57 | 97.26       | 110.40   |
| 2   | Bb    | 223 | ASN  | CB-CA-C | -6.57 | 97.26       | 110.40   |
| 2   | Bn    | 223 | ASN  | CB-CA-C | -6.57 | 97.27       | 110.40   |
| 2   | Bf    | 223 | ASN  | CB-CA-C | -6.57 | 97.27       | 110.40   |
| 2   | Bi    | 223 | ASN  | CB-CA-C | -6.57 | 97.27       | 110.40   |
| 1   | DH    | 87  | GLN  | N-CA-C  | 6.57  | 128.72      | 111.00   |
| 1   | DI    | 87  | GLN  | N-CA-C  | 6.57  | 128.73      | 111.00   |
| 1   | AH    | 87  | GLN  | N-CA-C  | 6.56  | 128.72      | 111.00   |
| 1   | AX    | 87  | GLN  | N-CA-C  | 6.56  | 128.72      | 111.00   |
| 1   | A0    | 87  | GLN  | N-CA-C  | 6.56  | 128.72      | 111.00   |
| 1   | A2    | 87  | GLN  | N-CA-C  | 6.56  | 128.72      | 111.00   |
| 1   | Af    | 87  | GLN  | N-CA-C  | 6.56  | 128.72      | 111.00   |
| 2   | Br    | 223 | ASN  | CB-CA-C | -6.56 | 97.27       | 110.40   |
| 1   | AN    | 87  | GLN  | N-CA-C  | 6.56  | 128.71      | 111.00   |
| 2   | Bp    | 223 | ASN  | CB-CA-C | -6.56 | 97.28       | 110.40   |
| 1   | DD    | 87  | GLN  | N-CA-C  | 6.56  | 128.72      | 111.00   |
| 2   | BA    | 223 | ASN  | CB-CA-C | -6.56 | 97.28       | 110.40   |
| 2   | Bm    | 223 | ASN  | CB-CA-C | -6.56 | 97.28       | 110.40   |
| 1   | AC    | 87  | GLN  | N-CA-C  | 6.56  | 128.70      | 111.00   |
| 1   | AS    | 87  | GLN  | N-CA-C  | 6.56  | 128.70      | 111.00   |
| 1   | AU    | 87  | GLN  | N-CA-C  | 6.56  | 128.70      | 111.00   |
| 1   | A1    | 87  | GLN  | N-CA-C  | 6.56  | 128.71      | 111.00   |
| 1   | A6    | 87  | GLN  | N-CA-C  | 6.56  | 128.70      | 111.00   |
| 1   | Ak    | 87  | GLN  | N-CA-C  | 6.56  | 128.71      | 111.00   |
| 1   | Am    | 87  | GLN  | N-CA-C  | 6.56  | 128.70      | 111.00   |
| 2   | Bc    | 223 | ASN  | CB-CA-C | -6.56 | 97.28       | 110.40   |
| 1   | AA    | 87  | GLN  | N-CA-C  | 6.56  | 128.70      | 111.00   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A7    | 87  | GLN  | N-CA-C  | 6.56  | 128.70      | 111.00   |
| 1   | Ae    | 87  | GLN  | N-CA-C  | 6.56  | 128.70      | 111.00   |
| 2   | Bw    | 223 | ASN  | CB-CA-C | -6.56 | 97.29       | 110.40   |
| 1   | AE    | 87  | GLN  | N-CA-C  | 6.55  | 128.70      | 111.00   |
| 2   | BE    | 223 | ASN  | CB-CA-C | -6.55 | 97.29       | 110.40   |
| 2   | BO    | 223 | ASN  | CB-CA-C | -6.55 | 97.29       | 110.40   |
| 2   | B1    | 223 | ASN  | CB-CA-C | -6.55 | 97.29       | 110.40   |
| 2   | Ba    | 223 | ASN  | CB-CA-C | -6.55 | 97.29       | 110.40   |
| 1   | DE    | 87  | GLN  | N-CA-C  | 6.55  | 128.70      | 111.00   |
| 1   | A9    | 87  | GLN  | N-CA-C  | 6.55  | 128.69      | 111.00   |
| 1   | AF    | 87  | GLN  | N-CA-C  | 6.55  | 128.69      | 111.00   |
| 1   | AT    | 87  | GLN  | N-CA-C  | 6.55  | 128.69      | 111.00   |
| 1   | AY    | 87  | GLN  | N-CA-C  | 6.55  | 128.69      | 111.00   |
| 1   | AZ    | 87  | GLN  | N-CA-C  | 6.55  | 128.69      | 111.00   |
| 1   | Ab    | 87  | GLN  | N-CA-C  | 6.55  | 128.69      | 111.00   |
| 2   | BP    | 223 | ASN  | CB-CA-C | -6.55 | 97.30       | 110.40   |
| 1   | AI    | 87  | GLN  | N-CA-C  | 6.55  | 128.68      | 111.00   |
| 1   | Aj    | 87  | GLN  | N-CA-C  | 6.55  | 128.68      | 111.00   |
| 1   | A8    | 87  | GLN  | N-CA-C  | 6.55  | 128.68      | 111.00   |
| 1   | DF    | 87  | GLN  | N-CA-C  | 6.55  | 128.68      | 111.00   |
| 2   | B7    | 223 | ASN  | CB-CA-C | -6.55 | 97.31       | 110.40   |
| 2   | Bk    | 223 | ASN  | CB-CA-C | -6.55 | 97.31       | 110.40   |
| 1   | DK    | 87  | GLN  | N-CA-C  | 6.55  | 128.68      | 111.00   |
| 1   | Ad    | 87  | GLN  | N-CA-C  | 6.54  | 128.67      | 111.00   |
| 1   | Ai    | 87  | GLN  | N-CA-C  | 6.54  | 128.67      | 111.00   |
| 1   | DC    | 87  | GLN  | N-CA-C  | 6.54  | 128.67      | 111.00   |
| 1   | AK    | 87  | GLN  | N-CA-C  | 6.54  | 128.67      | 111.00   |
| 1   | AD    | 87  | GLN  | N-CA-C  | 6.54  | 128.66      | 111.00   |
| 1   | AP    | 87  | GLN  | N-CA-C  | 6.54  | 128.66      | 111.00   |
| 1   | A3    | 87  | GLN  | N-CA-C  | 6.54  | 128.66      | 111.00   |
| 1   | Ac    | 87  | GLN  | N-CA-C  | 6.54  | 128.66      | 111.00   |
| 1   | Ao    | 87  | GLN  | N-CA-C  | 6.54  | 128.66      | 111.00   |
| 2   | BC    | 223 | ASN  | CB-CA-C | -6.54 | 97.32       | 110.40   |
| 1   | AJ    | 87  | GLN  | N-CA-C  | 6.54  | 128.65      | 111.00   |
| 1   | AV    | 87  | GLN  | N-CA-C  | 6.54  | 128.66      | 111.00   |
| 2   | BR    | 223 | ASN  | CB-CA-C | -6.54 | 97.33       | 110.40   |
| 1   | AB    | 87  | GLN  | N-CA-C  | 6.54  | 128.65      | 111.00   |
| 1   | A4    | 87  | GLN  | N-CA-C  | 6.53  | 128.64      | 111.00   |
| 1   | Ag    | 203 | ASP  | N-CA-C  | -6.53 | 93.37       | 111.00   |
| 1   | AG    | 87  | GLN  | N-CA-C  | 6.53  | 128.63      | 111.00   |
| 1   | DG    | 87  | GLN  | N-CA-C  | 6.53  | 128.63      | 111.00   |
| 1   | AM    | 203 | ASP  | N-CA-C  | -6.53 | 93.38       | 111.00   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | Ab    | 203 | ASP  | N-CA-C | -6.52 | 93.39       | 111.00   |
| 1   | Al    | 203 | ASP  | N-CA-C | -6.52 | 93.39       | 111.00   |
| 1   | AD    | 203 | ASP  | N-CA-C | -6.52 | 93.40       | 111.00   |
| 1   | DI    | 203 | ASP  | N-CA-C | -6.52 | 93.40       | 111.00   |
| 1   | AG    | 203 | ASP  | N-CA-C | -6.52 | 93.40       | 111.00   |
| 1   | AZ    | 203 | ASP  | N-CA-C | -6.52 | 93.41       | 111.00   |
| 1   | AI    | 203 | ASP  | N-CA-C | -6.51 | 93.41       | 111.00   |
| 1   | AU    | 203 | ASP  | N-CA-C | -6.51 | 93.42       | 111.00   |
| 1   | A3    | 203 | ASP  | N-CA-C | -6.51 | 93.42       | 111.00   |
| 1   | A9    | 203 | ASP  | N-CA-C | -6.51 | 93.42       | 111.00   |
| 1   | Ai    | 203 | ASP  | N-CA-C | -6.51 | 93.43       | 111.00   |
| 1   | Ao    | 203 | ASP  | N-CA-C | -6.51 | 93.43       | 111.00   |
| 1   | Ah    | 203 | ASP  | N-CA-C | -6.51 | 93.43       | 111.00   |
| 1   | AN    | 203 | ASP  | N-CA-C | -6.51 | 93.43       | 111.00   |
| 1   | AP    | 203 | ASP  | N-CA-C | -6.51 | 93.43       | 111.00   |
| 1   | AW    | 203 | ASP  | N-CA-C | -6.51 | 93.43       | 111.00   |
| 1   | AY    | 203 | ASP  | N-CA-C | -6.51 | 93.43       | 111.00   |
| 1   | AR    | 203 | ASP  | N-CA-C | -6.50 | 93.44       | 111.00   |
| 1   | A6    | 203 | ASP  | N-CA-C | -6.50 | 93.44       | 111.00   |
| 1   | Ad    | 203 | ASP  | N-CA-C | -6.50 | 93.44       | 111.00   |
| 1   | AJ    | 203 | ASP  | N-CA-C | -6.50 | 93.45       | 111.00   |
| 1   | AK    | 203 | ASP  | N-CA-C | -6.50 | 93.44       | 111.00   |
| 1   | AX    | 203 | ASP  | N-CA-C | -6.50 | 93.45       | 111.00   |
| 1   | A1    | 203 | ASP  | N-CA-C | -6.50 | 93.44       | 111.00   |
| 1   | Ac    | 203 | ASP  | N-CA-C | -6.50 | 93.44       | 111.00   |
| 1   | DD    | 203 | ASP  | N-CA-C | -6.50 | 93.45       | 111.00   |
| 1   | AE    | 203 | ASP  | N-CA-C | -6.50 | 93.45       | 111.00   |
| 1   | A0    | 203 | ASP  | N-CA-C | -6.50 | 93.45       | 111.00   |
| 1   | A4    | 203 | ASP  | N-CA-C | -6.50 | 93.45       | 111.00   |
| 1   | AB    | 203 | ASP  | N-CA-C | -6.50 | 93.46       | 111.00   |
| 1   | AO    | 203 | ASP  | N-CA-C | -6.50 | 93.46       | 111.00   |
| 1   | AS    | 203 | ASP  | N-CA-C | -6.50 | 93.46       | 111.00   |
| 1   | AT    | 203 | ASP  | N-CA-C | -6.50 | 93.46       | 111.00   |
| 1   | Ae    | 203 | ASP  | N-CA-C | -6.50 | 93.46       | 111.00   |
| 1   | Aj    | 203 | ASP  | N-CA-C | -6.50 | 93.46       | 111.00   |
| 1   | DE    | 203 | ASP  | N-CA-C | -6.50 | 93.46       | 111.00   |
| 1   | Am    | 203 | ASP  | N-CA-C | -6.50 | 93.46       | 111.00   |
| 1   | AA    | 203 | ASP  | N-CA-C | -6.49 | 93.47       | 111.00   |
| 1   | AC    | 203 | ASP  | N-CA-C | -6.49 | 93.47       | 111.00   |
| 1   | A2    | 203 | ASP  | N-CA-C | -6.49 | 93.47       | 111.00   |
| 1   | DF    | 203 | ASP  | N-CA-C | -6.49 | 93.47       | 111.00   |
| 1   | AQ    | 203 | ASP  | N-CA-C | -6.49 | 93.47       | 111.00   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A5    | 203 | ASP  | N-CA-C  | -6.49 | 93.47       | 111.00   |
| 1   | DG    | 203 | ASP  | N-CA-C  | -6.49 | 93.47       | 111.00   |
| 1   | A8    | 203 | ASP  | N-CA-C  | -6.49 | 93.48       | 111.00   |
| 1   | An    | 203 | ASP  | N-CA-C  | -6.49 | 93.47       | 111.00   |
| 1   | DK    | 203 | ASP  | N-CA-C  | -6.49 | 93.48       | 111.00   |
| 1   | AF    | 203 | ASP  | N-CA-C  | -6.49 | 93.48       | 111.00   |
| 1   | A7    | 203 | ASP  | N-CA-C  | -6.49 | 93.49       | 111.00   |
| 1   | AL    | 203 | ASP  | N-CA-C  | -6.49 | 93.49       | 111.00   |
| 1   | AV    | 203 | ASP  | N-CA-C  | -6.49 | 93.49       | 111.00   |
| 1   | Aa    | 203 | ASP  | N-CA-C  | -6.49 | 93.49       | 111.00   |
| 1   | DH    | 203 | ASP  | N-CA-C  | -6.49 | 93.49       | 111.00   |
| 1   | DJ    | 203 | ASP  | N-CA-C  | -6.49 | 93.49       | 111.00   |
| 1   | Ak    | 203 | ASP  | N-CA-C  | -6.48 | 93.50       | 111.00   |
| 1   | Af    | 203 | ASP  | N-CA-C  | -6.48 | 93.50       | 111.00   |
| 1   | AH    | 203 | ASP  | N-CA-C  | -6.48 | 93.51       | 111.00   |
| 1   | DC    | 203 | ASP  | N-CA-C  | -6.47 | 93.53       | 111.00   |
| 1   | Ai    | 146 | ILE  | CB-CA-C | -6.39 | 98.82       | 111.60   |
| 1   | AJ    | 146 | ILE  | CB-CA-C | -6.39 | 98.83       | 111.60   |
| 1   | AY    | 146 | ILE  | CB-CA-C | -6.38 | 98.84       | 111.60   |
| 1   | Ad    | 146 | ILE  | CB-CA-C | -6.38 | 98.84       | 111.60   |
| 1   | AO    | 146 | ILE  | CB-CA-C | -6.38 | 98.85       | 111.60   |
| 1   | AF    | 146 | ILE  | CB-CA-C | -6.37 | 98.86       | 111.60   |
| 1   | AA    | 146 | ILE  | CB-CA-C | -6.37 | 98.86       | 111.60   |
| 1   | Ae    | 146 | ILE  | CB-CA-C | -6.37 | 98.87       | 111.60   |
| 1   | A8    | 146 | ILE  | CB-CA-C | -6.37 | 98.87       | 111.60   |
| 1   | AQ    | 146 | ILE  | CB-CA-C | -6.36 | 98.87       | 111.60   |
| 1   | A9    | 146 | ILE  | CB-CA-C | -6.36 | 98.87       | 111.60   |
| 1   | Ao    | 146 | ILE  | CB-CA-C | -6.36 | 98.87       | 111.60   |
| 1   | AB    | 146 | ILE  | CB-CA-C | -6.36 | 98.88       | 111.60   |
| 1   | A6    | 146 | ILE  | CB-CA-C | -6.36 | 98.88       | 111.60   |
| 1   | AT    | 146 | ILE  | CB-CA-C | -6.36 | 98.88       | 111.60   |
| 1   | AE    | 146 | ILE  | CB-CA-C | -6.36 | 98.89       | 111.60   |
| 1   | A3    | 146 | ILE  | CB-CA-C | -6.36 | 98.89       | 111.60   |
| 1   | Al    | 146 | ILE  | CB-CA-C | -6.35 | 98.89       | 111.60   |
| 1   | AG    | 146 | ILE  | CB-CA-C | -6.35 | 98.90       | 111.60   |
| 1   | AL    | 146 | ILE  | CB-CA-C | -6.35 | 98.90       | 111.60   |
| 1   | DG    | 146 | ILE  | CB-CA-C | -6.35 | 98.90       | 111.60   |
| 1   | AP    | 146 | ILE  | CB-CA-C | -6.35 | 98.90       | 111.60   |
| 1   | Am    | 146 | ILE  | CB-CA-C | -6.35 | 98.90       | 111.60   |
| 1   | DF    | 146 | ILE  | CB-CA-C | -6.35 | 98.90       | 111.60   |
| 1   | DH    | 146 | ILE  | CB-CA-C | -6.35 | 98.90       | 111.60   |
| 1   | Ak    | 146 | ILE  | CB-CA-C | -6.35 | 98.91       | 111.60   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | An    | 146 | ILE  | CB-CA-C | -6.35 | 98.91       | 111.60   |
| 1   | AC    | 146 | ILE  | CB-CA-C | -6.34 | 98.91       | 111.60   |
| 1   | DK    | 146 | ILE  | CB-CA-C | -6.34 | 98.91       | 111.60   |
| 1   | DC    | 146 | ILE  | CB-CA-C | -6.34 | 98.92       | 111.60   |
| 1   | AX    | 146 | ILE  | CB-CA-C | -6.34 | 98.92       | 111.60   |
| 1   | Ag    | 146 | ILE  | CB-CA-C | -6.34 | 98.92       | 111.60   |
| 1   | A2    | 146 | ILE  | CB-CA-C | -6.34 | 98.93       | 111.60   |
| 1   | Ah    | 146 | ILE  | CB-CA-C | -6.34 | 98.93       | 111.60   |
| 1   | Aj    | 146 | ILE  | CB-CA-C | -6.34 | 98.93       | 111.60   |
| 1   | AD    | 146 | ILE  | CB-CA-C | -6.33 | 98.93       | 111.60   |
| 1   | AW    | 146 | ILE  | CB-CA-C | -6.33 | 98.93       | 111.60   |
| 1   | A0    | 146 | ILE  | CB-CA-C | -6.33 | 98.94       | 111.60   |
| 1   | AV    | 146 | ILE  | CB-CA-C | -6.33 | 98.94       | 111.60   |
| 1   | A7    | 146 | ILE  | CB-CA-C | -6.33 | 98.94       | 111.60   |
| 1   | DE    | 146 | ILE  | CB-CA-C | -6.33 | 98.94       | 111.60   |
| 1   | AM    | 146 | ILE  | CB-CA-C | -6.33 | 98.95       | 111.60   |
| 1   | A5    | 146 | ILE  | CB-CA-C | -6.33 | 98.95       | 111.60   |
| 1   | AH    | 146 | ILE  | CB-CA-C | -6.33 | 98.95       | 111.60   |
| 1   | AK    | 146 | ILE  | CB-CA-C | -6.33 | 98.95       | 111.60   |
| 1   | Af    | 146 | ILE  | CB-CA-C | -6.33 | 98.95       | 111.60   |
| 1   | AZ    | 146 | ILE  | CB-CA-C | -6.32 | 98.95       | 111.60   |
| 1   | Aa    | 146 | ILE  | CB-CA-C | -6.32 | 98.95       | 111.60   |
| 1   | Ac    | 146 | ILE  | CB-CA-C | -6.32 | 98.95       | 111.60   |
| 1   | DD    | 146 | ILE  | CB-CA-C | -6.32 | 98.95       | 111.60   |
| 1   | AN    | 146 | ILE  | CB-CA-C | -6.32 | 98.96       | 111.60   |
| 1   | A1    | 146 | ILE  | CB-CA-C | -6.32 | 98.96       | 111.60   |
| 1   | AR    | 146 | ILE  | CB-CA-C | -6.32 | 98.96       | 111.60   |
| 1   | AS    | 146 | ILE  | CB-CA-C | -6.32 | 98.97       | 111.60   |
| 1   | DI    | 146 | ILE  | CB-CA-C | -6.32 | 98.97       | 111.60   |
| 1   | DJ    | 146 | ILE  | CB-CA-C | -6.30 | 98.99       | 111.60   |
| 1   | Ab    | 146 | ILE  | CB-CA-C | -6.30 | 99.00       | 111.60   |
| 1   | AI    | 146 | ILE  | CB-CA-C | -6.30 | 99.01       | 111.60   |
| 1   | A4    | 146 | ILE  | CB-CA-C | -6.30 | 99.01       | 111.60   |
| 1   | AU    | 146 | ILE  | CB-CA-C | -6.29 | 99.02       | 111.60   |
| 3   | CX    | 70  | ASP  | N-CA-C  | 6.25  | 127.87      | 111.00   |
| 3   | Cd    | 70  | ASP  | N-CA-C  | 6.24  | 127.84      | 111.00   |
| 3   | Cs    | 70  | ASP  | N-CA-C  | 6.24  | 127.84      | 111.00   |
| 3   | CT    | 70  | ASP  | N-CA-C  | 6.23  | 127.83      | 111.00   |
| 3   | CM    | 70  | ASP  | N-CA-C  | 6.23  | 127.82      | 111.00   |
| 3   | C0    | 70  | ASP  | N-CA-C  | 6.23  | 127.81      | 111.00   |
| 3   | Cn    | 70  | ASP  | N-CA-C  | 6.23  | 127.81      | 111.00   |
| 3   | CS    | 70  | ASP  | N-CA-C  | 6.22  | 127.81      | 111.00   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | C3    | 70  | ASP  | N-CA-C | 6.22  | 127.80      | 111.00   |
| 3   | CI    | 70  | ASP  | N-CA-C | 6.22  | 127.80      | 111.00   |
| 3   | C1    | 70  | ASP  | N-CA-C | 6.22  | 127.80      | 111.00   |
| 3   | C9    | 70  | ASP  | N-CA-C | 6.22  | 127.80      | 111.00   |
| 3   | CF    | 70  | ASP  | N-CA-C | 6.22  | 127.80      | 111.00   |
| 3   | CE    | 70  | ASP  | N-CA-C | 6.22  | 127.79      | 111.00   |
| 3   | C4    | 70  | ASP  | N-CA-C | 6.22  | 127.79      | 111.00   |
| 3   | Cj    | 70  | ASP  | N-CA-C | 6.22  | 127.79      | 111.00   |
| 3   | Cx    | 70  | ASP  | N-CA-C | 6.22  | 127.80      | 111.00   |
| 3   | C8    | 70  | ASP  | N-CA-C | 6.22  | 127.79      | 111.00   |
| 3   | Cm    | 70  | ASP  | N-CA-C | 6.22  | 127.79      | 111.00   |
| 3   | Ch    | 70  | ASP  | N-CA-C | 6.22  | 127.78      | 111.00   |
| 3   | Ct    | 70  | ASP  | N-CA-C | 6.22  | 127.78      | 111.00   |
| 3   | CJ    | 70  | ASP  | N-CA-C | 6.21  | 127.78      | 111.00   |
| 3   | CY    | 70  | ASP  | N-CA-C | 6.21  | 127.77      | 111.00   |
| 3   | Cr    | 70  | ASP  | N-CA-C | 6.21  | 127.77      | 111.00   |
| 3   | DB    | 70  | ASP  | N-CA-C | 6.21  | 127.77      | 111.00   |
| 3   | CD    | 70  | ASP  | N-CA-C | 6.21  | 127.76      | 111.00   |
| 3   | Cl    | 70  | ASP  | N-CA-C | 6.21  | 127.76      | 111.00   |
| 3   | CN    | 70  | ASP  | N-CA-C | 6.21  | 127.76      | 111.00   |
| 3   | CW    | 70  | ASP  | N-CA-C | 6.21  | 127.75      | 111.00   |
| 3   | C2    | 70  | ASP  | N-CA-C | 6.21  | 127.75      | 111.00   |
| 3   | Ce    | 70  | ASP  | N-CA-C | 6.21  | 127.75      | 111.00   |
| 3   | DA    | 70  | ASP  | N-CA-C | 6.21  | 127.75      | 111.00   |
| 2   | BT    | 85  | SER  | N-CA-C | 6.20  | 127.75      | 111.00   |
| 3   | CQ    | 70  | ASP  | N-CA-C | 6.20  | 127.75      | 111.00   |
| 3   | C6    | 70  | ASP  | N-CA-C | 6.20  | 127.75      | 111.00   |
| 3   | Cf    | 70  | ASP  | N-CA-C | 6.20  | 127.75      | 111.00   |
| 3   | Cu    | 70  | ASP  | N-CA-C | 6.20  | 127.75      | 111.00   |
| 3   | CU    | 70  | ASP  | N-CA-C | 6.20  | 127.75      | 111.00   |
| 2   | B5    | 134 | HIS  | N-CA-C | -6.20 | 94.26       | 111.00   |
| 3   | CB    | 70  | ASP  | N-CA-C | 6.20  | 127.74      | 111.00   |
| 3   | Ci    | 70  | ASP  | N-CA-C | 6.20  | 127.74      | 111.00   |
| 3   | CC    | 70  | ASP  | N-CA-C | 6.20  | 127.74      | 111.00   |
| 3   | C5    | 70  | ASP  | N-CA-C | 6.20  | 127.74      | 111.00   |
| 3   | Cw    | 70  | ASP  | N-CA-C | 6.20  | 127.74      | 111.00   |
| 3   | CV    | 70  | ASP  | N-CA-C | 6.20  | 127.73      | 111.00   |
| 3   | C7    | 70  | ASP  | N-CA-C | 6.20  | 127.73      | 111.00   |
| 3   | Cv    | 70  | ASP  | N-CA-C | 6.20  | 127.73      | 111.00   |
| 3   | CG    | 70  | ASP  | N-CA-C | 6.20  | 127.73      | 111.00   |
| 3   | Co    | 70  | ASP  | N-CA-C | 6.20  | 127.73      | 111.00   |
| 3   | CL    | 70  | ASP  | N-CA-C | 6.19  | 127.72      | 111.00   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | Bn    | 85  | SER  | N-CA-C | 6.19  | 127.72      | 111.00   |
| 3   | CA    | 70  | ASP  | N-CA-C | 6.19  | 127.72      | 111.00   |
| 3   | CH    | 70  | ASP  | N-CA-C | 6.19  | 127.72      | 111.00   |
| 3   | CZ    | 70  | ASP  | N-CA-C | 6.19  | 127.72      | 111.00   |
| 2   | B7    | 85  | SER  | N-CA-C | 6.19  | 127.72      | 111.00   |
| 2   | B8    | 85  | SER  | N-CA-C | 6.19  | 127.72      | 111.00   |
| 3   | CK    | 70  | ASP  | N-CA-C | 6.19  | 127.72      | 111.00   |
| 3   | CO    | 70  | ASP  | N-CA-C | 6.19  | 127.72      | 111.00   |
| 3   | CP    | 70  | ASP  | N-CA-C | 6.19  | 127.71      | 111.00   |
| 3   | Cc    | 70  | ASP  | N-CA-C | 6.19  | 127.71      | 111.00   |
| 2   | BC    | 134 | HIS  | N-CA-C | -6.19 | 94.29       | 111.00   |
| 3   | Cq    | 70  | ASP  | N-CA-C | 6.19  | 127.71      | 111.00   |
| 2   | BY    | 85  | SER  | N-CA-C | 6.19  | 127.71      | 111.00   |
| 2   | Bt    | 134 | HIS  | N-CA-C | -6.19 | 94.30       | 111.00   |
| 2   | BN    | 134 | HIS  | N-CA-C | -6.18 | 94.30       | 111.00   |
| 2   | Bq    | 85  | SER  | N-CA-C | 6.18  | 127.70      | 111.00   |
| 2   | BH    | 134 | HIS  | N-CA-C | -6.18 | 94.31       | 111.00   |
| 2   | Bh    | 85  | SER  | N-CA-C | 6.18  | 127.69      | 111.00   |
| 3   | CR    | 70  | ASP  | N-CA-C | 6.18  | 127.69      | 111.00   |
| 3   | Cg    | 70  | ASP  | N-CA-C | 6.18  | 127.69      | 111.00   |
| 2   | Bm    | 85  | SER  | N-CA-C | 6.18  | 127.69      | 111.00   |
| 2   | Ba    | 134 | HIS  | N-CA-C | -6.18 | 94.31       | 111.00   |
| 2   | Bb    | 134 | HIS  | N-CA-C | -6.18 | 94.31       | 111.00   |
| 2   | Bf    | 134 | HIS  | N-CA-C | -6.18 | 94.32       | 111.00   |
| 3   | Ck    | 70  | ASP  | N-CA-C | 6.18  | 127.68      | 111.00   |
| 2   | BF    | 134 | HIS  | N-CA-C | -6.18 | 94.32       | 111.00   |
| 2   | BP    | 134 | HIS  | N-CA-C | -6.18 | 94.32       | 111.00   |
| 2   | BZ    | 134 | HIS  | N-CA-C | -6.18 | 94.33       | 111.00   |
| 2   | Bn    | 134 | HIS  | N-CA-C | -6.18 | 94.32       | 111.00   |
| 2   | Bp    | 134 | HIS  | N-CA-C | -6.18 | 94.32       | 111.00   |
| 2   | BI    | 134 | HIS  | N-CA-C | -6.17 | 94.33       | 111.00   |
| 2   | BX    | 134 | HIS  | N-CA-C | -6.17 | 94.33       | 111.00   |
| 2   | Bs    | 85  | SER  | N-CA-C | 6.17  | 127.67      | 111.00   |
| 2   | BV    | 134 | HIS  | N-CA-C | -6.17 | 94.33       | 111.00   |
| 3   | Cp    | 70  | ASP  | N-CA-C | 6.17  | 127.67      | 111.00   |
| 2   | BD    | 134 | HIS  | N-CA-C | -6.17 | 94.34       | 111.00   |
| 2   | BR    | 134 | HIS  | N-CA-C | -6.17 | 94.34       | 111.00   |
| 2   | BU    | 134 | HIS  | N-CA-C | -6.17 | 94.34       | 111.00   |
| 2   | BZ    | 85  | SER  | N-CA-C | 6.17  | 127.66      | 111.00   |
| 2   | B1    | 134 | HIS  | N-CA-C | -6.17 | 94.34       | 111.00   |
| 2   | Bu    | 134 | HIS  | N-CA-C | -6.17 | 94.34       | 111.00   |
| 2   | Bi    | 85  | SER  | N-CA-C | 6.17  | 127.66      | 111.00   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | BE    | 85  | SER  | N-CA-C | 6.17  | 127.66      | 111.00   |
| 2   | BJ    | 85  | SER  | N-CA-C | 6.17  | 127.66      | 111.00   |
| 2   | B2    | 134 | HIS  | N-CA-C | -6.17 | 94.34       | 111.00   |
| 2   | Bw    | 134 | HIS  | N-CA-C | -6.17 | 94.35       | 111.00   |
| 2   | BA    | 134 | HIS  | N-CA-C | -6.17 | 94.35       | 111.00   |
| 2   | BW    | 134 | HIS  | N-CA-C | -6.17 | 94.35       | 111.00   |
| 2   | B3    | 85  | SER  | N-CA-C | 6.17  | 127.65      | 111.00   |
| 2   | Bq    | 134 | HIS  | N-CA-C | -6.17 | 94.35       | 111.00   |
| 2   | BK    | 134 | HIS  | N-CA-C | -6.17 | 94.36       | 111.00   |
| 2   | BQ    | 134 | HIS  | N-CA-C | -6.17 | 94.35       | 111.00   |
| 2   | Bd    | 85  | SER  | N-CA-C | 6.17  | 127.64      | 111.00   |
| 2   | Bh    | 134 | HIS  | N-CA-C | -6.17 | 94.36       | 111.00   |
| 2   | Bi    | 134 | HIS  | N-CA-C | -6.17 | 94.36       | 111.00   |
| 2   | BA    | 85  | SER  | N-CA-C | 6.16  | 127.64      | 111.00   |
| 2   | BE    | 134 | HIS  | N-CA-C | -6.16 | 94.36       | 111.00   |
| 2   | BH    | 85  | SER  | N-CA-C | 6.16  | 127.64      | 111.00   |
| 2   | BO    | 85  | SER  | N-CA-C | 6.16  | 127.64      | 111.00   |
| 2   | Bc    | 85  | SER  | N-CA-C | 6.16  | 127.64      | 111.00   |
| 2   | Bg    | 134 | HIS  | N-CA-C | -6.16 | 94.36       | 111.00   |
| 2   | Bl    | 134 | HIS  | N-CA-C | -6.16 | 94.36       | 111.00   |
| 2   | Bv    | 85  | SER  | N-CA-C | 6.16  | 127.64      | 111.00   |
| 2   | BK    | 85  | SER  | N-CA-C | 6.16  | 127.64      | 111.00   |
| 2   | BU    | 85  | SER  | N-CA-C | 6.16  | 127.64      | 111.00   |
| 2   | B1    | 85  | SER  | N-CA-C | 6.16  | 127.64      | 111.00   |
| 2   | B6    | 85  | SER  | N-CA-C | 6.16  | 127.64      | 111.00   |
| 2   | Bk    | 85  | SER  | N-CA-C | 6.16  | 127.64      | 111.00   |
| 2   | BM    | 134 | HIS  | N-CA-C | -6.16 | 94.37       | 111.00   |
| 2   | BS    | 85  | SER  | N-CA-C | 6.16  | 127.63      | 111.00   |
| 2   | BF    | 85  | SER  | N-CA-C | 6.16  | 127.63      | 111.00   |
| 2   | BS    | 134 | HIS  | N-CA-C | -6.16 | 94.37       | 111.00   |
| 2   | BX    | 85  | SER  | N-CA-C | 6.16  | 127.63      | 111.00   |
| 2   | B4    | 134 | HIS  | N-CA-C | -6.16 | 94.37       | 111.00   |
| 2   | B6    | 134 | HIS  | N-CA-C | -6.16 | 94.37       | 111.00   |
| 2   | Bs    | 134 | HIS  | N-CA-C | -6.16 | 94.37       | 111.00   |
| 2   | Bx    | 85  | SER  | N-CA-C | 6.16  | 127.63      | 111.00   |
| 2   | BP    | 85  | SER  | N-CA-C | 6.16  | 127.62      | 111.00   |
| 2   | BT    | 134 | HIS  | N-CA-C | -6.16 | 94.38       | 111.00   |
| 2   | B3    | 134 | HIS  | N-CA-C | -6.16 | 94.38       | 111.00   |
| 2   | Be    | 134 | HIS  | N-CA-C | -6.16 | 94.38       | 111.00   |
| 2   | Bw    | 85  | SER  | N-CA-C | 6.16  | 127.62      | 111.00   |
| 2   | BB    | 134 | HIS  | N-CA-C | -6.16 | 94.38       | 111.00   |
| 2   | BG    | 85  | SER  | N-CA-C | 6.16  | 127.62      | 111.00   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | BI    | 85  | SER  | N-CA-C | 6.16  | 127.62      | 111.00   |
| 2   | B5    | 85  | SER  | N-CA-C | 6.16  | 127.62      | 111.00   |
| 2   | Ba    | 85  | SER  | N-CA-C | 6.16  | 127.62      | 111.00   |
| 2   | Bc    | 134 | HIS  | N-CA-C | -6.16 | 94.38       | 111.00   |
| 2   | BR    | 85  | SER  | N-CA-C | 6.15  | 127.61      | 111.00   |
| 2   | BO    | 134 | HIS  | N-CA-C | -6.15 | 94.38       | 111.00   |
| 2   | BW    | 85  | SER  | N-CA-C | 6.15  | 127.61      | 111.00   |
| 2   | B0    | 85  | SER  | N-CA-C | 6.15  | 127.61      | 111.00   |
| 2   | B0    | 134 | HIS  | N-CA-C | -6.15 | 94.39       | 111.00   |
| 2   | Bk    | 134 | HIS  | N-CA-C | -6.15 | 94.39       | 111.00   |
| 2   | Bv    | 134 | HIS  | N-CA-C | -6.15 | 94.39       | 111.00   |
| 2   | BG    | 134 | HIS  | N-CA-C | -6.15 | 94.39       | 111.00   |
| 2   | BQ    | 85  | SER  | N-CA-C | 6.15  | 127.61      | 111.00   |
| 2   | Bg    | 85  | SER  | N-CA-C | 6.15  | 127.61      | 111.00   |
| 2   | Bj    | 134 | HIS  | N-CA-C | -6.15 | 94.40       | 111.00   |
| 2   | Bo    | 134 | HIS  | N-CA-C | -6.15 | 94.39       | 111.00   |
| 2   | Bp    | 85  | SER  | N-CA-C | 6.15  | 127.61      | 111.00   |
| 2   | Br    | 134 | HIS  | N-CA-C | -6.15 | 94.39       | 111.00   |
| 2   | B4    | 85  | SER  | N-CA-C | 6.15  | 127.60      | 111.00   |
| 2   | B9    | 134 | HIS  | N-CA-C | -6.15 | 94.40       | 111.00   |
| 2   | BD    | 85  | SER  | N-CA-C | 6.15  | 127.60      | 111.00   |
| 2   | BJ    | 134 | HIS  | N-CA-C | -6.15 | 94.40       | 111.00   |
| 2   | Bb    | 85  | SER  | N-CA-C | 6.15  | 127.60      | 111.00   |
| 2   | Bd    | 134 | HIS  | N-CA-C | -6.15 | 94.40       | 111.00   |
| 2   | Bo    | 85  | SER  | N-CA-C | 6.15  | 127.60      | 111.00   |
| 2   | BL    | 134 | HIS  | N-CA-C | -6.15 | 94.41       | 111.00   |
| 2   | B9    | 85  | SER  | N-CA-C | 6.15  | 127.59      | 111.00   |
| 2   | BY    | 134 | HIS  | N-CA-C | -6.14 | 94.41       | 111.00   |
| 2   | B7    | 134 | HIS  | N-CA-C | -6.14 | 94.41       | 111.00   |
| 2   | Bj    | 85  | SER  | N-CA-C | 6.14  | 127.59      | 111.00   |
| 2   | Bx    | 134 | HIS  | N-CA-C | -6.14 | 94.41       | 111.00   |
| 2   | BC    | 85  | SER  | N-CA-C | 6.14  | 127.58      | 111.00   |
| 2   | BL    | 85  | SER  | N-CA-C | 6.14  | 127.58      | 111.00   |
| 2   | BM    | 85  | SER  | N-CA-C | 6.14  | 127.58      | 111.00   |
| 2   | B8    | 134 | HIS  | N-CA-C | -6.14 | 94.41       | 111.00   |
| 2   | Br    | 85  | SER  | N-CA-C | 6.14  | 127.59      | 111.00   |
| 2   | Bt    | 85  | SER  | N-CA-C | 6.14  | 127.58      | 111.00   |
| 2   | BN    | 85  | SER  | N-CA-C | 6.14  | 127.58      | 111.00   |
| 2   | Bu    | 85  | SER  | N-CA-C | 6.14  | 127.57      | 111.00   |
| 2   | Bf    | 85  | SER  | N-CA-C | 6.14  | 127.57      | 111.00   |
| 2   | Bl    | 85  | SER  | N-CA-C | 6.14  | 127.57      | 111.00   |
| 2   | Bm    | 134 | HIS  | N-CA-C | -6.14 | 94.43       | 111.00   |

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| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 2   | BB    | 85  | SER  | N-CA-C   | 6.13 | 127.56      | 111.00   |
| 2   | B2    | 85  | SER  | N-CA-C   | 6.13 | 127.56      | 111.00   |
| 2   | Be    | 85  | SER  | N-CA-C   | 6.13 | 127.56      | 111.00   |
| 3   | CR    | 216 | LEU  | CA-CB-CG | 6.13 | 129.40      | 115.30   |
| 3   | Cx    | 216 | LEU  | CA-CB-CG | 6.13 | 129.39      | 115.30   |
| 2   | BV    | 85  | SER  | N-CA-C   | 6.12 | 127.53      | 111.00   |
| 3   | Ct    | 216 | LEU  | CA-CB-CG | 6.12 | 129.37      | 115.30   |
| 3   | DB    | 216 | LEU  | CA-CB-CG | 6.11 | 129.36      | 115.30   |
| 3   | CM    | 216 | LEU  | CA-CB-CG | 6.11 | 129.35      | 115.30   |
| 3   | CW    | 216 | LEU  | CA-CB-CG | 6.11 | 129.36      | 115.30   |
| 3   | C3    | 216 | LEU  | CA-CB-CG | 6.11 | 129.34      | 115.30   |
| 3   | C6    | 216 | LEU  | CA-CB-CG | 6.11 | 129.34      | 115.30   |
| 3   | Ci    | 216 | LEU  | CA-CB-CG | 6.10 | 129.33      | 115.30   |
| 3   | CJ    | 216 | LEU  | CA-CB-CG | 6.10 | 129.33      | 115.30   |
| 3   | CV    | 216 | LEU  | CA-CB-CG | 6.10 | 129.33      | 115.30   |
| 3   | CZ    | 216 | LEU  | CA-CB-CG | 6.10 | 129.33      | 115.30   |
| 3   | Cn    | 216 | LEU  | CA-CB-CG | 6.10 | 129.33      | 115.30   |
| 3   | C1    | 216 | LEU  | CA-CB-CG | 6.10 | 129.33      | 115.30   |
| 3   | Ck    | 216 | LEU  | CA-CB-CG | 6.10 | 129.33      | 115.30   |
| 3   | Cg    | 216 | LEU  | CA-CB-CG | 6.10 | 129.32      | 115.30   |
| 3   | Cd    | 216 | LEU  | CA-CB-CG | 6.09 | 129.32      | 115.30   |
| 3   | Cj    | 216 | LEU  | CA-CB-CG | 6.09 | 129.32      | 115.30   |
| 3   | CL    | 216 | LEU  | CA-CB-CG | 6.09 | 129.31      | 115.30   |
| 3   | CQ    | 216 | LEU  | CA-CB-CG | 6.09 | 129.31      | 115.30   |
| 3   | Cr    | 216 | LEU  | CA-CB-CG | 6.09 | 129.31      | 115.30   |
| 3   | CC    | 216 | LEU  | CA-CB-CG | 6.09 | 129.31      | 115.30   |
| 3   | Cq    | 216 | LEU  | CA-CB-CG | 6.09 | 129.31      | 115.30   |
| 3   | CA    | 216 | LEU  | CA-CB-CG | 6.09 | 129.31      | 115.30   |
| 3   | CI    | 216 | LEU  | CA-CB-CG | 6.09 | 129.31      | 115.30   |
| 3   | Cs    | 216 | LEU  | CA-CB-CG | 6.09 | 129.31      | 115.30   |
| 3   | Cv    | 216 | LEU  | CA-CB-CG | 6.09 | 129.31      | 115.30   |
| 3   | C7    | 216 | LEU  | CA-CB-CG | 6.09 | 129.30      | 115.30   |
| 3   | CE    | 216 | LEU  | CA-CB-CG | 6.09 | 129.30      | 115.30   |
| 3   | CT    | 216 | LEU  | CA-CB-CG | 6.09 | 129.30      | 115.30   |
| 3   | C4    | 216 | LEU  | CA-CB-CG | 6.09 | 129.30      | 115.30   |
| 3   | C9    | 216 | LEU  | CA-CB-CG | 6.09 | 129.30      | 115.30   |
| 3   | Cf    | 216 | LEU  | CA-CB-CG | 6.09 | 129.30      | 115.30   |
| 3   | Cp    | 216 | LEU  | CA-CB-CG | 6.09 | 129.30      | 115.30   |
| 3   | C0    | 216 | LEU  | CA-CB-CG | 6.08 | 129.29      | 115.30   |
| 3   | C5    | 216 | LEU  | CA-CB-CG | 6.08 | 129.29      | 115.30   |
| 1   | Al    | 4   | VAL  | N-CA-C   | 6.08 | 127.42      | 111.00   |
| 3   | CG    | 216 | LEU  | CA-CB-CG | 6.08 | 129.29      | 115.30   |

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| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 3   | CS    | 216 | LEU  | CA-CB-CG | 6.08 | 129.29      | 115.30   |
| 3   | C2    | 216 | LEU  | CA-CB-CG | 6.08 | 129.28      | 115.30   |
| 1   | An    | 4   | VAL  | N-CA-C   | 6.08 | 127.41      | 111.00   |
| 3   | DA    | 216 | LEU  | CA-CB-CG | 6.08 | 129.28      | 115.30   |
| 3   | CF    | 216 | LEU  | CA-CB-CG | 6.08 | 129.28      | 115.30   |
| 3   | CH    | 216 | LEU  | CA-CB-CG | 6.08 | 129.28      | 115.30   |
| 1   | DF    | 4   | VAL  | N-CA-C   | 6.08 | 127.40      | 111.00   |
| 3   | Cc    | 216 | LEU  | CA-CB-CG | 6.07 | 129.27      | 115.30   |
| 1   | DI    | 4   | VAL  | N-CA-C   | 6.07 | 127.40      | 111.00   |
| 1   | Af    | 4   | VAL  | N-CA-C   | 6.07 | 127.39      | 111.00   |
| 3   | CX    | 216 | LEU  | CA-CB-CG | 6.07 | 129.26      | 115.30   |
| 1   | AO    | 4   | VAL  | N-CA-C   | 6.07 | 127.39      | 111.00   |
| 1   | AQ    | 4   | VAL  | N-CA-C   | 6.07 | 127.39      | 111.00   |
| 1   | AY    | 4   | VAL  | N-CA-C   | 6.07 | 127.39      | 111.00   |
| 1   | A0    | 4   | VAL  | N-CA-C   | 6.07 | 127.39      | 111.00   |
| 1   | Aj    | 4   | VAL  | N-CA-C   | 6.07 | 127.39      | 111.00   |
| 3   | Co    | 216 | LEU  | CA-CB-CG | 6.07 | 129.26      | 115.30   |
| 3   | Cw    | 216 | LEU  | CA-CB-CG | 6.07 | 129.26      | 115.30   |
| 1   | AG    | 4   | VAL  | N-CA-C   | 6.07 | 127.39      | 111.00   |
| 3   | CB    | 216 | LEU  | CA-CB-CG | 6.07 | 129.26      | 115.30   |
| 3   | CD    | 216 | LEU  | CA-CB-CG | 6.07 | 129.26      | 115.30   |
| 3   | CP    | 216 | LEU  | CA-CB-CG | 6.07 | 129.26      | 115.30   |
| 3   | Ce    | 216 | LEU  | CA-CB-CG | 6.07 | 129.26      | 115.30   |
| 1   | AB    | 4   | VAL  | N-CA-C   | 6.07 | 127.38      | 111.00   |
| 1   | A9    | 4   | VAL  | N-CA-C   | 6.07 | 127.38      | 111.00   |
| 3   | CN    | 216 | LEU  | CA-CB-CG | 6.07 | 129.25      | 115.30   |
| 3   | CU    | 216 | LEU  | CA-CB-CG | 6.07 | 129.25      | 115.30   |
| 3   | CY    | 216 | LEU  | CA-CB-CG | 6.07 | 129.25      | 115.30   |
| 3   | C8    | 216 | LEU  | CA-CB-CG | 6.07 | 129.25      | 115.30   |
| 3   | Cm    | 216 | LEU  | CA-CB-CG | 6.07 | 129.25      | 115.30   |
| 1   | AE    | 4   | VAL  | N-CA-C   | 6.06 | 127.37      | 111.00   |
| 1   | A2    | 4   | VAL  | N-CA-C   | 6.06 | 127.37      | 111.00   |
| 1   | A3    | 4   | VAL  | N-CA-C   | 6.06 | 127.37      | 111.00   |
| 1   | AC    | 4   | VAL  | N-CA-C   | 6.06 | 127.37      | 111.00   |
| 1   | Ae    | 4   | VAL  | N-CA-C   | 6.06 | 127.37      | 111.00   |
| 1   | Ag    | 4   | VAL  | N-CA-C   | 6.06 | 127.37      | 111.00   |
| 3   | Ch    | 216 | LEU  | CA-CB-CG | 6.06 | 129.24      | 115.30   |
| 3   | Cl    | 216 | LEU  | CA-CB-CG | 6.06 | 129.24      | 115.30   |
| 1   | AR    | 4   | VAL  | N-CA-C   | 6.06 | 127.37      | 111.00   |
| 1   | Am    | 4   | VAL  | N-CA-C   | 6.06 | 127.36      | 111.00   |
| 1   | A4    | 4   | VAL  | N-CA-C   | 6.06 | 127.36      | 111.00   |
| 1   | Ah    | 4   | VAL  | N-CA-C   | 6.06 | 127.36      | 111.00   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | CO    | 216 | LEU  | CA-CB-CG | 6.06  | 129.24      | 115.30   |
| 3   | Cu    | 216 | LEU  | CA-CB-CG | 6.06  | 129.24      | 115.30   |
| 1   | DG    | 4   | VAL  | N-CA-C   | 6.06  | 127.36      | 111.00   |
| 1   | AW    | 4   | VAL  | N-CA-C   | 6.06  | 127.36      | 111.00   |
| 1   | A7    | 4   | VAL  | N-CA-C   | 6.06  | 127.35      | 111.00   |
| 3   | CK    | 216 | LEU  | CA-CB-CG | 6.06  | 129.23      | 115.30   |
| 1   | AN    | 4   | VAL  | N-CA-C   | 6.05  | 127.35      | 111.00   |
| 1   | AU    | 4   | VAL  | N-CA-C   | 6.05  | 127.35      | 111.00   |
| 1   | AZ    | 4   | VAL  | N-CA-C   | 6.05  | 127.35      | 111.00   |
| 1   | Ad    | 4   | VAL  | N-CA-C   | 6.05  | 127.35      | 111.00   |
| 1   | DD    | 4   | VAL  | N-CA-C   | 6.05  | 127.34      | 111.00   |
| 1   | Ao    | 4   | VAL  | N-CA-C   | 6.05  | 127.34      | 111.00   |
| 1   | AD    | 4   | VAL  | N-CA-C   | 6.05  | 127.34      | 111.00   |
| 1   | AI    | 4   | VAL  | N-CA-C   | 6.05  | 127.34      | 111.00   |
| 1   | AJ    | 4   | VAL  | N-CA-C   | 6.05  | 127.34      | 111.00   |
| 1   | A8    | 4   | VAL  | N-CA-C   | 6.05  | 127.34      | 111.00   |
| 1   | AP    | 4   | VAL  | N-CA-C   | 6.05  | 127.33      | 111.00   |
| 1   | AS    | 4   | VAL  | N-CA-C   | 6.05  | 127.34      | 111.00   |
| 1   | AT    | 4   | VAL  | N-CA-C   | 6.05  | 127.33      | 111.00   |
| 1   | A1    | 4   | VAL  | N-CA-C   | 6.05  | 127.33      | 111.00   |
| 1   | A6    | 4   | VAL  | N-CA-C   | 6.05  | 127.33      | 111.00   |
| 1   | DJ    | 4   | VAL  | N-CA-C   | 6.05  | 127.32      | 111.00   |
| 1   | AK    | 4   | VAL  | N-CA-C   | 6.04  | 127.32      | 111.00   |
| 1   | AA    | 4   | VAL  | N-CA-C   | 6.04  | 127.31      | 111.00   |
| 1   | AF    | 4   | VAL  | N-CA-C   | 6.04  | 127.31      | 111.00   |
| 1   | AM    | 4   | VAL  | N-CA-C   | 6.04  | 127.31      | 111.00   |
| 1   | AV    | 4   | VAL  | N-CA-C   | 6.04  | 127.31      | 111.00   |
| 1   | Ac    | 4   | VAL  | N-CA-C   | 6.04  | 127.31      | 111.00   |
| 1   | Ai    | 4   | VAL  | N-CA-C   | 6.04  | 127.31      | 111.00   |
| 1   | Ak    | 4   | VAL  | N-CA-C   | 6.04  | 127.30      | 111.00   |
| 1   | DH    | 4   | VAL  | N-CA-C   | 6.04  | 127.30      | 111.00   |
| 1   | DK    | 4   | VAL  | N-CA-C   | 6.04  | 127.30      | 111.00   |
| 1   | Aa    | 4   | VAL  | N-CA-C   | 6.04  | 127.30      | 111.00   |
| 1   | AX    | 4   | VAL  | N-CA-C   | 6.04  | 127.30      | 111.00   |
| 1   | Ab    | 4   | VAL  | N-CA-C   | 6.04  | 127.30      | 111.00   |
| 1   | A5    | 4   | VAL  | N-CA-C   | 6.03  | 127.29      | 111.00   |
| 1   | AH    | 4   | VAL  | N-CA-C   | 6.03  | 127.29      | 111.00   |
| 1   | AL    | 4   | VAL  | N-CA-C   | 6.03  | 127.28      | 111.00   |
| 1   | DE    | 4   | VAL  | N-CA-C   | 6.03  | 127.28      | 111.00   |
| 1   | DC    | 4   | VAL  | N-CA-C   | 6.03  | 127.27      | 111.00   |
| 1   | Al    | 151 | SER  | N-CA-C   | -5.76 | 95.45       | 111.00   |
| 1   | AM    | 151 | SER  | N-CA-C   | -5.76 | 95.46       | 111.00   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | DD    | 151 | SER  | N-CA-C | -5.75 | 95.47       | 111.00   |
| 1   | AR    | 151 | SER  | N-CA-C | -5.74 | 95.50       | 111.00   |
| 1   | AW    | 151 | SER  | N-CA-C | -5.74 | 95.49       | 111.00   |
| 1   | DI    | 151 | SER  | N-CA-C | -5.74 | 95.49       | 111.00   |
| 1   | Aa    | 151 | SER  | N-CA-C | -5.74 | 95.50       | 111.00   |
| 1   | AI    | 151 | SER  | N-CA-C | -5.74 | 95.50       | 111.00   |
| 1   | AH    | 151 | SER  | N-CA-C | -5.74 | 95.51       | 111.00   |
| 1   | AX    | 151 | SER  | N-CA-C | -5.74 | 95.51       | 111.00   |
| 1   | Ab    | 151 | SER  | N-CA-C | -5.74 | 95.50       | 111.00   |
| 1   | AD    | 151 | SER  | N-CA-C | -5.74 | 95.51       | 111.00   |
| 1   | AL    | 151 | SER  | N-CA-C | -5.74 | 95.51       | 111.00   |
| 1   | DF    | 151 | SER  | N-CA-C | -5.74 | 95.52       | 111.00   |
| 1   | A6    | 151 | SER  | N-CA-C | -5.73 | 95.52       | 111.00   |
| 1   | AC    | 151 | SER  | N-CA-C | -5.73 | 95.52       | 111.00   |
| 1   | AV    | 151 | SER  | N-CA-C | -5.73 | 95.52       | 111.00   |
| 1   | AE    | 151 | SER  | N-CA-C | -5.73 | 95.53       | 111.00   |
| 1   | AJ    | 151 | SER  | N-CA-C | -5.73 | 95.53       | 111.00   |
| 1   | Ac    | 151 | SER  | N-CA-C | -5.73 | 95.53       | 111.00   |
| 1   | Ah    | 151 | SER  | N-CA-C | -5.73 | 95.53       | 111.00   |
| 1   | DJ    | 151 | SER  | N-CA-C | -5.73 | 95.53       | 111.00   |
| 1   | DK    | 151 | SER  | N-CA-C | -5.73 | 95.53       | 111.00   |
| 1   | A2    | 151 | SER  | N-CA-C | -5.73 | 95.53       | 111.00   |
| 1   | A7    | 151 | SER  | N-CA-C | -5.73 | 95.53       | 111.00   |
| 1   | AS    | 151 | SER  | N-CA-C | -5.73 | 95.54       | 111.00   |
| 1   | AT    | 151 | SER  | N-CA-C | -5.73 | 95.53       | 111.00   |
| 1   | Af    | 151 | SER  | N-CA-C | -5.73 | 95.54       | 111.00   |
| 1   | Ag    | 151 | SER  | N-CA-C | -5.73 | 95.53       | 111.00   |
| 1   | Ak    | 151 | SER  | N-CA-C | -5.73 | 95.53       | 111.00   |
| 1   | An    | 151 | SER  | N-CA-C | -5.73 | 95.53       | 111.00   |
| 1   | Ao    | 151 | SER  | N-CA-C | -5.73 | 95.53       | 111.00   |
| 1   | AY    | 151 | SER  | N-CA-C | -5.73 | 95.54       | 111.00   |
| 1   | A1    | 151 | SER  | N-CA-C | -5.72 | 95.55       | 111.00   |
| 1   | AQ    | 151 | SER  | N-CA-C | -5.72 | 95.55       | 111.00   |
| 1   | Am    | 151 | SER  | N-CA-C | -5.72 | 95.55       | 111.00   |
| 1   | AN    | 151 | SER  | N-CA-C | -5.72 | 95.56       | 111.00   |
| 1   | AA    | 151 | SER  | N-CA-C | -5.72 | 95.56       | 111.00   |
| 1   | AK    | 151 | SER  | N-CA-C | -5.72 | 95.56       | 111.00   |
| 1   | DE    | 151 | SER  | N-CA-C | -5.72 | 95.56       | 111.00   |
| 1   | AO    | 151 | SER  | N-CA-C | -5.72 | 95.56       | 111.00   |
| 1   | A5    | 151 | SER  | N-CA-C | -5.72 | 95.56       | 111.00   |
| 1   | A8    | 151 | SER  | N-CA-C | -5.72 | 95.56       | 111.00   |
| 1   | Ai    | 151 | SER  | N-CA-C | -5.72 | 95.57       | 111.00   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | DG    | 151 | SER  | N-CA-C | -5.72 | 95.56       | 111.00   |
| 1   | A0    | 151 | SER  | N-CA-C | -5.71 | 95.57       | 111.00   |
| 1   | Aj    | 151 | SER  | N-CA-C | -5.71 | 95.57       | 111.00   |
| 1   | AG    | 151 | SER  | N-CA-C | -5.71 | 95.58       | 111.00   |
| 1   | AF    | 151 | SER  | N-CA-C | -5.71 | 95.58       | 111.00   |
| 1   | DC    | 151 | SER  | N-CA-C | -5.71 | 95.58       | 111.00   |
| 1   | AP    | 151 | SER  | N-CA-C | -5.71 | 95.59       | 111.00   |
| 1   | Ae    | 151 | SER  | N-CA-C | -5.71 | 95.59       | 111.00   |
| 1   | AB    | 151 | SER  | N-CA-C | -5.71 | 95.59       | 111.00   |
| 1   | Ad    | 151 | SER  | N-CA-C | -5.71 | 95.59       | 111.00   |
| 1   | AU    | 151 | SER  | N-CA-C | -5.70 | 95.61       | 111.00   |
| 1   | AZ    | 151 | SER  | N-CA-C | -5.70 | 95.60       | 111.00   |
| 1   | DH    | 151 | SER  | N-CA-C | -5.70 | 95.61       | 111.00   |
| 1   | A3    | 151 | SER  | N-CA-C | -5.70 | 95.61       | 111.00   |
| 1   | A4    | 151 | SER  | N-CA-C | -5.70 | 95.62       | 111.00   |
| 1   | A9    | 151 | SER  | N-CA-C | -5.70 | 95.62       | 111.00   |
| 1   | Af    | 181 | LYS  | N-CA-C | -5.67 | 95.68       | 111.00   |
| 1   | Ao    | 181 | LYS  | N-CA-C | -5.67 | 95.69       | 111.00   |
| 1   | AQ    | 181 | LYS  | N-CA-C | -5.67 | 95.69       | 111.00   |
| 1   | AU    | 181 | LYS  | N-CA-C | -5.67 | 95.70       | 111.00   |
| 1   | A4    | 181 | LYS  | N-CA-C | -5.67 | 95.70       | 111.00   |
| 1   | An    | 181 | LYS  | N-CA-C | -5.67 | 95.70       | 111.00   |
| 1   | AB    | 181 | LYS  | N-CA-C | -5.66 | 95.71       | 111.00   |
| 1   | AG    | 181 | LYS  | N-CA-C | -5.66 | 95.71       | 111.00   |
| 1   | AH    | 181 | LYS  | N-CA-C | -5.66 | 95.71       | 111.00   |
| 1   | A0    | 181 | LYS  | N-CA-C | -5.66 | 95.71       | 111.00   |
| 1   | AS    | 181 | LYS  | N-CA-C | -5.66 | 95.71       | 111.00   |
| 1   | DG    | 181 | LYS  | N-CA-C | -5.66 | 95.72       | 111.00   |
| 1   | DH    | 181 | LYS  | N-CA-C | -5.66 | 95.72       | 111.00   |
| 1   | AC    | 181 | LYS  | N-CA-C | -5.66 | 95.73       | 111.00   |
| 1   | A6    | 181 | LYS  | N-CA-C | -5.66 | 95.73       | 111.00   |
| 1   | Ah    | 181 | LYS  | N-CA-C | -5.66 | 95.73       | 111.00   |
| 1   | Ae    | 181 | LYS  | N-CA-C | -5.66 | 95.73       | 111.00   |
| 1   | AF    | 181 | LYS  | N-CA-C | -5.65 | 95.74       | 111.00   |
| 1   | AL    | 181 | LYS  | N-CA-C | -5.65 | 95.74       | 111.00   |
| 1   | AO    | 181 | LYS  | N-CA-C | -5.65 | 95.74       | 111.00   |
| 1   | DJ    | 181 | LYS  | N-CA-C | -5.65 | 95.74       | 111.00   |
| 1   | AN    | 181 | LYS  | N-CA-C | -5.65 | 95.74       | 111.00   |
| 1   | A2    | 181 | LYS  | N-CA-C | -5.65 | 95.75       | 111.00   |
| 1   | AI    | 181 | LYS  | N-CA-C | -5.65 | 95.74       | 111.00   |
| 1   | DI    | 181 | LYS  | N-CA-C | -5.65 | 95.75       | 111.00   |
| 1   | AI    | 181 | LYS  | N-CA-C | -5.65 | 95.75       | 111.00   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | AK    | 181 | LYS  | N-CA-C | -5.65 | 95.75       | 111.00   |
| 1   | AV    | 181 | LYS  | N-CA-C | -5.65 | 95.75       | 111.00   |
| 1   | Ab    | 181 | LYS  | N-CA-C | -5.65 | 95.75       | 111.00   |
| 1   | Aa    | 181 | LYS  | N-CA-C | -5.65 | 95.75       | 111.00   |
| 1   | AY    | 181 | LYS  | N-CA-C | -5.64 | 95.76       | 111.00   |
| 1   | A3    | 181 | LYS  | N-CA-C | -5.64 | 95.76       | 111.00   |
| 1   | Aj    | 181 | LYS  | N-CA-C | -5.64 | 95.76       | 111.00   |
| 1   | Ak    | 181 | LYS  | N-CA-C | -5.64 | 95.76       | 111.00   |
| 1   | AP    | 181 | LYS  | N-CA-C | -5.64 | 95.76       | 111.00   |
| 1   | AX    | 181 | LYS  | N-CA-C | -5.64 | 95.76       | 111.00   |
| 1   | Ai    | 181 | LYS  | N-CA-C | -5.64 | 95.77       | 111.00   |
| 1   | AA    | 181 | LYS  | N-CA-C | -5.64 | 95.77       | 111.00   |
| 1   | AT    | 181 | LYS  | N-CA-C | -5.64 | 95.77       | 111.00   |
| 1   | A9    | 181 | LYS  | N-CA-C | -5.64 | 95.78       | 111.00   |
| 1   | DK    | 181 | LYS  | N-CA-C | -5.64 | 95.77       | 111.00   |
| 1   | AD    | 181 | LYS  | N-CA-C | -5.64 | 95.78       | 111.00   |
| 1   | AZ    | 181 | LYS  | N-CA-C | -5.64 | 95.78       | 111.00   |
| 1   | DF    | 181 | LYS  | N-CA-C | -5.64 | 95.78       | 111.00   |
| 1   | AM    | 181 | LYS  | N-CA-C | -5.64 | 95.78       | 111.00   |
| 1   | Ac    | 181 | LYS  | N-CA-C | -5.64 | 95.78       | 111.00   |
| 1   | Ad    | 181 | LYS  | N-CA-C | -5.63 | 95.79       | 111.00   |
| 1   | DD    | 181 | LYS  | N-CA-C | -5.63 | 95.79       | 111.00   |
| 1   | A5    | 181 | LYS  | N-CA-C | -5.63 | 95.79       | 111.00   |
| 1   | Am    | 181 | LYS  | N-CA-C | -5.63 | 95.79       | 111.00   |
| 1   | AE    | 181 | LYS  | N-CA-C | -5.63 | 95.80       | 111.00   |
| 1   | DE    | 181 | LYS  | N-CA-C | -5.63 | 95.81       | 111.00   |
| 1   | AJ    | 181 | LYS  | N-CA-C | -5.63 | 95.81       | 111.00   |
| 1   | A7    | 181 | LYS  | N-CA-C | -5.63 | 95.81       | 111.00   |
| 1   | AW    | 181 | LYS  | N-CA-C | -5.62 | 95.82       | 111.00   |
| 1   | DC    | 181 | LYS  | N-CA-C | -5.62 | 95.82       | 111.00   |
| 1   | A1    | 181 | LYS  | N-CA-C | -5.62 | 95.83       | 111.00   |
| 1   | A8    | 181 | LYS  | N-CA-C | -5.62 | 95.83       | 111.00   |
| 1   | Ag    | 181 | LYS  | N-CA-C | -5.62 | 95.84       | 111.00   |
| 1   | AR    | 181 | LYS  | N-CA-C | -5.61 | 95.86       | 111.00   |
| 1   | AV    | 226 | PRO  | N-CA-C | 5.60  | 126.66      | 112.10   |
| 1   | Af    | 226 | PRO  | N-CA-C | 5.59  | 126.63      | 112.10   |
| 1   | A1    | 226 | PRO  | N-CA-C | 5.58  | 126.62      | 112.10   |
| 1   | A5    | 226 | PRO  | N-CA-C | 5.58  | 126.62      | 112.10   |
| 1   | AC    | 226 | PRO  | N-CA-C | 5.58  | 126.61      | 112.10   |
| 1   | Aa    | 226 | PRO  | N-CA-C | 5.58  | 126.61      | 112.10   |
| 1   | Ag    | 226 | PRO  | N-CA-C | 5.58  | 126.61      | 112.10   |
| 1   | AQ    | 226 | PRO  | N-CA-C | 5.58  | 126.61      | 112.10   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | DC    | 226 | PRO  | N-CA-C | 5.58 | 126.60      | 112.10   |
| 1   | AX    | 226 | PRO  | N-CA-C | 5.58 | 126.60      | 112.10   |
| 1   | Am    | 226 | PRO  | N-CA-C | 5.58 | 126.60      | 112.10   |
| 1   | DI    | 226 | PRO  | N-CA-C | 5.58 | 126.60      | 112.10   |
| 1   | AR    | 226 | PRO  | N-CA-C | 5.57 | 126.59      | 112.10   |
| 1   | A0    | 226 | PRO  | N-CA-C | 5.57 | 126.59      | 112.10   |
| 1   | Ae    | 226 | PRO  | N-CA-C | 5.57 | 126.59      | 112.10   |
| 1   | DD    | 226 | PRO  | N-CA-C | 5.57 | 126.59      | 112.10   |
| 1   | A6    | 226 | PRO  | N-CA-C | 5.57 | 126.58      | 112.10   |
| 1   | A9    | 226 | PRO  | N-CA-C | 5.57 | 126.58      | 112.10   |
| 1   | DG    | 226 | PRO  | N-CA-C | 5.57 | 126.58      | 112.10   |
| 1   | AZ    | 226 | PRO  | N-CA-C | 5.57 | 126.57      | 112.10   |
| 1   | A3    | 226 | PRO  | N-CA-C | 5.57 | 126.57      | 112.10   |
| 1   | A7    | 226 | PRO  | N-CA-C | 5.57 | 126.57      | 112.10   |
| 1   | Ab    | 226 | PRO  | N-CA-C | 5.57 | 126.57      | 112.10   |
| 1   | Aj    | 226 | PRO  | N-CA-C | 5.57 | 126.57      | 112.10   |
| 1   | DH    | 226 | PRO  | N-CA-C | 5.57 | 126.57      | 112.10   |
| 1   | AF    | 226 | PRO  | N-CA-C | 5.56 | 126.56      | 112.10   |
| 1   | AI    | 226 | PRO  | N-CA-C | 5.56 | 126.56      | 112.10   |
| 1   | AL    | 226 | PRO  | N-CA-C | 5.56 | 126.56      | 112.10   |
| 1   | AO    | 226 | PRO  | N-CA-C | 5.56 | 126.56      | 112.10   |
| 1   | AA    | 226 | PRO  | N-CA-C | 5.56 | 126.56      | 112.10   |
| 1   | AD    | 226 | PRO  | N-CA-C | 5.56 | 126.56      | 112.10   |
| 1   | AP    | 226 | PRO  | N-CA-C | 5.56 | 126.56      | 112.10   |
| 1   | AS    | 226 | PRO  | N-CA-C | 5.56 | 126.55      | 112.10   |
| 1   | AH    | 226 | PRO  | N-CA-C | 5.56 | 126.55      | 112.10   |
| 1   | AW    | 226 | PRO  | N-CA-C | 5.56 | 126.55      | 112.10   |
| 1   | Al    | 226 | PRO  | N-CA-C | 5.56 | 126.55      | 112.10   |
| 1   | AK    | 226 | PRO  | N-CA-C | 5.56 | 126.55      | 112.10   |
| 1   | Ak    | 226 | PRO  | N-CA-C | 5.56 | 126.55      | 112.10   |
| 1   | AE    | 226 | PRO  | N-CA-C | 5.55 | 126.54      | 112.10   |
| 1   | AJ    | 226 | PRO  | N-CA-C | 5.55 | 126.54      | 112.10   |
| 1   | AM    | 226 | PRO  | N-CA-C | 5.55 | 126.54      | 112.10   |
| 1   | Ac    | 226 | PRO  | N-CA-C | 5.55 | 126.54      | 112.10   |
| 1   | A4    | 226 | PRO  | N-CA-C | 5.55 | 126.54      | 112.10   |
| 1   | Ao    | 226 | PRO  | N-CA-C | 5.55 | 126.54      | 112.10   |
| 1   | A8    | 226 | PRO  | N-CA-C | 5.55 | 126.53      | 112.10   |
| 1   | DE    | 226 | PRO  | N-CA-C | 5.55 | 126.53      | 112.10   |
| 1   | DJ    | 226 | PRO  | N-CA-C | 5.55 | 126.54      | 112.10   |
| 1   | AB    | 226 | PRO  | N-CA-C | 5.55 | 126.53      | 112.10   |
| 1   | AT    | 226 | PRO  | N-CA-C | 5.55 | 126.53      | 112.10   |
| 1   | AY    | 226 | PRO  | N-CA-C | 5.55 | 126.53      | 112.10   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | Ad    | 226 | PRO  | N-CA-C  | 5.55  | 126.53      | 112.10   |
| 1   | DK    | 226 | PRO  | N-CA-C  | 5.55  | 126.52      | 112.10   |
| 1   | AN    | 226 | PRO  | N-CA-C  | 5.54  | 126.52      | 112.10   |
| 1   | A2    | 226 | PRO  | N-CA-C  | 5.54  | 126.52      | 112.10   |
| 1   | Ah    | 226 | PRO  | N-CA-C  | 5.54  | 126.51      | 112.10   |
| 1   | DF    | 226 | PRO  | N-CA-C  | 5.54  | 126.51      | 112.10   |
| 1   | DK    | 186 | TRP  | N-CA-C  | 5.54  | 125.96      | 111.00   |
| 1   | AU    | 226 | PRO  | N-CA-C  | 5.54  | 126.50      | 112.10   |
| 3   | Ci    | 64  | VAL  | CB-CA-C | -5.54 | 100.88      | 111.40   |
| 3   | CR    | 64  | VAL  | CB-CA-C | -5.53 | 100.89      | 111.40   |
| 3   | C4    | 18  | VAL  | CB-CA-C | -5.53 | 100.89      | 111.40   |
| 3   | Cq    | 64  | VAL  | CB-CA-C | -5.53 | 100.89      | 111.40   |
| 3   | C1    | 64  | VAL  | CB-CA-C | -5.53 | 100.89      | 111.40   |
| 3   | Co    | 64  | VAL  | CB-CA-C | -5.53 | 100.89      | 111.40   |
| 3   | Cp    | 64  | VAL  | CB-CA-C | -5.53 | 100.89      | 111.40   |
| 3   | CQ    | 208 | VAL  | CB-CA-C | -5.53 | 100.89      | 111.40   |
| 1   | DH    | 186 | TRP  | N-CA-C  | 5.53  | 125.93      | 111.00   |
| 1   | AG    | 226 | PRO  | N-CA-C  | 5.53  | 126.47      | 112.10   |
| 1   | Ai    | 226 | PRO  | N-CA-C  | 5.53  | 126.47      | 112.10   |
| 3   | C6    | 64  | VAL  | CB-CA-C | -5.52 | 100.90      | 111.40   |
| 1   | An    | 226 | PRO  | N-CA-C  | 5.52  | 126.46      | 112.10   |
| 3   | Ct    | 64  | VAL  | CB-CA-C | -5.52 | 100.91      | 111.40   |
| 1   | Aj    | 186 | TRP  | N-CA-C  | 5.52  | 125.90      | 111.00   |
| 3   | C4    | 64  | VAL  | CB-CA-C | -5.52 | 100.91      | 111.40   |
| 3   | Cj    | 64  | VAL  | CB-CA-C | -5.52 | 100.91      | 111.40   |
| 3   | Cl    | 64  | VAL  | CB-CA-C | -5.52 | 100.92      | 111.40   |
| 3   | CM    | 64  | VAL  | CB-CA-C | -5.52 | 100.92      | 111.40   |
| 3   | Cf    | 64  | VAL  | CB-CA-C | -5.52 | 100.92      | 111.40   |
| 3   | CB    | 64  | VAL  | CB-CA-C | -5.51 | 100.92      | 111.40   |
| 3   | CK    | 64  | VAL  | CB-CA-C | -5.51 | 100.92      | 111.40   |
| 3   | CQ    | 64  | VAL  | CB-CA-C | -5.51 | 100.92      | 111.40   |
| 3   | Cn    | 64  | VAL  | CB-CA-C | -5.51 | 100.92      | 111.40   |
| 1   | AH    | 186 | TRP  | N-CA-C  | 5.51  | 125.89      | 111.00   |
| 1   | AR    | 186 | TRP  | N-CA-C  | 5.51  | 125.88      | 111.00   |
| 1   | AS    | 186 | TRP  | N-CA-C  | 5.51  | 125.89      | 111.00   |
| 3   | CE    | 64  | VAL  | CB-CA-C | -5.51 | 100.92      | 111.40   |
| 3   | CJ    | 64  | VAL  | CB-CA-C | -5.51 | 100.93      | 111.40   |
| 3   | CU    | 18  | VAL  | CB-CA-C | -5.51 | 100.92      | 111.40   |
| 3   | Cd    | 64  | VAL  | CB-CA-C | -5.51 | 100.93      | 111.40   |
| 1   | DG    | 186 | TRP  | N-CA-C  | 5.51  | 125.88      | 111.00   |
| 1   | AP    | 186 | TRP  | N-CA-C  | 5.51  | 125.88      | 111.00   |
| 3   | C1    | 208 | VAL  | CB-CA-C | -5.51 | 100.93      | 111.40   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | AK    | 186 | TRP  | N-CA-C  | 5.51  | 125.88      | 111.00   |
| 1   | AQ    | 186 | TRP  | N-CA-C  | 5.51  | 125.88      | 111.00   |
| 1   | AU    | 186 | TRP  | N-CA-C  | 5.51  | 125.88      | 111.00   |
| 1   | A5    | 186 | TRP  | N-CA-C  | 5.51  | 125.88      | 111.00   |
| 3   | CR    | 18  | VAL  | CB-CA-C | -5.51 | 100.93      | 111.40   |
| 3   | C3    | 64  | VAL  | CB-CA-C | -5.51 | 100.93      | 111.40   |
| 3   | CL    | 208 | VAL  | CB-CA-C | -5.51 | 100.93      | 111.40   |
| 3   | CU    | 64  | VAL  | CB-CA-C | -5.51 | 100.94      | 111.40   |
| 3   | CW    | 18  | VAL  | CB-CA-C | -5.51 | 100.93      | 111.40   |
| 1   | AX    | 186 | TRP  | N-CA-C  | 5.51  | 125.87      | 111.00   |
| 1   | Al    | 186 | TRP  | N-CA-C  | 5.51  | 125.87      | 111.00   |
| 3   | CA    | 64  | VAL  | CB-CA-C | -5.51 | 100.94      | 111.40   |
| 3   | CJ    | 208 | VAL  | CB-CA-C | -5.51 | 100.94      | 111.40   |
| 3   | Ce    | 208 | VAL  | CB-CA-C | -5.51 | 100.94      | 111.40   |
| 1   | DC    | 186 | TRP  | N-CA-C  | 5.51  | 125.87      | 111.00   |
| 1   | DJ    | 186 | TRP  | N-CA-C  | 5.51  | 125.87      | 111.00   |
| 1   | A9    | 186 | TRP  | N-CA-C  | 5.50  | 125.86      | 111.00   |
| 1   | Aa    | 186 | TRP  | N-CA-C  | 5.50  | 125.86      | 111.00   |
| 1   | Ag    | 186 | TRP  | N-CA-C  | 5.50  | 125.86      | 111.00   |
| 1   | AF    | 186 | TRP  | N-CA-C  | 5.50  | 125.86      | 111.00   |
| 1   | AG    | 186 | TRP  | N-CA-C  | 5.50  | 125.86      | 111.00   |
| 1   | AM    | 186 | TRP  | N-CA-C  | 5.50  | 125.86      | 111.00   |
| 1   | A0    | 186 | TRP  | N-CA-C  | 5.50  | 125.86      | 111.00   |
| 3   | CY    | 64  | VAL  | CB-CA-C | -5.50 | 100.94      | 111.40   |
| 3   | DA    | 64  | VAL  | CB-CA-C | -5.50 | 100.94      | 111.40   |
| 1   | AB    | 186 | TRP  | N-CA-C  | 5.50  | 125.86      | 111.00   |
| 1   | AY    | 186 | TRP  | N-CA-C  | 5.50  | 125.85      | 111.00   |
| 1   | Ad    | 186 | TRP  | N-CA-C  | 5.50  | 125.85      | 111.00   |
| 1   | Ai    | 186 | TRP  | N-CA-C  | 5.50  | 125.86      | 111.00   |
| 3   | CH    | 64  | VAL  | CB-CA-C | -5.50 | 100.95      | 111.40   |
| 3   | Cq    | 18  | VAL  | CB-CA-C | -5.50 | 100.95      | 111.40   |
| 1   | AL    | 186 | TRP  | N-CA-C  | 5.50  | 125.85      | 111.00   |
| 1   | Ao    | 186 | TRP  | N-CA-C  | 5.50  | 125.85      | 111.00   |
| 3   | CZ    | 18  | VAL  | CB-CA-C | -5.50 | 100.95      | 111.40   |
| 3   | C7    | 208 | VAL  | CB-CA-C | -5.50 | 100.95      | 111.40   |
| 3   | Ce    | 64  | VAL  | CB-CA-C | -5.50 | 100.95      | 111.40   |
| 3   | Cp    | 208 | VAL  | CB-CA-C | -5.50 | 100.95      | 111.40   |
| 1   | AI    | 186 | TRP  | N-CA-C  | 5.50  | 125.85      | 111.00   |
| 1   | Am    | 186 | TRP  | N-CA-C  | 5.50  | 125.85      | 111.00   |
| 1   | An    | 186 | TRP  | N-CA-C  | 5.50  | 125.85      | 111.00   |
| 3   | CA    | 18  | VAL  | CB-CA-C | -5.50 | 100.95      | 111.40   |
| 3   | C8    | 64  | VAL  | CB-CA-C | -5.50 | 100.95      | 111.40   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | Cl    | 18  | VAL  | CB-CA-C | -5.50 | 100.95      | 111.40   |
| 3   | Cv    | 64  | VAL  | CB-CA-C | -5.50 | 100.95      | 111.40   |
| 3   | Cw    | 64  | VAL  | CB-CA-C | -5.50 | 100.95      | 111.40   |
| 1   | AE    | 186 | TRP  | N-CA-C  | 5.50  | 125.84      | 111.00   |
| 1   | Ak    | 186 | TRP  | N-CA-C  | 5.50  | 125.84      | 111.00   |
| 3   | CL    | 64  | VAL  | CB-CA-C | -5.50 | 100.96      | 111.40   |
| 3   | C9    | 18  | VAL  | CB-CA-C | -5.50 | 100.96      | 111.40   |
| 3   | Cj    | 208 | VAL  | CB-CA-C | -5.50 | 100.96      | 111.40   |
| 3   | Cu    | 208 | VAL  | CB-CA-C | -5.50 | 100.96      | 111.40   |
| 3   | DB    | 18  | VAL  | CB-CA-C | -5.50 | 100.96      | 111.40   |
| 1   | AC    | 186 | TRP  | N-CA-C  | 5.50  | 125.84      | 111.00   |
| 1   | AV    | 186 | TRP  | N-CA-C  | 5.50  | 125.84      | 111.00   |
| 3   | CB    | 208 | VAL  | CB-CA-C | -5.50 | 100.96      | 111.40   |
| 3   | CF    | 64  | VAL  | CB-CA-C | -5.50 | 100.96      | 111.40   |
| 3   | CO    | 64  | VAL  | CB-CA-C | -5.50 | 100.96      | 111.40   |
| 3   | CV    | 64  | VAL  | CB-CA-C | -5.50 | 100.96      | 111.40   |
| 3   | Cs    | 64  | VAL  | CB-CA-C | -5.50 | 100.96      | 111.40   |
| 3   | Ct    | 18  | VAL  | CB-CA-C | -5.50 | 100.96      | 111.40   |
| 1   | A3    | 186 | TRP  | N-CA-C  | 5.49  | 125.83      | 111.00   |
| 1   | A8    | 186 | TRP  | N-CA-C  | 5.49  | 125.83      | 111.00   |
| 1   | Ae    | 186 | TRP  | N-CA-C  | 5.49  | 125.83      | 111.00   |
| 1   | Ah    | 186 | TRP  | N-CA-C  | 5.49  | 125.83      | 111.00   |
| 3   | CZ    | 64  | VAL  | CB-CA-C | -5.49 | 100.96      | 111.40   |
| 3   | C2    | 64  | VAL  | CB-CA-C | -5.49 | 100.96      | 111.40   |
| 3   | Cc    | 18  | VAL  | CB-CA-C | -5.49 | 100.96      | 111.40   |
| 3   | DA    | 18  | VAL  | CB-CA-C | -5.49 | 100.96      | 111.40   |
| 1   | Ab    | 186 | TRP  | N-CA-C  | 5.49  | 125.83      | 111.00   |
| 3   | CP    | 18  | VAL  | CB-CA-C | -5.49 | 100.97      | 111.40   |
| 3   | C0    | 64  | VAL  | CB-CA-C | -5.49 | 100.97      | 111.40   |
| 3   | Cg    | 64  | VAL  | CB-CA-C | -5.49 | 100.96      | 111.40   |
| 3   | Cx    | 18  | VAL  | CB-CA-C | -5.49 | 100.97      | 111.40   |
| 1   | AT    | 186 | TRP  | N-CA-C  | 5.49  | 125.83      | 111.00   |
| 1   | A4    | 186 | TRP  | N-CA-C  | 5.49  | 125.82      | 111.00   |
| 3   | CE    | 18  | VAL  | CB-CA-C | -5.49 | 100.97      | 111.40   |
| 3   | CG    | 64  | VAL  | CB-CA-C | -5.49 | 100.97      | 111.40   |
| 3   | CH    | 18  | VAL  | CB-CA-C | -5.49 | 100.97      | 111.40   |
| 3   | CK    | 18  | VAL  | CB-CA-C | -5.49 | 100.97      | 111.40   |
| 3   | CM    | 18  | VAL  | CB-CA-C | -5.49 | 100.97      | 111.40   |
| 3   | CX    | 208 | VAL  | CB-CA-C | -5.49 | 100.97      | 111.40   |
| 3   | C1    | 18  | VAL  | CB-CA-C | -5.49 | 100.97      | 111.40   |
| 3   | C5    | 208 | VAL  | CB-CA-C | -5.49 | 100.97      | 111.40   |
| 3   | C9    | 64  | VAL  | CB-CA-C | -5.49 | 100.97      | 111.40   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | Cc    | 64  | VAL  | CB-CA-C | -5.49 | 100.97      | 111.40   |
| 3   | Cf    | 18  | VAL  | CB-CA-C | -5.49 | 100.97      | 111.40   |
| 3   | Ck    | 208 | VAL  | CB-CA-C | -5.49 | 100.97      | 111.40   |
| 3   | Co    | 208 | VAL  | CB-CA-C | -5.49 | 100.97      | 111.40   |
| 3   | Cr    | 208 | VAL  | CB-CA-C | -5.49 | 100.97      | 111.40   |
| 1   | DF    | 186 | TRP  | N-CA-C  | 5.49  | 125.82      | 111.00   |
| 1   | Ac    | 186 | TRP  | N-CA-C  | 5.49  | 125.82      | 111.00   |
| 3   | CC    | 64  | VAL  | CB-CA-C | -5.49 | 100.97      | 111.40   |
| 3   | CT    | 64  | VAL  | CB-CA-C | -5.49 | 100.97      | 111.40   |
| 3   | C6    | 18  | VAL  | CB-CA-C | -5.49 | 100.97      | 111.40   |
| 3   | Ch    | 64  | VAL  | CB-CA-C | -5.49 | 100.97      | 111.40   |
| 1   | DI    | 186 | TRP  | N-CA-C  | 5.49  | 125.82      | 111.00   |
| 1   | AZ    | 186 | TRP  | N-CA-C  | 5.49  | 125.81      | 111.00   |
| 3   | CG    | 208 | VAL  | CB-CA-C | -5.49 | 100.97      | 111.40   |
| 3   | CP    | 64  | VAL  | CB-CA-C | -5.49 | 100.97      | 111.40   |
| 1   | AA    | 186 | TRP  | N-CA-C  | 5.49  | 125.81      | 111.00   |
| 1   | AD    | 186 | TRP  | N-CA-C  | 5.49  | 125.81      | 111.00   |
| 1   | AN    | 186 | TRP  | N-CA-C  | 5.49  | 125.81      | 111.00   |
| 1   | AO    | 186 | TRP  | N-CA-C  | 5.49  | 125.81      | 111.00   |
| 1   | A2    | 186 | TRP  | N-CA-C  | 5.49  | 125.81      | 111.00   |
| 1   | A6    | 186 | TRP  | N-CA-C  | 5.49  | 125.81      | 111.00   |
| 3   | CJ    | 18  | VAL  | CB-CA-C | -5.49 | 100.98      | 111.40   |
| 3   | CW    | 208 | VAL  | CB-CA-C | -5.49 | 100.98      | 111.40   |
| 3   | Cj    | 18  | VAL  | CB-CA-C | -5.49 | 100.98      | 111.40   |
| 1   | DD    | 186 | TRP  | N-CA-C  | 5.49  | 125.81      | 111.00   |
| 3   | CC    | 18  | VAL  | CB-CA-C | -5.48 | 100.98      | 111.40   |
| 3   | CD    | 18  | VAL  | CB-CA-C | -5.48 | 100.98      | 111.40   |
| 3   | CF    | 18  | VAL  | CB-CA-C | -5.48 | 100.98      | 111.40   |
| 3   | CV    | 208 | VAL  | CB-CA-C | -5.48 | 100.98      | 111.40   |
| 3   | Co    | 18  | VAL  | CB-CA-C | -5.48 | 100.98      | 111.40   |
| 1   | AJ    | 186 | TRP  | N-CA-C  | 5.48  | 125.80      | 111.00   |
| 1   | Af    | 186 | TRP  | N-CA-C  | 5.48  | 125.80      | 111.00   |
| 3   | CG    | 18  | VAL  | CB-CA-C | -5.48 | 100.98      | 111.40   |
| 3   | CL    | 18  | VAL  | CB-CA-C | -5.48 | 100.98      | 111.40   |
| 3   | CP    | 208 | VAL  | CB-CA-C | -5.48 | 100.98      | 111.40   |
| 3   | CR    | 208 | VAL  | CB-CA-C | -5.48 | 100.98      | 111.40   |
| 3   | C0    | 208 | VAL  | CB-CA-C | -5.48 | 100.98      | 111.40   |
| 3   | C8    | 18  | VAL  | CB-CA-C | -5.48 | 100.98      | 111.40   |
| 3   | Ce    | 18  | VAL  | CB-CA-C | -5.48 | 100.98      | 111.40   |
| 3   | Ck    | 18  | VAL  | CB-CA-C | -5.48 | 100.98      | 111.40   |
| 3   | Cp    | 18  | VAL  | CB-CA-C | -5.48 | 100.98      | 111.40   |
| 3   | Cw    | 18  | VAL  | CB-CA-C | -5.48 | 100.98      | 111.40   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | DB    | 64  | VAL  | CB-CA-C | -5.48 | 100.98      | 111.40   |
| 3   | Cl    | 208 | VAL  | CB-CA-C | -5.48 | 100.99      | 111.40   |
| 3   | Cu    | 64  | VAL  | CB-CA-C | -5.48 | 100.99      | 111.40   |
| 3   | Cx    | 64  | VAL  | CB-CA-C | -5.48 | 100.99      | 111.40   |
| 3   | C2    | 208 | VAL  | CB-CA-C | -5.48 | 100.99      | 111.40   |
| 3   | Ct    | 208 | VAL  | CB-CA-C | -5.48 | 100.99      | 111.40   |
| 3   | CF    | 208 | VAL  | CB-CA-C | -5.48 | 101.00      | 111.40   |
| 3   | CQ    | 18  | VAL  | CB-CA-C | -5.48 | 100.99      | 111.40   |
| 3   | C9    | 208 | VAL  | CB-CA-C | -5.48 | 100.99      | 111.40   |
| 3   | Cf    | 208 | VAL  | CB-CA-C | -5.48 | 100.99      | 111.40   |
| 3   | Ck    | 64  | VAL  | CB-CA-C | -5.48 | 100.99      | 111.40   |
| 3   | Cm    | 18  | VAL  | CB-CA-C | -5.48 | 100.99      | 111.40   |
| 3   | Cx    | 208 | VAL  | CB-CA-C | -5.48 | 100.99      | 111.40   |
| 3   | DA    | 208 | VAL  | CB-CA-C | -5.48 | 100.99      | 111.40   |
| 1   | DE    | 186 | TRP  | N-CA-C  | 5.48  | 125.79      | 111.00   |
| 3   | CH    | 208 | VAL  | CB-CA-C | -5.48 | 101.00      | 111.40   |
| 3   | C5    | 64  | VAL  | CB-CA-C | -5.48 | 101.00      | 111.40   |
| 3   | Cr    | 64  | VAL  | CB-CA-C | -5.48 | 101.00      | 111.40   |
| 3   | C3    | 18  | VAL  | CB-CA-C | -5.47 | 101.00      | 111.40   |
| 3   | Cd    | 18  | VAL  | CB-CA-C | -5.47 | 101.00      | 111.40   |
| 3   | Cg    | 18  | VAL  | CB-CA-C | -5.47 | 101.00      | 111.40   |
| 3   | Ch    | 18  | VAL  | CB-CA-C | -5.47 | 101.00      | 111.40   |
| 3   | Cm    | 64  | VAL  | CB-CA-C | -5.47 | 101.00      | 111.40   |
| 3   | CA    | 208 | VAL  | CB-CA-C | -5.47 | 101.00      | 111.40   |
| 3   | CD    | 64  | VAL  | CB-CA-C | -5.47 | 101.00      | 111.40   |
| 3   | CN    | 18  | VAL  | CB-CA-C | -5.47 | 101.00      | 111.40   |
| 3   | CS    | 64  | VAL  | CB-CA-C | -5.47 | 101.00      | 111.40   |
| 3   | CW    | 64  | VAL  | CB-CA-C | -5.47 | 101.00      | 111.40   |
| 3   | DB    | 208 | VAL  | CB-CA-C | -5.47 | 101.00      | 111.40   |
| 1   | AW    | 186 | TRP  | N-CA-C  | 5.47  | 125.77      | 111.00   |
| 3   | CI    | 208 | VAL  | CB-CA-C | -5.47 | 101.01      | 111.40   |
| 3   | CX    | 64  | VAL  | CB-CA-C | -5.47 | 101.01      | 111.40   |
| 3   | C7    | 64  | VAL  | CB-CA-C | -5.47 | 101.01      | 111.40   |
| 3   | Cs    | 18  | VAL  | CB-CA-C | -5.47 | 101.01      | 111.40   |
| 1   | A1    | 186 | TRP  | N-CA-C  | 5.47  | 125.76      | 111.00   |
| 3   | CZ    | 208 | VAL  | CB-CA-C | -5.47 | 101.01      | 111.40   |
| 3   | Cn    | 18  | VAL  | CB-CA-C | -5.47 | 101.01      | 111.40   |
| 3   | CC    | 208 | VAL  | CB-CA-C | -5.47 | 101.01      | 111.40   |
| 3   | CO    | 208 | VAL  | CB-CA-C | -5.47 | 101.01      | 111.40   |
| 3   | C2    | 18  | VAL  | CB-CA-C | -5.47 | 101.01      | 111.40   |
| 3   | C6    | 208 | VAL  | CB-CA-C | -5.47 | 101.02      | 111.40   |
| 3   | Cv    | 18  | VAL  | CB-CA-C | -5.47 | 101.01      | 111.40   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | CN    | 208 | VAL  | CB-CA-C | -5.46 | 101.02      | 111.40   |
| 3   | CS    | 18  | VAL  | CB-CA-C | -5.46 | 101.02      | 111.40   |
| 3   | CY    | 18  | VAL  | CB-CA-C | -5.46 | 101.02      | 111.40   |
| 3   | Cd    | 208 | VAL  | CB-CA-C | -5.46 | 101.02      | 111.40   |
| 3   | CM    | 208 | VAL  | CB-CA-C | -5.46 | 101.02      | 111.40   |
| 3   | Ci    | 208 | VAL  | CB-CA-C | -5.46 | 101.02      | 111.40   |
| 3   | CD    | 208 | VAL  | CB-CA-C | -5.46 | 101.02      | 111.40   |
| 3   | CX    | 18  | VAL  | CB-CA-C | -5.46 | 101.03      | 111.40   |
| 3   | C5    | 18  | VAL  | CB-CA-C | -5.46 | 101.02      | 111.40   |
| 3   | Cw    | 208 | VAL  | CB-CA-C | -5.46 | 101.02      | 111.40   |
| 1   | A7    | 186 | TRP  | N-CA-C  | 5.46  | 125.74      | 111.00   |
| 3   | CI    | 18  | VAL  | CB-CA-C | -5.46 | 101.03      | 111.40   |
| 3   | C7    | 18  | VAL  | CB-CA-C | -5.46 | 101.03      | 111.40   |
| 3   | Cr    | 18  | VAL  | CB-CA-C | -5.46 | 101.03      | 111.40   |
| 3   | CO    | 18  | VAL  | CB-CA-C | -5.46 | 101.03      | 111.40   |
| 3   | C4    | 208 | VAL  | CB-CA-C | -5.46 | 101.03      | 111.40   |
| 3   | Cu    | 18  | VAL  | CB-CA-C | -5.46 | 101.03      | 111.40   |
| 3   | CI    | 64  | VAL  | CB-CA-C | -5.45 | 101.04      | 111.40   |
| 3   | CT    | 208 | VAL  | CB-CA-C | -5.45 | 101.04      | 111.40   |
| 3   | CY    | 208 | VAL  | CB-CA-C | -5.45 | 101.04      | 111.40   |
| 3   | CK    | 208 | VAL  | CB-CA-C | -5.45 | 101.04      | 111.40   |
| 3   | CU    | 208 | VAL  | CB-CA-C | -5.45 | 101.04      | 111.40   |
| 3   | CV    | 18  | VAL  | CB-CA-C | -5.45 | 101.04      | 111.40   |
| 3   | Cq    | 208 | VAL  | CB-CA-C | -5.45 | 101.04      | 111.40   |
| 3   | CN    | 64  | VAL  | CB-CA-C | -5.45 | 101.05      | 111.40   |
| 3   | Cm    | 208 | VAL  | CB-CA-C | -5.45 | 101.04      | 111.40   |
| 3   | Cv    | 208 | VAL  | CB-CA-C | -5.45 | 101.05      | 111.40   |
| 3   | CB    | 18  | VAL  | CB-CA-C | -5.45 | 101.05      | 111.40   |
| 3   | Cg    | 208 | VAL  | CB-CA-C | -5.45 | 101.05      | 111.40   |
| 3   | Cc    | 208 | VAL  | CB-CA-C | -5.45 | 101.05      | 111.40   |
| 3   | Cn    | 208 | VAL  | CB-CA-C | -5.45 | 101.05      | 111.40   |
| 3   | Ci    | 18  | VAL  | CB-CA-C | -5.45 | 101.05      | 111.40   |
| 3   | C8    | 208 | VAL  | CB-CA-C | -5.44 | 101.06      | 111.40   |
| 3   | CE    | 208 | VAL  | CB-CA-C | -5.44 | 101.06      | 111.40   |
| 3   | CT    | 18  | VAL  | CB-CA-C | -5.44 | 101.06      | 111.40   |
| 3   | Cs    | 208 | VAL  | CB-CA-C | -5.44 | 101.06      | 111.40   |
| 3   | C0    | 18  | VAL  | CB-CA-C | -5.43 | 101.08      | 111.40   |
| 3   | C3    | 208 | VAL  | CB-CA-C | -5.43 | 101.08      | 111.40   |
| 3   | CS    | 208 | VAL  | CB-CA-C | -5.43 | 101.09      | 111.40   |
| 3   | Ch    | 208 | VAL  | CB-CA-C | -5.43 | 101.09      | 111.40   |
| 1   | DJ    | 242 | ASN  | CB-CA-C | -5.35 | 99.71       | 110.40   |
| 1   | A5    | 242 | ASN  | CB-CA-C | -5.34 | 99.71       | 110.40   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | AH    | 242 | ASN  | CB-CA-C | -5.34 | 99.72       | 110.40   |
| 1   | Aa    | 242 | ASN  | CB-CA-C | -5.34 | 99.72       | 110.40   |
| 1   | AX    | 242 | ASN  | CB-CA-C | -5.34 | 99.72       | 110.40   |
| 1   | Ag    | 242 | ASN  | CB-CA-C | -5.34 | 99.72       | 110.40   |
| 1   | An    | 242 | ASN  | CB-CA-C | -5.34 | 99.73       | 110.40   |
| 1   | Am    | 242 | ASN  | CB-CA-C | -5.33 | 99.73       | 110.40   |
| 1   | AA    | 242 | ASN  | CB-CA-C | -5.33 | 99.73       | 110.40   |
| 1   | AU    | 242 | ASN  | CB-CA-C | -5.33 | 99.74       | 110.40   |
| 1   | A2    | 242 | ASN  | CB-CA-C | -5.33 | 99.74       | 110.40   |
| 1   | A8    | 242 | ASN  | CB-CA-C | -5.33 | 99.74       | 110.40   |
| 1   | AN    | 242 | ASN  | CB-CA-C | -5.33 | 99.74       | 110.40   |
| 1   | AV    | 242 | ASN  | CB-CA-C | -5.33 | 99.74       | 110.40   |
| 1   | A6    | 242 | ASN  | CB-CA-C | -5.33 | 99.74       | 110.40   |
| 1   | Ac    | 242 | ASN  | CB-CA-C | -5.33 | 99.74       | 110.40   |
| 1   | DF    | 242 | ASN  | CB-CA-C | -5.33 | 99.74       | 110.40   |
| 1   | Ad    | 242 | ASN  | CB-CA-C | -5.33 | 99.75       | 110.40   |
| 1   | DE    | 242 | ASN  | CB-CA-C | -5.33 | 99.75       | 110.40   |
| 1   | A0    | 242 | ASN  | CB-CA-C | -5.32 | 99.75       | 110.40   |
| 1   | A9    | 242 | ASN  | CB-CA-C | -5.32 | 99.75       | 110.40   |
| 1   | Ak    | 242 | ASN  | CB-CA-C | -5.32 | 99.75       | 110.40   |
| 1   | DG    | 242 | ASN  | CB-CA-C | -5.32 | 99.75       | 110.40   |
| 1   | A3    | 242 | ASN  | CB-CA-C | -5.32 | 99.75       | 110.40   |
| 1   | AL    | 242 | ASN  | CB-CA-C | -5.32 | 99.76       | 110.40   |
| 1   | AT    | 242 | ASN  | CB-CA-C | -5.32 | 99.76       | 110.40   |
| 1   | A4    | 242 | ASN  | CB-CA-C | -5.32 | 99.76       | 110.40   |
| 1   | DH    | 242 | ASN  | CB-CA-C | -5.32 | 99.76       | 110.40   |
| 1   | AG    | 242 | ASN  | CB-CA-C | -5.32 | 99.77       | 110.40   |
| 1   | AK    | 242 | ASN  | CB-CA-C | -5.32 | 99.77       | 110.40   |
| 1   | Af    | 242 | ASN  | CB-CA-C | -5.32 | 99.77       | 110.40   |
| 1   | Ao    | 242 | ASN  | CB-CA-C | -5.32 | 99.76       | 110.40   |
| 1   | AY    | 242 | ASN  | CB-CA-C | -5.32 | 99.77       | 110.40   |
| 1   | AE    | 242 | ASN  | CB-CA-C | -5.31 | 99.77       | 110.40   |
| 1   | AS    | 242 | ASN  | CB-CA-C | -5.31 | 99.77       | 110.40   |
| 1   | AZ    | 242 | ASN  | CB-CA-C | -5.31 | 99.78       | 110.40   |
| 1   | AB    | 242 | ASN  | CB-CA-C | -5.31 | 99.78       | 110.40   |
| 1   | AC    | 242 | ASN  | CB-CA-C | -5.31 | 99.78       | 110.40   |
| 1   | Aj    | 242 | ASN  | CB-CA-C | -5.31 | 99.78       | 110.40   |
| 1   | DK    | 242 | ASN  | CB-CA-C | -5.31 | 99.78       | 110.40   |
| 1   | AQ    | 242 | ASN  | CB-CA-C | -5.31 | 99.79       | 110.40   |
| 1   | AD    | 242 | ASN  | CB-CA-C | -5.31 | 99.79       | 110.40   |
| 1   | AW    | 242 | ASN  | CB-CA-C | -5.31 | 99.79       | 110.40   |
| 1   | AM    | 242 | ASN  | CB-CA-C | -5.30 | 99.79       | 110.40   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | AR    | 242 | ASN  | CB-CA-C | -5.30 | 99.79       | 110.40   |
| 1   | A1    | 242 | ASN  | CB-CA-C | -5.30 | 99.79       | 110.40   |
| 1   | Ai    | 242 | ASN  | CB-CA-C | -5.30 | 99.79       | 110.40   |
| 1   | AO    | 242 | ASN  | CB-CA-C | -5.30 | 99.80       | 110.40   |
| 1   | A7    | 242 | ASN  | CB-CA-C | -5.30 | 99.80       | 110.40   |
| 1   | Ab    | 242 | ASN  | CB-CA-C | -5.30 | 99.80       | 110.40   |
| 1   | Al    | 242 | ASN  | CB-CA-C | -5.30 | 99.80       | 110.40   |
| 1   | AI    | 242 | ASN  | CB-CA-C | -5.30 | 99.81       | 110.40   |
| 1   | AJ    | 242 | ASN  | CB-CA-C | -5.30 | 99.81       | 110.40   |
| 1   | AP    | 242 | ASN  | CB-CA-C | -5.30 | 99.81       | 110.40   |
| 1   | DC    | 242 | ASN  | CB-CA-C | -5.29 | 99.81       | 110.40   |
| 1   | DI    | 242 | ASN  | CB-CA-C | -5.29 | 99.82       | 110.40   |
| 1   | AF    | 242 | ASN  | CB-CA-C | -5.29 | 99.82       | 110.40   |
| 1   | DD    | 242 | ASN  | CB-CA-C | -5.28 | 99.84       | 110.40   |
| 1   | Ah    | 242 | ASN  | CB-CA-C | -5.27 | 99.86       | 110.40   |
| 1   | Ae    | 242 | ASN  | CB-CA-C | -5.27 | 99.86       | 110.40   |
| 1   | Ao    | 6   | GLU  | N-CA-C  | 5.25  | 125.17      | 111.00   |
| 1   | A3    | 6   | GLU  | N-CA-C  | 5.24  | 125.14      | 111.00   |
| 1   | AM    | 6   | GLU  | N-CA-C  | 5.24  | 125.13      | 111.00   |
| 1   | AU    | 6   | GLU  | N-CA-C  | 5.24  | 125.13      | 111.00   |
| 1   | Ac    | 6   | GLU  | N-CA-C  | 5.24  | 125.13      | 111.00   |
| 1   | Ah    | 6   | GLU  | N-CA-C  | 5.24  | 125.14      | 111.00   |
| 1   | A0    | 6   | GLU  | N-CA-C  | 5.23  | 125.13      | 111.00   |
| 1   | AB    | 6   | GLU  | N-CA-C  | 5.23  | 125.13      | 111.00   |
| 1   | AO    | 6   | GLU  | N-CA-C  | 5.23  | 125.13      | 111.00   |
| 1   | Ai    | 6   | GLU  | N-CA-C  | 5.23  | 125.13      | 111.00   |
| 1   | Am    | 6   | GLU  | N-CA-C  | 5.23  | 125.13      | 111.00   |
| 1   | AP    | 6   | GLU  | N-CA-C  | 5.23  | 125.12      | 111.00   |
| 1   | AT    | 6   | GLU  | N-CA-C  | 5.23  | 125.12      | 111.00   |
| 1   | DI    | 6   | GLU  | N-CA-C  | 5.23  | 125.12      | 111.00   |
| 1   | A5    | 6   | GLU  | N-CA-C  | 5.23  | 125.11      | 111.00   |
| 1   | DJ    | 6   | GLU  | N-CA-C  | 5.23  | 125.12      | 111.00   |
| 1   | Ae    | 6   | GLU  | N-CA-C  | 5.23  | 125.11      | 111.00   |
| 1   | AF    | 6   | GLU  | N-CA-C  | 5.22  | 125.11      | 111.00   |
| 1   | AS    | 6   | GLU  | N-CA-C  | 5.22  | 125.10      | 111.00   |
| 1   | A1    | 6   | GLU  | N-CA-C  | 5.22  | 125.10      | 111.00   |
| 1   | A4    | 6   | GLU  | N-CA-C  | 5.22  | 125.10      | 111.00   |
| 1   | Aa    | 6   | GLU  | N-CA-C  | 5.22  | 125.10      | 111.00   |
| 1   | DC    | 6   | GLU  | N-CA-C  | 5.22  | 125.10      | 111.00   |
| 1   | DF    | 6   | GLU  | N-CA-C  | 5.22  | 125.10      | 111.00   |
| 1   | DH    | 6   | GLU  | N-CA-C  | 5.22  | 125.10      | 111.00   |
| 1   | Ag    | 6   | GLU  | N-CA-C  | 5.22  | 125.10      | 111.00   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | AW    | 6   | GLU  | N-CA-C | 5.22  | 125.09      | 111.00   |
| 1   | AZ    | 6   | GLU  | N-CA-C | 5.22  | 125.09      | 111.00   |
| 1   | Af    | 6   | GLU  | N-CA-C | 5.22  | 125.09      | 111.00   |
| 1   | A8    | 6   | GLU  | N-CA-C | 5.22  | 125.08      | 111.00   |
| 1   | AC    | 6   | GLU  | N-CA-C | 5.21  | 125.08      | 111.00   |
| 1   | Aj    | 6   | GLU  | N-CA-C | 5.21  | 125.08      | 111.00   |
| 1   | Ab    | 6   | GLU  | N-CA-C | 5.21  | 125.08      | 111.00   |
| 1   | Ad    | 6   | GLU  | N-CA-C | 5.21  | 125.08      | 111.00   |
| 1   | AR    | 6   | GLU  | N-CA-C | 5.21  | 125.07      | 111.00   |
| 1   | DG    | 6   | GLU  | N-CA-C | 5.21  | 125.07      | 111.00   |
| 1   | AI    | 6   | GLU  | N-CA-C | 5.21  | 125.07      | 111.00   |
| 1   | A2    | 6   | GLU  | N-CA-C | 5.21  | 125.07      | 111.00   |
| 1   | Ak    | 6   | GLU  | N-CA-C | 5.21  | 125.07      | 111.00   |
| 1   | DD    | 6   | GLU  | N-CA-C | 5.21  | 125.07      | 111.00   |
| 1   | AH    | 6   | GLU  | N-CA-C | 5.21  | 125.06      | 111.00   |
| 1   | AN    | 6   | GLU  | N-CA-C | 5.21  | 125.06      | 111.00   |
| 1   | AQ    | 6   | GLU  | N-CA-C | 5.21  | 125.06      | 111.00   |
| 1   | A9    | 6   | GLU  | N-CA-C | 5.21  | 125.06      | 111.00   |
| 1   | DE    | 6   | GLU  | N-CA-C | 5.21  | 125.06      | 111.00   |
| 1   | AE    | 6   | GLU  | N-CA-C | 5.21  | 125.06      | 111.00   |
| 1   | AL    | 6   | GLU  | N-CA-C | 5.21  | 125.06      | 111.00   |
| 1   | AV    | 6   | GLU  | N-CA-C | 5.21  | 125.06      | 111.00   |
| 1   | AX    | 6   | GLU  | N-CA-C | 5.21  | 125.06      | 111.00   |
| 1   | A6    | 6   | GLU  | N-CA-C | 5.21  | 125.06      | 111.00   |
| 1   | A7    | 6   | GLU  | N-CA-C | 5.21  | 125.05      | 111.00   |
| 1   | AJ    | 6   | GLU  | N-CA-C | 5.20  | 125.04      | 111.00   |
| 1   | DK    | 6   | GLU  | N-CA-C | 5.20  | 125.05      | 111.00   |
| 1   | AT    | 70  | ARG  | N-CA-C | -5.20 | 96.96       | 111.00   |
| 1   | Al    | 6   | GLU  | N-CA-C | 5.20  | 125.04      | 111.00   |
| 1   | AG    | 6   | GLU  | N-CA-C | 5.20  | 125.04      | 111.00   |
| 1   | AK    | 6   | GLU  | N-CA-C | 5.20  | 125.04      | 111.00   |
| 1   | AA    | 6   | GLU  | N-CA-C | 5.20  | 125.03      | 111.00   |
| 1   | AF    | 70  | ARG  | N-CA-C | -5.20 | 96.97       | 111.00   |
| 1   | AO    | 70  | ARG  | N-CA-C | -5.20 | 96.97       | 111.00   |
| 1   | Ad    | 70  | ARG  | N-CA-C | -5.20 | 96.97       | 111.00   |
| 1   | DH    | 4   | VAL  | C-N-CA | 5.20  | 133.21      | 122.30   |
| 1   | DI    | 70  | ARG  | N-CA-C | -5.20 | 96.97       | 111.00   |
| 1   | AD    | 6   | GLU  | N-CA-C | 5.19  | 125.01      | 111.00   |
| 1   | Ac    | 70  | ARG  | N-CA-C | -5.19 | 96.99       | 111.00   |
| 1   | An    | 6   | GLU  | N-CA-C | 5.19  | 125.01      | 111.00   |
| 1   | A3    | 4   | VAL  | C-N-CA | 5.19  | 133.19      | 122.30   |
| 1   | AB    | 70  | ARG  | N-CA-C | -5.18 | 97.00       | 111.00   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | Af    | 4   | VAL  | C-N-CA    | 5.18  | 133.19      | 122.30   |
| 1   | AJ    | 70  | ARG  | N-CA-C    | -5.18 | 97.01       | 111.00   |
| 1   | AM    | 70  | ARG  | N-CA-C    | -5.18 | 97.01       | 111.00   |
| 2   | Bq    | 60  | ARG  | NE-CZ-NH1 | 5.18  | 122.89      | 120.30   |
| 1   | DF    | 70  | ARG  | N-CA-C    | -5.18 | 97.00       | 111.00   |
| 1   | AD    | 70  | ARG  | N-CA-C    | -5.18 | 97.01       | 111.00   |
| 1   | AR    | 70  | ARG  | N-CA-C    | -5.18 | 97.01       | 111.00   |
| 1   | A0    | 70  | ARG  | N-CA-C    | -5.18 | 97.01       | 111.00   |
| 1   | Af    | 70  | ARG  | N-CA-C    | -5.18 | 97.01       | 111.00   |
| 1   | DE    | 70  | ARG  | N-CA-C    | -5.18 | 97.01       | 111.00   |
| 1   | AA    | 70  | ARG  | N-CA-C    | -5.18 | 97.01       | 111.00   |
| 1   | AY    | 70  | ARG  | N-CA-C    | -5.18 | 97.01       | 111.00   |
| 1   | A8    | 70  | ARG  | N-CA-C    | -5.18 | 97.02       | 111.00   |
| 1   | An    | 4   | VAL  | C-N-CA    | 5.18  | 133.18      | 122.30   |
| 1   | An    | 70  | ARG  | N-CA-C    | -5.18 | 97.02       | 111.00   |
| 1   | AT    | 4   | VAL  | C-N-CA    | 5.18  | 133.18      | 122.30   |
| 1   | Ao    | 4   | VAL  | C-N-CA    | 5.18  | 133.17      | 122.30   |
| 1   | AG    | 70  | ARG  | N-CA-C    | -5.18 | 97.02       | 111.00   |
| 1   | AK    | 4   | VAL  | C-N-CA    | 5.18  | 133.17      | 122.30   |
| 1   | AY    | 6   | GLU  | N-CA-C    | 5.18  | 124.98      | 111.00   |
| 1   | Ai    | 70  | ARG  | N-CA-C    | -5.18 | 97.02       | 111.00   |
| 1   | AG    | 62  | SER  | N-CA-C    | 5.17  | 124.97      | 111.00   |
| 1   | AK    | 70  | ARG  | N-CA-C    | -5.17 | 97.03       | 111.00   |
| 1   | AN    | 70  | ARG  | N-CA-C    | -5.17 | 97.03       | 111.00   |
| 1   | A1    | 70  | ARG  | N-CA-C    | -5.17 | 97.03       | 111.00   |
| 1   | A9    | 4   | VAL  | C-N-CA    | 5.17  | 133.16      | 122.30   |
| 1   | Ae    | 70  | ARG  | N-CA-C    | -5.17 | 97.03       | 111.00   |
| 1   | Ao    | 70  | ARG  | N-CA-C    | -5.17 | 97.03       | 111.00   |
| 1   | DD    | 70  | ARG  | N-CA-C    | -5.17 | 97.03       | 111.00   |
| 1   | AL    | 70  | ARG  | N-CA-C    | -5.17 | 97.03       | 111.00   |
| 1   | AW    | 70  | ARG  | N-CA-C    | -5.17 | 97.04       | 111.00   |
| 1   | A4    | 70  | ARG  | N-CA-C    | -5.17 | 97.04       | 111.00   |
| 1   | A7    | 70  | ARG  | N-CA-C    | -5.17 | 97.04       | 111.00   |
| 1   | Aj    | 70  | ARG  | N-CA-C    | -5.17 | 97.03       | 111.00   |
| 1   | Am    | 70  | ARG  | N-CA-C    | -5.17 | 97.03       | 111.00   |
| 1   | AL    | 4   | VAL  | C-N-CA    | 5.17  | 133.15      | 122.30   |
| 1   | AP    | 70  | ARG  | N-CA-C    | -5.17 | 97.05       | 111.00   |
| 1   | Aa    | 70  | ARG  | N-CA-C    | -5.17 | 97.05       | 111.00   |
| 1   | Ab    | 70  | ARG  | N-CA-C    | -5.17 | 97.05       | 111.00   |
| 1   | AQ    | 4   | VAL  | C-N-CA    | 5.17  | 133.15      | 122.30   |
| 1   | AV    | 4   | VAL  | C-N-CA    | 5.17  | 133.15      | 122.30   |
| 1   | A3    | 70  | ARG  | N-CA-C    | -5.17 | 97.05       | 111.00   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | Ag    | 70  | ARG  | N-CA-C    | -5.17 | 97.05       | 111.00   |
| 1   | DK    | 70  | ARG  | N-CA-C    | -5.17 | 97.05       | 111.00   |
| 1   | A0    | 4   | VAL  | C-N-CA    | 5.17  | 133.15      | 122.30   |
| 1   | A6    | 70  | ARG  | N-CA-C    | -5.17 | 97.06       | 111.00   |
| 1   | AA    | 4   | VAL  | C-N-CA    | 5.16  | 133.14      | 122.30   |
| 1   | AP    | 4   | VAL  | C-N-CA    | 5.16  | 133.14      | 122.30   |
| 1   | AU    | 62  | SER  | N-CA-C    | 5.16  | 124.94      | 111.00   |
| 1   | AY    | 4   | VAL  | C-N-CA    | 5.16  | 133.14      | 122.30   |
| 1   | A9    | 70  | ARG  | N-CA-C    | -5.16 | 97.06       | 111.00   |
| 2   | Bb    | 60  | ARG  | NE-CZ-NH1 | 5.16  | 122.88      | 120.30   |
| 1   | DG    | 70  | ARG  | N-CA-C    | -5.16 | 97.06       | 111.00   |
| 1   | AF    | 4   | VAL  | C-N-CA    | 5.16  | 133.14      | 122.30   |
| 1   | Ah    | 70  | ARG  | N-CA-C    | -5.16 | 97.06       | 111.00   |
| 1   | Ak    | 70  | ARG  | N-CA-C    | -5.16 | 97.06       | 111.00   |
| 1   | AB    | 4   | VAL  | C-N-CA    | 5.16  | 133.14      | 122.30   |
| 1   | AS    | 70  | ARG  | N-CA-C    | -5.16 | 97.07       | 111.00   |
| 1   | AV    | 70  | ARG  | N-CA-C    | -5.16 | 97.07       | 111.00   |
| 1   | AW    | 4   | VAL  | C-N-CA    | 5.16  | 133.14      | 122.30   |
| 1   | AZ    | 70  | ARG  | N-CA-C    | -5.16 | 97.06       | 111.00   |
| 1   | A2    | 70  | ARG  | N-CA-C    | -5.16 | 97.07       | 111.00   |
| 1   | Aj    | 4   | VAL  | C-N-CA    | 5.16  | 133.14      | 122.30   |
| 1   | AE    | 70  | ARG  | N-CA-C    | -5.16 | 97.07       | 111.00   |
| 1   | A8    | 62  | SER  | N-CA-C    | 5.16  | 124.93      | 111.00   |
| 1   | A9    | 62  | SER  | N-CA-C    | 5.16  | 124.93      | 111.00   |
| 1   | DC    | 70  | ARG  | N-CA-C    | -5.16 | 97.07       | 111.00   |
| 1   | DG    | 4   | VAL  | C-N-CA    | 5.16  | 133.13      | 122.30   |
| 1   | DJ    | 70  | ARG  | N-CA-C    | -5.16 | 97.07       | 111.00   |
| 1   | Al    | 70  | ARG  | N-CA-C    | -5.16 | 97.08       | 111.00   |
| 1   | DH    | 62  | SER  | N-CA-C    | 5.16  | 124.92      | 111.00   |
| 1   | AB    | 62  | SER  | N-CA-C    | 5.16  | 124.92      | 111.00   |
| 1   | AH    | 70  | ARG  | N-CA-C    | -5.16 | 97.08       | 111.00   |
| 1   | AQ    | 70  | ARG  | N-CA-C    | -5.16 | 97.08       | 111.00   |
| 1   | AU    | 70  | ARG  | N-CA-C    | -5.16 | 97.08       | 111.00   |
| 1   | A5    | 70  | ARG  | N-CA-C    | -5.16 | 97.08       | 111.00   |
| 1   | Ae    | 62  | SER  | N-CA-C    | 5.16  | 124.92      | 111.00   |
| 1   | Aj    | 62  | SER  | N-CA-C    | 5.16  | 124.92      | 111.00   |
| 1   | DC    | 4   | VAL  | C-N-CA    | 5.16  | 133.12      | 122.30   |
| 1   | DG    | 62  | SER  | N-CA-C    | 5.16  | 124.92      | 111.00   |
| 1   | AJ    | 62  | SER  | N-CA-C    | 5.15  | 124.92      | 111.00   |
| 1   | AT    | 62  | SER  | N-CA-C    | 5.15  | 124.92      | 111.00   |
| 1   | AX    | 70  | ARG  | N-CA-C    | -5.15 | 97.08       | 111.00   |
| 1   | AI    | 70  | ARG  | N-CA-C    | -5.15 | 97.09       | 111.00   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | AO    | 4   | VAL  | C-N-CA    | 5.15  | 133.12      | 122.30   |
| 1   | AP    | 62  | SER  | N-CA-C    | 5.15  | 124.91      | 111.00   |
| 1   | AZ    | 4   | VAL  | C-N-CA    | 5.15  | 133.12      | 122.30   |
| 1   | AZ    | 62  | SER  | N-CA-C    | 5.15  | 124.91      | 111.00   |
| 1   | AH    | 62  | SER  | N-CA-C    | 5.15  | 124.91      | 111.00   |
| 1   | A1    | 62  | SER  | N-CA-C    | 5.15  | 124.91      | 111.00   |
| 1   | A4    | 4   | VAL  | C-N-CA    | 5.15  | 133.12      | 122.30   |
| 1   | Ai    | 62  | SER  | N-CA-C    | 5.15  | 124.91      | 111.00   |
| 2   | Bl    | 60  | ARG  | NE-CZ-NH1 | 5.15  | 122.88      | 120.30   |
| 1   | AG    | 4   | VAL  | C-N-CA    | 5.15  | 133.11      | 122.30   |
| 1   | AH    | 4   | VAL  | C-N-CA    | 5.15  | 133.11      | 122.30   |
| 1   | AJ    | 4   | VAL  | C-N-CA    | 5.15  | 133.11      | 122.30   |
| 1   | A4    | 62  | SER  | N-CA-C    | 5.15  | 124.90      | 111.00   |
| 1   | Ak    | 4   | VAL  | C-N-CA    | 5.15  | 133.11      | 122.30   |
| 1   | AC    | 70  | ARG  | N-CA-C    | -5.15 | 97.10       | 111.00   |
| 1   | AQ    | 62  | SER  | N-CA-C    | 5.15  | 124.90      | 111.00   |
| 1   | AS    | 4   | VAL  | C-N-CA    | 5.15  | 133.11      | 122.30   |
| 1   | DF    | 62  | SER  | N-CA-C    | 5.15  | 124.90      | 111.00   |
| 1   | AC    | 4   | VAL  | C-N-CA    | 5.15  | 133.11      | 122.30   |
| 1   | AU    | 4   | VAL  | C-N-CA    | 5.15  | 133.11      | 122.30   |
| 1   | AY    | 62  | SER  | N-CA-C    | 5.15  | 124.89      | 111.00   |
| 1   | A6    | 62  | SER  | N-CA-C    | 5.15  | 124.89      | 111.00   |
| 1   | Ae    | 4   | VAL  | C-N-CA    | 5.15  | 133.11      | 122.30   |
| 1   | An    | 62  | SER  | N-CA-C    | 5.15  | 124.89      | 111.00   |
| 1   | AI    | 4   | VAL  | C-N-CA    | 5.14  | 133.10      | 122.30   |
| 1   | A5    | 4   | VAL  | C-N-CA    | 5.14  | 133.10      | 122.30   |
| 1   | A8    | 4   | VAL  | C-N-CA    | 5.14  | 133.10      | 122.30   |
| 1   | DF    | 4   | VAL  | C-N-CA    | 5.14  | 133.10      | 122.30   |
| 1   | DH    | 70  | ARG  | N-CA-C    | -5.14 | 97.11       | 111.00   |
| 1   | DI    | 62  | SER  | N-CA-C    | 5.14  | 124.89      | 111.00   |
| 1   | AF    | 62  | SER  | N-CA-C    | 5.14  | 124.89      | 111.00   |
| 1   | AI    | 62  | SER  | N-CA-C    | 5.14  | 124.89      | 111.00   |
| 1   | AM    | 62  | SER  | N-CA-C    | 5.14  | 124.88      | 111.00   |
| 1   | Ab    | 62  | SER  | N-CA-C    | 5.14  | 124.89      | 111.00   |
| 1   | Ak    | 62  | SER  | N-CA-C    | 5.14  | 124.89      | 111.00   |
| 1   | AR    | 4   | VAL  | C-N-CA    | 5.14  | 133.10      | 122.30   |
| 1   | AX    | 4   | VAL  | C-N-CA    | 5.14  | 133.10      | 122.30   |
| 1   | Ad    | 62  | SER  | N-CA-C    | 5.14  | 124.88      | 111.00   |
| 1   | AD    | 62  | SER  | N-CA-C    | 5.14  | 124.88      | 111.00   |
| 1   | Ac    | 4   | VAL  | C-N-CA    | 5.14  | 133.09      | 122.30   |
| 1   | AR    | 62  | SER  | N-CA-C    | 5.14  | 124.87      | 111.00   |
| 1   | AX    | 62  | SER  | N-CA-C    | 5.14  | 124.87      | 111.00   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | A6    | 4   | VAL  | C-N-CA | 5.14 | 133.09      | 122.30   |
| 1   | Aa    | 4   | VAL  | C-N-CA | 5.14 | 133.09      | 122.30   |
| 1   | Al    | 4   | VAL  | C-N-CA | 5.14 | 133.09      | 122.30   |
| 1   | Ao    | 62  | SER  | N-CA-C | 5.14 | 124.87      | 111.00   |
| 1   | AA    | 62  | SER  | N-CA-C | 5.13 | 124.86      | 111.00   |
| 1   | AK    | 62  | SER  | N-CA-C | 5.13 | 124.86      | 111.00   |
| 1   | A3    | 62  | SER  | N-CA-C | 5.13 | 124.86      | 111.00   |
| 1   | Al    | 62  | SER  | N-CA-C | 5.13 | 124.87      | 111.00   |
| 1   | DJ    | 4   | VAL  | C-N-CA | 5.13 | 133.08      | 122.30   |
| 1   | DK    | 4   | VAL  | C-N-CA | 5.13 | 133.08      | 122.30   |
| 1   | Ad    | 4   | VAL  | C-N-CA | 5.13 | 133.08      | 122.30   |
| 1   | DC    | 62  | SER  | N-CA-C | 5.13 | 124.86      | 111.00   |
| 1   | Ai    | 4   | VAL  | C-N-CA | 5.13 | 133.07      | 122.30   |
| 1   | AO    | 62  | SER  | N-CA-C | 5.13 | 124.84      | 111.00   |
| 1   | A1    | 4   | VAL  | C-N-CA | 5.13 | 133.07      | 122.30   |
| 1   | A5    | 62  | SER  | N-CA-C | 5.13 | 124.84      | 111.00   |
| 1   | A7    | 62  | SER  | N-CA-C | 5.13 | 124.84      | 111.00   |
| 1   | Ag    | 62  | SER  | N-CA-C | 5.13 | 124.84      | 111.00   |
| 1   | AD    | 4   | VAL  | C-N-CA | 5.12 | 133.06      | 122.30   |
| 1   | AL    | 62  | SER  | N-CA-C | 5.12 | 124.84      | 111.00   |
| 1   | AC    | 62  | SER  | N-CA-C | 5.12 | 124.83      | 111.00   |
| 1   | AW    | 62  | SER  | N-CA-C | 5.12 | 124.83      | 111.00   |
| 1   | Af    | 62  | SER  | N-CA-C | 5.12 | 124.84      | 111.00   |
| 1   | DD    | 4   | VAL  | C-N-CA | 5.12 | 133.06      | 122.30   |
| 1   | DD    | 62  | SER  | N-CA-C | 5.12 | 124.83      | 111.00   |
| 1   | DK    | 62  | SER  | N-CA-C | 5.12 | 124.83      | 111.00   |
| 1   | AE    | 4   | VAL  | C-N-CA | 5.12 | 133.06      | 122.30   |
| 1   | AV    | 62  | SER  | N-CA-C | 5.12 | 124.83      | 111.00   |
| 1   | Ah    | 62  | SER  | N-CA-C | 5.12 | 124.82      | 111.00   |
| 1   | Ac    | 62  | SER  | N-CA-C | 5.12 | 124.82      | 111.00   |
| 1   | Am    | 62  | SER  | N-CA-C | 5.12 | 124.82      | 111.00   |
| 1   | AE    | 62  | SER  | N-CA-C | 5.11 | 124.80      | 111.00   |
| 1   | A7    | 4   | VAL  | C-N-CA | 5.11 | 133.04      | 122.30   |
| 1   | Aa    | 62  | SER  | N-CA-C | 5.11 | 124.81      | 111.00   |
| 1   | DE    | 62  | SER  | N-CA-C | 5.11 | 124.81      | 111.00   |
| 1   | AM    | 4   | VAL  | C-N-CA | 5.11 | 133.03      | 122.30   |
| 1   | AN    | 4   | VAL  | C-N-CA | 5.11 | 133.03      | 122.30   |
| 1   | AS    | 62  | SER  | N-CA-C | 5.11 | 124.80      | 111.00   |
| 1   | DJ    | 62  | SER  | N-CA-C | 5.11 | 124.80      | 111.00   |
| 1   | Ab    | 4   | VAL  | C-N-CA | 5.11 | 133.03      | 122.30   |
| 1   | DE    | 4   | VAL  | C-N-CA | 5.11 | 133.03      | 122.30   |
| 1   | A2    | 4   | VAL  | C-N-CA | 5.11 | 133.02      | 122.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | Ag    | 4   | VAL  | C-N-CA    | 5.11  | 133.02      | 122.30   |
| 1   | AN    | 62  | SER  | N-CA-C    | 5.10  | 124.78      | 111.00   |
| 2   | BQ    | 60  | ARG  | NE-CZ-NH1 | 5.10  | 122.85      | 120.30   |
| 1   | DI    | 4   | VAL  | C-N-CA    | 5.10  | 133.01      | 122.30   |
| 1   | A0    | 62  | SER  | N-CA-C    | 5.10  | 124.77      | 111.00   |
| 1   | Ah    | 4   | VAL  | C-N-CA    | 5.10  | 133.00      | 122.30   |
| 1   | A2    | 62  | SER  | N-CA-C    | 5.09  | 124.75      | 111.00   |
| 1   | Am    | 4   | VAL  | C-N-CA    | 5.09  | 133.00      | 122.30   |
| 1   | A5    | 113 | THR  | N-CA-C    | 5.09  | 124.75      | 111.00   |
| 1   | Aa    | 113 | THR  | N-CA-C    | 5.09  | 124.74      | 111.00   |
| 1   | AI    | 113 | THR  | N-CA-C    | 5.08  | 124.72      | 111.00   |
| 1   | AQ    | 113 | THR  | N-CA-C    | 5.08  | 124.72      | 111.00   |
| 2   | Bl    | 60  | ARG  | NE-CZ-NH2 | -5.08 | 117.76      | 120.30   |
| 2   | Bs    | 60  | ARG  | NE-CZ-NH1 | 5.08  | 122.84      | 120.30   |
| 1   | DD    | 113 | THR  | N-CA-C    | 5.08  | 124.72      | 111.00   |
| 1   | AA    | 113 | THR  | N-CA-C    | 5.08  | 124.71      | 111.00   |
| 1   | AP    | 113 | THR  | N-CA-C    | 5.08  | 124.71      | 111.00   |
| 1   | A3    | 113 | THR  | N-CA-C    | 5.08  | 124.71      | 111.00   |
| 1   | Ak    | 113 | THR  | N-CA-C    | 5.08  | 124.71      | 111.00   |
| 1   | DC    | 113 | THR  | N-CA-C    | 5.08  | 124.71      | 111.00   |
| 1   | AW    | 113 | THR  | N-CA-C    | 5.08  | 124.71      | 111.00   |
| 2   | BF    | 60  | ARG  | NE-CZ-NH1 | 5.08  | 122.84      | 120.30   |
| 1   | AJ    | 113 | THR  | N-CA-C    | 5.08  | 124.70      | 111.00   |
| 1   | A4    | 113 | THR  | N-CA-C    | 5.08  | 124.70      | 111.00   |
| 1   | Ab    | 113 | THR  | N-CA-C    | 5.08  | 124.70      | 111.00   |
| 2   | BT    | 60  | ARG  | NE-CZ-NH1 | 5.08  | 122.84      | 120.30   |
| 1   | DH    | 113 | THR  | N-CA-C    | 5.08  | 124.71      | 111.00   |
| 1   | AY    | 113 | THR  | N-CA-C    | 5.07  | 124.70      | 111.00   |
| 1   | AC    | 113 | THR  | N-CA-C    | 5.07  | 124.69      | 111.00   |
| 1   | A8    | 113 | THR  | N-CA-C    | 5.07  | 124.69      | 111.00   |
| 1   | Ah    | 113 | THR  | N-CA-C    | 5.07  | 124.69      | 111.00   |
| 1   | AV    | 113 | THR  | N-CA-C    | 5.07  | 124.68      | 111.00   |
| 1   | AX    | 113 | THR  | N-CA-C    | 5.07  | 124.68      | 111.00   |
| 1   | AZ    | 113 | THR  | N-CA-C    | 5.07  | 124.68      | 111.00   |
| 1   | A0    | 113 | THR  | N-CA-C    | 5.07  | 124.68      | 111.00   |
| 1   | An    | 113 | THR  | N-CA-C    | 5.07  | 124.68      | 111.00   |
| 1   | AT    | 113 | THR  | N-CA-C    | 5.07  | 124.68      | 111.00   |
| 2   | Bv    | 59  | SER  | N-CA-C    | -5.07 | 97.32       | 111.00   |
| 1   | AG    | 113 | THR  | N-CA-C    | 5.06  | 124.67      | 111.00   |
| 1   | A9    | 113 | THR  | N-CA-C    | 5.06  | 124.67      | 111.00   |
| 1   | Ag    | 113 | THR  | N-CA-C    | 5.06  | 124.67      | 111.00   |
| 2   | BI    | 59  | SER  | N-CA-C    | -5.06 | 97.33       | 111.00   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | AK    | 113 | THR  | N-CA-C    | 5.06  | 124.67      | 111.00   |
| 1   | AN    | 113 | THR  | N-CA-C    | 5.06  | 124.67      | 111.00   |
| 1   | DI    | 113 | THR  | N-CA-C    | 5.06  | 124.67      | 111.00   |
| 1   | AF    | 113 | THR  | N-CA-C    | 5.06  | 124.66      | 111.00   |
| 1   | AL    | 113 | THR  | N-CA-C    | 5.06  | 124.66      | 111.00   |
| 1   | AR    | 113 | THR  | N-CA-C    | 5.06  | 124.66      | 111.00   |
| 2   | BA    | 59  | SER  | N-CA-C    | -5.06 | 97.34       | 111.00   |
| 2   | BQ    | 59  | SER  | N-CA-C    | -5.06 | 97.34       | 111.00   |
| 2   | BZ    | 59  | SER  | N-CA-C    | -5.06 | 97.35       | 111.00   |
| 2   | B6    | 59  | SER  | N-CA-C    | -5.06 | 97.35       | 111.00   |
| 2   | Bb    | 59  | SER  | N-CA-C    | -5.06 | 97.34       | 111.00   |
| 1   | DE    | 113 | THR  | N-CA-C    | 5.06  | 124.66      | 111.00   |
| 1   | Ad    | 113 | THR  | N-CA-C    | 5.06  | 124.65      | 111.00   |
| 2   | BF    | 59  | SER  | N-CA-C    | -5.06 | 97.35       | 111.00   |
| 2   | BK    | 59  | SER  | N-CA-C    | -5.06 | 97.35       | 111.00   |
| 2   | BL    | 59  | SER  | N-CA-C    | -5.06 | 97.35       | 111.00   |
| 2   | BW    | 59  | SER  | N-CA-C    | -5.06 | 97.35       | 111.00   |
| 2   | Bd    | 59  | SER  | N-CA-C    | -5.06 | 97.35       | 111.00   |
| 1   | AD    | 113 | THR  | N-CA-C    | 5.05  | 124.64      | 111.00   |
| 1   | AE    | 113 | THR  | N-CA-C    | 5.05  | 124.64      | 111.00   |
| 1   | Af    | 113 | THR  | N-CA-C    | 5.05  | 124.65      | 111.00   |
| 1   | Ao    | 113 | THR  | N-CA-C    | 5.05  | 124.64      | 111.00   |
| 2   | BA    | 60  | ARG  | NE-CZ-NH1 | 5.05  | 122.83      | 120.30   |
| 2   | BB    | 60  | ARG  | NE-CZ-NH1 | 5.05  | 122.83      | 120.30   |
| 2   | B0    | 59  | SER  | N-CA-C    | -5.05 | 97.36       | 111.00   |
| 2   | B4    | 60  | ARG  | NE-CZ-NH1 | 5.05  | 122.83      | 120.30   |
| 2   | Bn    | 59  | SER  | N-CA-C    | -5.05 | 97.36       | 111.00   |
| 2   | Bu    | 59  | SER  | N-CA-C    | -5.05 | 97.36       | 111.00   |
| 1   | AH    | 113 | THR  | N-CA-C    | 5.05  | 124.64      | 111.00   |
| 2   | BD    | 59  | SER  | N-CA-C    | -5.05 | 97.36       | 111.00   |
| 2   | B8    | 59  | SER  | N-CA-C    | -5.05 | 97.36       | 111.00   |
| 2   | Bj    | 59  | SER  | N-CA-C    | -5.05 | 97.36       | 111.00   |
| 2   | Bk    | 59  | SER  | N-CA-C    | -5.05 | 97.36       | 111.00   |
| 2   | Bq    | 59  | SER  | N-CA-C    | -5.05 | 97.36       | 111.00   |
| 1   | AO    | 113 | THR  | N-CA-C    | 5.05  | 124.63      | 111.00   |
| 1   | A1    | 113 | THR  | N-CA-C    | 5.05  | 124.64      | 111.00   |
| 1   | Am    | 113 | THR  | N-CA-C    | 5.05  | 124.63      | 111.00   |
| 2   | BB    | 59  | SER  | N-CA-C    | -5.05 | 97.37       | 111.00   |
| 1   | AM    | 113 | THR  | N-CA-C    | 5.05  | 124.63      | 111.00   |
| 2   | Bp    | 59  | SER  | N-CA-C    | -5.05 | 97.37       | 111.00   |
| 2   | Bs    | 59  | SER  | N-CA-C    | -5.05 | 97.37       | 111.00   |
| 1   | DF    | 113 | THR  | N-CA-C    | 5.05  | 124.63      | 111.00   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | AB    | 113 | THR  | N-CA-C    | 5.05  | 124.62      | 111.00   |
| 1   | A6    | 113 | THR  | N-CA-C    | 5.05  | 124.63      | 111.00   |
| 1   | Aj    | 113 | THR  | N-CA-C    | 5.05  | 124.62      | 111.00   |
| 2   | BC    | 59  | SER  | N-CA-C    | -5.05 | 97.37       | 111.00   |
| 2   | BM    | 59  | SER  | N-CA-C    | -5.05 | 97.37       | 111.00   |
| 2   | BN    | 59  | SER  | N-CA-C    | -5.05 | 97.38       | 111.00   |
| 2   | B2    | 59  | SER  | N-CA-C    | -5.05 | 97.38       | 111.00   |
| 2   | Ba    | 59  | SER  | N-CA-C    | -5.05 | 97.37       | 111.00   |
| 2   | Bo    | 59  | SER  | N-CA-C    | -5.05 | 97.37       | 111.00   |
| 1   | DG    | 113 | THR  | N-CA-C    | 5.05  | 124.62      | 111.00   |
| 1   | DK    | 113 | THR  | N-CA-C    | 5.05  | 124.62      | 111.00   |
| 2   | BH    | 59  | SER  | N-CA-C    | -5.04 | 97.38       | 111.00   |
| 2   | B4    | 59  | SER  | N-CA-C    | -5.04 | 97.38       | 111.00   |
| 1   | Ac    | 113 | THR  | N-CA-C    | 5.04  | 124.61      | 111.00   |
| 1   | Ae    | 113 | THR  | N-CA-C    | 5.04  | 124.61      | 111.00   |
| 2   | BE    | 60  | ARG  | NE-CZ-NH1 | 5.04  | 122.82      | 120.30   |
| 2   | Bt    | 59  | SER  | N-CA-C    | -5.04 | 97.39       | 111.00   |
| 2   | Bx    | 59  | SER  | N-CA-C    | -5.04 | 97.39       | 111.00   |
| 1   | Al    | 113 | THR  | N-CA-C    | 5.04  | 124.61      | 111.00   |
| 1   | A2    | 113 | THR  | N-CA-C    | 5.04  | 124.61      | 111.00   |
| 2   | BI    | 60  | ARG  | NE-CZ-NH1 | 5.04  | 122.82      | 120.30   |
| 2   | BN    | 60  | ARG  | NE-CZ-NH1 | 5.04  | 122.82      | 120.30   |
| 2   | B3    | 59  | SER  | N-CA-C    | -5.04 | 97.39       | 111.00   |
| 1   | Ac    | 71  | LEU  | N-CA-C    | -5.04 | 97.40       | 111.00   |
| 2   | BO    | 59  | SER  | N-CA-C    | -5.04 | 97.40       | 111.00   |
| 2   | B7    | 59  | SER  | N-CA-C    | -5.04 | 97.40       | 111.00   |
| 1   | Ai    | 113 | THR  | N-CA-C    | 5.04  | 124.59      | 111.00   |
| 2   | BJ    | 59  | SER  | N-CA-C    | -5.04 | 97.41       | 111.00   |
| 2   | BP    | 59  | SER  | N-CA-C    | -5.04 | 97.40       | 111.00   |
| 2   | Be    | 60  | ARG  | NE-CZ-NH2 | -5.04 | 117.78      | 120.30   |
| 2   | Bf    | 59  | SER  | N-CA-C    | -5.04 | 97.40       | 111.00   |
| 2   | Bg    | 59  | SER  | N-CA-C    | -5.04 | 97.40       | 111.00   |
| 2   | Bl    | 59  | SER  | N-CA-C    | -5.04 | 97.41       | 111.00   |
| 1   | DJ    | 113 | THR  | N-CA-C    | 5.04  | 124.59      | 111.00   |
| 1   | AU    | 113 | THR  | N-CA-C    | 5.03  | 124.59      | 111.00   |
| 2   | BJ    | 60  | ARG  | NE-CZ-NH1 | 5.03  | 122.82      | 120.30   |
| 2   | BS    | 59  | SER  | N-CA-C    | -5.03 | 97.41       | 111.00   |
| 2   | B5    | 59  | SER  | N-CA-C    | -5.03 | 97.41       | 111.00   |
| 2   | BU    | 59  | SER  | N-CA-C    | -5.03 | 97.41       | 111.00   |
| 1   | AS    | 113 | THR  | N-CA-C    | 5.03  | 124.58      | 111.00   |
| 2   | B1    | 59  | SER  | N-CA-C    | -5.03 | 97.42       | 111.00   |
| 2   | B6    | 60  | ARG  | NE-CZ-NH1 | 5.03  | 122.81      | 120.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | Bh    | 59  | SER  | N-CA-C    | -5.03 | 97.42       | 111.00   |
| 2   | Br    | 59  | SER  | N-CA-C    | -5.03 | 97.42       | 111.00   |
| 2   | BV    | 59  | SER  | N-CA-C    | -5.03 | 97.42       | 111.00   |
| 2   | BX    | 59  | SER  | N-CA-C    | -5.03 | 97.42       | 111.00   |
| 2   | BG    | 59  | SER  | N-CA-C    | -5.03 | 97.42       | 111.00   |
| 2   | Bq    | 60  | ARG  | NE-CZ-NH2 | -5.03 | 117.79      | 120.30   |
| 2   | Bi    | 59  | SER  | N-CA-C    | -5.03 | 97.43       | 111.00   |
| 2   | Bj    | 60  | ARG  | NE-CZ-NH1 | 5.03  | 122.81      | 120.30   |
| 1   | A7    | 71  | LEU  | N-CA-C    | -5.02 | 97.44       | 111.00   |
| 1   | A7    | 113 | THR  | N-CA-C    | 5.02  | 124.56      | 111.00   |
| 2   | BE    | 59  | SER  | N-CA-C    | -5.02 | 97.44       | 111.00   |
| 2   | BT    | 59  | SER  | N-CA-C    | -5.02 | 97.44       | 111.00   |
| 2   | Be    | 59  | SER  | N-CA-C    | -5.02 | 97.45       | 111.00   |
| 2   | BD    | 60  | ARG  | NE-CZ-NH1 | 5.02  | 122.81      | 120.30   |
| 2   | BY    | 59  | SER  | N-CA-C    | -5.02 | 97.45       | 111.00   |
| 2   | B9    | 59  | SER  | N-CA-C    | -5.02 | 97.45       | 111.00   |
| 2   | Bc    | 59  | SER  | N-CA-C    | -5.02 | 97.45       | 111.00   |
| 1   | AO    | 71  | LEU  | N-CA-C    | -5.02 | 97.46       | 111.00   |
| 2   | Bw    | 59  | SER  | N-CA-C    | -5.02 | 97.46       | 111.00   |
| 1   | AX    | 71  | LEU  | N-CA-C    | -5.01 | 97.47       | 111.00   |
| 1   | Ai    | 71  | LEU  | N-CA-C    | -5.01 | 97.47       | 111.00   |
| 2   | Bm    | 59  | SER  | N-CA-C    | -5.01 | 97.47       | 111.00   |
| 1   | Ah    | 71  | LEU  | N-CA-C    | -5.01 | 97.48       | 111.00   |
| 3   | Ck    | 178 | ASN  | CB-CA-C   | -5.01 | 100.38      | 110.40   |
| 1   | AF    | 71  | LEU  | N-CA-C    | -5.01 | 97.48       | 111.00   |
| 1   | AK    | 71  | LEU  | N-CA-C    | -5.01 | 97.48       | 111.00   |
| 1   | AS    | 71  | LEU  | N-CA-C    | -5.01 | 97.48       | 111.00   |
| 1   | AE    | 71  | LEU  | N-CA-C    | -5.00 | 97.49       | 111.00   |
| 2   | BR    | 59  | SER  | N-CA-C    | -5.00 | 97.49       | 111.00   |

There are no chirality outliers.

All (180) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A0    | 208 | TYR  | Sidechain |
| 1   | A1    | 208 | TYR  | Sidechain |
| 1   | A2    | 208 | TYR  | Sidechain |
| 1   | A3    | 208 | TYR  | Sidechain |
| 1   | A4    | 208 | TYR  | Sidechain |
| 1   | A5    | 208 | TYR  | Sidechain |
| 1   | A6    | 208 | TYR  | Sidechain |
| 1   | A7    | 208 | TYR  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A8    | 208 | TYR  | Sidechain |
| 1   | A9    | 208 | TYR  | Sidechain |
| 1   | AA    | 208 | TYR  | Sidechain |
| 1   | AB    | 208 | TYR  | Sidechain |
| 1   | AC    | 208 | TYR  | Sidechain |
| 1   | AD    | 208 | TYR  | Sidechain |
| 1   | AE    | 208 | TYR  | Sidechain |
| 1   | AF    | 208 | TYR  | Sidechain |
| 1   | AG    | 208 | TYR  | Sidechain |
| 1   | AH    | 208 | TYR  | Sidechain |
| 1   | AI    | 208 | TYR  | Sidechain |
| 1   | AJ    | 208 | TYR  | Sidechain |
| 1   | AK    | 208 | TYR  | Sidechain |
| 1   | AL    | 208 | TYR  | Sidechain |
| 1   | AM    | 208 | TYR  | Sidechain |
| 1   | AN    | 208 | TYR  | Sidechain |
| 1   | AO    | 208 | TYR  | Sidechain |
| 1   | AP    | 208 | TYR  | Sidechain |
| 1   | AQ    | 208 | TYR  | Sidechain |
| 1   | AR    | 208 | TYR  | Sidechain |
| 1   | AS    | 208 | TYR  | Sidechain |
| 1   | AT    | 208 | TYR  | Sidechain |
| 1   | AU    | 208 | TYR  | Sidechain |
| 1   | AV    | 208 | TYR  | Sidechain |
| 1   | AW    | 208 | TYR  | Sidechain |
| 1   | AX    | 208 | TYR  | Sidechain |
| 1   | AY    | 208 | TYR  | Sidechain |
| 1   | AZ    | 208 | TYR  | Sidechain |
| 1   | Aa    | 208 | TYR  | Sidechain |
| 1   | Ab    | 208 | TYR  | Sidechain |
| 1   | Ac    | 208 | TYR  | Sidechain |
| 1   | Ad    | 208 | TYR  | Sidechain |
| 1   | Ae    | 208 | TYR  | Sidechain |
| 1   | Af    | 208 | TYR  | Sidechain |
| 1   | Ag    | 208 | TYR  | Sidechain |
| 1   | Ah    | 208 | TYR  | Sidechain |
| 1   | Ai    | 208 | TYR  | Sidechain |
| 1   | Aj    | 208 | TYR  | Sidechain |
| 1   | Ak    | 208 | TYR  | Sidechain |
| 1   | Al    | 208 | TYR  | Sidechain |
| 1   | Am    | 208 | TYR  | Sidechain |
| 1   | An    | 208 | TYR  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | Ao    | 208 | TYR  | Sidechain |
| 2   | B0    | 177 | TYR  | Sidechain |
| 2   | B0    | 86  | ASP  | Mainchain |
| 2   | B1    | 177 | TYR  | Sidechain |
| 2   | B1    | 86  | ASP  | Mainchain |
| 2   | B2    | 177 | TYR  | Sidechain |
| 2   | B2    | 86  | ASP  | Mainchain |
| 2   | B3    | 177 | TYR  | Sidechain |
| 2   | B3    | 86  | ASP  | Mainchain |
| 2   | B4    | 177 | TYR  | Sidechain |
| 2   | B4    | 86  | ASP  | Mainchain |
| 2   | B5    | 177 | TYR  | Sidechain |
| 2   | B5    | 86  | ASP  | Mainchain |
| 2   | B6    | 177 | TYR  | Sidechain |
| 2   | B6    | 86  | ASP  | Mainchain |
| 2   | B7    | 177 | TYR  | Sidechain |
| 2   | B7    | 86  | ASP  | Mainchain |
| 2   | B8    | 177 | TYR  | Sidechain |
| 2   | B8    | 86  | ASP  | Mainchain |
| 2   | B9    | 177 | TYR  | Sidechain |
| 2   | B9    | 86  | ASP  | Mainchain |
| 2   | BA    | 177 | TYR  | Sidechain |
| 2   | BA    | 86  | ASP  | Mainchain |
| 2   | BB    | 177 | TYR  | Sidechain |
| 2   | BB    | 86  | ASP  | Mainchain |
| 2   | BC    | 177 | TYR  | Sidechain |
| 2   | BC    | 86  | ASP  | Mainchain |
| 2   | BD    | 177 | TYR  | Sidechain |
| 2   | BD    | 86  | ASP  | Mainchain |
| 2   | BE    | 177 | TYR  | Sidechain |
| 2   | BE    | 86  | ASP  | Mainchain |
| 2   | BF    | 177 | TYR  | Sidechain |
| 2   | BF    | 86  | ASP  | Mainchain |
| 2   | BG    | 177 | TYR  | Sidechain |
| 2   | BG    | 86  | ASP  | Mainchain |
| 2   | BH    | 177 | TYR  | Sidechain |
| 2   | BH    | 86  | ASP  | Mainchain |
| 2   | BI    | 177 | TYR  | Sidechain |
| 2   | BI    | 86  | ASP  | Mainchain |
| 2   | BJ    | 177 | TYR  | Sidechain |
| 2   | BJ    | 86  | ASP  | Mainchain |
| 2   | BK    | 177 | TYR  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 2   | BK    | 86  | ASP  | Mainchain |
| 2   | BL    | 177 | TYR  | Sidechain |
| 2   | BL    | 86  | ASP  | Mainchain |
| 2   | BM    | 177 | TYR  | Sidechain |
| 2   | BM    | 86  | ASP  | Mainchain |
| 2   | BN    | 177 | TYR  | Sidechain |
| 2   | BN    | 86  | ASP  | Mainchain |
| 2   | BO    | 177 | TYR  | Sidechain |
| 2   | BO    | 86  | ASP  | Mainchain |
| 2   | BP    | 177 | TYR  | Sidechain |
| 2   | BP    | 86  | ASP  | Mainchain |
| 2   | BQ    | 177 | TYR  | Sidechain |
| 2   | BQ    | 86  | ASP  | Mainchain |
| 2   | BR    | 177 | TYR  | Sidechain |
| 2   | BR    | 86  | ASP  | Mainchain |
| 2   | BS    | 177 | TYR  | Sidechain |
| 2   | BS    | 86  | ASP  | Mainchain |
| 2   | BT    | 177 | TYR  | Sidechain |
| 2   | BT    | 86  | ASP  | Mainchain |
| 2   | BU    | 177 | TYR  | Sidechain |
| 2   | BU    | 86  | ASP  | Mainchain |
| 2   | BV    | 177 | TYR  | Sidechain |
| 2   | BV    | 86  | ASP  | Mainchain |
| 2   | BW    | 177 | TYR  | Sidechain |
| 2   | BW    | 86  | ASP  | Mainchain |
| 2   | BX    | 177 | TYR  | Sidechain |
| 2   | BX    | 86  | ASP  | Mainchain |
| 2   | BY    | 177 | TYR  | Sidechain |
| 2   | BY    | 86  | ASP  | Mainchain |
| 2   | BZ    | 177 | TYR  | Sidechain |
| 2   | BZ    | 86  | ASP  | Mainchain |
| 2   | Ba    | 177 | TYR  | Sidechain |
| 2   | Ba    | 86  | ASP  | Mainchain |
| 2   | Bb    | 177 | TYR  | Sidechain |
| 2   | Bb    | 86  | ASP  | Mainchain |
| 2   | Bc    | 177 | TYR  | Sidechain |
| 2   | Bc    | 86  | ASP  | Mainchain |
| 2   | Bd    | 177 | TYR  | Sidechain |
| 2   | Bd    | 86  | ASP  | Mainchain |
| 2   | Be    | 177 | TYR  | Sidechain |
| 2   | Be    | 86  | ASP  | Mainchain |
| 2   | Bf    | 177 | TYR  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 2   | Bf    | 86  | ASP  | Mainchain |
| 2   | Bg    | 177 | TYR  | Sidechain |
| 2   | Bg    | 86  | ASP  | Mainchain |
| 2   | Bh    | 177 | TYR  | Sidechain |
| 2   | Bh    | 86  | ASP  | Mainchain |
| 2   | Bi    | 177 | TYR  | Sidechain |
| 2   | Bi    | 86  | ASP  | Mainchain |
| 2   | Bj    | 177 | TYR  | Sidechain |
| 2   | Bj    | 86  | ASP  | Mainchain |
| 2   | Bk    | 177 | TYR  | Sidechain |
| 2   | Bk    | 86  | ASP  | Mainchain |
| 2   | Bl    | 177 | TYR  | Sidechain |
| 2   | Bl    | 86  | ASP  | Mainchain |
| 2   | Bm    | 177 | TYR  | Sidechain |
| 2   | Bm    | 86  | ASP  | Mainchain |
| 2   | Bn    | 177 | TYR  | Sidechain |
| 2   | Bn    | 86  | ASP  | Mainchain |
| 2   | Bo    | 177 | TYR  | Sidechain |
| 2   | Bo    | 86  | ASP  | Mainchain |
| 2   | Bp    | 177 | TYR  | Sidechain |
| 2   | Bp    | 86  | ASP  | Mainchain |
| 2   | Bq    | 177 | TYR  | Sidechain |
| 2   | Bq    | 86  | ASP  | Mainchain |
| 2   | Br    | 177 | TYR  | Sidechain |
| 2   | Br    | 86  | ASP  | Mainchain |
| 2   | Bs    | 177 | TYR  | Sidechain |
| 2   | Bs    | 86  | ASP  | Mainchain |
| 2   | Bt    | 177 | TYR  | Sidechain |
| 2   | Bt    | 86  | ASP  | Mainchain |
| 2   | Bu    | 177 | TYR  | Sidechain |
| 2   | Bu    | 86  | ASP  | Mainchain |
| 2   | Bv    | 177 | TYR  | Sidechain |
| 2   | Bv    | 86  | ASP  | Mainchain |
| 2   | Bw    | 177 | TYR  | Sidechain |
| 2   | Bw    | 86  | ASP  | Mainchain |
| 2   | Bx    | 177 | TYR  | Sidechain |
| 2   | Bx    | 86  | ASP  | Mainchain |
| 1   | DC    | 208 | TYR  | Sidechain |
| 1   | DD    | 208 | TYR  | Sidechain |
| 1   | DE    | 208 | TYR  | Sidechain |
| 1   | DF    | 208 | TYR  | Sidechain |
| 1   | DG    | 208 | TYR  | Sidechain |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | DH    | 208 | TYR  | Sidechain |
| 1   | DI    | 208 | TYR  | Sidechain |
| 1   | DJ    | 208 | TYR  | Sidechain |
| 1   | DK    | 208 | TYR  | Sidechain |

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A0    | 1928  | 0        | 1864     | 92      | 0            |
| 1   | A1    | 1928  | 0        | 1864     | 93      | 0            |
| 1   | A2    | 1928  | 0        | 1864     | 94      | 0            |
| 1   | A3    | 1928  | 0        | 1864     | 92      | 0            |
| 1   | A4    | 1928  | 0        | 1864     | 92      | 0            |
| 1   | A5    | 1928  | 0        | 1864     | 90      | 0            |
| 1   | A6    | 1928  | 0        | 1864     | 92      | 0            |
| 1   | A7    | 1928  | 0        | 1864     | 93      | 0            |
| 1   | A8    | 1928  | 0        | 1864     | 91      | 0            |
| 1   | A9    | 1928  | 0        | 1864     | 93      | 0            |
| 1   | AA    | 1928  | 0        | 1864     | 119     | 0            |
| 1   | AB    | 1928  | 0        | 1864     | 122     | 0            |
| 1   | AC    | 1928  | 0        | 1864     | 133     | 0            |
| 1   | AD    | 1928  | 0        | 1864     | 136     | 0            |
| 1   | AE    | 1928  | 0        | 1864     | 133     | 0            |
| 1   | AF    | 1928  | 0        | 1864     | 120     | 0            |
| 1   | AG    | 1928  | 0        | 1864     | 123     | 0            |
| 1   | AH    | 1928  | 0        | 1864     | 135     | 0            |
| 1   | AI    | 1928  | 0        | 1864     | 131     | 0            |
| 1   | AJ    | 1928  | 0        | 1864     | 129     | 0            |
| 1   | AK    | 1928  | 0        | 1864     | 132     | 0            |
| 1   | AL    | 1928  | 0        | 1864     | 133     | 0            |
| 1   | AM    | 1928  | 0        | 1864     | 127     | 0            |
| 1   | AN    | 1928  | 0        | 1864     | 130     | 0            |
| 1   | AO    | 1928  | 0        | 1864     | 123     | 0            |
| 1   | AP    | 1928  | 0        | 1864     | 94      | 0            |
| 1   | AQ    | 1928  | 0        | 1864     | 90      | 0            |
| 1   | AR    | 1928  | 0        | 1864     | 93      | 0            |
| 1   | AS    | 1928  | 0        | 1864     | 91      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | AT    | 1928  | 0        | 1864     | 92      | 0            |
| 1   | AU    | 1928  | 0        | 1864     | 92      | 0            |
| 1   | AV    | 1928  | 0        | 1864     | 91      | 0            |
| 1   | AW    | 1928  | 0        | 1864     | 94      | 0            |
| 1   | AX    | 1928  | 0        | 1864     | 92      | 0            |
| 1   | AY    | 1928  | 0        | 1864     | 92      | 0            |
| 1   | AZ    | 1928  | 0        | 1864     | 90      | 0            |
| 1   | Aa    | 1928  | 0        | 1864     | 0       | 0            |
| 1   | Ab    | 1928  | 0        | 1864     | 0       | 0            |
| 1   | Ac    | 1928  | 0        | 1864     | 0       | 0            |
| 1   | Ad    | 1928  | 0        | 1864     | 0       | 0            |
| 1   | Ae    | 1928  | 0        | 1864     | 0       | 0            |
| 1   | Af    | 1928  | 0        | 1864     | 0       | 0            |
| 1   | Ag    | 1928  | 0        | 1864     | 0       | 0            |
| 1   | Ah    | 1928  | 0        | 1864     | 0       | 0            |
| 1   | Ai    | 1928  | 0        | 1864     | 0       | 0            |
| 1   | Aj    | 1928  | 0        | 1864     | 0       | 0            |
| 1   | Ak    | 1928  | 0        | 1864     | 0       | 0            |
| 1   | Al    | 1928  | 0        | 1864     | 0       | 0            |
| 1   | Am    | 1928  | 0        | 1864     | 0       | 0            |
| 1   | An    | 1928  | 0        | 1864     | 0       | 0            |
| 1   | Ao    | 1928  | 0        | 1864     | 0       | 0            |
| 1   | DC    | 1928  | 0        | 1864     | 90      | 0            |
| 1   | DD    | 1928  | 0        | 1864     | 93      | 0            |
| 1   | DE    | 1928  | 0        | 1864     | 90      | 0            |
| 1   | DF    | 1928  | 0        | 1864     | 90      | 0            |
| 1   | DG    | 1928  | 0        | 1864     | 91      | 0            |
| 1   | DH    | 1928  | 0        | 1864     | 92      | 0            |
| 1   | DI    | 1928  | 0        | 1864     | 92      | 0            |
| 1   | DJ    | 1928  | 0        | 1864     | 91      | 0            |
| 1   | DK    | 1928  | 0        | 1864     | 92      | 0            |
| 2   | B0    | 1553  | 0        | 1523     | 59      | 0            |
| 2   | B1    | 1553  | 0        | 1523     | 57      | 0            |
| 2   | B2    | 1553  | 0        | 1523     | 57      | 0            |
| 2   | B3    | 1553  | 0        | 1523     | 58      | 0            |
| 2   | B4    | 1553  | 0        | 1523     | 58      | 0            |
| 2   | B5    | 1553  | 0        | 1523     | 58      | 0            |
| 2   | B6    | 1553  | 0        | 1523     | 57      | 0            |
| 2   | B7    | 1553  | 0        | 1523     | 57      | 0            |
| 2   | B8    | 1553  | 0        | 1523     | 58      | 0            |
| 2   | B9    | 1553  | 0        | 1523     | 55      | 0            |
| 2   | BA    | 1553  | 0        | 1523     | 65      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | BB    | 1553  | 0        | 1523     | 67      | 0            |
| 2   | BC    | 1553  | 0        | 1523     | 69      | 0            |
| 2   | BD    | 1553  | 0        | 1523     | 67      | 0            |
| 2   | BE    | 1553  | 0        | 1523     | 70      | 0            |
| 2   | BF    | 1553  | 0        | 1523     | 66      | 0            |
| 2   | BG    | 1553  | 0        | 1523     | 70      | 0            |
| 2   | BH    | 1553  | 0        | 1523     | 68      | 0            |
| 2   | BI    | 1553  | 0        | 1523     | 70      | 0            |
| 2   | BJ    | 1553  | 0        | 1523     | 74      | 0            |
| 2   | BK    | 1553  | 0        | 1523     | 71      | 0            |
| 2   | BL    | 1553  | 0        | 1523     | 75      | 0            |
| 2   | BM    | 1553  | 0        | 1523     | 76      | 0            |
| 2   | BN    | 1553  | 0        | 1523     | 76      | 0            |
| 2   | BO    | 1553  | 0        | 1523     | 66      | 0            |
| 2   | BP    | 1553  | 0        | 1523     | 74      | 0            |
| 2   | BQ    | 1553  | 0        | 1523     | 76      | 0            |
| 2   | BR    | 1553  | 0        | 1523     | 76      | 0            |
| 2   | BS    | 1553  | 0        | 1523     | 75      | 0            |
| 2   | BT    | 1553  | 0        | 1523     | 74      | 0            |
| 2   | BU    | 1553  | 0        | 1523     | 72      | 0            |
| 2   | BV    | 1553  | 0        | 1523     | 74      | 0            |
| 2   | BW    | 1553  | 0        | 1523     | 74      | 0            |
| 2   | BX    | 1553  | 0        | 1523     | 75      | 0            |
| 2   | BY    | 1553  | 0        | 1523     | 56      | 0            |
| 2   | BZ    | 1553  | 0        | 1523     | 57      | 0            |
| 2   | Ba    | 1553  | 0        | 1523     | 0       | 0            |
| 2   | Bb    | 1553  | 0        | 1523     | 0       | 0            |
| 2   | Bc    | 1553  | 0        | 1523     | 0       | 0            |
| 2   | Bd    | 1553  | 0        | 1523     | 0       | 0            |
| 2   | Be    | 1553  | 0        | 1523     | 0       | 0            |
| 2   | Bf    | 1553  | 0        | 1523     | 0       | 0            |
| 2   | Bg    | 1553  | 0        | 1523     | 0       | 0            |
| 2   | Bh    | 1553  | 0        | 1523     | 0       | 0            |
| 2   | Bi    | 1553  | 0        | 1523     | 0       | 0            |
| 2   | Bj    | 1553  | 0        | 1523     | 0       | 0            |
| 2   | Bk    | 1553  | 0        | 1523     | 0       | 0            |
| 2   | Bl    | 1553  | 0        | 1523     | 0       | 0            |
| 2   | Bm    | 1553  | 0        | 1523     | 0       | 0            |
| 2   | Bn    | 1553  | 0        | 1523     | 0       | 0            |
| 2   | Bo    | 1553  | 0        | 1523     | 0       | 0            |
| 2   | Bp    | 1553  | 0        | 1523     | 0       | 0            |
| 2   | Bq    | 1553  | 0        | 1523     | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | Br    | 1553  | 0        | 1523     | 0       | 0            |
| 2   | Bs    | 1553  | 0        | 1523     | 0       | 0            |
| 2   | Bt    | 1553  | 0        | 1523     | 0       | 0            |
| 2   | Bu    | 1553  | 0        | 1523     | 0       | 0            |
| 2   | Bv    | 1553  | 0        | 1523     | 0       | 0            |
| 2   | Bw    | 1553  | 0        | 1523     | 0       | 0            |
| 2   | Bx    | 1553  | 0        | 1523     | 0       | 0            |
| 3   | C0    | 1718  | 0        | 1677     | 54      | 0            |
| 3   | C1    | 1718  | 0        | 1677     | 56      | 0            |
| 3   | C2    | 1718  | 0        | 1677     | 56      | 0            |
| 3   | C3    | 1718  | 0        | 1677     | 54      | 0            |
| 3   | C4    | 1718  | 0        | 1677     | 56      | 0            |
| 3   | C5    | 1718  | 0        | 1677     | 59      | 0            |
| 3   | C6    | 1718  | 0        | 1677     | 56      | 0            |
| 3   | C7    | 1718  | 0        | 1677     | 54      | 0            |
| 3   | C8    | 1718  | 0        | 1677     | 59      | 0            |
| 3   | C9    | 1718  | 0        | 1677     | 57      | 0            |
| 3   | CA    | 1718  | 0        | 1677     | 57      | 0            |
| 3   | CB    | 1718  | 0        | 1677     | 58      | 0            |
| 3   | CC    | 1718  | 0        | 1677     | 86      | 0            |
| 3   | CD    | 1718  | 0        | 1677     | 85      | 0            |
| 3   | CE    | 1718  | 0        | 1677     | 88      | 0            |
| 3   | CF    | 1718  | 0        | 1677     | 86      | 0            |
| 3   | CG    | 1718  | 0        | 1677     | 87      | 0            |
| 3   | CH    | 1718  | 0        | 1677     | 85      | 0            |
| 3   | CI    | 1718  | 0        | 1677     | 82      | 0            |
| 3   | CJ    | 1718  | 0        | 1677     | 86      | 0            |
| 3   | CK    | 1718  | 0        | 1677     | 75      | 0            |
| 3   | CL    | 1718  | 0        | 1677     | 76      | 0            |
| 3   | CM    | 1718  | 0        | 1677     | 78      | 0            |
| 3   | CN    | 1718  | 0        | 1677     | 72      | 0            |
| 3   | CO    | 1718  | 0        | 1677     | 75      | 0            |
| 3   | CP    | 1718  | 0        | 1677     | 71      | 0            |
| 3   | CQ    | 1718  | 0        | 1677     | 85      | 0            |
| 3   | CR    | 1718  | 0        | 1677     | 86      | 0            |
| 3   | CS    | 1718  | 0        | 1677     | 85      | 0            |
| 3   | CT    | 1718  | 0        | 1677     | 88      | 0            |
| 3   | CU    | 1718  | 0        | 1677     | 85      | 0            |
| 3   | CV    | 1718  | 0        | 1677     | 85      | 0            |
| 3   | CW    | 1718  | 0        | 1677     | 81      | 0            |
| 3   | CX    | 1718  | 0        | 1677     | 82      | 0            |
| 3   | CY    | 1718  | 0        | 1677     | 56      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 3   | CZ    | 1718   | 0        | 1677     | 52      | 0            |
| 3   | Cc    | 1718   | 0        | 1677     | 0       | 0            |
| 3   | Cd    | 1718   | 0        | 1677     | 0       | 0            |
| 3   | Ce    | 1718   | 0        | 1677     | 0       | 0            |
| 3   | Cf    | 1718   | 0        | 1677     | 0       | 0            |
| 3   | Cg    | 1718   | 0        | 1677     | 0       | 0            |
| 3   | Ch    | 1718   | 0        | 1677     | 0       | 0            |
| 3   | Ci    | 1718   | 0        | 1677     | 0       | 0            |
| 3   | Cj    | 1718   | 0        | 1677     | 0       | 0            |
| 3   | Ck    | 1718   | 0        | 1677     | 0       | 0            |
| 3   | Cl    | 1718   | 0        | 1677     | 0       | 0            |
| 3   | Cm    | 1718   | 0        | 1677     | 0       | 0            |
| 3   | Cn    | 1718   | 0        | 1677     | 0       | 0            |
| 3   | Co    | 1718   | 0        | 1677     | 0       | 0            |
| 3   | Cp    | 1718   | 0        | 1677     | 0       | 0            |
| 3   | Cq    | 1718   | 0        | 1677     | 0       | 0            |
| 3   | Cr    | 1718   | 0        | 1677     | 0       | 0            |
| 3   | Cs    | 1718   | 0        | 1677     | 0       | 0            |
| 3   | Ct    | 1718   | 0        | 1677     | 0       | 0            |
| 3   | Cu    | 1718   | 0        | 1677     | 0       | 0            |
| 3   | Cv    | 1718   | 0        | 1677     | 0       | 0            |
| 3   | Cw    | 1718   | 0        | 1677     | 0       | 0            |
| 3   | Cx    | 1718   | 0        | 1677     | 0       | 0            |
| 3   | DA    | 1718   | 0        | 1677     | 55      | 0            |
| 3   | DB    | 1718   | 0        | 1677     | 59      | 0            |
| All | All   | 311940 | 0        | 303840   | 7281    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (7281) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:AN:115:THR:HG21 | 1:AN:131:GLN:HB3 | 1.44                     | 1.00              |
| 1:AF:115:THR:HG21 | 1:AF:131:GLN:HB3 | 1.44                     | 1.00              |
| 1:AP:115:THR:HG21 | 1:AP:131:GLN:HB3 | 1.44                     | 1.00              |
| 1:AV:115:THR:HG21 | 1:AV:131:GLN:HB3 | 1.44                     | 1.00              |
| 1:AA:115:THR:HG21 | 1:AA:131:GLN:HB3 | 1.44                     | 1.00              |
| 1:AD:115:THR:HG21 | 1:AD:131:GLN:HB3 | 1.44                     | 0.99              |
| 1:A7:115:THR:HG21 | 1:A7:131:GLN:HB3 | 1.44                     | 0.99              |
| 1:AK:115:THR:HG21 | 1:AK:131:GLN:HB3 | 1.44                     | 0.99              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:DJ:115:THR:HG21 | 1:DJ:131:GLN:HB3  | 1.44                     | 0.99              |
| 1:DI:115:THR:HG21 | 1:DI:131:GLN:HB3  | 1.44                     | 0.99              |
| 1:AR:115:THR:HG21 | 1:AR:131:GLN:HB3  | 1.44                     | 0.99              |
| 1:AY:115:THR:HG21 | 1:AY:131:GLN:HB3  | 1.44                     | 0.99              |
| 1:A5:115:THR:HG21 | 1:A5:131:GLN:HB3  | 1.44                     | 0.99              |
| 1:A2:115:THR:HG21 | 1:A2:131:GLN:HB3  | 1.44                     | 0.99              |
| 1:DK:115:THR:HG21 | 1:DK:131:GLN:HB3  | 1.44                     | 0.99              |
| 1:AW:115:THR:HG21 | 1:AW:131:GLN:HB3  | 1.44                     | 0.99              |
| 1:AO:115:THR:HG21 | 1:AO:131:GLN:HB3  | 1.44                     | 0.99              |
| 1:AM:115:THR:HG21 | 1:AM:131:GLN:HB3  | 1.44                     | 0.99              |
| 1:AC:115:THR:HG21 | 1:AC:131:GLN:HB3  | 1.44                     | 0.99              |
| 1:DF:115:THR:HG21 | 1:DF:131:GLN:HB3  | 1.44                     | 0.99              |
| 1:AG:115:THR:HG21 | 1:AG:131:GLN:HB3  | 1.44                     | 0.98              |
| 1:A8:115:THR:HG21 | 1:A8:131:GLN:HB3  | 1.44                     | 0.98              |
| 1:AL:115:THR:HG21 | 1:AL:131:GLN:HB3  | 1.44                     | 0.98              |
| 1:A0:115:THR:HG21 | 1:A0:131:GLN:HB3  | 1.44                     | 0.98              |
| 1:AB:115:THR:HG21 | 1:AB:131:GLN:HB3  | 1.44                     | 0.98              |
| 1:AU:115:THR:HG21 | 1:AU:131:GLN:HB3  | 1.44                     | 0.98              |
| 1:AT:115:THR:HG21 | 1:AT:131:GLN:HB3  | 1.44                     | 0.98              |
| 1:A9:115:THR:HG21 | 1:A9:131:GLN:HB3  | 1.44                     | 0.98              |
| 1:A3:115:THR:HG21 | 1:A3:131:GLN:HB3  | 1.44                     | 0.98              |
| 1:AE:115:THR:HG21 | 1:AE:131:GLN:HB3  | 1.44                     | 0.98              |
| 1:AJ:115:THR:HG21 | 1:AJ:131:GLN:HB3  | 1.44                     | 0.97              |
| 1:A1:115:THR:HG21 | 1:A1:131:GLN:HB3  | 1.44                     | 0.97              |
| 1:A4:115:THR:HG21 | 1:A4:131:GLN:HB3  | 1.44                     | 0.97              |
| 1:AS:115:THR:HG21 | 1:AS:131:GLN:HB3  | 1.44                     | 0.97              |
| 1:AQ:115:THR:HG21 | 1:AQ:131:GLN:HB3  | 1.44                     | 0.97              |
| 1:AZ:115:THR:HG21 | 1:AZ:131:GLN:HB3  | 1.44                     | 0.97              |
| 1:A6:115:THR:HG21 | 1:A6:131:GLN:HB3  | 1.44                     | 0.97              |
| 1:AI:115:THR:HG21 | 1:AI:131:GLN:HB3  | 1.44                     | 0.97              |
| 1:AH:115:THR:HG21 | 1:AH:131:GLN:HB3  | 1.44                     | 0.96              |
| 1:DD:115:THR:HG21 | 1:DD:131:GLN:HB3  | 1.44                     | 0.96              |
| 1:DG:115:THR:HG21 | 1:DG:131:GLN:HB3  | 1.44                     | 0.96              |
| 1:DH:115:THR:HG21 | 1:DH:131:GLN:HB3  | 1.44                     | 0.96              |
| 1:AX:115:THR:HG21 | 1:AX:131:GLN:HB3  | 1.44                     | 0.95              |
| 1:DC:115:THR:HG21 | 1:DC:131:GLN:HB3  | 1.44                     | 0.95              |
| 1:DE:115:THR:HG21 | 1:DE:131:GLN:HB3  | 1.44                     | 0.95              |
| 1:AM:112:PRO:HD2  | 3:CK:220:VAL:HG11 | 67.79                    | 0.85              |
| 1:A1:112:PRO:HD2  | 3:C1:220:VAL:HG11 | 1.58                     | 0.85              |
| 1:A0:112:PRO:HD2  | 3:C3:220:VAL:HG11 | 1.59                     | 0.85              |
| 1:AT:112:PRO:HD2  | 3:CX:220:VAL:HG11 | 1.59                     | 0.85              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:CT:220:VAL:HG11 | 1:DG:112:PRO:HD2  | 273.99                   | 0.85              |
| 3:CU:220:VAL:HG11 | 1:DJ:112:PRO:HD2  | 291.28                   | 0.85              |
| 1:AM:112:PRO:HD2  | 3:CM:220:VAL:HG11 | 1.58                     | 0.85              |
| 1:AL:112:PRO:HD2  | 3:CO:220:VAL:HG11 | 1.58                     | 0.85              |
| 1:A8:112:PRO:HD2  | 3:CC:220:VAL:HG11 | 260.52                   | 0.85              |
| 3:CW:220:VAL:HG11 | 1:DF:112:PRO:HD2  | 227.69                   | 0.85              |
| 1:A6:112:PRO:HD2  | 3:C6:220:VAL:HG11 | 1.59                     | 0.85              |
| 3:CG:220:VAL:HG11 | 1:DK:112:PRO:HD2  | 1.59                     | 0.85              |
| 1:AC:112:PRO:HD2  | 3:DA:220:VAL:HG11 | 271.86                   | 0.85              |
| 1:A7:112:PRO:HD2  | 3:C5:220:VAL:HG11 | 1.59                     | 0.85              |
| 1:AK:112:PRO:HD2  | 3:CN:220:VAL:HG11 | 42.63                    | 0.84              |
| 1:AX:112:PRO:HD2  | 3:CV:220:VAL:HG11 | 1.59                     | 0.84              |
| 1:AP:112:PRO:HD2  | 3:CP:220:VAL:HG11 | 1.58                     | 0.84              |
| 1:AJ:112:PRO:HD2  | 3:CN:220:VAL:HG11 | 1.59                     | 0.84              |
| 1:AY:112:PRO:HD2  | 3:C2:220:VAL:HG11 | 1.59                     | 0.84              |
| 1:AO:112:PRO:HD2  | 3:CS:220:VAL:HG11 | 1.59                     | 0.84              |
| 3:CV:220:VAL:HG11 | 1:DI:112:PRO:HD2  | 285.15                   | 0.84              |
| 1:AW:112:PRO:HD2  | 3:CW:220:VAL:HG11 | 1.58                     | 0.84              |
| 3:CP:220:VAL:HG11 | 1:DE:112:PRO:HD2  | 286.05                   | 0.84              |
| 1:A2:112:PRO:HD2  | 3:C0:220:VAL:HG11 | 1.59                     | 0.84              |
| 1:AK:112:PRO:HD2  | 3:CK:220:VAL:HG11 | 1.58                     | 0.84              |
| 1:A4:112:PRO:HD2  | 3:C4:220:VAL:HG11 | 1.59                     | 0.84              |
| 2:BG:134:HIS:HD2  | 2:BG:145:LEU:HD13 | 1.43                     | 0.84              |
| 2:BA:134:HIS:HD2  | 2:BA:145:LEU:HD13 | 1.43                     | 0.84              |
| 1:AJ:112:PRO:HD2  | 3:CJ:220:VAL:HG11 | 210.33                   | 0.84              |
| 1:AG:112:PRO:HD2  | 3:CF:220:VAL:HG11 | 1.59                     | 0.84              |
| 1:AE:112:PRO:HD2  | 3:CB:220:VAL:HG11 | 1.58                     | 0.84              |
| 2:B3:134:HIS:HD2  | 2:B3:145:LEU:HD13 | 1.43                     | 0.84              |
| 2:BE:134:HIS:HD2  | 2:BE:145:LEU:HD13 | 1.43                     | 0.84              |
| 2:BH:134:HIS:HD2  | 2:BH:145:LEU:HD13 | 1.43                     | 0.84              |
| 2:BI:134:HIS:HD2  | 2:BI:145:LEU:HD13 | 1.43                     | 0.84              |
| 3:CQ:220:VAL:HG11 | 1:DD:112:PRO:HD2  | 227.70                   | 0.84              |
| 1:AU:112:PRO:HD2  | 3:CU:220:VAL:HG11 | 1.59                     | 0.84              |
| 2:B4:134:HIS:HD2  | 2:B4:145:LEU:HD13 | 1.43                     | 0.84              |
| 2:BK:134:HIS:HD2  | 2:BK:145:LEU:HD13 | 1.43                     | 0.84              |
| 1:A9:112:PRO:HD2  | 3:C9:220:VAL:HG11 | 1.58                     | 0.84              |
| 2:BD:134:HIS:HD2  | 2:BD:145:LEU:HD13 | 1.43                     | 0.84              |
| 2:BC:134:HIS:HD2  | 2:BC:145:LEU:HD13 | 1.43                     | 0.84              |
| 2:BL:134:HIS:HD2  | 2:BL:145:LEU:HD13 | 1.43                     | 0.84              |
| 1:AD:112:PRO:HD2  | 3:CC:220:VAL:HG11 | 1.59                     | 0.83              |
| 1:AI:112:PRO:HD2  | 3:CM:220:VAL:HG11 | 144.43                   | 0.83              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AI:112:PRO:HD2  | 3:CH:220:VAL:HG11 | 1.59                     | 0.83              |
| 1:AN:112:PRO:HD2  | 3:CL:220:VAL:HG11 | 1.58                     | 0.83              |
| 1:AL:112:PRO:HD2  | 3:CL:220:VAL:HG11 | 42.63                    | 0.83              |
| 2:BU:134:HIS:HD2  | 2:BU:145:LEU:HD13 | 1.43                     | 0.83              |
| 2:BP:134:HIS:HD2  | 2:BP:145:LEU:HD13 | 1.43                     | 0.83              |
| 1:A5:112:PRO:HD2  | 3:C8:220:VAL:HG11 | 1.59                     | 0.83              |
| 1:AD:112:PRO:HD2  | 3:CH:220:VAL:HG11 | 181.11                   | 0.83              |
| 1:AQ:112:PRO:HD2  | 3:CT:220:VAL:HG11 | 1.59                     | 0.83              |
| 2:BO:134:HIS:HD2  | 2:BO:145:LEU:HD13 | 1.43                     | 0.83              |
| 2:B7:134:HIS:HD2  | 2:B7:145:LEU:HD13 | 1.43                     | 0.83              |
| 2:BR:134:HIS:HD2  | 2:BR:145:LEU:HD13 | 1.43                     | 0.83              |
| 1:AB:112:PRO:HD2  | 3:CA:220:VAL:HG11 | 1.59                     | 0.83              |
| 3:CS:220:VAL:HG11 | 1:DC:112:PRO:HD2  | 285.17                   | 0.83              |
| 2:BY:134:HIS:HD2  | 2:BY:145:LEU:HD13 | 1.43                     | 0.83              |
| 2:BV:134:HIS:HD2  | 2:BV:145:LEU:HD13 | 1.43                     | 0.83              |
| 1:AN:112:PRO:HD2  | 3:CR:220:VAL:HG11 | 227.67                   | 0.83              |
| 2:BS:134:HIS:HD2  | 2:BS:145:LEU:HD13 | 1.43                     | 0.83              |
| 2:BM:134:HIS:HD2  | 2:BM:145:LEU:HD13 | 1.43                     | 0.83              |
| 1:AG:112:PRO:HD2  | 3:CG:220:VAL:HG11 | 41.47                    | 0.83              |
| 1:AB:112:PRO:HD2  | 3:DB:220:VAL:HG11 | 271.44                   | 0.83              |
| 2:BW:134:HIS:HD2  | 2:BW:145:LEU:HD13 | 1.43                     | 0.83              |
| 2:BF:134:HIS:HD2  | 2:BF:145:LEU:HD13 | 1.43                     | 0.83              |
| 2:BX:134:HIS:HD2  | 2:BX:145:LEU:HD13 | 1.43                     | 0.83              |
| 1:AZ:112:PRO:HD2  | 3:CZ:220:VAL:HG11 | 1.59                     | 0.83              |
| 1:AH:112:PRO:HD2  | 3:CJ:220:VAL:HG11 | 1.59                     | 0.83              |
| 1:AA:112:PRO:HD2  | 3:CD:220:VAL:HG11 | 1.59                     | 0.83              |
| 1:AC:112:PRO:HD2  | 3:CE:220:VAL:HG11 | 1.59                     | 0.83              |
| 1:AV:112:PRO:HD2  | 3:CY:220:VAL:HG11 | 1.59                     | 0.83              |
| 1:AH:112:PRO:HD2  | 3:CF:220:VAL:HG11 | 68.24                    | 0.83              |
| 2:B0:134:HIS:HD2  | 2:B0:145:LEU:HD13 | 1.43                     | 0.83              |
| 2:BB:134:HIS:HD2  | 2:BB:145:LEU:HD13 | 1.43                     | 0.83              |
| 1:AO:112:PRO:HD2  | 3:CO:220:VAL:HG11 | 248.57                   | 0.82              |
| 2:BZ:134:HIS:HD2  | 2:BZ:145:LEU:HD13 | 1.43                     | 0.82              |
| 2:BT:134:HIS:HD2  | 2:BT:145:LEU:HD13 | 1.43                     | 0.82              |
| 3:CX:220:VAL:HG11 | 1:DH:112:PRO:HD2  | 274.60                   | 0.82              |
| 2:BJ:134:HIS:HD2  | 2:BJ:145:LEU:HD13 | 1.43                     | 0.82              |
| 2:BQ:134:HIS:HD2  | 2:BQ:145:LEU:HD13 | 1.43                     | 0.82              |
| 1:AR:112:PRO:HD2  | 3:CR:220:VAL:HG11 | 1.59                     | 0.82              |
| 1:A3:112:PRO:HD2  | 3:C7:220:VAL:HG11 | 1.59                     | 0.82              |
| 2:B9:134:HIS:HD2  | 2:B9:145:LEU:HD13 | 1.43                     | 0.82              |
| 2:B2:134:HIS:HD2  | 2:B2:145:LEU:HD13 | 1.43                     | 0.82              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:BN:134:HIS:HD2 | 2:BN:145:LEU:HD13 | 1.43                     | 0.82              |
| 1:AF:112:PRO:HD2 | 3:CI:220:VAL:HG11 | 1.59                     | 0.82              |
| 1:AS:112:PRO:HD2 | 3:CQ:220:VAL:HG11 | 1.59                     | 0.82              |
| 1:AE:112:PRO:HD2 | 3:CE:220:VAL:HG11 | 41.47                    | 0.81              |
| 2:B5:134:HIS:HD2 | 2:B5:145:LEU:HD13 | 1.43                     | 0.81              |
| 2:B1:134:HIS:HD2 | 2:B1:145:LEU:HD13 | 1.43                     | 0.81              |
| 2:B8:134:HIS:HD2 | 2:B8:145:LEU:HD13 | 1.43                     | 0.81              |
| 1:DC:70:ARG:O    | 1:DC:71:LEU:HB2   | 1.81                     | 0.81              |
| 1:AH:70:ARG:O    | 1:AH:71:LEU:HB2   | 1.81                     | 0.81              |
| 1:A2:70:ARG:O    | 1:A2:71:LEU:HB2   | 1.81                     | 0.81              |
| 1:AL:70:ARG:O    | 1:AL:71:LEU:HB2   | 1.81                     | 0.81              |
| 1:AD:70:ARG:O    | 1:AD:71:LEU:HB2   | 1.81                     | 0.81              |
| 1:AR:70:ARG:O    | 1:AR:71:LEU:HB2   | 1.81                     | 0.81              |
| 1:AP:70:ARG:O    | 1:AP:71:LEU:HB2   | 1.81                     | 0.81              |
| 2:B6:134:HIS:HD2 | 2:B6:145:LEU:HD13 | 1.43                     | 0.80              |
| 1:AV:70:ARG:O    | 1:AV:71:LEU:HB2   | 1.81                     | 0.80              |
| 1:AC:70:ARG:O    | 1:AC:71:LEU:HB2   | 1.81                     | 0.80              |
| 1:AI:70:ARG:O    | 1:AI:71:LEU:HB2   | 1.81                     | 0.80              |
| 1:DH:70:ARG:O    | 1:DH:71:LEU:HB2   | 1.81                     | 0.80              |
| 1:AM:70:ARG:O    | 1:AM:71:LEU:HB2   | 1.81                     | 0.80              |
| 1:DK:70:ARG:O    | 1:DK:71:LEU:HB2   | 1.81                     | 0.80              |
| 1:AT:70:ARG:O    | 1:AT:71:LEU:HB2   | 1.81                     | 0.80              |
| 1:AF:70:ARG:O    | 1:AF:71:LEU:HB2   | 1.81                     | 0.80              |
| 1:AK:70:ARG:O    | 1:AK:71:LEU:HB2   | 1.81                     | 0.80              |
| 1:AW:70:ARG:O    | 1:AW:71:LEU:HB2   | 1.81                     | 0.80              |
| 1:DF:70:ARG:O    | 1:DF:71:LEU:HB2   | 1.81                     | 0.80              |
| 1:A8:70:ARG:O    | 1:A8:71:LEU:HB2   | 1.81                     | 0.80              |
| 1:AA:70:ARG:O    | 1:AA:71:LEU:HB2   | 1.81                     | 0.80              |
| 1:AN:70:ARG:O    | 1:AN:71:LEU:HB2   | 1.81                     | 0.80              |
| 1:DI:70:ARG:O    | 1:DI:71:LEU:HB2   | 1.81                     | 0.80              |
| 1:AS:70:ARG:O    | 1:AS:71:LEU:HB2   | 1.81                     | 0.80              |
| 1:DD:70:ARG:O    | 1:DD:71:LEU:HB2   | 1.81                     | 0.80              |
| 1:AG:70:ARG:O    | 1:AG:71:LEU:HB2   | 1.81                     | 0.79              |
| 1:AE:70:ARG:O    | 1:AE:71:LEU:HB2   | 1.81                     | 0.79              |
| 1:AU:70:ARG:O    | 1:AU:71:LEU:HB2   | 1.81                     | 0.79              |
| 1:A6:70:ARG:O    | 1:A6:71:LEU:HB2   | 1.81                     | 0.79              |
| 1:AO:70:ARG:O    | 1:AO:71:LEU:HB2   | 1.81                     | 0.79              |
| 1:A7:70:ARG:O    | 1:A7:71:LEU:HB2   | 1.81                     | 0.79              |
| 1:A5:70:ARG:O    | 1:A5:71:LEU:HB2   | 1.81                     | 0.79              |
| 1:A9:70:ARG:O    | 1:A9:71:LEU:HB2   | 1.81                     | 0.79              |
| 1:DG:70:ARG:O    | 1:DG:71:LEU:HB2   | 1.81                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:AZ:70:ARG:O    | 1:AZ:71:LEU:HB2  | 1.81                     | 0.79              |
| 1:AQ:70:ARG:O    | 1:AQ:71:LEU:HB2  | 1.81                     | 0.79              |
| 1:A1:70:ARG:O    | 1:A1:71:LEU:HB2  | 1.81                     | 0.79              |
| 1:AY:70:ARG:O    | 1:AY:71:LEU:HB2  | 1.81                     | 0.79              |
| 1:AB:70:ARG:O    | 1:AB:71:LEU:HB2  | 1.81                     | 0.78              |
| 1:DE:70:ARG:O    | 1:DE:71:LEU:HB2  | 1.81                     | 0.78              |
| 1:DJ:70:ARG:O    | 1:DJ:71:LEU:HB2  | 1.81                     | 0.78              |
| 1:AJ:70:ARG:O    | 1:AJ:71:LEU:HB2  | 1.81                     | 0.78              |
| 1:A4:70:ARG:O    | 1:A4:71:LEU:HB2  | 1.81                     | 0.78              |
| 1:A0:70:ARG:O    | 1:A0:71:LEU:HB2  | 1.81                     | 0.78              |
| 1:AX:70:ARG:O    | 1:AX:71:LEU:HB2  | 1.81                     | 0.77              |
| 1:A3:70:ARG:O    | 1:A3:71:LEU:HB2  | 1.81                     | 0.77              |
| 2:BV:137:GLU:HB2 | 1:DI:181:LYS:HE3 | 291.18                   | 0.77              |
| 1:AQ:181:LYS:HE3 | 2:BP:137:GLU:HB2 | 1.67                     | 0.77              |
| 1:A6:181:LYS:HE3 | 2:B6:137:GLU:HB2 | 1.67                     | 0.77              |
| 1:A8:181:LYS:HE3 | 2:B8:137:GLU:HB2 | 1.67                     | 0.77              |
| 1:AL:181:LYS:HE3 | 2:BL:137:GLU:HB2 | 105.01                   | 0.77              |
| 1:AM:181:LYS:HE3 | 2:BN:137:GLU:HB2 | 1.67                     | 0.77              |
| 1:AP:181:LYS:HE3 | 2:BS:137:GLU:HB2 | 1.67                     | 0.77              |
| 1:AI:191:HIS:HD2 | 1:AI:193:GLY:H   | 1.33                     | 0.77              |
| 1:AJ:191:HIS:HD2 | 1:AJ:193:GLY:H   | 1.33                     | 0.77              |
| 1:AA:181:LYS:HE3 | 2:BA:137:GLU:HB2 | 1.67                     | 0.77              |
| 2:BJ:137:GLU:HB2 | 1:DK:181:LYS:HE3 | 1.67                     | 0.77              |
| 1:AZ:191:HIS:HD2 | 1:AZ:193:GLY:H   | 1.33                     | 0.77              |
| 1:AH:181:LYS:HE3 | 2:BH:137:GLU:HB2 | 1.67                     | 0.77              |
| 1:A7:191:HIS:HD2 | 1:A7:193:GLY:H   | 1.33                     | 0.77              |
| 1:AU:181:LYS:HE3 | 2:BV:137:GLU:HB2 | 1.67                     | 0.77              |
| 1:AD:181:LYS:HE3 | 2:BD:137:GLU:HB2 | 1.67                     | 0.77              |
| 1:A4:181:LYS:HE3 | 2:BX:137:GLU:HB2 | 292.29                   | 0.77              |
| 1:AW:191:HIS:HD2 | 1:AW:193:GLY:H   | 1.33                     | 0.77              |
| 1:AZ:181:LYS:HE3 | 2:B0:137:GLU:HB2 | 1.67                     | 0.77              |
| 1:AA:191:HIS:HD2 | 1:AA:193:GLY:H   | 1.33                     | 0.77              |
| 1:AZ:207:CYS:O   | 1:AZ:208:TYR:HB2 | 1.85                     | 0.77              |
| 1:AN:191:HIS:HD2 | 1:AN:193:GLY:H   | 1.33                     | 0.77              |
| 1:AG:191:HIS:HD2 | 1:AG:193:GLY:H   | 1.33                     | 0.77              |
| 1:AT:181:LYS:HE3 | 2:BU:137:GLU:HB2 | 1.67                     | 0.77              |
| 1:AI:181:LYS:HE3 | 2:BI:137:GLU:HB2 | 1.67                     | 0.76              |
| 1:AJ:181:LYS:HE3 | 2:BJ:137:GLU:HB2 | 259.30                   | 0.76              |
| 1:DH:191:HIS:HD2 | 1:DH:193:GLY:H   | 1.33                     | 0.76              |
| 1:AM:191:HIS:HD2 | 1:AM:193:GLY:H   | 1.33                     | 0.76              |
| 1:AX:181:LYS:HE3 | 2:BY:137:GLU:HB2 | 1.67                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:AY:181:LYS:HE3 | 2:BZ:137:GLU:HB2 | 1.67                     | 0.76              |
| 2:BQ:137:GLU:HB2 | 1:DD:181:LYS:HE3 | 285.66                   | 0.76              |
| 1:AL:181:LYS:HE3 | 2:BM:137:GLU:HB2 | 1.67                     | 0.76              |
| 1:DF:191:HIS:HD2 | 1:DF:193:GLY:H   | 1.33                     | 0.76              |
| 1:A2:181:LYS:HE3 | 2:B3:137:GLU:HB2 | 1.67                     | 0.76              |
| 1:A2:207:CYS:O   | 1:A2:208:TYR:HB2 | 1.86                     | 0.76              |
| 2:BU:137:GLU:HB2 | 1:DH:181:LYS:HE3 | 288.74                   | 0.76              |
| 2:BW:137:GLU:HB2 | 1:DJ:181:LYS:HE3 | 290.71                   | 0.76              |
| 1:A1:207:CYS:O   | 1:A1:208:TYR:HB2 | 1.86                     | 0.76              |
| 1:A6:207:CYS:O   | 1:A6:208:TYR:HB2 | 1.86                     | 0.76              |
| 1:AN:181:LYS:HE3 | 2:BR:137:GLU:HB2 | 1.67                     | 0.76              |
| 1:AI:207:CYS:O   | 1:AI:208:TYR:HB2 | 1.86                     | 0.76              |
| 1:AC:191:HIS:HD2 | 1:AC:193:GLY:H   | 1.33                     | 0.76              |
| 1:AO:191:HIS:HD2 | 1:AO:193:GLY:H   | 1.33                     | 0.76              |
| 1:A4:207:CYS:O   | 1:A4:208:TYR:HB2 | 1.86                     | 0.76              |
| 1:DC:207:CYS:O   | 1:DC:208:TYR:HB2 | 1.86                     | 0.76              |
| 1:A0:191:HIS:HD2 | 1:A0:193:GLY:H   | 1.33                     | 0.76              |
| 1:AK:191:HIS:HD2 | 1:AK:193:GLY:H   | 1.33                     | 0.76              |
| 1:AK:207:CYS:O   | 1:AK:208:TYR:HB2 | 1.86                     | 0.76              |
| 1:AC:207:CYS:O   | 1:AC:208:TYR:HB2 | 1.86                     | 0.76              |
| 1:A4:191:HIS:HD2 | 1:A4:193:GLY:H   | 1.33                     | 0.76              |
| 1:DK:207:CYS:O   | 1:DK:208:TYR:HB2 | 1.86                     | 0.76              |
| 1:DI:207:CYS:O   | 1:DI:208:TYR:HB2 | 1.86                     | 0.76              |
| 3:CY:46:VAL:O    | 3:CY:50:THR:HB   | 1.86                     | 0.76              |
| 1:AO:207:CYS:O   | 1:AO:208:TYR:HB2 | 1.86                     | 0.76              |
| 1:AP:207:CYS:O   | 1:AP:208:TYR:HB2 | 1.85                     | 0.76              |
| 2:BP:137:GLU:HB2 | 1:DC:181:LYS:HE3 | 253.86                   | 0.76              |
| 1:AK:181:LYS:HE3 | 2:BK:137:GLU:HB2 | 64.94                    | 0.76              |
| 3:C2:46:VAL:O    | 3:C2:50:THR:HB   | 1.86                     | 0.76              |
| 3:CZ:46:VAL:O    | 3:CZ:50:THR:HB   | 1.86                     | 0.76              |
| 1:AL:191:HIS:HD2 | 1:AL:193:GLY:H   | 1.33                     | 0.76              |
| 1:A8:207:CYS:O   | 1:A8:208:TYR:HB2 | 1.86                     | 0.76              |
| 1:DG:207:CYS:O   | 1:DG:208:TYR:HB2 | 1.86                     | 0.76              |
| 3:CI:46:VAL:O    | 3:CI:50:THR:HB   | 1.86                     | 0.76              |
| 3:CQ:46:VAL:O    | 3:CQ:50:THR:HB   | 1.86                     | 0.76              |
| 1:AW:207:CYS:O   | 1:AW:208:TYR:HB2 | 1.86                     | 0.76              |
| 1:AJ:181:LYS:HE3 | 2:BK:137:GLU:HB2 | 1.67                     | 0.76              |
| 3:CR:46:VAL:O    | 3:CR:50:THR:HB   | 1.86                     | 0.76              |
| 3:CS:46:VAL:O    | 3:CS:50:THR:HB   | 1.86                     | 0.76              |
| 1:AQ:207:CYS:O   | 1:AQ:208:TYR:HB2 | 1.86                     | 0.76              |
| 1:AU:191:HIS:HD2 | 1:AU:193:GLY:H   | 1.33                     | 0.76              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:C9:46:VAL:O     | 3:C9:50:THR:HB   | 1.86                     | 0.76              |
| 1:A5:181:LYS:HE3  | 2:B5:137:GLU:HB2 | 1.67                     | 0.76              |
| 1:AS:181:LYS:HE3  | 2:BT:137:GLU:HB2 | 1.67                     | 0.76              |
| 1:A7:181:LYS:HE3  | 2:B7:137:GLU:HB2 | 1.67                     | 0.76              |
| 1:AE:181:LYS:HE3  | 2:BE:137:GLU:HB2 | 1.67                     | 0.76              |
| 3:CC:46:VAL:O     | 3:CC:50:THR:HB   | 1.86                     | 0.76              |
| 3:CD:46:VAL:O     | 3:CD:50:THR:HB   | 1.86                     | 0.76              |
| 3:CF:46:VAL:O     | 3:CF:50:THR:HB   | 1.86                     | 0.76              |
| 3:CM:46:VAL:O     | 3:CM:50:THR:HB   | 1.86                     | 0.76              |
| 3:CN:46:VAL:O     | 3:CN:50:THR:HB   | 1.86                     | 0.76              |
| 3:CW:46:VAL:O     | 3:CW:50:THR:HB   | 1.86                     | 0.76              |
| 3:CX:46:VAL:O     | 3:CX:50:THR:HB   | 1.86                     | 0.76              |
| 1:AB:181:LYS:HE3  | 2:BB:137:GLU:HB2 | 1.67                     | 0.76              |
| 1:DG:191:HIS:HD2  | 1:DG:193:GLY:H   | 1.33                     | 0.76              |
| 1:AA:207:CYS:O    | 1:AA:208:TYR:HB2 | 1.86                     | 0.76              |
| 1:AB:207:CYS:O    | 1:AB:208:TYR:HB2 | 1.85                     | 0.76              |
| 3:C0:46:VAL:O     | 3:C0:50:THR:HB   | 1.86                     | 0.76              |
| 1:AF:207:CYS:O    | 1:AF:208:TYR:HB2 | 1.86                     | 0.76              |
| 1:AV:181:LYS:HE3  | 2:BW:137:GLU:HB2 | 1.67                     | 0.76              |
| 3:C5:46:VAL:O     | 3:C5:50:THR:HB   | 1.86                     | 0.76              |
| 2:BF:157:VAL:HG23 | 3:CF:50:THR:HG21 | 1.68                     | 0.76              |
| 3:CJ:46:VAL:O     | 3:CJ:50:THR:HB   | 1.86                     | 0.76              |
| 3:CT:46:VAL:O     | 3:CT:50:THR:HB   | 1.86                     | 0.76              |
| 1:AH:207:CYS:O    | 1:AH:208:TYR:HB2 | 1.86                     | 0.76              |
| 1:AJ:207:CYS:O    | 1:AJ:208:TYR:HB2 | 1.86                     | 0.76              |
| 1:AV:207:CYS:O    | 1:AV:208:TYR:HB2 | 1.86                     | 0.76              |
| 1:AT:207:CYS:O    | 1:AT:208:TYR:HB2 | 1.86                     | 0.76              |
| 1:DJ:191:HIS:HD2  | 1:DJ:193:GLY:H   | 1.33                     | 0.76              |
| 1:DJ:207:CYS:O    | 1:DJ:208:TYR:HB2 | 1.86                     | 0.76              |
| 2:BW:157:VAL:HG23 | 3:CW:50:THR:HG21 | 1.68                     | 0.75              |
| 2:BC:157:VAL:HG23 | 3:CC:50:THR:HG21 | 1.68                     | 0.75              |
| 2:BO:157:VAL:HG23 | 3:CP:50:THR:HG21 | 1.68                     | 0.75              |
| 1:A9:191:HIS:HD2  | 1:A9:193:GLY:H   | 1.33                     | 0.75              |
| 1:A3:181:LYS:HE3  | 2:B4:137:GLU:HB2 | 1.67                     | 0.75              |
| 1:AD:191:HIS:HD2  | 1:AD:193:GLY:H   | 1.33                     | 0.75              |
| 1:A3:207:CYS:O    | 1:A3:208:TYR:HB2 | 1.86                     | 0.75              |
| 1:AG:207:CYS:O    | 1:AG:208:TYR:HB2 | 1.86                     | 0.75              |
| 1:A9:181:LYS:HE3  | 2:B9:137:GLU:HB2 | 1.67                     | 0.75              |
| 1:A8:191:HIS:HD2  | 1:A8:193:GLY:H   | 1.33                     | 0.75              |
| 1:AC:181:LYS:HE3  | 2:BC:137:GLU:HB2 | 1.67                     | 0.75              |
| 2:BM:157:VAL:HG23 | 3:CM:50:THR:HG21 | 1.68                     | 0.75              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:BW:157:VAL:HG23 | 3:CX:50:THR:HG21 | 57.59                    | 0.75              |
| 2:BB:157:VAL:HG23 | 3:CB:50:THR:HG21 | 1.69                     | 0.75              |
| 2:BD:157:VAL:HG23 | 3:CE:50:THR:HG21 | 91.26                    | 0.75              |
| 2:BS:157:VAL:HG23 | 3:CQ:50:THR:HG21 | 1.69                     | 0.75              |
| 1:DE:207:CYS:O    | 1:DE:208:TYR:HB2 | 1.86                     | 0.75              |
| 1:A1:191:HIS:HD2  | 1:A1:193:GLY:H   | 1.33                     | 0.75              |
| 3:DA:46:VAL:O     | 3:DA:50:THR:HB   | 1.86                     | 0.75              |
| 1:AK:181:LYS:HE3  | 2:BL:137:GLU:HB2 | 1.67                     | 0.75              |
| 2:BF:157:VAL:HG23 | 3:CG:50:THR:HG21 | 57.59                    | 0.75              |
| 2:BP:157:VAL:HG23 | 3:CQ:50:THR:HG21 | 91.25                    | 0.75              |
| 1:DD:207:CYS:O    | 1:DD:208:TYR:HB2 | 1.86                     | 0.75              |
| 1:A1:181:LYS:HE3  | 2:B2:137:GLU:HB2 | 1.67                     | 0.75              |
| 1:AX:207:CYS:O    | 1:AX:208:TYR:HB2 | 1.86                     | 0.75              |
| 1:DD:191:HIS:HD2  | 1:DD:193:GLY:H   | 1.33                     | 0.75              |
| 1:AO:181:LYS:HE3  | 2:BO:137:GLU:HB2 | 1.67                     | 0.75              |
| 2:BR:137:GLU:HB2  | 1:DE:181:LYS:HE3 | 273.00                   | 0.75              |
| 3:CE:46:VAL:O     | 3:CE:50:THR:HB   | 1.86                     | 0.75              |
| 3:CV:46:VAL:O     | 3:CV:50:THR:HB   | 1.86                     | 0.75              |
| 1:AS:207:CYS:O    | 1:AS:208:TYR:HB2 | 1.86                     | 0.75              |
| 3:C7:46:VAL:O     | 3:C7:50:THR:HB   | 1.86                     | 0.75              |
| 3:DB:46:VAL:O     | 3:DB:50:THR:HB   | 1.86                     | 0.75              |
| 1:AY:207:CYS:O    | 1:AY:208:TYR:HB2 | 1.86                     | 0.75              |
| 2:BJ:157:VAL:HG23 | 3:CJ:50:THR:HG21 | 1.68                     | 0.75              |
| 3:CL:46:VAL:O     | 3:CL:50:THR:HB   | 1.86                     | 0.75              |
| 3:CO:46:VAL:O     | 3:CO:50:THR:HB   | 1.86                     | 0.75              |
| 3:CU:46:VAL:O     | 3:CU:50:THR:HB   | 1.86                     | 0.75              |
| 2:B0:157:VAL:HG23 | 3:C0:50:THR:HG21 | 1.69                     | 0.75              |
| 1:AE:191:HIS:HD2  | 1:AE:193:GLY:H   | 1.33                     | 0.75              |
| 1:AL:207:CYS:O    | 1:AL:208:TYR:HB2 | 1.86                     | 0.75              |
| 1:DH:207:CYS:O    | 1:DH:208:TYR:HB2 | 1.86                     | 0.75              |
| 1:AD:207:CYS:O    | 1:AD:208:TYR:HB2 | 1.86                     | 0.75              |
| 1:AQ:191:HIS:HD2  | 1:AQ:193:GLY:H   | 1.33                     | 0.75              |
| 1:AR:191:HIS:HD2  | 1:AR:193:GLY:H   | 1.33                     | 0.75              |
| 1:AS:191:HIS:HD2  | 1:AS:193:GLY:H   | 1.33                     | 0.75              |
| 1:AM:181:LYS:HE3  | 2:BM:137:GLU:HB2 | 64.94                    | 0.75              |
| 2:BK:157:VAL:HG23 | 3:CK:50:THR:HG21 | 1.69                     | 0.75              |
| 2:BL:157:VAL:HG23 | 3:CL:50:THR:HG21 | 1.69                     | 0.75              |
| 1:A0:181:LYS:HE3  | 2:B1:137:GLU:HB2 | 1.67                     | 0.75              |
| 1:AN:181:LYS:HE3  | 2:BN:137:GLU:HB2 | 104.99                   | 0.75              |
| 2:BZ:157:VAL:HG23 | 3:CZ:50:THR:HG21 | 1.68                     | 0.75              |
| 2:BC:157:VAL:HG23 | 3:CD:50:THR:HG21 | 57.59                    | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BG:157:VAL:HG23 | 3:CH:50:THR:HG21  | 91.99                    | 0.75              |
| 3:CK:46:VAL:O     | 3:CK:50:THR:HB    | 1.86                     | 0.75              |
| 2:BL:157:VAL:HG23 | 3:CM:50:THR:HG21  | 91.99                    | 0.75              |
| 2:BN:157:VAL:HG23 | 3:CO:50:THR:HG21  | 91.25                    | 0.75              |
| 3:CA:46:VAL:O     | 3:CA:50:THR:HB    | 1.86                     | 0.75              |
| 1:AU:207:CYS:O    | 1:AU:208:TYR:HB2  | 1.86                     | 0.75              |
| 1:AN:207:CYS:O    | 1:AN:208:TYR:HB2  | 1.86                     | 0.75              |
| 1:A5:207:CYS:O    | 1:A5:208:TYR:HB2  | 1.86                     | 0.75              |
| 1:AF:181:LYS:HE3  | 2:BF:137:GLU:HB2  | 1.67                     | 0.75              |
| 1:AW:181:LYS:HE3  | 2:BX:137:GLU:HB2  | 1.67                     | 0.75              |
| 2:BJ:157:VAL:HG23 | 3:CK:50:THR:HG21  | 221.75                   | 0.75              |
| 2:BB:157:VAL:HG23 | 3:CC:50:THR:HG21  | 91.99                    | 0.75              |
| 1:AV:191:HIS:HD2  | 1:AV:193:GLY:H    | 1.33                     | 0.75              |
| 1:AE:207:CYS:O    | 1:AE:208:TYR:HB2  | 1.86                     | 0.75              |
| 2:BX:157:VAL:HG23 | 3:C5:50:THR:HG21  | 243.10                   | 0.75              |
| 2:BX:157:VAL:HG23 | 3:CX:50:THR:HG21  | 1.69                     | 0.75              |
| 2:BQ:157:VAL:HG23 | 3:CS:50:THR:HG21  | 1.68                     | 0.75              |
| 2:BU:157:VAL:HG23 | 3:CU:50:THR:HG21  | 1.69                     | 0.75              |
| 1:A0:207:CYS:O    | 1:A0:208:TYR:HB2  | 1.86                     | 0.75              |
| 1:A3:191:HIS:HD2  | 1:A3:193:GLY:H    | 1.33                     | 0.75              |
| 1:AF:191:HIS:HD2  | 1:AF:193:GLY:H    | 1.33                     | 0.75              |
| 1:AX:191:HIS:HD2  | 1:AX:193:GLY:H    | 1.33                     | 0.75              |
| 1:DC:191:HIS:HD2  | 1:DC:193:GLY:H    | 1.33                     | 0.75              |
| 1:AH:191:HIS:HD2  | 1:AH:193:GLY:H    | 1.33                     | 0.75              |
| 1:AB:243:ILE:HG23 | 1:A8:188:PRO:HB2  | 214.07                   | 0.75              |
| 1:AG:243:ILE:HG23 | 1:DK:188:PRO:HB2  | 1.69                     | 0.75              |
| 2:BY:157:VAL:HG23 | 3:CY:50:THR:HG21  | 1.68                     | 0.74              |
| 3:CH:46:VAL:O     | 3:CH:50:THR:HB    | 1.86                     | 0.74              |
| 2:BT:137:GLU:HB2  | 1:DG:181:LYS:HE3  | 253.84                   | 0.74              |
| 1:AJ:188:PRO:HB2  | 1:AM:243:ILE:HG23 | 1.69                     | 0.74              |
| 1:A7:207:CYS:O    | 1:A7:208:TYR:HB2  | 1.86                     | 0.74              |
| 3:C3:46:VAL:O     | 3:C3:50:THR:HB    | 1.86                     | 0.74              |
| 1:A5:243:ILE:HG23 | 1:A6:188:PRO:HB2  | 1.70                     | 0.74              |
| 1:DG:243:ILE:HG23 | 1:DJ:188:PRO:HB2  | 1.69                     | 0.74              |
| 1:A4:243:ILE:HG23 | 1:A7:188:PRO:HB2  | 1.70                     | 0.74              |
| 2:BK:157:VAL:HG23 | 3:CL:50:THR:HG21  | 57.59                    | 0.74              |
| 2:BR:157:VAL:HG23 | 3:CS:50:THR:HG21  | 207.50                   | 0.74              |
| 2:B9:157:VAL:HG23 | 3:DA:50:THR:HG21  | 1.69                     | 0.74              |
| 1:AA:188:PRO:HB2  | 1:AC:243:ILE:HG23 | 51.83                    | 0.74              |
| 1:AJ:243:ILE:HG23 | 1:AM:188:PRO:HB2  | 82.20                    | 0.74              |
| 1:AK:243:ILE:HG23 | 1:AL:188:PRO:HB2  | 51.83                    | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AK:243:ILE:HG23 | 1:AN:188:PRO:HB2  | 1.69                     | 0.74              |
| 3:C6:46:VAL:O     | 3:C6:50:THR:HB    | 1.86                     | 0.74              |
| 2:B5:157:VAL:HG23 | 3:C6:50:THR:HG21  | 1.69                     | 0.74              |
| 2:BO:184:THR:HG21 | 2:BO:189:HIS:ND1  | 2.03                     | 0.74              |
| 3:C8:46:VAL:O     | 3:C8:50:THR:HB    | 1.86                     | 0.74              |
| 1:A9:207:CYS:O    | 1:A9:208:TYR:HB2  | 1.86                     | 0.74              |
| 1:AG:181:LYS:HE3  | 2:BG:137:GLU:HB2  | 1.67                     | 0.74              |
| 1:DH:243:ILE:HG23 | 1:DI:188:PRO:HB2  | 1.69                     | 0.74              |
| 1:AY:243:ILE:HG23 | 1:AZ:188:PRO:HB2  | 1.69                     | 0.74              |
| 1:AR:181:LYS:HE3  | 2:BQ:137:GLU:HB2  | 1.67                     | 0.74              |
| 2:BN:157:VAL:HG23 | 3:CN:50:THR:HG21  | 1.69                     | 0.74              |
| 3:CG:46:VAL:O     | 3:CG:50:THR:HB    | 1.86                     | 0.74              |
| 2:BU:157:VAL:HG23 | 3:CV:50:THR:HG21  | 57.59                    | 0.74              |
| 1:AC:243:ILE:HG23 | 1:AD:188:PRO:HB2  | 1.69                     | 0.74              |
| 1:AF:243:ILE:HG23 | 1:AG:188:PRO:HB2  | 1.69                     | 0.74              |
| 1:AI:243:ILE:HG23 | 1:AJ:188:PRO:HB2  | 174.22                   | 0.74              |
| 1:DC:188:PRO:HB2  | 1:DE:243:ILE:HG23 | 1.70                     | 0.74              |
| 1:AO:243:ILE:HG23 | 1:DE:188:PRO:HB2  | 283.03                   | 0.74              |
| 1:AV:243:ILE:HG23 | 1:AW:188:PRO:HB2  | 1.69                     | 0.74              |
| 1:AT:188:PRO:HB2  | 1:AW:243:ILE:HG23 | 1.69                     | 0.74              |
| 1:DE:191:HIS:HD2  | 1:DE:193:GLY:H    | 1.33                     | 0.74              |
| 2:BS:157:VAL:HG23 | 3:CT:50:THR:HG21  | 57.59                    | 0.74              |
| 1:AL:243:ILE:HG23 | 1:AM:188:PRO:HB2  | 1.70                     | 0.74              |
| 1:AU:243:ILE:HG23 | 1:AX:188:PRO:HB2  | 1.69                     | 0.74              |
| 1:AB:191:HIS:HD2  | 1:AB:193:GLY:H    | 1.33                     | 0.74              |
| 2:BF:184:THR:HG21 | 2:BF:189:HIS:ND1  | 2.03                     | 0.74              |
| 2:B1:157:VAL:HG23 | 3:C1:50:THR:HG21  | 1.69                     | 0.74              |
| 2:BP:184:THR:HG21 | 2:BP:189:HIS:ND1  | 2.03                     | 0.74              |
| 1:AY:188:PRO:HB2  | 1:A1:243:ILE:HG23 | 1.70                     | 0.74              |
| 1:A8:243:ILE:HG23 | 1:A9:188:PRO:HB2  | 1.70                     | 0.74              |
| 2:BI:184:THR:HG21 | 2:BI:189:HIS:ND1  | 2.03                     | 0.74              |
| 2:BR:184:THR:HG21 | 2:BR:189:HIS:ND1  | 2.03                     | 0.74              |
| 2:BP:157:VAL:HG23 | 3:CR:50:THR:HG21  | 1.68                     | 0.74              |
| 3:CB:46:VAL:O     | 3:CB:50:THR:HB    | 1.86                     | 0.74              |
| 2:BA:157:VAL:HG23 | 3:CA:50:THR:HG21  | 1.68                     | 0.74              |
| 1:AC:188:PRO:HB2  | 1:A9:243:ILE:HG23 | 281.58                   | 0.74              |
| 1:AC:188:PRO:HB2  | 1:AE:243:ILE:HG23 | 1.70                     | 0.74              |
| 1:AE:243:ILE:HG23 | 1:AH:188:PRO:HB2  | 174.22                   | 0.74              |
| 1:AF:188:PRO:HB2  | 1:AH:243:ILE:HG23 | 51.83                    | 0.74              |
| 1:AI:188:PRO:HB2  | 1:AL:243:ILE:HG23 | 143.74                   | 0.74              |
| 1:AF:188:PRO:HB2  | 1:AI:243:ILE:HG23 | 1.70                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AQ:243:ILE:HG23 | 1:AR:188:PRO:HB2  | 1.70                     | 0.74              |
| 1:DF:188:PRO:HB2  | 1:DI:243:ILE:HG23 | 1.70                     | 0.74              |
| 1:AQ:188:PRO:HB2  | 1:AS:243:ILE:HG23 | 1.70                     | 0.74              |
| 2:BJ:184:THR:HG21 | 2:BJ:189:HIS:ND1  | 2.03                     | 0.74              |
| 2:BT:184:THR:HG21 | 2:BT:189:HIS:ND1  | 2.03                     | 0.74              |
| 2:BX:184:THR:HG21 | 2:BX:189:HIS:ND1  | 2.03                     | 0.74              |
| 1:A3:243:ILE:HG23 | 1:A4:188:PRO:HB2  | 1.70                     | 0.74              |
| 2:B4:184:THR:HG21 | 2:B4:189:HIS:ND1  | 2.03                     | 0.74              |
| 3:C4:46:VAL:O     | 3:C4:50:THR:HB    | 1.86                     | 0.74              |
| 2:B2:157:VAL:HG23 | 3:C2:50:THR:HG21  | 1.69                     | 0.74              |
| 1:DH:188:PRO:HB2  | 1:DJ:243:ILE:HG23 | 1.70                     | 0.74              |
| 2:B8:184:THR:HG21 | 2:B8:189:HIS:ND1  | 2.03                     | 0.74              |
| 2:BA:184:THR:HG21 | 2:BA:189:HIS:ND1  | 2.03                     | 0.74              |
| 1:AV:188:PRO:HB2  | 1:AX:243:ILE:HG23 | 1.70                     | 0.74              |
| 2:BC:184:THR:HG21 | 2:BC:189:HIS:ND1  | 2.03                     | 0.74              |
| 2:BU:184:THR:HG21 | 2:BU:189:HIS:ND1  | 2.03                     | 0.74              |
| 1:A3:188:PRO:HB2  | 1:A6:243:ILE:HG23 | 1.70                     | 0.74              |
| 1:DI:191:HIS:HD2  | 1:DI:193:GLY:H    | 1.33                     | 0.74              |
| 1:AZ:243:ILE:HG23 | 1:A2:188:PRO:HB2  | 1.69                     | 0.74              |
| 2:BD:184:THR:HG21 | 2:BD:189:HIS:ND1  | 2.03                     | 0.74              |
| 2:BE:184:THR:HG21 | 2:BE:189:HIS:ND1  | 2.03                     | 0.74              |
| 1:A0:188:PRO:HB2  | 1:A2:243:ILE:HG23 | 1.69                     | 0.74              |
| 1:AM:207:CYS:O    | 1:AM:208:TYR:HB2  | 1.85                     | 0.74              |
| 1:A0:243:ILE:HG23 | 1:A1:188:PRO:HB2  | 1.69                     | 0.74              |
| 1:DK:191:HIS:HD2  | 1:DK:193:GLY:H    | 1.33                     | 0.74              |
| 2:BQ:184:THR:HG21 | 2:BQ:189:HIS:ND1  | 2.03                     | 0.74              |
| 3:CP:46:VAL:O     | 3:CP:50:THR:HB    | 1.86                     | 0.74              |
| 2:B6:157:VAL:HG23 | 3:C7:50:THR:HG21  | 1.69                     | 0.74              |
| 1:AH:243:ILE:HG23 | 1:AI:188:PRO:HB2  | 1.70                     | 0.74              |
| 3:C1:46:VAL:O     | 3:C1:50:THR:HB    | 1.86                     | 0.74              |
| 2:BK:184:THR:HG21 | 2:BK:189:HIS:ND1  | 2.03                     | 0.74              |
| 2:BL:184:THR:HG21 | 2:BL:189:HIS:ND1  | 2.03                     | 0.74              |
| 2:BM:184:THR:HG21 | 2:BM:189:HIS:ND1  | 2.03                     | 0.74              |
| 2:BW:184:THR:HG21 | 2:BW:189:HIS:ND1  | 2.03                     | 0.74              |
| 2:BZ:184:THR:HG21 | 2:BZ:189:HIS:ND1  | 2.02                     | 0.74              |
| 2:BD:157:VAL:HG23 | 3:CD:50:THR:HG21  | 1.69                     | 0.74              |
| 2:BV:157:VAL:HG23 | 3:CV:50:THR:HG21  | 1.69                     | 0.74              |
| 1:AJ:243:ILE:HG23 | 1:AK:188:PRO:HB2  | 1.70                     | 0.74              |
| 1:AT:243:ILE:HG23 | 1:AU:188:PRO:HB2  | 1.69                     | 0.74              |
| 2:BS:184:THR:HG21 | 2:BS:189:HIS:ND1  | 2.03                     | 0.74              |
| 1:AT:191:HIS:HD2  | 1:AT:193:GLY:H    | 1.33                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B0:184:THR:HG21 | 2:B0:189:HIS:ND1  | 2.03                     | 0.74              |
| 2:BV:184:THR:HG21 | 2:BV:189:HIS:ND1  | 2.02                     | 0.74              |
| 1:DC:243:ILE:HG23 | 1:DD:188:PRO:HB2  | 1.70                     | 0.74              |
| 2:BG:184:THR:HG21 | 2:BG:189:HIS:ND1  | 2.03                     | 0.74              |
| 2:BS:137:GLU:HB2  | 1:DF:181:LYS:HE3  | 272.37                   | 0.74              |
| 1:AB:243:ILE:HG23 | 1:AE:188:PRO:HB2  | 1.69                     | 0.74              |
| 1:AO:188:PRO:HB2  | 1:AR:243:ILE:HG23 | 1.69                     | 0.74              |
| 1:AP:243:ILE:HG23 | 1:AS:188:PRO:HB2  | 1.69                     | 0.74              |
| 2:BB:184:THR:HG21 | 2:BB:189:HIS:ND1  | 2.03                     | 0.74              |
| 1:DF:207:CYS:O    | 1:DF:208:TYR:HB2  | 1.86                     | 0.74              |
| 1:A5:191:HIS:HD2  | 1:A5:193:GLY:H    | 1.33                     | 0.74              |
| 2:BV:157:VAL:HG23 | 3:CW:50:THR:HG21  | 91.99                    | 0.74              |
| 1:DF:243:ILE:HG23 | 1:DG:188:PRO:HB2  | 1.69                     | 0.74              |
| 2:BH:157:VAL:HG23 | 3:CI:50:THR:HG21  | 57.59                    | 0.73              |
| 2:BT:157:VAL:HG23 | 3:CU:50:THR:HG21  | 243.09                   | 0.73              |
| 1:AD:243:ILE:HG23 | 1:AE:188:PRO:HB2  | 82.83                    | 0.73              |
| 1:AD:188:PRO:HB2  | 1:AG:243:ILE:HG23 | 199.91                   | 0.73              |
| 2:B4:157:VAL:HG23 | 3:C4:50:THR:HG21  | 1.68                     | 0.73              |
| 1:AR:207:CYS:O    | 1:AR:208:TYR:HB2  | 1.86                     | 0.73              |
| 1:A6:191:HIS:HD2  | 1:A6:193:GLY:H    | 1.33                     | 0.73              |
| 1:AF:115:THR:CG2  | 1:AF:131:GLN:HB3  | 2.19                     | 0.73              |
| 1:A3:115:THR:CG2  | 1:A3:131:GLN:HB3  | 2.19                     | 0.73              |
| 2:BE:157:VAL:HG23 | 3:CE:50:THR:HG21  | 1.68                     | 0.73              |
| 2:B8:157:VAL:HG23 | 3:C9:50:THR:HG21  | 1.68                     | 0.73              |
| 1:AH:188:PRO:HB2  | 1:DK:243:ILE:HG23 | 1.70                     | 0.73              |
| 2:B2:184:THR:HG21 | 2:B2:189:HIS:ND1  | 2.03                     | 0.73              |
| 2:B3:184:THR:HG21 | 2:B3:189:HIS:ND1  | 2.03                     | 0.73              |
| 1:AP:191:HIS:HD2  | 1:AP:193:GLY:H    | 1.33                     | 0.73              |
| 2:B6:184:THR:HG21 | 2:B6:189:HIS:ND1  | 2.03                     | 0.73              |
| 1:A2:115:THR:CG2  | 1:A2:131:GLN:HB3  | 2.19                     | 0.73              |
| 2:BM:157:VAL:HG23 | 3:CN:50:THR:HG21  | 57.59                    | 0.73              |
| 1:AK:188:PRO:HB2  | 1:AM:243:ILE:HG23 | 51.83                    | 0.73              |
| 1:AN:243:ILE:HG23 | 1:AO:188:PRO:HB2  | 258.06                   | 0.73              |
| 1:AO:243:ILE:HG23 | 1:AP:188:PRO:HB2  | 1.69                     | 0.73              |
| 1:DK:115:THR:CG2  | 1:DK:131:GLN:HB3  | 2.19                     | 0.73              |
| 1:AO:115:THR:CG2  | 1:AO:131:GLN:HB3  | 2.19                     | 0.73              |
| 1:DF:115:THR:CG2  | 1:DF:131:GLN:HB3  | 2.19                     | 0.73              |
| 1:AB:115:THR:CG2  | 1:AB:131:GLN:HB3  | 2.19                     | 0.73              |
| 1:AE:115:THR:CG2  | 1:AE:131:GLN:HB3  | 2.19                     | 0.73              |
| 2:BE:157:VAL:HG23 | 3:CF:50:THR:HG21  | 66.46                    | 0.73              |
| 2:BH:157:VAL:HG23 | 3:CH:50:THR:HG21  | 1.68                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B9:184:THR:HG21 | 2:B9:189:HIS:ND1  | 2.03                     | 0.73              |
| 2:BN:184:THR:HG21 | 2:BN:189:HIS:ND1  | 2.03                     | 0.73              |
| 2:BY:184:THR:HG21 | 2:BY:189:HIS:ND1  | 2.03                     | 0.73              |
| 2:B7:184:THR:HG21 | 2:B7:189:HIS:ND1  | 2.03                     | 0.73              |
| 1:AT:115:THR:CG2  | 1:AT:131:GLN:HB3  | 2.19                     | 0.73              |
| 1:AJ:115:THR:CG2  | 1:AJ:131:GLN:HB3  | 2.19                     | 0.73              |
| 2:BI:157:VAL:HG23 | 3:CJ:50:THR:HG21  | 91.26                    | 0.73              |
| 2:BA:157:VAL:HG23 | 3:DB:50:THR:HG21  | 271.34                   | 0.73              |
| 1:AA:188:PRO:HB2  | 1:AD:243:ILE:HG23 | 1.70                     | 0.73              |
| 2:B3:157:VAL:HG23 | 3:C3:50:THR:HG21  | 1.68                     | 0.73              |
| 1:AY:191:HIS:HD2  | 1:AY:193:GLY:H    | 1.33                     | 0.73              |
| 2:BH:184:THR:HG21 | 2:BH:189:HIS:ND1  | 2.03                     | 0.73              |
| 2:BI:157:VAL:HG23 | 3:CI:50:THR:HG21  | 1.68                     | 0.73              |
| 1:AL:188:PRO:HB2  | 1:AN:243:ILE:HG23 | 1.69                     | 0.73              |
| 2:B1:184:THR:HG21 | 2:B1:189:HIS:ND1  | 2.03                     | 0.73              |
| 1:AA:243:ILE:HG23 | 1:AB:188:PRO:HB2  | 1.69                     | 0.73              |
| 1:AD:115:THR:CG2  | 1:AD:131:GLN:HB3  | 2.19                     | 0.73              |
| 1:AL:115:THR:CG2  | 1:AL:131:GLN:HB3  | 2.19                     | 0.73              |
| 2:BQ:157:VAL:HG23 | 3:CR:50:THR:HG21  | 55.68                    | 0.73              |
| 2:B5:184:THR:HG21 | 2:B5:189:HIS:ND1  | 2.03                     | 0.73              |
| 1:AN:115:THR:CG2  | 1:AN:131:GLN:HB3  | 2.19                     | 0.73              |
| 2:BG:157:VAL:HG23 | 3:CG:50:THR:HG21  | 1.69                     | 0.73              |
| 1:AN:188:PRO:HB2  | 1:DD:243:ILE:HG23 | 301.19                   | 0.73              |
| 1:AM:115:THR:CG2  | 1:AM:131:GLN:HB3  | 2.19                     | 0.72              |
| 1:AH:115:THR:CG2  | 1:AH:131:GLN:HB3  | 2.19                     | 0.72              |
| 1:AK:115:THR:CG2  | 1:AK:131:GLN:HB3  | 2.19                     | 0.72              |
| 1:DH:115:THR:CG2  | 1:DH:131:GLN:HB3  | 2.19                     | 0.72              |
| 2:BR:157:VAL:HG23 | 3:CO:50:THR:HG21  | 1.69                     | 0.72              |
| 1:AU:115:THR:CG2  | 1:AU:131:GLN:HB3  | 2.19                     | 0.72              |
| 2:BT:157:VAL:HG23 | 3:CT:50:THR:HG21  | 1.69                     | 0.72              |
| 1:DI:115:THR:CG2  | 1:DI:131:GLN:HB3  | 2.19                     | 0.72              |
| 1:A8:115:THR:CG2  | 1:A8:131:GLN:HB3  | 2.19                     | 0.72              |
| 2:B7:157:VAL:HG23 | 3:C8:50:THR:HG21  | 1.68                     | 0.72              |
| 1:A5:188:PRO:HB2  | 1:A7:243:ILE:HG23 | 1.70                     | 0.72              |
| 1:AA:115:THR:CG2  | 1:AA:131:GLN:HB3  | 2.19                     | 0.72              |
| 1:AZ:115:THR:CG2  | 1:AZ:131:GLN:HB3  | 2.19                     | 0.72              |
| 1:A2:191:HIS:HD2  | 1:A2:193:GLY:H    | 1.33                     | 0.72              |
| 1:AP:115:THR:CG2  | 1:AP:131:GLN:HB3  | 2.19                     | 0.72              |
| 1:AS:115:THR:CG2  | 1:AS:131:GLN:HB3  | 2.19                     | 0.72              |
| 1:AC:115:THR:CG2  | 1:AC:131:GLN:HB3  | 2.19                     | 0.72              |
| 1:AX:115:THR:CG2  | 1:AX:131:GLN:HB3  | 2.19                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A3:242:ASN:HD22 | 1:A4:110:GLY:H    | 1.38                     | 0.72              |
| 1:A0:110:GLY:H    | 1:A2:242:ASN:HD22 | 1.38                     | 0.72              |
| 1:A8:242:ASN:HD22 | 1:A9:110:GLY:H    | 1.38                     | 0.72              |
| 1:A7:115:THR:CG2  | 1:A7:131:GLN:HB3  | 2.19                     | 0.72              |
| 1:AI:242:ASN:HD22 | 1:AJ:110:GLY:H    | 171.53                   | 0.72              |
| 1:DH:242:ASN:HD22 | 1:DI:110:GLY:H    | 1.38                     | 0.72              |
| 1:AI:115:THR:CG2  | 1:AI:131:GLN:HB3  | 2.19                     | 0.72              |
| 1:AJ:110:GLY:H    | 1:AM:242:ASN:HD22 | 1.38                     | 0.72              |
| 1:AJ:242:ASN:HD22 | 1:AK:110:GLY:H    | 1.38                     | 0.72              |
| 1:AL:242:ASN:HD22 | 1:AM:110:GLY:H    | 1.38                     | 0.72              |
| 1:AO:242:ASN:HD22 | 1:DE:110:GLY:H    | 280.63                   | 0.72              |
| 1:DF:110:GLY:H    | 1:DI:242:ASN:HD22 | 1.38                     | 0.72              |
| 1:A4:115:THR:CG2  | 1:A4:131:GLN:HB3  | 2.19                     | 0.72              |
| 1:AC:110:GLY:H    | 1:A9:242:ASN:HD22 | 275.53                   | 0.72              |
| 1:AC:110:GLY:H    | 1:AE:242:ASN:HD22 | 1.38                     | 0.72              |
| 1:AE:242:ASN:HD22 | 1:AH:110:GLY:H    | 171.53                   | 0.72              |
| 1:AB:242:ASN:HD22 | 1:AE:110:GLY:H    | 1.38                     | 0.72              |
| 1:A9:115:THR:CG2  | 1:A9:131:GLN:HB3  | 2.19                     | 0.71              |
| 2:BR:134:HIS:CD2  | 2:BR:145:LEU:HD13 | 2.26                     | 0.71              |
| 1:AN:242:ASN:HD22 | 1:AO:110:GLY:H    | 254.56                   | 0.71              |
| 1:DJ:115:THR:CG2  | 1:DJ:131:GLN:HB3  | 2.19                     | 0.71              |
| 1:DD:115:THR:CG2  | 1:DD:131:GLN:HB3  | 2.19                     | 0.71              |
| 2:B3:134:HIS:CD2  | 2:B3:145:LEU:HD13 | 2.26                     | 0.71              |
| 2:BX:134:HIS:CD2  | 2:BX:145:LEU:HD13 | 2.26                     | 0.71              |
| 2:B6:134:HIS:CD2  | 2:B6:145:LEU:HD13 | 2.26                     | 0.71              |
| 1:AQ:110:GLY:H    | 1:AS:242:ASN:HD22 | 1.38                     | 0.71              |
| 1:AF:242:ASN:HD22 | 1:AG:110:GLY:H    | 1.38                     | 0.71              |
| 1:AU:242:ASN:HD22 | 1:AX:110:GLY:H    | 1.38                     | 0.71              |
| 1:DG:115:THR:CG2  | 1:DG:131:GLN:HB3  | 2.19                     | 0.71              |
| 2:B0:134:HIS:CD2  | 2:B0:145:LEU:HD13 | 2.26                     | 0.71              |
| 1:AZ:242:ASN:HD22 | 1:A2:110:GLY:H    | 1.38                     | 0.71              |
| 1:AT:242:ASN:HD22 | 1:AU:110:GLY:H    | 1.38                     | 0.71              |
| 1:AR:115:THR:CG2  | 1:AR:131:GLN:HB3  | 2.19                     | 0.71              |
| 1:A0:115:THR:CG2  | 1:A0:131:GLN:HB3  | 2.19                     | 0.71              |
| 1:DF:242:ASN:HD22 | 1:DG:110:GLY:H    | 1.38                     | 0.71              |
| 1:AQ:242:ASN:HD22 | 1:AR:110:GLY:H    | 1.38                     | 0.71              |
| 1:DC:110:GLY:H    | 1:DE:242:ASN:HD22 | 1.38                     | 0.71              |
| 1:AG:115:THR:CG2  | 1:AG:131:GLN:HB3  | 2.19                     | 0.71              |
| 1:DC:115:THR:CG2  | 1:DC:131:GLN:HB3  | 2.19                     | 0.71              |
| 2:BA:134:HIS:CD2  | 2:BA:145:LEU:HD13 | 2.26                     | 0.71              |
| 2:BK:134:HIS:CD2  | 2:BK:145:LEU:HD13 | 2.26                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BT:134:HIS:CD2  | 2:BT:145:LEU:HD13 | 2.26                     | 0.71              |
| 2:BJ:134:HIS:CD2  | 2:BJ:145:LEU:HD13 | 2.26                     | 0.71              |
| 1:AB:242:ASN:HD22 | 1:A8:110:GLY:H    | 222.98                   | 0.71              |
| 1:AA:242:ASN:HD22 | 1:AB:110:GLY:H    | 1.38                     | 0.71              |
| 1:A6:115:THR:CG2  | 1:A6:131:GLN:HB3  | 2.19                     | 0.71              |
| 2:BG:134:HIS:CD2  | 2:BG:145:LEU:HD13 | 2.25                     | 0.71              |
| 2:BO:134:HIS:CD2  | 2:BO:145:LEU:HD13 | 2.26                     | 0.71              |
| 2:BS:134:HIS:CD2  | 2:BS:145:LEU:HD13 | 2.26                     | 0.71              |
| 2:BB:134:HIS:CD2  | 2:BB:145:LEU:HD13 | 2.26                     | 0.71              |
| 2:BN:134:HIS:CD2  | 2:BN:145:LEU:HD13 | 2.26                     | 0.71              |
| 1:AI:110:GLY:H    | 1:AL:242:ASN:HD22 | 146.06                   | 0.71              |
| 1:AL:110:GLY:H    | 1:AN:242:ASN:HD22 | 1.38                     | 0.71              |
| 1:AU:87:GLN:HE21  | 1:AU:210:ARG:HH22 | 1.39                     | 0.71              |
| 1:AV:110:GLY:H    | 1:AX:242:ASN:HD22 | 1.38                     | 0.71              |
| 1:A5:115:THR:CG2  | 1:A5:131:GLN:HB3  | 2.19                     | 0.71              |
| 2:BV:134:HIS:CD2  | 2:BV:145:LEU:HD13 | 2.26                     | 0.71              |
| 2:B2:134:HIS:CD2  | 2:B2:145:LEU:HD13 | 2.26                     | 0.71              |
| 1:AH:242:ASN:HD22 | 1:AI:110:GLY:H    | 1.38                     | 0.71              |
| 1:AC:87:GLN:HE21  | 1:AC:210:ARG:HH22 | 1.39                     | 0.71              |
| 1:AY:115:THR:CG2  | 1:AY:131:GLN:HB3  | 2.19                     | 0.71              |
| 1:AW:115:THR:CG2  | 1:AW:131:GLN:HB3  | 2.19                     | 0.71              |
| 2:BC:134:HIS:CD2  | 2:BC:145:LEU:HD13 | 2.26                     | 0.71              |
| 2:BY:134:HIS:CD2  | 2:BY:145:LEU:HD13 | 2.26                     | 0.71              |
| 2:B9:134:HIS:CD2  | 2:B9:145:LEU:HD13 | 2.25                     | 0.71              |
| 1:AH:110:GLY:H    | 1:DK:242:ASN:HD22 | 1.38                     | 0.71              |
| 1:AT:110:GLY:H    | 1:AW:242:ASN:HD22 | 1.38                     | 0.71              |
| 1:AH:87:GLN:HE21  | 1:AH:210:ARG:HH22 | 1.39                     | 0.71              |
| 1:A3:110:GLY:H    | 1:A6:242:ASN:HD22 | 1.38                     | 0.71              |
| 1:AV:87:GLN:HE21  | 1:AV:210:ARG:HH22 | 1.39                     | 0.71              |
| 1:DE:115:THR:CG2  | 1:DE:131:GLN:HB3  | 2.19                     | 0.71              |
| 2:BE:134:HIS:CD2  | 2:BE:145:LEU:HD13 | 2.26                     | 0.71              |
| 2:BM:134:HIS:CD2  | 2:BM:145:LEU:HD13 | 2.26                     | 0.71              |
| 2:BZ:134:HIS:CD2  | 2:BZ:145:LEU:HD13 | 2.26                     | 0.71              |
| 2:B8:134:HIS:CD2  | 2:B8:145:LEU:HD13 | 2.26                     | 0.71              |
| 1:AF:110:GLY:H    | 1:AH:242:ASN:HD22 | 42.38                    | 0.71              |
| 1:AF:110:GLY:H    | 1:AI:242:ASN:HD22 | 1.38                     | 0.71              |
| 1:AN:110:GLY:H    | 1:DD:242:ASN:HD22 | 296.00                   | 0.71              |
| 1:AA:87:GLN:HE21  | 1:AA:210:ARG:HH22 | 1.39                     | 0.71              |
| 1:AN:87:GLN:HE21  | 1:AN:210:ARG:HH22 | 1.39                     | 0.71              |
| 2:B7:134:HIS:CD2  | 2:B7:145:LEU:HD13 | 2.26                     | 0.70              |
| 1:AG:242:ASN:HD22 | 1:DK:110:GLY:H    | 1.38                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AJ:87:GLN:HE21  | 1:AJ:210:ARG:HH22 | 1.39                     | 0.70              |
| 1:AW:87:GLN:HE21  | 1:AW:210:ARG:HH22 | 1.39                     | 0.70              |
| 2:BD:134:HIS:CD2  | 2:BD:145:LEU:HD13 | 2.26                     | 0.70              |
| 1:AA:110:GLY:H    | 1:AD:242:ASN:HD22 | 1.38                     | 0.70              |
| 1:AI:87:GLN:HE21  | 1:AI:210:ARG:HH22 | 1.39                     | 0.70              |
| 1:A5:110:GLY:H    | 1:A7:242:ASN:HD22 | 1.38                     | 0.70              |
| 1:A0:242:ASN:HD22 | 1:A1:110:GLY:H    | 1.38                     | 0.70              |
| 1:A8:87:GLN:HE21  | 1:A8:210:ARG:HH22 | 1.39                     | 0.70              |
| 1:AB:87:GLN:HE21  | 1:AB:210:ARG:HH22 | 1.39                     | 0.70              |
| 1:A6:87:GLN:HE21  | 1:A6:210:ARG:HH22 | 1.39                     | 0.70              |
| 1:A5:87:GLN:HE21  | 1:A5:210:ARG:HH22 | 1.39                     | 0.70              |
| 2:BW:134:HIS:CD2  | 2:BW:145:LEU:HD13 | 2.26                     | 0.70              |
| 1:AG:87:GLN:HE21  | 1:AG:210:ARG:HH22 | 1.39                     | 0.70              |
| 1:AM:87:GLN:HE21  | 1:AM:210:ARG:HH22 | 1.39                     | 0.70              |
| 1:AK:87:GLN:HE21  | 1:AK:210:ARG:HH22 | 1.39                     | 0.70              |
| 1:A9:150:ARG:H    | 1:A9:150:ARG:HE   | 1.39                     | 0.70              |
| 2:BU:134:HIS:CD2  | 2:BU:145:LEU:HD13 | 2.26                     | 0.70              |
| 2:BP:134:HIS:CD2  | 2:BP:145:LEU:HD13 | 2.26                     | 0.70              |
| 2:BF:134:HIS:CD2  | 2:BF:145:LEU:HD13 | 2.26                     | 0.70              |
| 1:AC:242:ASN:HD22 | 1:AD:110:GLY:H    | 1.38                     | 0.70              |
| 1:AO:87:GLN:HE21  | 1:AO:210:ARG:HH22 | 1.39                     | 0.70              |
| 1:DC:242:ASN:HD22 | 1:DD:110:GLY:H    | 1.38                     | 0.70              |
| 1:AE:150:ARG:H    | 1:AE:150:ARG:HE   | 1.39                     | 0.70              |
| 1:A4:87:GLN:HE21  | 1:A4:210:ARG:HH22 | 1.39                     | 0.70              |
| 2:BH:134:HIS:CD2  | 2:BH:145:LEU:HD13 | 2.26                     | 0.70              |
| 1:AJ:150:ARG:H    | 1:AJ:150:ARG:HE   | 1.40                     | 0.70              |
| 1:DG:150:ARG:H    | 1:DG:150:ARG:HE   | 1.40                     | 0.70              |
| 1:DJ:150:ARG:H    | 1:DJ:150:ARG:HE   | 1.40                     | 0.70              |
| 1:DK:150:ARG:HE   | 1:DK:150:ARG:H    | 1.40                     | 0.70              |
| 1:AE:87:GLN:HE21  | 1:AE:210:ARG:HH22 | 1.39                     | 0.70              |
| 1:AL:87:GLN:HE21  | 1:AL:210:ARG:HH22 | 1.39                     | 0.70              |
| 1:AS:87:GLN:HE21  | 1:AS:210:ARG:HH22 | 1.39                     | 0.70              |
| 1:AS:150:ARG:HE   | 1:AS:150:ARG:H    | 1.40                     | 0.70              |
| 1:A3:150:ARG:HE   | 1:A3:150:ARG:H    | 1.40                     | 0.70              |
| 1:AX:150:ARG:HE   | 1:AX:150:ARG:H    | 1.40                     | 0.70              |
| 1:AP:150:ARG:H    | 1:AP:150:ARG:HE   | 1.39                     | 0.70              |
| 1:AC:92:THR:HG22  | 1:AC:93:THR:H     | 1.57                     | 0.70              |
| 1:A3:87:GLN:HE21  | 1:A3:210:ARG:HH22 | 1.39                     | 0.70              |
| 2:B4:134:HIS:CD2  | 2:B4:145:LEU:HD13 | 2.26                     | 0.70              |
| 1:DH:87:GLN:HE21  | 1:DH:210:ARG:HH22 | 1.39                     | 0.70              |
| 1:A7:87:GLN:HE21  | 1:A7:210:ARG:HH22 | 1.39                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AC:150:ARG:HE   | 1:AC:150:ARG:H    | 1.40                     | 0.70              |
| 1:AG:150:ARG:H    | 1:AG:150:ARG:HE   | 1.40                     | 0.70              |
| 1:AB:92:THR:HG22  | 1:AB:93:THR:H     | 1.57                     | 0.70              |
| 1:AG:92:THR:HG22  | 1:AG:93:THR:H     | 1.57                     | 0.70              |
| 1:AE:74:THR:HG21  | 3:CF:43:PHE:HE2   | 87.59                    | 0.70              |
| 1:AB:74:THR:HG21  | 3:CB:43:PHE:HE1   | 1.57                     | 0.70              |
| 1:AG:74:THR:HG21  | 3:CG:43:PHE:HE1   | 1.57                     | 0.70              |
| 1:A5:242:ASN:HD22 | 1:A6:110:GLY:H    | 1.38                     | 0.70              |
| 1:A2:150:ARG:HE   | 1:A2:150:ARG:H    | 1.40                     | 0.70              |
| 1:AD:150:ARG:HE   | 1:AD:150:ARG:H    | 1.40                     | 0.70              |
| 1:A4:74:THR:HG21  | 3:C5:43:PHE:HE2   | 1.57                     | 0.70              |
| 1:AE:92:THR:HG22  | 1:AE:93:THR:H     | 1.57                     | 0.70              |
| 1:AF:87:GLN:HE21  | 1:AF:210:ARG:HH22 | 1.39                     | 0.70              |
| 2:B5:134:HIS:CD2  | 2:B5:145:LEU:HD13 | 2.26                     | 0.70              |
| 1:AH:92:THR:HG22  | 1:AH:93:THR:H     | 1.57                     | 0.70              |
| 1:AZ:92:THR:HG22  | 1:AZ:93:THR:H     | 1.57                     | 0.70              |
| 1:AF:150:ARG:H    | 1:AF:150:ARG:HE   | 1.40                     | 0.70              |
| 1:AI:150:ARG:H    | 1:AI:150:ARG:HE   | 1.39                     | 0.70              |
| 1:AR:150:ARG:HE   | 1:AR:150:ARG:H    | 1.40                     | 0.70              |
| 1:DE:150:ARG:H    | 1:DE:150:ARG:HE   | 1.40                     | 0.70              |
| 1:AL:92:THR:HG22  | 1:AL:93:THR:H     | 1.57                     | 0.70              |
| 1:AK:110:GLY:H    | 1:AM:242:ASN:HD22 | 42.38                    | 0.69              |
| 1:AD:110:GLY:H    | 1:AG:242:ASN:HD22 | 188.47                   | 0.69              |
| 1:AC:74:THR:HG21  | 3:CD:43:PHE:HE2   | 45.90                    | 0.69              |
| 1:AZ:74:THR:HG21  | 3:C0:43:PHE:HE2   | 1.57                     | 0.69              |
| 1:AQ:92:THR:HG22  | 1:AQ:93:THR:H     | 1.57                     | 0.69              |
| 1:AO:150:ARG:H    | 1:AO:150:ARG:HE   | 1.40                     | 0.69              |
| 1:A2:87:GLN:HE21  | 1:A2:210:ARG:HH22 | 1.39                     | 0.69              |
| 1:DI:92:THR:HG22  | 1:DI:93:THR:H     | 1.57                     | 0.69              |
| 1:AZ:87:GLN:HE21  | 1:AZ:210:ARG:HH22 | 1.39                     | 0.69              |
| 1:AY:74:THR:HG21  | 3:CZ:43:PHE:HE2   | 1.57                     | 0.69              |
| 1:AK:74:THR:HG21  | 3:CL:43:PHE:HE1   | 1.57                     | 0.69              |
| 1:DI:150:ARG:H    | 1:DI:150:ARG:HE   | 1.40                     | 0.69              |
| 3:CX:43:PHE:HE2   | 1:DJ:74:THR:HG21  | 259.35                   | 0.69              |
| 1:AD:92:THR:HG22  | 1:AD:93:THR:H     | 1.57                     | 0.69              |
| 1:A5:74:THR:HG21  | 3:C6:43:PHE:HE2   | 1.57                     | 0.69              |
| 1:A2:74:THR:HG21  | 3:C3:43:PHE:HE2   | 1.57                     | 0.69              |
| 1:A1:115:THR:CG2  | 1:A1:131:GLN:HB3  | 2.19                     | 0.69              |
| 1:AR:87:GLN:HE21  | 1:AR:210:ARG:HH22 | 1.39                     | 0.69              |
| 1:DE:92:THR:HG22  | 1:DE:93:THR:H     | 1.57                     | 0.69              |
| 1:A0:87:GLN:HE21  | 1:A0:210:ARG:HH22 | 1.39                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AS:92:THR:HG22  | 1:AS:93:THR:H     | 1.57                     | 0.69              |
| 1:AK:150:ARG:H    | 1:AK:150:ARG:HE   | 1.39                     | 0.69              |
| 1:DH:150:ARG:H    | 1:DH:150:ARG:HE   | 1.40                     | 0.69              |
| 1:AN:150:ARG:H    | 1:AN:150:ARG:HE   | 1.39                     | 0.69              |
| 1:DC:150:ARG:H    | 1:DC:150:ARG:HE   | 1.40                     | 0.69              |
| 1:AU:92:THR:HG22  | 1:AU:93:THR:H     | 1.57                     | 0.69              |
| 1:AT:92:THR:HG22  | 1:AT:93:THR:H     | 1.57                     | 0.69              |
| 1:AK:242:ASN:HD22 | 1:AN:110:GLY:H    | 1.38                     | 0.69              |
| 1:AG:74:THR:HG21  | 3:CH:43:PHE:HE2   | 72.79                    | 0.69              |
| 3:CV:43:PHE:HE2   | 1:DH:74:THR:HG21  | 278.03                   | 0.69              |
| 1:AM:92:THR:HG22  | 1:AM:93:THR:H     | 1.57                     | 0.69              |
| 1:AO:74:THR:HG21  | 3:CP:43:PHE:HE2   | 5.35                     | 0.69              |
| 1:DJ:92:THR:HG22  | 1:DJ:93:THR:H     | 1.57                     | 0.69              |
| 1:AD:242:ASN:HD22 | 1:AE:110:GLY:H    | 68.90                    | 0.69              |
| 1:AO:110:GLY:H    | 1:AR:242:ASN:HD22 | 1.38                     | 0.69              |
| 1:AC:74:THR:HG21  | 3:CC:43:PHE:HE1   | 1.57                     | 0.69              |
| 1:A6:74:THR:HG21  | 3:C7:43:PHE:HE2   | 1.57                     | 0.69              |
| 1:DK:92:THR:HG22  | 1:DK:93:THR:H     | 1.57                     | 0.69              |
| 1:AJ:74:THR:HG21  | 3:CK:43:PHE:HE2   | 5.35                     | 0.69              |
| 1:AL:150:ARG:H    | 1:AL:150:ARG:HE   | 1.40                     | 0.69              |
| 3:CW:43:PHE:HE2   | 1:DI:74:THR:HG21  | 219.01                   | 0.69              |
| 1:DJ:87:GLN:HE21  | 1:DJ:210:ARG:HH22 | 1.39                     | 0.69              |
| 1:AV:92:THR:HG22  | 1:AV:93:THR:H     | 1.57                     | 0.69              |
| 1:AW:92:THR:HG22  | 1:AW:93:THR:H     | 1.57                     | 0.69              |
| 1:AP:74:THR:HG21  | 3:CQ:43:PHE:HE1   | 1.57                     | 0.69              |
| 2:B1:134:HIS:CD2  | 2:B1:145:LEU:HD13 | 2.26                     | 0.69              |
| 1:DD:87:GLN:HE21  | 1:DD:210:ARG:HH22 | 1.39                     | 0.69              |
| 1:AF:92:THR:HG22  | 1:AF:93:THR:H     | 1.57                     | 0.69              |
| 1:AO:92:THR:HG22  | 1:AO:93:THR:H     | 1.57                     | 0.69              |
| 1:A5:92:THR:HG22  | 1:A5:93:THR:H     | 1.57                     | 0.69              |
| 1:DE:87:GLN:HE21  | 1:DE:210:ARG:HH22 | 1.39                     | 0.69              |
| 1:AA:74:THR:HG21  | 3:DB:43:PHE:HE1   | 271.58                   | 0.69              |
| 1:AL:74:THR:HG21  | 3:CM:43:PHE:HE1   | 1.57                     | 0.69              |
| 1:AH:150:ARG:HE   | 1:AH:150:ARG:H    | 1.40                     | 0.69              |
| 1:DI:87:GLN:HE21  | 1:DI:210:ARG:HH22 | 1.39                     | 0.69              |
| 1:AM:74:THR:HG21  | 3:CN:43:PHE:HE1   | 1.57                     | 0.69              |
| 1:A2:92:THR:HG22  | 1:A2:93:THR:H     | 1.57                     | 0.69              |
| 1:AO:242:ASN:HD22 | 1:AP:110:GLY:H    | 1.38                     | 0.69              |
| 1:AW:74:THR:HG21  | 3:CX:43:PHE:HE2   | 1.58                     | 0.69              |
| 1:A7:74:THR:HG21  | 3:C8:43:PHE:HE2   | 1.57                     | 0.69              |
| 1:DF:92:THR:HG22  | 1:DF:93:THR:H     | 1.57                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:DG:87:GLN:HE21  | 1:DG:210:ARG:HH22 | 1.39                     | 0.69              |
| 1:AZ:150:ARG:H    | 1:AZ:150:ARG:HE   | 1.40                     | 0.69              |
| 2:BL:134:HIS:CD2  | 2:BL:145:LEU:HD13 | 2.26                     | 0.69              |
| 2:BQ:134:HIS:CD2  | 2:BQ:145:LEU:HD13 | 2.26                     | 0.69              |
| 1:A9:87:GLN:HE21  | 1:A9:210:ARG:HH22 | 1.39                     | 0.69              |
| 1:AH:74:THR:HG21  | 3:CH:43:PHE:HE1   | 1.57                     | 0.69              |
| 1:AU:74:THR:HG21  | 3:CV:43:PHE:HE2   | 1.57                     | 0.69              |
| 1:AM:74:THR:HG21  | 3:CN:43:PHE:HE2   | 5.35                     | 0.69              |
| 2:BR:82:PRO:HA    | 2:BR:193:THR:HB   | 1.75                     | 0.69              |
| 1:AP:92:THR:HG22  | 1:AP:93:THR:H     | 1.57                     | 0.69              |
| 1:A0:92:THR:HG22  | 1:A0:93:THR:H     | 1.57                     | 0.69              |
| 1:AI:92:THR:HG22  | 1:AI:93:THR:H     | 1.57                     | 0.69              |
| 1:A1:87:GLN:HE21  | 1:A1:210:ARG:HH22 | 1.39                     | 0.69              |
| 3:CU:43:PHE:HE2   | 1:DG:74:THR:HG21  | 269.41                   | 0.69              |
| 1:DF:150:ARG:H    | 1:DF:150:ARG:HE   | 1.39                     | 0.69              |
| 1:A4:242:ASN:HD22 | 1:A7:110:GLY:H    | 1.38                     | 0.69              |
| 2:BY:82:PRO:HA    | 2:BY:193:THR:HB   | 1.75                     | 0.69              |
| 1:DD:92:THR:HG22  | 1:DD:93:THR:H     | 1.57                     | 0.69              |
| 1:A1:74:THR:HG21  | 3:C2:43:PHE:HE2   | 1.57                     | 0.69              |
| 1:AM:150:ARG:H    | 1:AM:150:ARG:HE   | 1.40                     | 0.69              |
| 1:A1:92:THR:HG22  | 1:A1:93:THR:H     | 1.57                     | 0.69              |
| 1:AV:242:ASN:HD22 | 1:AW:110:GLY:H    | 1.38                     | 0.69              |
| 1:AV:115:THR:CG2  | 1:AV:131:GLN:HB3  | 2.19                     | 0.69              |
| 1:AK:74:THR:HG21  | 3:CL:43:PHE:HE2   | 5.35                     | 0.69              |
| 1:AV:74:THR:HG21  | 3:CW:43:PHE:HE2   | 1.57                     | 0.69              |
| 2:BW:82:PRO:HA    | 2:BW:193:THR:HB   | 1.75                     | 0.69              |
| 3:CG:1:ALA:HB2    | 3:CI:21:ASN:OD1   | 1.93                     | 0.69              |
| 3:CQ:21:ASN:OD1   | 3:CR:1:ALA:HB2    | 1.93                     | 0.69              |
| 3:CS:43:PHE:HE2   | 1:DE:74:THR:HG21  | 278.05                   | 0.69              |
| 1:AY:242:ASN:HD22 | 1:AZ:110:GLY:H    | 1.38                     | 0.69              |
| 1:DF:87:GLN:HE21  | 1:DF:210:ARG:HH22 | 1.39                     | 0.69              |
| 1:AA:92:THR:HG22  | 1:AA:93:THR:H     | 1.57                     | 0.69              |
| 2:BL:82:PRO:HA    | 2:BL:193:THR:HB   | 1.75                     | 0.69              |
| 1:AK:92:THR:HG22  | 1:AK:93:THR:H     | 1.57                     | 0.69              |
| 1:AY:110:GLY:H    | 1:A1:242:ASN:HD22 | 1.38                     | 0.69              |
| 1:AN:92:THR:HG22  | 1:AN:93:THR:H     | 1.57                     | 0.69              |
| 1:AA:110:GLY:H    | 1:AC:242:ASN:HD22 | 42.38                    | 0.69              |
| 2:B0:82:PRO:HA    | 2:B0:193:THR:HB   | 1.75                     | 0.69              |
| 1:DG:242:ASN:HD22 | 1:DJ:110:GLY:H    | 1.38                     | 0.69              |
| 3:CU:1:ALA:HB2    | 3:CW:21:ASN:OD1   | 1.93                     | 0.69              |
| 2:BE:82:PRO:HA    | 2:BE:193:THR:HB   | 1.75                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:CZ:21:ASN:OD1   | 3:C3:1:ALA:HB2    | 1.93                     | 0.69              |
| 1:AQ:115:THR:CG2  | 1:AQ:131:GLN:HB3  | 2.19                     | 0.68              |
| 1:AJ:152:GLN:NE2  | 1:AM:145:LYS:HE3  | 21.01                    | 0.68              |
| 1:AD:74:THR:HG21  | 3:CE:43:PHE:HE2   | 72.05                    | 0.68              |
| 1:AI:74:THR:HG21  | 3:CJ:43:PHE:HE2   | 72.05                    | 0.68              |
| 3:CQ:1:ALA:HB2    | 3:CS:21:ASN:OD1   | 1.93                     | 0.68              |
| 1:AR:74:THR:HG21  | 3:CS:43:PHE:HE2   | 1.57                     | 0.68              |
| 1:AY:92:THR:HG22  | 1:AY:93:THR:H     | 1.57                     | 0.68              |
| 3:CS:1:ALA:HB2    | 3:CT:21:ASN:OD1   | 1.93                     | 0.68              |
| 1:AQ:87:GLN:HE21  | 1:AQ:210:ARG:HH22 | 1.39                     | 0.68              |
| 2:BA:82:PRO:HA    | 2:BA:193:THR:HB   | 1.75                     | 0.68              |
| 1:AA:150:ARG:HE   | 1:AA:150:ARG:H    | 1.40                     | 0.68              |
| 1:AB:150:ARG:H    | 1:AB:150:ARG:HE   | 1.40                     | 0.68              |
| 1:AV:150:ARG:H    | 1:AV:150:ARG:HE   | 1.40                     | 0.68              |
| 1:AQ:150:ARG:HE   | 1:AQ:150:ARG:H    | 1.40                     | 0.68              |
| 1:AN:74:THR:HG21  | 3:CO:43:PHE:HE2   | 5.35                     | 0.68              |
| 1:AX:87:GLN:HE21  | 1:AX:210:ARG:HH22 | 1.39                     | 0.68              |
| 1:AD:145:LYS:HE3  | 1:AG:152:GLN:NE2  | 171.41                   | 0.68              |
| 1:AJ:152:GLN:NE2  | 1:AK:145:LYS:HE3  | 2.08                     | 0.68              |
| 1:AH:145:LYS:HE3  | 1:DK:152:GLN:NE2  | 2.09                     | 0.68              |
| 1:AF:152:GLN:NE2  | 1:AG:145:LYS:HE3  | 2.09                     | 0.68              |
| 3:CQ:43:PHE:HE2   | 1:DC:74:THR:HG21  | 219.52                   | 0.68              |
| 3:CF:21:ASN:OD1   | 3:CG:1:ALA:HB2    | 16.87                    | 0.68              |
| 3:CG:21:ASN:OD1   | 3:CH:1:ALA:HB2    | 1.93                     | 0.68              |
| 3:CK:21:ASN:OD1   | 3:CO:1:ALA:HB2    | 1.93                     | 0.68              |
| 1:A4:92:THR:HG22  | 1:A4:93:THR:H     | 1.57                     | 0.68              |
| 1:DH:110:GLY:H    | 1:DJ:242:ASN:HD22 | 1.38                     | 0.68              |
| 3:CZ:1:ALA:HB2    | 3:C1:21:ASN:OD1   | 1.93                     | 0.68              |
| 1:A9:74:THR:HG21  | 3:DA:43:PHE:HE1   | 1.57                     | 0.68              |
| 3:CK:1:ALA:HB2    | 3:CM:21:ASN:OD1   | 1.93                     | 0.68              |
| 2:BF:82:PRO:HA    | 2:BF:193:THR:HB   | 1.75                     | 0.68              |
| 3:C4:1:ALA:HB2    | 3:C6:21:ASN:OD1   | 1.93                     | 0.68              |
| 1:AJ:242:ASN:HD22 | 1:AM:110:GLY:H    | 69.12                    | 0.68              |
| 1:AF:145:LYS:HE3  | 1:AH:152:GLN:NE2  | 14.85                    | 0.68              |
| 1:AC:145:LYS:HE3  | 1:A9:152:GLN:NE2  | 284.57                   | 0.68              |
| 1:A5:145:LYS:HE3  | 1:A7:152:GLN:NE2  | 2.09                     | 0.68              |
| 3:CJ:43:PHE:HE1   | 1:DK:74:THR:HG21  | 1.57                     | 0.68              |
| 3:CM:1:ALA:HB2    | 3:CN:21:ASN:OD1   | 27.30                    | 0.68              |
| 3:CT:21:ASN:OD1   | 3:CX:1:ALA:HB2    | 234.03                   | 0.68              |
| 1:AQ:152:GLN:NE2  | 1:AR:145:LYS:HE3  | 2.09                     | 0.68              |
| 2:B7:82:PRO:HA    | 2:B7:193:THR:HB   | 1.75                     | 0.68              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:DC:92:THR:HG22 | 1:DC:93:THR:H     | 1.57                     | 0.68              |
| 3:C0:21:ASN:OD1  | 3:C1:1:ALA:HB2    | 1.93                     | 0.68              |
| 1:DG:92:THR:HG22 | 1:DG:93:THR:H     | 1.57                     | 0.68              |
| 2:BK:82:PRO:HA   | 2:BK:193:THR:HB   | 1.75                     | 0.68              |
| 1:AW:150:ARG:HE  | 1:AW:150:ARG:H    | 1.40                     | 0.68              |
| 1:DH:92:THR:HG22 | 1:DH:93:THR:H     | 1.57                     | 0.68              |
| 1:AX:74:THR:HG21 | 3:CY:43:PHE:HE2   | 1.57                     | 0.68              |
| 1:A3:92:THR:HG22 | 1:A3:93:THR:H     | 1.57                     | 0.68              |
| 1:AI:145:LYS:HE3 | 1:AL:152:GLN:NE2  | 170.22                   | 0.68              |
| 1:A3:152:GLN:NE2 | 1:A4:145:LYS:HE3  | 2.09                     | 0.68              |
| 1:AB:74:THR:HG21 | 3:CC:43:PHE:HE2   | 72.79                    | 0.68              |
| 1:DC:145:LYS:HE3 | 1:DE:152:GLN:NE2  | 2.09                     | 0.68              |
| 3:CE:1:ALA:HB2   | 3:CG:21:ASN:OD1   | 155.17                   | 0.68              |
| 3:CK:21:ASN:OD1  | 3:CL:1:ALA:HB2    | 16.87                    | 0.68              |
| 3:CU:21:ASN:OD1  | 3:CV:1:ALA:HB2    | 16.87                    | 0.68              |
| 3:CI:1:ALA:HB2   | 3:CJ:21:ASN:OD1   | 1.93                     | 0.68              |
| 1:AQ:74:THR:HG21 | 3:CR:43:PHE:HE1   | 1.57                     | 0.68              |
| 1:AS:74:THR:HG21 | 3:CT:43:PHE:HE2   | 1.57                     | 0.68              |
| 3:CT:43:PHE:HE2  | 1:DF:74:THR:HG21  | 259.79                   | 0.68              |
| 1:A8:92:THR:HG22 | 1:A8:93:THR:H     | 1.57                     | 0.68              |
| 3:C9:1:ALA:HB2   | 3:DB:21:ASN:OD1   | 1.93                     | 0.68              |
| 1:AD:87:GLN:HE21 | 1:AD:210:ARG:HH22 | 1.39                     | 0.68              |
| 1:AG:152:GLN:NE2 | 1:DK:145:LYS:HE3  | 2.09                     | 0.68              |
| 1:AL:152:GLN:NE2 | 1:AM:145:LYS:HE3  | 2.09                     | 0.68              |
| 1:AT:145:LYS:HE3 | 1:AW:152:GLN:NE2  | 2.09                     | 0.68              |
| 1:A3:145:LYS:HE3 | 1:A6:152:GLN:NE2  | 2.09                     | 0.68              |
| 1:AF:74:THR:HG21 | 3:CF:43:PHE:HE1   | 1.57                     | 0.68              |
| 1:DF:145:LYS:HE3 | 1:DI:152:GLN:NE2  | 2.09                     | 0.68              |
| 3:CH:1:ALA:HB2   | 3:CI:21:ASN:OD1   | 27.30                    | 0.68              |
| 2:BJ:82:PRO:HA   | 2:BJ:193:THR:HB   | 1.75                     | 0.68              |
| 1:A6:92:THR:HG22 | 1:A6:93:THR:H     | 1.57                     | 0.68              |
| 3:C7:1:ALA:HB2   | 3:C8:21:ASN:OD1   | 1.93                     | 0.68              |
| 3:CC:21:ASN:OD1  | 3:DA:1:ALA:HB2    | 241.07                   | 0.68              |
| 1:AY:150:ARG:HE  | 1:AY:150:ARG:H    | 1.39                     | 0.68              |
| 3:DA:21:ASN:OD1  | 3:DB:1:ALA:HB2    | 1.93                     | 0.68              |
| 1:AC:152:GLN:NE2 | 1:AD:145:LYS:HE3  | 2.09                     | 0.68              |
| 1:AF:145:LYS:HE3 | 1:AI:152:GLN:NE2  | 2.09                     | 0.68              |
| 1:AA:152:GLN:NE2 | 1:AB:145:LYS:HE3  | 2.09                     | 0.68              |
| 1:AO:152:GLN:NE2 | 1:AP:145:LYS:HE3  | 2.09                     | 0.68              |
| 1:DF:152:GLN:NE2 | 1:DG:145:LYS:HE3  | 2.09                     | 0.68              |
| 1:AX:92:THR:HG22 | 1:AX:93:THR:H     | 1.57                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:CP:1:ALA:HB2    | 3:CR:21:ASN:OD1   | 1.93                     | 0.68              |
| 2:BB:82:PRO:HA    | 2:BB:193:THR:HB   | 1.75                     | 0.68              |
| 2:BM:82:PRO:HA    | 2:BM:193:THR:HB   | 1.75                     | 0.68              |
| 1:AA:145:LYS:HE3  | 1:AC:152:GLN:NE2  | 14.85                    | 0.68              |
| 1:AV:152:GLN:NE2  | 1:AW:145:LYS:HE3  | 2.09                     | 0.68              |
| 1:A8:152:GLN:NE2  | 1:A9:145:LYS:HE3  | 2.09                     | 0.68              |
| 1:AC:145:LYS:HE3  | 1:AE:152:GLN:NE2  | 2.09                     | 0.68              |
| 1:A0:145:LYS:HE3  | 1:A2:152:GLN:NE2  | 2.09                     | 0.68              |
| 3:CJ:1:ALA:HB2    | 3:CL:21:ASN:OD1   | 145.06                   | 0.68              |
| 3:CP:21:ASN:OD1   | 3:CT:1:ALA:HB2    | 1.93                     | 0.68              |
| 2:BS:82:PRO:HA    | 2:BS:193:THR:HB   | 1.75                     | 0.68              |
| 2:BU:82:PRO:HA    | 2:BU:193:THR:HB   | 1.75                     | 0.68              |
| 2:BT:82:PRO:HA    | 2:BT:193:THR:HB   | 1.75                     | 0.68              |
| 1:A7:150:ARG:HE   | 1:A7:150:ARG:H    | 1.40                     | 0.68              |
| 2:BI:134:HIS:CD2  | 2:BI:145:LEU:HD13 | 2.26                     | 0.68              |
| 1:AK:242:ASN:HD22 | 1:AL:110:GLY:H    | 42.38                    | 0.68              |
| 1:AD:152:GLN:NE2  | 1:AE:145:LYS:HE3  | 22.15                    | 0.68              |
| 1:AJ:74:THR:HG21  | 3:CK:43:PHE:HE1   | 1.57                     | 0.68              |
| 1:AA:74:THR:HG21  | 3:CA:43:PHE:HE1   | 1.57                     | 0.68              |
| 1:AL:74:THR:HG21  | 3:CM:43:PHE:HE2   | 5.35                     | 0.68              |
| 3:CL:1:ALA:HB2    | 3:CN:21:ASN:OD1   | 1.93                     | 0.68              |
| 3:CO:1:ALA:HB2    | 3:CQ:21:ASN:OD1   | 257.08                   | 0.68              |
| 3:CP:21:ASN:OD1   | 3:CQ:1:ALA:HB2    | 16.87                    | 0.68              |
| 3:CV:1:ALA:HB2    | 3:CX:21:ASN:OD1   | 1.93                     | 0.68              |
| 3:CX:1:ALA:HB2    | 3:CY:21:ASN:OD1   | 1.93                     | 0.68              |
| 2:BI:82:PRO:HA    | 2:BI:193:THR:HB   | 1.75                     | 0.68              |
| 3:CB:1:ALA:HB2    | 3:CD:21:ASN:OD1   | 1.93                     | 0.68              |
| 1:AP:242:ASN:HD22 | 1:AS:110:GLY:H    | 1.38                     | 0.68              |
| 1:A7:92:THR:HG22  | 1:A7:93:THR:H     | 1.57                     | 0.68              |
| 1:AJ:92:THR:HG22  | 1:AJ:93:THR:H     | 1.57                     | 0.68              |
| 1:AU:150:ARG:HE   | 1:AU:150:ARG:H    | 1.40                     | 0.68              |
| 1:DD:150:ARG:HE   | 1:DD:150:ARG:H    | 1.40                     | 0.68              |
| 2:BC:82:PRO:HA    | 2:BC:193:THR:HB   | 1.75                     | 0.68              |
| 2:BQ:82:PRO:HA    | 2:BQ:193:THR:HB   | 1.75                     | 0.68              |
| 1:AB:152:GLN:NE2  | 1:A8:145:LYS:HE3  | 279.01                   | 0.68              |
| 1:AF:74:THR:HG21  | 3:CG:43:PHE:HE2   | 45.91                    | 0.68              |
| 1:AY:145:LYS:HE3  | 1:A1:152:GLN:NE2  | 2.09                     | 0.68              |
| 1:AT:74:THR:HG21  | 3:CU:43:PHE:HE2   | 1.57                     | 0.68              |
| 3:CF:21:ASN:OD1   | 3:CJ:1:ALA:HB2    | 1.93                     | 0.68              |
| 3:CD:1:ALA:HB2    | 3:CE:21:ASN:OD1   | 1.93                     | 0.68              |
| 1:AN:74:THR:HG21  | 3:CO:43:PHE:HE1   | 1.57                     | 0.68              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C5:1:ALA:HB2   | 3:C7:21:ASN:OD1   | 1.93                     | 0.68              |
| 1:DC:87:GLN:HE21 | 1:DC:210:ARG:HH22 | 1.39                     | 0.68              |
| 1:AR:92:THR:HG22 | 1:AR:93:THR:H     | 1.57                     | 0.68              |
| 1:AI:152:GLN:NE2 | 1:AJ:145:LYS:HE3  | 175.62                   | 0.68              |
| 1:AK:145:LYS:HE3 | 1:AM:152:GLN:NE2  | 14.85                    | 0.68              |
| 1:AO:152:GLN:NE2 | 1:DE:145:LYS:HE3  | 296.45                   | 0.68              |
| 1:A4:152:GLN:NE2 | 1:A7:145:LYS:HE3  | 2.09                     | 0.68              |
| 1:AO:74:THR:HG21 | 3:CP:43:PHE:HE1   | 1.57                     | 0.68              |
| 3:CL:21:ASN:OD1  | 3:CM:1:ALA:HB2    | 1.93                     | 0.68              |
| 3:CT:1:ALA:HB2   | 3:CV:21:ASN:OD1   | 248.02                   | 0.68              |
| 3:CV:21:ASN:OD1  | 3:CW:1:ALA:HB2    | 1.93                     | 0.68              |
| 3:CU:21:ASN:OD1  | 3:CY:1:ALA:HB2    | 1.93                     | 0.68              |
| 3:CB:21:ASN:OD1  | 3:CC:1:ALA:HB2    | 1.93                     | 0.68              |
| 2:BO:82:PRO:HA   | 2:BO:193:THR:HB   | 1.75                     | 0.68              |
| 3:C5:21:ASN:OD1  | 3:C6:1:ALA:HB2    | 1.93                     | 0.68              |
| 2:BP:82:PRO:HA   | 2:BP:193:THR:HB   | 1.75                     | 0.68              |
| 3:CF:1:ALA:HB2   | 3:CH:21:ASN:OD1   | 1.93                     | 0.68              |
| 2:BN:82:PRO:HA   | 2:BN:193:THR:HB   | 1.75                     | 0.68              |
| 1:AE:74:THR:HG21 | 3:CE:43:PHE:HE1   | 1.57                     | 0.67              |
| 1:AD:74:THR:HG21 | 3:CD:43:PHE:HE1   | 1.57                     | 0.67              |
| 3:CA:21:ASN:OD1  | 3:CE:1:ALA:HB2    | 1.93                     | 0.67              |
| 1:AV:145:LYS:HE3 | 1:AX:152:GLN:NE2  | 2.09                     | 0.67              |
| 3:CR:43:PHE:HE2  | 1:DD:74:THR:HG21  | 243.97                   | 0.67              |
| 2:B8:82:PRO:HA   | 2:B8:193:THR:HB   | 1.75                     | 0.67              |
| 2:BG:82:PRO:HA   | 2:BG:193:THR:HB   | 1.75                     | 0.67              |
| 1:A9:92:THR:HG22 | 1:A9:93:THR:H     | 1.57                     | 0.67              |
| 1:AP:87:GLN:HE21 | 1:AP:210:ARG:HH22 | 1.39                     | 0.67              |
| 3:C0:1:ALA:HB2   | 3:C2:21:ASN:OD1   | 1.93                     | 0.67              |
| 1:A6:150:ARG:HE  | 1:A6:150:ARG:H    | 1.40                     | 0.67              |
| 2:B1:82:PRO:HA   | 2:B1:193:THR:HB   | 1.75                     | 0.67              |
| 1:AB:152:GLN:NE2 | 1:AE:145:LYS:HE3  | 2.09                     | 0.67              |
| 1:DK:87:GLN:HE21 | 1:DK:210:ARG:HH22 | 1.39                     | 0.67              |
| 1:AZ:152:GLN:NE2 | 1:A2:145:LYS:HE3  | 2.09                     | 0.67              |
| 2:BX:82:PRO:HA   | 2:BX:193:THR:HB   | 1.75                     | 0.67              |
| 2:BV:82:PRO:HA   | 2:BV:193:THR:HB   | 1.75                     | 0.67              |
| 1:A1:150:ARG:H   | 1:A1:150:ARG:HE   | 1.40                     | 0.67              |
| 1:A5:150:ARG:H   | 1:A5:150:ARG:HE   | 1.40                     | 0.67              |
| 3:CW:1:ALA:HB2   | 3:CX:21:ASN:OD1   | 27.29                    | 0.67              |
| 3:CJ:21:ASN:OD1  | 3:CN:1:ALA:HB2    | 154.09                   | 0.67              |
| 3:CC:1:ALA:HB2   | 3:CD:21:ASN:OD1   | 27.30                    | 0.67              |
| 1:DC:152:GLN:NE2 | 1:DD:145:LYS:HE3  | 2.09                     | 0.67              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:AY:87:GLN:HE21 | 1:AY:210:ARG:HH22 | 1.39                     | 0.67              |
| 1:A8:74:THR:HG21 | 3:C9:43:PHE:HE2   | 1.57                     | 0.67              |
| 2:BH:82:PRO:HA   | 2:BH:193:THR:HB   | 1.75                     | 0.67              |
| 1:AK:152:GLN:NE2 | 1:AL:145:LYS:HE3  | 14.85                    | 0.67              |
| 1:AW:150:ARG:NE  | 1:AW:150:ARG:H    | 1.93                     | 0.67              |
| 1:A0:150:ARG:H   | 1:A0:150:ARG:HE   | 1.40                     | 0.67              |
| 1:AN:145:LYS:HE3 | 1:DD:152:GLN:NE2  | 299.49                   | 0.67              |
| 1:A9:150:ARG:NE  | 1:A9:150:ARG:H    | 1.93                     | 0.67              |
| 1:AG:150:ARG:H   | 1:AG:150:ARG:NE   | 1.93                     | 0.67              |
| 1:AI:74:THR:HG21 | 3:CI:43:PHE:HE1   | 1.57                     | 0.67              |
| 1:DH:145:LYS:HE3 | 1:DJ:152:GLN:NE2  | 2.09                     | 0.67              |
| 3:CE:21:ASN:OD1  | 3:CI:1:ALA:HB2    | 146.34                   | 0.67              |
| 3:CA:1:ALA:HB2   | 3:CC:21:ASN:OD1   | 1.93                     | 0.67              |
| 1:AT:152:GLN:NE2 | 1:AU:145:LYS:HE3  | 2.09                     | 0.67              |
| 2:B5:82:PRO:HA   | 2:B5:193:THR:HB   | 1.75                     | 0.67              |
| 2:BD:82:PRO:HA   | 2:BD:193:THR:HB   | 1.75                     | 0.67              |
| 1:AT:150:ARG:H   | 1:AT:150:ARG:HE   | 1.39                     | 0.67              |
| 1:AO:145:LYS:HE3 | 1:AR:152:GLN:NE2  | 2.09                     | 0.67              |
| 1:AE:150:ARG:NE  | 1:AE:150:ARG:H    | 1.93                     | 0.67              |
| 1:AH:150:ARG:NE  | 1:AH:150:ARG:H    | 1.93                     | 0.67              |
| 1:DG:152:GLN:NE2 | 1:DJ:145:LYS:HE3  | 2.09                     | 0.67              |
| 3:CD:1:ALA:HB2   | 3:C9:21:ASN:OD1   | 230.90                   | 0.67              |
| 1:AA:150:ARG:NE  | 1:AA:150:ARG:H    | 1.93                     | 0.67              |
| 1:AT:87:GLN:HE21 | 1:AT:210:ARG:HH22 | 1.39                     | 0.67              |
| 1:A4:150:ARG:NE  | 1:A4:150:ARG:H    | 1.93                     | 0.67              |
| 1:AL:145:LYS:HE3 | 1:AN:152:GLN:NE2  | 2.09                     | 0.67              |
| 1:AQ:145:LYS:HE3 | 1:AS:152:GLN:NE2  | 2.09                     | 0.67              |
| 1:AS:150:ARG:H   | 1:AS:150:ARG:NE   | 1.93                     | 0.67              |
| 1:AH:74:THR:HG21 | 3:CI:43:PHE:HE2   | 45.91                    | 0.67              |
| 1:DE:150:ARG:H   | 1:DE:150:ARG:NE   | 1.93                     | 0.67              |
| 1:AO:150:ARG:H   | 1:AO:150:ARG:NE   | 1.93                     | 0.67              |
| 1:A0:152:GLN:NE2 | 1:A1:145:LYS:HE3  | 2.09                     | 0.67              |
| 1:AK:150:ARG:H   | 1:AK:150:ARG:NE   | 1.93                     | 0.67              |
| 1:AN:150:ARG:H   | 1:AN:150:ARG:NE   | 1.93                     | 0.67              |
| 3:CR:1:ALA:HB2   | 3:CS:21:ASN:OD1   | 27.30                    | 0.67              |
| 1:AP:152:GLN:NE2 | 1:AS:145:LYS:HE3  | 2.09                     | 0.67              |
| 1:A1:150:ARG:H   | 1:A1:150:ARG:NE   | 1.93                     | 0.67              |
| 1:A5:150:ARG:NE  | 1:A5:150:ARG:H    | 1.93                     | 0.67              |
| 1:AY:152:GLN:NE2 | 1:AZ:145:LYS:HE3  | 2.09                     | 0.67              |
| 1:A8:150:ARG:HE  | 1:A8:150:ARG:H    | 1.40                     | 0.67              |
| 3:C4:21:ASN:OD1  | 3:C8:1:ALA:HB2    | 1.93                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A3:74:THR:HG21 | 3:C4:43:PHE:HE2  | 1.57                     | 0.67              |
| 1:AA:145:LYS:HE3 | 1:AD:152:GLN:NE2 | 2.09                     | 0.67              |
| 1:AJ:145:LYS:HE3 | 1:AM:152:GLN:NE2 | 2.09                     | 0.67              |
| 1:AK:152:GLN:NE2 | 1:AN:145:LYS:HE3 | 2.09                     | 0.67              |
| 1:AJ:150:ARG:H   | 1:AJ:150:ARG:NE  | 1.93                     | 0.67              |
| 1:DH:152:GLN:NE2 | 1:DI:145:LYS:HE3 | 2.09                     | 0.67              |
| 3:CO:21:ASN:OD1  | 3:CS:1:ALA:HB2   | 242.50                   | 0.67              |
| 1:A8:150:ARG:NE  | 1:A8:150:ARG:H   | 1.93                     | 0.67              |
| 1:A0:74:THR:HG21 | 3:C1:43:PHE:HE2  | 1.57                     | 0.67              |
| 3:C2:1:ALA:HB2   | 3:C3:21:ASN:OD1  | 1.93                     | 0.67              |
| 2:B3:82:PRO:HA   | 2:B3:193:THR:HB  | 1.75                     | 0.67              |
| 1:AH:152:GLN:NE2 | 1:AI:145:LYS:HE3 | 2.09                     | 0.67              |
| 1:A5:152:GLN:NE2 | 1:A6:145:LYS:HE3 | 2.09                     | 0.67              |
| 1:AF:150:ARG:NE  | 1:AF:150:ARG:H   | 1.93                     | 0.67              |
| 1:AL:150:ARG:NE  | 1:AL:150:ARG:H   | 1.93                     | 0.67              |
| 3:CN:1:ALA:HB2   | 3:CO:21:ASN:OD1  | 1.93                     | 0.67              |
| 1:AU:150:ARG:H   | 1:AU:150:ARG:NE  | 1.93                     | 0.67              |
| 1:AY:231:PRO:HG2 | 3:CZ:83:ALA:HB2  | 1.77                     | 0.67              |
| 2:B9:82:PRO:HA   | 2:B9:193:THR:HB  | 1.75                     | 0.67              |
| 1:AA:231:PRO:HG2 | 3:CA:83:ALA:HB2  | 1.77                     | 0.67              |
| 1:AY:83:GLU:HB2  | 1:AY:212:ARG:HB3 | 1.77                     | 0.67              |
| 1:AM:231:PRO:HG2 | 3:CN:83:ALA:HB2  | 1.77                     | 0.67              |
| 1:AU:152:GLN:NE2 | 1:AX:145:LYS:HE3 | 2.09                     | 0.67              |
| 1:DG:150:ARG:H   | 1:DG:150:ARG:NE  | 1.93                     | 0.67              |
| 1:A2:150:ARG:H   | 1:A2:150:ARG:NE  | 1.93                     | 0.67              |
| 1:DF:150:ARG:H   | 1:DF:150:ARG:NE  | 1.93                     | 0.67              |
| 1:AB:150:ARG:NE  | 1:AB:150:ARG:H   | 1.93                     | 0.67              |
| 1:A4:150:ARG:HE  | 1:A4:150:ARG:H   | 1.40                     | 0.67              |
| 1:AB:231:PRO:HG2 | 3:CB:83:ALA:HB2  | 1.77                     | 0.67              |
| 1:A4:231:PRO:HG2 | 3:C5:83:ALA:HB2  | 1.77                     | 0.67              |
| 1:AJ:231:PRO:HG2 | 3:CK:83:ALA:HB2  | 1.77                     | 0.67              |
| 1:AS:231:PRO:HG2 | 3:CT:83:ALA:HB2  | 1.77                     | 0.67              |
| 1:DE:83:GLU:HB2  | 1:DE:212:ARG:HB3 | 1.77                     | 0.67              |
| 1:DJ:83:GLU:HB2  | 1:DJ:212:ARG:HB3 | 1.77                     | 0.67              |
| 1:AI:150:ARG:NE  | 1:AI:150:ARG:H   | 1.93                     | 0.66              |
| 1:AE:231:PRO:HG2 | 3:CF:83:ALA:HB2  | 79.38                    | 0.66              |
| 1:AO:231:PRO:HG2 | 3:CP:83:ALA:HB2  | 1.77                     | 0.66              |
| 2:B4:82:PRO:HA   | 2:B4:193:THR:HB  | 1.75                     | 0.66              |
| 1:DC:83:GLU:HB2  | 1:DC:212:ARG:HB3 | 1.77                     | 0.66              |
| 1:AC:83:GLU:HB2  | 1:AC:212:ARG:HB3 | 1.77                     | 0.66              |
| 1:AD:83:GLU:HB2  | 1:AD:212:ARG:HB3 | 1.77                     | 0.66              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B6:82:PRO:HA   | 2:B6:193:THR:HB   | 1.75                     | 0.66              |
| 1:AN:231:PRO:HG2 | 3:CO:83:ALA:HB2   | 1.78                     | 0.66              |
| 1:AP:83:GLU:HB2  | 1:AP:212:ARG:HB3  | 1.77                     | 0.66              |
| 1:AE:152:GLN:NE2 | 1:AH:145:LYS:HE3  | 175.63                   | 0.66              |
| 1:AC:150:ARG:H   | 1:AC:150:ARG:NE   | 1.93                     | 0.66              |
| 1:AR:150:ARG:NE  | 1:AR:150:ARG:H    | 1.93                     | 0.66              |
| 1:DH:150:ARG:H   | 1:DH:150:ARG:NE   | 1.93                     | 0.66              |
| 1:AV:150:ARG:NE  | 1:AV:150:ARG:H    | 1.93                     | 0.66              |
| 1:A7:150:ARG:NE  | 1:A7:150:ARG:H    | 1.93                     | 0.66              |
| 1:A6:150:ARG:NE  | 1:A6:150:ARG:H    | 1.93                     | 0.66              |
| 1:AC:231:PRO:HG2 | 3:CD:83:ALA:HB2   | 63.97                    | 0.66              |
| 1:AD:231:PRO:HG2 | 3:CE:83:ALA:HB2   | 103.28                   | 0.66              |
| 1:AE:83:GLU:HB2  | 1:AE:212:ARG:HB3  | 1.77                     | 0.66              |
| 1:AV:231:PRO:HG2 | 3:CW:83:ALA:HB2   | 1.77                     | 0.66              |
| 1:DD:83:GLU:HB2  | 1:DD:212:ARG:HB3  | 1.77                     | 0.66              |
| 1:AY:150:ARG:H   | 1:AY:150:ARG:NE   | 1.93                     | 0.66              |
| 1:A1:231:PRO:HG2 | 3:C2:83:ALA:HB2   | 1.77                     | 0.66              |
| 1:A1:83:GLU:HB2  | 1:A1:212:ARG:HB3  | 1.77                     | 0.66              |
| 1:AU:231:PRO:HG2 | 3:CV:83:ALA:HB2   | 1.77                     | 0.66              |
| 1:A0:231:PRO:HG2 | 3:C1:83:ALA:HB2   | 1.77                     | 0.66              |
| 1:A3:231:PRO:HG2 | 3:C4:83:ALA:HB2   | 1.77                     | 0.66              |
| 3:CR:83:ALA:HB2  | 1:DD:231:PRO:HG2  | 282.38                   | 0.66              |
| 1:AM:150:ARG:H   | 1:AM:150:ARG:NE   | 1.93                     | 0.66              |
| 1:DD:150:ARG:NE  | 1:DD:150:ARG:H    | 1.93                     | 0.66              |
| 1:AG:231:PRO:HG2 | 3:CH:83:ALA:HB2   | 103.36                   | 0.66              |
| 1:AE:231:PRO:HG2 | 3:CE:83:ALA:HB2   | 1.77                     | 0.66              |
| 3:CV:83:ALA:HB2  | 1:DH:231:PRO:HG2  | 305.08                   | 0.66              |
| 1:AK:83:GLU:HB2  | 1:AK:212:ARG:HB3  | 1.77                     | 0.66              |
| 1:AA:83:GLU:HB2  | 1:AA:212:ARG:HB3  | 1.77                     | 0.66              |
| 1:AD:103:TRP:HB2 | 1:AD:198:THR:HG22 | 1.78                     | 0.66              |
| 1:AF:103:TRP:HB2 | 1:AF:198:THR:HG22 | 1.78                     | 0.66              |
| 2:B2:82:PRO:HA   | 2:B2:193:THR:HB   | 1.75                     | 0.66              |
| 1:DC:150:ARG:NE  | 1:DC:150:ARG:H    | 1.93                     | 0.66              |
| 1:AQ:150:ARG:H   | 1:AQ:150:ARG:NE   | 1.93                     | 0.66              |
| 1:AG:231:PRO:HG2 | 3:CG:83:ALA:HB2   | 1.77                     | 0.66              |
| 1:AJ:103:TRP:HB2 | 1:AJ:198:THR:HG22 | 1.78                     | 0.66              |
| 1:AQ:42:THR:HG21 | 1:AR:120:GLN:O    | 1.96                     | 0.66              |
| 1:AB:103:TRP:HB2 | 1:AB:198:THR:HG22 | 1.78                     | 0.66              |
| 2:BZ:82:PRO:HA   | 2:BZ:193:THR:HB   | 1.75                     | 0.66              |
| 1:AV:103:TRP:HB2 | 1:AV:198:THR:HG22 | 1.78                     | 0.66              |
| 1:AM:83:GLU:HB2  | 1:AM:212:ARG:HB3  | 1.77                     | 0.66              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A3:83:GLU:HB2  | 1:A3:212:ARG:HB3  | 1.77                     | 0.66              |
| 1:AN:83:GLU:HB2  | 1:AN:212:ARG:HB3  | 1.78                     | 0.66              |
| 1:A6:103:TRP:HB2 | 1:A6:198:THR:HG22 | 1.78                     | 0.66              |
| 1:AK:231:PRO:HG2 | 3:CL:83:ALA:HB2   | 1.78                     | 0.66              |
| 1:DG:83:GLU:HB2  | 1:DG:212:ARG:HB3  | 1.77                     | 0.66              |
| 1:A7:231:PRO:HG2 | 3:C8:83:ALA:HB2   | 1.77                     | 0.66              |
| 1:AB:83:GLU:HB2  | 1:AB:212:ARG:HB3  | 1.78                     | 0.66              |
| 1:A8:231:PRO:HG2 | 3:C9:83:ALA:HB2   | 1.78                     | 0.66              |
| 1:AL:83:GLU:HB2  | 1:AL:212:ARG:HB3  | 1.78                     | 0.66              |
| 1:A9:231:PRO:HG2 | 3:DA:83:ALA:HB2   | 1.77                     | 0.66              |
| 1:AN:152:GLN:NE2 | 1:AO:145:LYS:HE3  | 277.59                   | 0.66              |
| 1:AI:231:PRO:HG2 | 3:CJ:83:ALA:HB2   | 103.27                   | 0.66              |
| 1:DH:83:GLU:HB2  | 1:DH:212:ARG:HB3  | 1.78                     | 0.66              |
| 1:AB:42:THR:HG21 | 1:AE:120:GLN:O    | 1.96                     | 0.66              |
| 1:AF:120:GLN:O   | 1:AI:42:THR:HG21  | 1.96                     | 0.66              |
| 1:AK:42:THR:HG21 | 1:AL:120:GLN:O    | 35.08                    | 0.66              |
| 1:AP:103:TRP:HB2 | 1:AP:198:THR:HG22 | 1.78                     | 0.66              |
| 1:DK:103:TRP:HB2 | 1:DK:198:THR:HG22 | 1.78                     | 0.66              |
| 1:AO:83:GLU:HB2  | 1:AO:212:ARG:HB3  | 1.77                     | 0.66              |
| 3:CX:83:ALA:HB2  | 1:DJ:231:PRO:HG2  | 284.87                   | 0.66              |
| 1:A0:150:ARG:H   | 1:A0:150:ARG:NE   | 1.93                     | 0.66              |
| 1:AF:231:PRO:HG2 | 3:CF:83:ALA:HB2   | 1.77                     | 0.66              |
| 1:AD:231:PRO:HG2 | 3:CD:83:ALA:HB2   | 1.77                     | 0.66              |
| 3:CT:83:ALA:HB2  | 1:DF:231:PRO:HG2  | 283.18                   | 0.66              |
| 1:AC:120:GLN:O   | 1:AE:42:THR:HG21  | 1.96                     | 0.66              |
| 1:AT:103:TRP:HB2 | 1:AT:198:THR:HG22 | 1.78                     | 0.66              |
| 1:DC:42:THR:HG21 | 1:DD:120:GLN:O    | 1.96                     | 0.66              |
| 1:AZ:83:GLU:HB2  | 1:AZ:212:ARG:HB3  | 1.78                     | 0.66              |
| 1:AL:103:TRP:HB2 | 1:AL:198:THR:HG22 | 1.78                     | 0.66              |
| 1:AO:42:THR:HG21 | 1:AP:120:GLN:O    | 1.96                     | 0.66              |
| 1:A2:83:GLU:HB2  | 1:A2:212:ARG:HB3  | 1.77                     | 0.66              |
| 1:AZ:231:PRO:HG2 | 3:C0:83:ALA:HB2   | 1.77                     | 0.66              |
| 1:AM:103:TRP:HB2 | 1:AM:198:THR:HG22 | 1.78                     | 0.66              |
| 1:A5:103:TRP:HB2 | 1:A5:198:THR:HG22 | 1.78                     | 0.66              |
| 1:AI:83:GLU:HB2  | 1:AI:212:ARG:HB3  | 1.77                     | 0.66              |
| 1:DK:150:ARG:NE  | 1:DK:150:ARG:H    | 1.93                     | 0.66              |
| 1:AD:150:ARG:NE  | 1:AD:150:ARG:H    | 1.93                     | 0.66              |
| 1:DI:150:ARG:NE  | 1:DI:150:ARG:H    | 1.93                     | 0.66              |
| 1:AZ:150:ARG:H   | 1:AZ:150:ARG:NE   | 1.93                     | 0.66              |
| 1:AA:120:GLN:O   | 1:AD:42:THR:HG21  | 1.96                     | 0.66              |
| 1:AA:120:GLN:O   | 1:AC:42:THR:HG21  | 35.08                    | 0.66              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:AJ:120:GLN:O   | 1:AM:42:THR:HG21  | 1.96                     | 0.66              |
| 1:AK:42:THR:HG21 | 1:AN:120:GLN:O    | 1.96                     | 0.66              |
| 1:AO:42:THR:HG21 | 1:DE:120:GLN:O    | 309.94                   | 0.66              |
| 1:DK:83:GLU:HB2  | 1:DK:212:ARG:HB3  | 1.77                     | 0.66              |
| 1:A6:83:GLU:HB2  | 1:A6:212:ARG:HB3  | 1.77                     | 0.66              |
| 1:A8:103:TRP:HB2 | 1:A8:198:THR:HG22 | 1.78                     | 0.66              |
| 1:AU:103:TRP:HB2 | 1:AU:198:THR:HG22 | 1.78                     | 0.66              |
| 1:A0:120:GLN:O   | 1:A2:42:THR:HG21  | 1.96                     | 0.66              |
| 1:AS:83:GLU:HB2  | 1:AS:212:ARG:HB3  | 1.77                     | 0.66              |
| 3:CS:83:ALA:HB2  | 1:DE:231:PRO:HG2  | 305.10                   | 0.66              |
| 1:DJ:103:TRP:HB2 | 1:DJ:198:THR:HG22 | 1.78                     | 0.66              |
| 1:AT:42:THR:HG21 | 1:AU:120:GLN:O    | 1.96                     | 0.66              |
| 1:AX:103:TRP:HB2 | 1:AX:198:THR:HG22 | 1.78                     | 0.66              |
| 1:AY:103:TRP:HB2 | 1:AY:198:THR:HG22 | 1.78                     | 0.66              |
| 1:AZ:103:TRP:HB2 | 1:AZ:198:THR:HG22 | 1.78                     | 0.66              |
| 1:AT:150:ARG:H   | 1:AT:150:ARG:NE   | 1.93                     | 0.66              |
| 1:AF:231:PRO:HG2 | 3:CG:83:ALA:HB2   | 63.97                    | 0.66              |
| 1:AJ:42:THR:HG21 | 1:AK:120:GLN:O    | 1.96                     | 0.66              |
| 1:AH:120:GLN:O   | 1:DK:42:THR:HG21  | 1.96                     | 0.66              |
| 1:AK:103:TRP:HB2 | 1:AK:198:THR:HG22 | 1.78                     | 0.66              |
| 1:A8:42:THR:HG21 | 1:A9:120:GLN:O    | 1.96                     | 0.66              |
| 1:AH:83:GLU:HB2  | 1:AH:212:ARG:HB3  | 1.78                     | 0.66              |
| 1:A7:83:GLU:HB2  | 1:A7:212:ARG:HB3  | 1.77                     | 0.66              |
| 1:DC:103:TRP:HB2 | 1:DC:198:THR:HG22 | 1.78                     | 0.66              |
| 1:AP:150:ARG:NE  | 1:AP:150:ARG:H    | 1.93                     | 0.65              |
| 1:AC:231:PRO:HG2 | 3:CC:83:ALA:HB2   | 1.77                     | 0.65              |
| 1:AG:42:THR:HG21 | 1:DK:120:GLN:O    | 1.96                     | 0.65              |
| 1:AR:231:PRO:HG2 | 3:CS:83:ALA:HB2   | 1.77                     | 0.65              |
| 1:AU:83:GLU:HB2  | 1:AU:212:ARG:HB3  | 1.77                     | 0.65              |
| 1:A9:103:TRP:HB2 | 1:A9:198:THR:HG22 | 1.78                     | 0.65              |
| 1:DF:83:GLU:HB2  | 1:DF:212:ARG:HB3  | 1.77                     | 0.65              |
| 1:AN:42:THR:HG21 | 1:AO:120:GLN:O    | 260.70                   | 0.65              |
| 1:A5:42:THR:HG21 | 1:A6:120:GLN:O    | 1.96                     | 0.65              |
| 1:AC:103:TRP:HB2 | 1:AC:198:THR:HG22 | 1.78                     | 0.65              |
| 1:AT:120:GLN:O   | 1:AW:42:THR:HG21  | 1.96                     | 0.65              |
| 1:AG:103:TRP:HB2 | 1:AG:198:THR:HG22 | 1.78                     | 0.65              |
| 1:AV:42:THR:HG21 | 1:AW:120:GLN:O    | 1.96                     | 0.65              |
| 3:CU:83:ALA:HB2  | 1:DG:231:PRO:HG2  | 309.57                   | 0.65              |
| 1:DJ:150:ARG:H   | 1:DJ:150:ARG:NE   | 1.93                     | 0.65              |
| 1:AI:231:PRO:HG2 | 3:CI:83:ALA:HB2   | 1.77                     | 0.65              |
| 1:AL:120:GLN:O   | 1:AN:42:THR:HG21  | 1.96                     | 0.65              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:AE:42:THR:HG21 | 1:AH:120:GLN:O    | 173.33                   | 0.65              |
| 1:AI:103:TRP:HB2 | 1:AI:198:THR:HG22 | 1.78                     | 0.65              |
| 1:A0:103:TRP:HB2 | 1:A0:198:THR:HG22 | 1.78                     | 0.65              |
| 1:A5:231:PRO:HG2 | 3:C6:83:ALA:HB2   | 1.77                     | 0.65              |
| 3:CQ:83:ALA:HB2  | 1:DC:231:PRO:HG2  | 215.14                   | 0.65              |
| 1:A1:103:TRP:HB2 | 1:A1:198:THR:HG22 | 1.78                     | 0.65              |
| 1:AR:83:GLU:HB2  | 1:AR:212:ARG:HB3  | 1.77                     | 0.65              |
| 1:AW:103:TRP:HB2 | 1:AW:198:THR:HG22 | 1.78                     | 0.65              |
| 1:DD:103:TRP:HB2 | 1:DD:198:THR:HG22 | 1.78                     | 0.65              |
| 1:A2:231:PRO:HG2 | 3:C3:83:ALA:HB2   | 1.77                     | 0.65              |
| 1:AF:42:THR:HG21 | 1:AG:120:GLN:O    | 1.96                     | 0.65              |
| 1:AQ:120:GLN:O   | 1:AS:42:THR:HG21  | 1.96                     | 0.65              |
| 1:A4:42:THR:HG21 | 1:A7:120:GLN:O    | 1.96                     | 0.65              |
| 1:A9:83:GLU:HB2  | 1:A9:212:ARG:HB3  | 1.78                     | 0.65              |
| 1:AX:83:GLU:HB2  | 1:AX:212:ARG:HB3  | 1.77                     | 0.65              |
| 1:AH:103:TRP:HB2 | 1:AH:198:THR:HG22 | 1.78                     | 0.65              |
| 1:AB:231:PRO:HG2 | 3:CC:83:ALA:HB2   | 103.36                   | 0.65              |
| 1:AB:42:THR:HG21 | 1:A8:120:GLN:O    | 269.04                   | 0.65              |
| 1:AC:42:THR:HG21 | 1:AD:120:GLN:O    | 1.96                     | 0.65              |
| 1:AH:42:THR:HG21 | 1:AI:120:GLN:O    | 1.96                     | 0.65              |
| 1:AL:42:THR:HG21 | 1:AM:120:GLN:O    | 1.96                     | 0.65              |
| 1:AC:120:GLN:O   | 1:A9:42:THR:HG21  | 278.91                   | 0.65              |
| 1:AY:120:GLN:O   | 1:A1:42:THR:HG21  | 1.96                     | 0.65              |
| 1:AA:103:TRP:HB2 | 1:AA:198:THR:HG22 | 1.78                     | 0.65              |
| 1:A3:150:ARG:NE  | 1:A3:150:ARG:H    | 1.93                     | 0.65              |
| 1:AW:231:PRO:HG2 | 3:CX:83:ALA:HB2   | 1.77                     | 0.65              |
| 1:A0:83:GLU:HB2  | 1:A0:212:ARG:HB3  | 1.77                     | 0.65              |
| 1:AU:42:THR:HG21 | 1:AX:120:GLN:O    | 1.96                     | 0.65              |
| 1:AP:42:THR:HG21 | 1:AS:120:GLN:O    | 1.96                     | 0.65              |
| 1:AA:42:THR:HG21 | 1:AB:120:GLN:O    | 1.96                     | 0.65              |
| 1:AH:231:PRO:HG2 | 3:CI:83:ALA:HB2   | 63.97                    | 0.65              |
| 1:AT:231:PRO:HG2 | 3:CU:83:ALA:HB2   | 1.77                     | 0.65              |
| 1:AP:231:PRO:HG2 | 3:CQ:83:ALA:HB2   | 1.77                     | 0.65              |
| 1:AG:83:GLU:HB2  | 1:AG:212:ARG:HB3  | 1.77                     | 0.65              |
| 1:DG:103:TRP:HB2 | 1:DG:198:THR:HG22 | 1.78                     | 0.65              |
| 1:A3:103:TRP:HB2 | 1:A3:198:THR:HG22 | 1.78                     | 0.65              |
| 1:AT:83:GLU:HB2  | 1:AT:212:ARG:HB3  | 1.77                     | 0.65              |
| 1:AO:103:TRP:HB2 | 1:AO:198:THR:HG22 | 1.78                     | 0.65              |
| 1:AQ:83:GLU:HB2  | 1:AQ:212:ARG:HB3  | 1.78                     | 0.65              |
| 1:AD:120:GLN:O   | 1:AG:42:THR:HG21  | 162.07                   | 0.65              |
| 1:AJ:42:THR:HG21 | 1:AM:120:GLN:O    | 53.76                    | 0.65              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:DC:120:GLN:O   | 1:DE:42:THR:HG21  | 1.96                     | 0.65              |
| 1:AR:103:TRP:HB2 | 1:AR:198:THR:HG22 | 1.78                     | 0.65              |
| 1:DH:103:TRP:HB2 | 1:DH:198:THR:HG22 | 1.78                     | 0.65              |
| 1:A6:231:PRO:HG2 | 3:C7:83:ALA:HB2   | 1.77                     | 0.65              |
| 1:AX:231:PRO:HG2 | 3:CY:83:ALA:HB2   | 1.77                     | 0.65              |
| 1:AX:150:ARG:NE  | 1:AX:150:ARG:H    | 1.93                     | 0.65              |
| 2:BY:132:TYR:HB3 | 2:BY:193:THR:HG21 | 1.79                     | 0.65              |
| 2:B7:132:TYR:HB3 | 2:B7:193:THR:HG21 | 1.79                     | 0.65              |
| 1:AH:231:PRO:HG2 | 3:CH:83:ALA:HB2   | 1.77                     | 0.65              |
| 1:AI:42:THR:HG21 | 1:AJ:120:GLN:O    | 173.32                   | 0.65              |
| 1:DF:103:TRP:HB2 | 1:DF:198:THR:HG22 | 1.78                     | 0.65              |
| 1:AV:83:GLU:HB2  | 1:AV:212:ARG:HB3  | 1.77                     | 0.65              |
| 1:DI:83:GLU:HB2  | 1:DI:212:ARG:HB3  | 1.77                     | 0.65              |
| 1:A8:83:GLU:HB2  | 1:A8:212:ARG:HB3  | 1.77                     | 0.65              |
| 1:DH:42:THR:HG21 | 1:DI:120:GLN:O    | 1.96                     | 0.65              |
| 1:AL:231:PRO:HG2 | 3:CM:83:ALA:HB2   | 1.77                     | 0.65              |
| 1:A3:120:GLN:O   | 1:A6:42:THR:HG21  | 1.96                     | 0.65              |
| 1:AJ:83:GLU:HB2  | 1:AJ:212:ARG:HB3  | 1.77                     | 0.65              |
| 1:AA:231:PRO:HG2 | 3:DB:83:ALA:HB2   | 289.04                   | 0.65              |
| 1:AY:42:THR:HG21 | 1:AZ:120:GLN:O    | 1.96                     | 0.65              |
| 1:DI:103:TRP:HB2 | 1:DI:198:THR:HG22 | 1.78                     | 0.65              |
| 1:DH:120:GLN:O   | 1:DJ:42:THR:HG21  | 1.96                     | 0.65              |
| 1:AN:103:TRP:HB2 | 1:AN:198:THR:HG22 | 1.78                     | 0.65              |
| 1:A5:120:GLN:O   | 1:A7:42:THR:HG21  | 1.96                     | 0.65              |
| 2:BW:132:TYR:HB3 | 2:BW:193:THR:HG21 | 1.79                     | 0.64              |
| 2:BF:132:TYR:HB3 | 2:BF:193:THR:HG21 | 1.79                     | 0.64              |
| 1:AQ:231:PRO:HG2 | 3:CR:83:ALA:HB2   | 1.77                     | 0.64              |
| 1:AO:120:GLN:O   | 1:AR:42:THR:HG21  | 1.96                     | 0.64              |
| 1:DF:42:THR:HG21 | 1:DG:120:GLN:O    | 1.96                     | 0.64              |
| 2:B0:132:TYR:HB3 | 2:B0:193:THR:HG21 | 1.80                     | 0.64              |
| 2:BA:132:TYR:HB3 | 2:BA:193:THR:HG21 | 1.79                     | 0.64              |
| 1:AD:42:THR:HG21 | 1:AE:120:GLN:O    | 54.90                    | 0.64              |
| 1:AK:120:GLN:O   | 1:AM:42:THR:HG21  | 35.08                    | 0.64              |
| 1:AF:83:GLU:HB2  | 1:AF:212:ARG:HB3  | 1.77                     | 0.64              |
| 1:A5:83:GLU:HB2  | 1:A5:212:ARG:HB3  | 1.78                     | 0.64              |
| 1:AS:103:TRP:HB2 | 1:AS:198:THR:HG22 | 1.78                     | 0.64              |
| 1:DG:42:THR:HG21 | 1:DJ:120:GLN:O    | 1.96                     | 0.64              |
| 2:BL:132:TYR:HB3 | 2:BL:193:THR:HG21 | 1.79                     | 0.64              |
| 2:B6:132:TYR:HB3 | 2:B6:193:THR:HG21 | 1.79                     | 0.64              |
| 1:A0:42:THR:HG21 | 1:A1:120:GLN:O    | 1.96                     | 0.64              |
| 1:DF:120:GLN:O   | 1:DI:42:THR:HG21  | 1.96                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AE:103:TRP:HB2  | 1:AE:198:THR:HG22 | 1.78                     | 0.64              |
| 2:BE:132:TYR:HB3  | 2:BE:193:THR:HG21 | 1.79                     | 0.64              |
| 2:BS:132:TYR:HB3  | 2:BS:193:THR:HG21 | 1.79                     | 0.64              |
| 3:CJ:83:ALA:HB2   | 1:DK:231:PRO:HG2  | 1.77                     | 0.64              |
| 2:BZ:132:TYR:HB3  | 2:BZ:193:THR:HG21 | 1.79                     | 0.64              |
| 1:AN:120:GLN:O    | 1:DD:42:THR:HG21  | 316.31                   | 0.64              |
| 1:A7:103:TRP:HB2  | 1:A7:198:THR:HG22 | 1.78                     | 0.64              |
| 1:AV:120:GLN:O    | 1:AX:42:THR:HG21  | 1.96                     | 0.64              |
| 1:A4:103:TRP:HB2  | 1:A4:198:THR:HG22 | 1.78                     | 0.64              |
| 1:AQ:103:TRP:HB2  | 1:AQ:198:THR:HG22 | 1.78                     | 0.64              |
| 2:BU:132:TYR:HB3  | 2:BU:193:THR:HG21 | 1.79                     | 0.64              |
| 2:BT:132:TYR:HB3  | 2:BT:193:THR:HG21 | 1.80                     | 0.64              |
| 1:DE:103:TRP:HB2  | 1:DE:198:THR:HG22 | 1.78                     | 0.64              |
| 1:AC:243:ILE:HG23 | 1:AD:188:PRO:CB   | 2.28                     | 0.64              |
| 1:AH:243:ILE:HG23 | 1:AI:188:PRO:CB   | 2.28                     | 0.64              |
| 2:BR:132:TYR:HB3  | 2:BR:193:THR:HG21 | 1.79                     | 0.64              |
| 2:BK:132:TYR:HB3  | 2:BK:193:THR:HG21 | 1.79                     | 0.64              |
| 2:BI:132:TYR:HB3  | 2:BI:193:THR:HG21 | 1.79                     | 0.64              |
| 1:AI:120:GLN:O    | 1:AL:42:THR:HG21  | 161.01                   | 0.64              |
| 1:A3:42:THR:HG21  | 1:A4:120:GLN:O    | 1.96                     | 0.64              |
| 1:AK:243:ILE:HG23 | 1:AN:188:PRO:CB   | 2.28                     | 0.64              |
| 3:CW:83:ALA:HB2   | 1:DI:231:PRO:HG2  | 215.13                   | 0.64              |
| 1:AC:188:PRO:CB   | 1:A9:243:ILE:HG23 | 282.16                   | 0.64              |
| 1:AA:188:PRO:CB   | 1:AD:243:ILE:HG23 | 2.28                     | 0.64              |
| 1:AB:243:ILE:HG23 | 1:AE:188:PRO:CB   | 2.28                     | 0.64              |
| 1:AI:243:ILE:HG23 | 1:AJ:188:PRO:CB   | 174.70                   | 0.64              |
| 1:AK:243:ILE:HG23 | 1:AL:188:PRO:CB   | 52.77                    | 0.64              |
| 1:AU:243:ILE:HG23 | 1:AX:188:PRO:CB   | 2.28                     | 0.64              |
| 1:AV:243:ILE:HG23 | 1:AW:188:PRO:CB   | 2.28                     | 0.64              |
| 2:BM:132:TYR:HB3  | 2:BM:193:THR:HG21 | 1.79                     | 0.64              |
| 2:BP:132:TYR:HB3  | 2:BP:193:THR:HG21 | 1.79                     | 0.64              |
| 1:AF:120:GLN:O    | 1:AH:42:THR:HG21  | 35.08                    | 0.64              |
| 1:A2:103:TRP:HB2  | 1:A2:198:THR:HG22 | 1.78                     | 0.64              |
| 1:AZ:42:THR:HG21  | 1:A2:120:GLN:O    | 1.96                     | 0.64              |
| 2:BA:226:LEU:HD23 | 3:CD:126:PRO:HG2  | 1.80                     | 0.64              |
| 1:A4:83:GLU:HB2   | 1:A4:212:ARG:HB3  | 1.78                     | 0.64              |
| 1:AC:188:PRO:CB   | 1:AE:243:ILE:HG23 | 2.28                     | 0.64              |
| 1:AT:188:PRO:CB   | 1:AW:243:ILE:HG23 | 2.28                     | 0.64              |
| 1:AZ:243:ILE:HG23 | 1:A2:188:PRO:CB   | 2.28                     | 0.64              |
| 1:AA:243:ILE:HG23 | 1:AB:188:PRO:CB   | 2.28                     | 0.64              |
| 2:BV:132:TYR:HB3  | 2:BV:193:THR:HG21 | 1.79                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BW:149:ALA:HA   | 2:BW:152:TYR:CE2  | 2.33                     | 0.64              |
| 2:BO:149:ALA:HA   | 2:BO:152:TYR:CE2  | 2.33                     | 0.64              |
| 2:BV:114:VAL:HG22 | 2:BV:209:VAL:CG1  | 2.28                     | 0.64              |
| 2:BC:149:ALA:HA   | 2:BC:152:TYR:CE2  | 2.33                     | 0.64              |
| 1:DH:188:PRO:CB   | 1:DJ:243:ILE:HG23 | 2.28                     | 0.64              |
| 2:BQ:132:TYR:HB3  | 2:BQ:193:THR:HG21 | 1.79                     | 0.64              |
| 2:B3:132:TYR:HB3  | 2:B3:193:THR:HG21 | 1.79                     | 0.64              |
| 2:BD:149:ALA:HA   | 2:BD:152:TYR:CE2  | 2.33                     | 0.64              |
| 2:BN:149:ALA:HA   | 2:BN:152:TYR:CE2  | 2.33                     | 0.64              |
| 2:B4:149:ALA:HA   | 2:B4:152:TYR:CE2  | 2.33                     | 0.64              |
| 1:AW:83:GLU:HB2   | 1:AW:212:ARG:HB3  | 1.77                     | 0.64              |
| 2:B5:149:ALA:HA   | 2:B5:152:TYR:CE2  | 2.33                     | 0.64              |
| 2:BI:149:ALA:HA   | 2:BI:152:TYR:CE2  | 2.33                     | 0.64              |
| 2:BN:114:VAL:HG22 | 2:BN:209:VAL:CG1  | 2.29                     | 0.64              |
| 2:B9:149:ALA:HA   | 2:B9:152:TYR:CE2  | 2.33                     | 0.64              |
| 2:BT:149:ALA:HA   | 2:BT:152:TYR:CE2  | 2.33                     | 0.64              |
| 1:AE:243:ILE:HG23 | 1:AH:188:PRO:CB   | 174.70                   | 0.63              |
| 1:AG:243:ILE:HG23 | 1:DK:188:PRO:CB   | 2.28                     | 0.63              |
| 1:AL:188:PRO:CB   | 1:AN:243:ILE:HG23 | 2.28                     | 0.63              |
| 1:DH:243:ILE:HG23 | 1:DI:188:PRO:CB   | 2.28                     | 0.63              |
| 1:AV:188:PRO:CB   | 1:AX:243:ILE:HG23 | 2.28                     | 0.63              |
| 2:BC:132:TYR:HB3  | 2:BC:193:THR:HG21 | 1.79                     | 0.63              |
| 2:BO:132:TYR:HB3  | 2:BO:193:THR:HG21 | 1.79                     | 0.63              |
| 2:BX:132:TYR:HB3  | 2:BX:193:THR:HG21 | 1.79                     | 0.63              |
| 2:BD:132:TYR:HB3  | 2:BD:193:THR:HG21 | 1.79                     | 0.63              |
| 2:B4:132:TYR:HB3  | 2:B4:193:THR:HG21 | 1.80                     | 0.63              |
| 2:BG:114:VAL:HG22 | 2:BG:209:VAL:CG1  | 2.29                     | 0.63              |
| 2:BC:114:VAL:HG22 | 2:BC:209:VAL:CG1  | 2.28                     | 0.63              |
| 2:BU:226:LEU:HD23 | 3:CX:126:PRO:HG2  | 1.80                     | 0.63              |
| 2:BJ:226:LEU:HD23 | 3:CG:126:PRO:HG2  | 1.80                     | 0.63              |
| 2:BF:149:ALA:HA   | 2:BF:152:TYR:CE2  | 2.33                     | 0.63              |
| 2:BB:114:VAL:HG22 | 2:BB:209:VAL:CG1  | 2.28                     | 0.63              |
| 2:BH:149:ALA:HA   | 2:BH:152:TYR:CE2  | 2.33                     | 0.63              |
| 2:BA:149:ALA:HA   | 2:BA:152:TYR:CE2  | 2.33                     | 0.63              |
| 2:BS:149:ALA:HA   | 2:BS:152:TYR:CE2  | 2.33                     | 0.63              |
| 2:BE:114:VAL:HG22 | 2:BE:209:VAL:CG1  | 2.29                     | 0.63              |
| 2:BU:149:ALA:HA   | 2:BU:152:TYR:CE2  | 2.33                     | 0.63              |
| 2:BF:114:VAL:HG22 | 2:BF:209:VAL:CG1  | 2.29                     | 0.63              |
| 1:AA:188:PRO:CB   | 1:AC:243:ILE:HG23 | 52.77                    | 0.63              |
| 1:AI:188:PRO:CB   | 1:AL:243:ILE:HG23 | 143.23                   | 0.63              |
| 2:B5:132:TYR:HB3  | 2:B5:193:THR:HG21 | 1.79                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BK:226:LEU:HD23 | 3:CN:126:PRO:HG2  | 1.80                     | 0.63              |
| 2:BL:114:VAL:HG22 | 2:BL:209:VAL:CG1  | 2.28                     | 0.63              |
| 2:B8:114:VAL:HG22 | 2:B8:209:VAL:CG1  | 2.29                     | 0.63              |
| 2:B2:149:ALA:HA   | 2:B2:152:TYR:CE2  | 2.34                     | 0.63              |
| 2:BM:149:ALA:HA   | 2:BM:152:TYR:CE2  | 2.33                     | 0.63              |
| 2:BQ:149:ALA:HA   | 2:BQ:152:TYR:CE2  | 2.34                     | 0.63              |
| 2:BM:226:LEU:HD23 | 3:CK:126:PRO:HG2  | 115.39                   | 0.63              |
| 2:BN:226:LEU:HD23 | 3:CR:126:PRO:HG2  | 253.75                   | 0.63              |
| 2:BR:226:LEU:HD23 | 3:CP:126:PRO:HG2  | 252.65                   | 0.63              |
| 1:AO:243:ILE:HG23 | 1:DE:188:PRO:CB   | 283.40                   | 0.63              |
| 1:DF:188:PRO:CB   | 1:DI:243:ILE:HG23 | 2.28                     | 0.63              |
| 2:BN:132:TYR:HB3  | 2:BN:193:THR:HG21 | 1.79                     | 0.63              |
| 2:BG:132:TYR:HB3  | 2:BG:193:THR:HG21 | 1.79                     | 0.63              |
| 2:BH:132:TYR:HB3  | 2:BH:193:THR:HG21 | 1.79                     | 0.63              |
| 2:BW:226:LEU:HD23 | 3:CY:126:PRO:HG2  | 1.80                     | 0.63              |
| 2:B6:114:VAL:HG22 | 2:B6:209:VAL:CG1  | 2.29                     | 0.63              |
| 2:B5:226:LEU:HD23 | 3:C8:126:PRO:HG2  | 1.80                     | 0.63              |
| 2:BL:149:ALA:HA   | 2:BL:152:TYR:CE2  | 2.34                     | 0.63              |
| 2:BJ:114:VAL:HG22 | 2:BJ:209:VAL:CG1  | 2.29                     | 0.63              |
| 2:BS:114:VAL:HG22 | 2:BS:209:VAL:CG1  | 2.28                     | 0.63              |
| 2:BG:149:ALA:HA   | 2:BG:152:TYR:CE2  | 2.33                     | 0.63              |
| 2:B6:149:ALA:HA   | 2:B6:152:TYR:CE2  | 2.33                     | 0.63              |
| 2:BT:114:VAL:HG22 | 2:BT:209:VAL:CG1  | 2.29                     | 0.63              |
| 1:AJ:146:ILE:O    | 1:AJ:147:ALA:HB2  | 1.99                     | 0.63              |
| 2:BD:114:VAL:HG22 | 2:BD:209:VAL:CG1  | 2.29                     | 0.63              |
| 2:BW:114:VAL:HG22 | 2:BW:209:VAL:CG1  | 2.29                     | 0.63              |
| 2:BB:149:ALA:HA   | 2:BB:152:TYR:CE2  | 2.33                     | 0.63              |
| 2:B2:226:LEU:HD23 | 3:C1:126:PRO:HG2  | 1.80                     | 0.63              |
| 1:AD:188:PRO:CB   | 1:AG:243:ILE:HG23 | 200.83                   | 0.63              |
| 1:AF:188:PRO:CB   | 1:AI:243:ILE:HG23 | 2.28                     | 0.63              |
| 1:AJ:243:ILE:HG23 | 1:AK:188:PRO:CB   | 2.28                     | 0.63              |
| 1:AT:243:ILE:HG23 | 1:AU:188:PRO:CB   | 2.28                     | 0.63              |
| 1:AO:188:PRO:CB   | 1:AR:243:ILE:HG23 | 2.28                     | 0.63              |
| 2:BJ:132:TYR:HB3  | 2:BJ:193:THR:HG21 | 1.80                     | 0.63              |
| 2:B2:132:TYR:HB3  | 2:B2:193:THR:HG21 | 1.79                     | 0.63              |
| 2:BD:226:LEU:HD23 | 3:CH:126:PRO:HG2  | 182.27                   | 0.63              |
| 2:BS:226:LEU:HD23 | 3:CP:126:PRO:HG2  | 1.80                     | 0.63              |
| 1:A9:146:ILE:O    | 1:A9:147:ALA:HB2  | 1.99                     | 0.63              |
| 2:BH:114:VAL:HG22 | 2:BH:209:VAL:CG1  | 2.29                     | 0.63              |
| 1:AH:146:ILE:O    | 1:AH:147:ALA:HB2  | 1.99                     | 0.63              |
| 2:B9:114:VAL:HG22 | 2:B9:209:VAL:CG1  | 2.29                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BR:149:ALA:HA   | 2:BR:152:TYR:CE2  | 2.33                     | 0.63              |
| 1:DH:146:ILE:O    | 1:DH:147:ALA:HB2  | 1.99                     | 0.63              |
| 2:BZ:149:ALA:HA   | 2:BZ:152:TYR:CE2  | 2.33                     | 0.63              |
| 1:AF:188:PRO:CB   | 1:AH:243:ILE:HG23 | 52.77                    | 0.63              |
| 1:AJ:188:PRO:CB   | 1:AM:243:ILE:HG23 | 2.28                     | 0.63              |
| 1:A0:243:ILE:HG23 | 1:A1:188:PRO:CB   | 2.28                     | 0.63              |
| 1:A5:188:PRO:CB   | 1:A7:243:ILE:HG23 | 2.28                     | 0.63              |
| 2:B8:132:TYR:HB3  | 2:B8:193:THR:HG21 | 1.79                     | 0.63              |
| 2:BQ:226:LEU:HD23 | 3:CQ:126:PRO:HG2  | 115.40                   | 0.63              |
| 2:BK:149:ALA:HA   | 2:BK:152:TYR:CE2  | 2.33                     | 0.63              |
| 2:B7:226:LEU:HD23 | 3:C5:126:PRO:HG2  | 1.80                     | 0.63              |
| 2:BP:149:ALA:HA   | 2:BP:152:TYR:CE2  | 2.33                     | 0.63              |
| 2:BB:226:LEU:HD23 | 3:CA:126:PRO:HG2  | 1.80                     | 0.63              |
| 2:B3:149:ALA:HA   | 2:B3:152:TYR:CE2  | 2.34                     | 0.63              |
| 2:BC:226:LEU:HD23 | 3:CE:126:PRO:HG2  | 1.81                     | 0.63              |
| 1:A3:146:ILE:O    | 1:A3:147:ALA:HB2  | 1.99                     | 0.63              |
| 1:AN:146:ILE:O    | 1:AN:147:ALA:HB2  | 1.99                     | 0.63              |
| 1:AW:146:ILE:O    | 1:AW:147:ALA:HB2  | 1.99                     | 0.63              |
| 1:AF:243:ILE:HG23 | 1:AG:188:PRO:CB   | 2.28                     | 0.63              |
| 1:AJ:243:ILE:HG23 | 1:AM:188:PRO:CB   | 82.48                    | 0.63              |
| 1:A4:243:ILE:HG23 | 1:A7:188:PRO:CB   | 2.28                     | 0.63              |
| 1:AN:243:ILE:HG23 | 1:AO:188:PRO:CB   | 258.74                   | 0.63              |
| 1:A3:188:PRO:CB   | 1:A6:243:ILE:HG23 | 2.28                     | 0.63              |
| 2:BY:226:LEU:HD23 | 3:CV:126:PRO:HG2  | 1.80                     | 0.63              |
| 2:BV:149:ALA:HA   | 2:BV:152:TYR:CE2  | 2.33                     | 0.63              |
| 1:AF:146:ILE:O    | 1:AF:147:ALA:HB2  | 1.99                     | 0.63              |
| 1:AG:146:ILE:O    | 1:AG:147:ALA:HB2  | 1.99                     | 0.63              |
| 1:DE:146:ILE:O    | 1:DE:147:ALA:HB2  | 1.99                     | 0.63              |
| 1:DF:146:ILE:O    | 1:DF:147:ALA:HB2  | 1.99                     | 0.63              |
| 1:AL:146:ILE:O    | 1:AL:147:ALA:HB2  | 1.99                     | 0.63              |
| 2:B4:114:VAL:HG22 | 2:B4:209:VAL:CG1  | 2.29                     | 0.63              |
| 1:AE:146:ILE:O    | 1:AE:147:ALA:HB2  | 1.99                     | 0.63              |
| 2:BX:114:VAL:HG22 | 2:BX:209:VAL:CG1  | 2.29                     | 0.63              |
| 1:AB:243:ILE:HG23 | 1:A8:188:PRO:CB   | 213.94                   | 0.63              |
| 1:AK:188:PRO:CB   | 1:AM:243:ILE:HG23 | 52.77                    | 0.63              |
| 1:A5:243:ILE:HG23 | 1:A6:188:PRO:CB   | 2.28                     | 0.63              |
| 1:DF:243:ILE:HG23 | 1:DG:188:PRO:CB   | 2.28                     | 0.63              |
| 2:BX:226:LEU:HD23 | 3:C4:126:PRO:HG2  | 282.10                   | 0.63              |
| 2:BC:226:LEU:HD23 | 3:DA:126:PRO:HG2  | 277.00                   | 0.63              |
| 1:A4:146:ILE:O    | 1:A4:147:ALA:HB2  | 1.99                     | 0.63              |
| 2:BP:114:VAL:HG22 | 2:BP:209:VAL:CG1  | 2.29                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B3:114:VAL:HG22 | 2:B3:209:VAL:CG1  | 2.29                     | 0.63              |
| 2:BY:149:ALA:HA   | 2:BY:152:TYR:CE2  | 2.33                     | 0.63              |
| 1:AD:146:ILE:O    | 1:AD:147:ALA:HB2  | 1.99                     | 0.63              |
| 2:B1:114:VAL:HG22 | 2:B1:209:VAL:CG1  | 2.29                     | 0.63              |
| 1:A8:243:ILE:HG23 | 1:A9:188:PRO:CB   | 2.28                     | 0.63              |
| 2:BI:226:LEU:HD23 | 3:CM:126:PRO:HG2  | 126.33                   | 0.63              |
| 2:BN:226:LEU:HD23 | 3:CM:126:PRO:HG2  | 1.80                     | 0.63              |
| 2:BJ:149:ALA:HA   | 2:BJ:152:TYR:CE2  | 2.34                     | 0.63              |
| 1:AP:146:ILE:O    | 1:AP:147:ALA:HB2  | 1.99                     | 0.63              |
| 2:BE:149:ALA:HA   | 2:BE:152:TYR:CE2  | 2.34                     | 0.63              |
| 2:BU:114:VAL:HG22 | 2:BU:209:VAL:CG1  | 2.29                     | 0.63              |
| 1:AQ:146:ILE:O    | 1:AQ:147:ALA:HB2  | 1.99                     | 0.63              |
| 1:AT:146:ILE:O    | 1:AT:147:ALA:HB2  | 1.99                     | 0.63              |
| 2:BA:114:VAL:HG22 | 2:BA:209:VAL:CG1  | 2.29                     | 0.63              |
| 2:B7:149:ALA:HA   | 2:B7:152:TYR:CE2  | 2.34                     | 0.63              |
| 1:AI:146:ILE:O    | 1:AI:147:ALA:HB2  | 1.99                     | 0.63              |
| 2:B0:114:VAL:HG22 | 2:B0:209:VAL:CG1  | 2.29                     | 0.63              |
| 2:BX:149:ALA:HA   | 2:BX:152:TYR:CE2  | 2.34                     | 0.63              |
| 1:AC:146:ILE:O    | 1:AC:147:ALA:HB2  | 1.99                     | 0.63              |
| 1:AV:146:ILE:O    | 1:AV:147:ALA:HB2  | 1.99                     | 0.63              |
| 1:DI:146:ILE:O    | 1:DI:147:ALA:HB2  | 1.99                     | 0.63              |
| 2:BO:114:VAL:HG22 | 2:BO:209:VAL:CG1  | 2.29                     | 0.63              |
| 1:DG:243:ILE:HG23 | 1:DJ:188:PRO:CB   | 2.28                     | 0.63              |
| 1:DC:188:PRO:CB   | 1:DE:243:ILE:HG23 | 2.28                     | 0.63              |
| 1:AQ:188:PRO:CB   | 1:AS:243:ILE:HG23 | 2.28                     | 0.63              |
| 1:A3:243:ILE:HG23 | 1:A4:188:PRO:CB   | 2.28                     | 0.63              |
| 2:B1:132:TYR:HB3  | 2:B1:193:THR:HG21 | 1.80                     | 0.63              |
| 2:BM:226:LEU:HD23 | 3:CO:126:PRO:HG2  | 1.80                     | 0.63              |
| 2:BT:226:LEU:HD23 | 3:CT:126:PRO:HG2  | 69.91                    | 0.63              |
| 2:BV:226:LEU:HD23 | 3:CU:126:PRO:HG2  | 1.80                     | 0.63              |
| 2:BE:226:LEU:HD23 | 3:CB:126:PRO:HG2  | 1.80                     | 0.63              |
| 1:A6:146:ILE:O    | 1:A6:147:ALA:HB2  | 1.99                     | 0.63              |
| 1:A7:146:ILE:O    | 1:A7:147:ALA:HB2  | 1.99                     | 0.63              |
| 2:BK:114:VAL:HG22 | 2:BK:209:VAL:CG1  | 2.29                     | 0.63              |
| 2:BM:114:VAL:HG22 | 2:BM:209:VAL:CG1  | 2.28                     | 0.63              |
| 1:AU:146:ILE:O    | 1:AU:147:ALA:HB2  | 1.99                     | 0.63              |
| 1:AD:243:ILE:HG23 | 1:AE:188:PRO:CB   | 83.58                    | 0.62              |
| 1:AY:243:ILE:HG23 | 1:AZ:188:PRO:CB   | 2.28                     | 0.62              |
| 1:AZ:74:THR:O     | 1:AZ:74:THR:HG22  | 1.99                     | 0.62              |
| 1:A5:74:THR:O     | 1:A5:74:THR:HG22  | 2.00                     | 0.62              |
| 1:A6:74:THR:HG22  | 1:A6:74:THR:O     | 2.00                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AP:74:THR:HG22  | 1:AP:74:THR:O     | 1.99                     | 0.62              |
| 2:BB:132:TYR:HB3  | 2:BB:193:THR:HG21 | 1.80                     | 0.62              |
| 2:BI:226:LEU:HD23 | 3:CH:126:PRO:HG2  | 1.80                     | 0.62              |
| 1:AB:146:ILE:O    | 1:AB:147:ALA:HB2  | 1.99                     | 0.62              |
| 2:B0:149:ALA:HA   | 2:B0:152:TYR:CE2  | 2.33                     | 0.62              |
| 2:BI:114:VAL:HG22 | 2:BI:209:VAL:CG1  | 2.29                     | 0.62              |
| 1:AK:146:ILE:O    | 1:AK:147:ALA:HB2  | 1.99                     | 0.62              |
| 1:AM:146:ILE:O    | 1:AM:147:ALA:HB2  | 1.99                     | 0.62              |
| 1:AL:243:ILE:HG23 | 1:AM:188:PRO:CB   | 2.28                     | 0.62              |
| 1:AY:188:PRO:CB   | 1:A1:243:ILE:HG23 | 2.28                     | 0.62              |
| 1:AH:74:THR:HG22  | 1:AH:74:THR:O     | 2.00                     | 0.62              |
| 1:A4:74:THR:O     | 1:A4:74:THR:HG22  | 1.99                     | 0.62              |
| 2:B9:132:TYR:HB3  | 2:B9:193:THR:HG21 | 1.80                     | 0.62              |
| 2:B8:226:LEU:HD23 | 3:CC:126:PRO:HG2  | 252.65                   | 0.62              |
| 2:BX:226:LEU:HD23 | 3:CW:126:PRO:HG2  | 1.80                     | 0.62              |
| 2:BW:226:LEU:HD23 | 3:CU:126:PRO:HG2  | 115.39                   | 0.62              |
| 1:AX:146:ILE:O    | 1:AX:147:ALA:HB2  | 1.99                     | 0.62              |
| 2:B1:149:ALA:HA   | 2:B1:152:TYR:CE2  | 2.33                     | 0.62              |
| 1:AA:146:ILE:O    | 1:AA:147:ALA:HB2  | 1.99                     | 0.62              |
| 2:BF:226:LEU:HD23 | 3:CI:126:PRO:HG2  | 1.80                     | 0.62              |
| 1:AN:188:PRO:CB   | 1:DD:243:ILE:HG23 | 301.51                   | 0.62              |
| 1:AQ:243:ILE:HG23 | 1:AR:188:PRO:CB   | 2.28                     | 0.62              |
| 1:A0:188:PRO:CB   | 1:A2:243:ILE:HG23 | 2.28                     | 0.62              |
| 1:DC:243:ILE:HG23 | 1:DD:188:PRO:CB   | 2.28                     | 0.62              |
| 1:AJ:74:THR:O     | 1:AJ:74:THR:HG22  | 1.99                     | 0.62              |
| 1:AR:74:THR:O     | 1:AR:74:THR:HG22  | 1.99                     | 0.62              |
| 2:BO:226:LEU:HD23 | 3:CS:126:PRO:HG2  | 1.80                     | 0.62              |
| 2:BY:114:VAL:HG22 | 2:BY:209:VAL:CG1  | 2.29                     | 0.62              |
| 1:DC:146:ILE:O    | 1:DC:147:ALA:HB2  | 1.99                     | 0.62              |
| 2:B7:114:VAL:HG22 | 2:B7:209:VAL:CG1  | 2.29                     | 0.62              |
| 1:AS:146:ILE:O    | 1:AS:147:ALA:HB2  | 1.99                     | 0.62              |
| 2:BZ:226:LEU:HD23 | 3:C2:126:PRO:HG2  | 1.80                     | 0.62              |
| 1:AO:243:ILE:HG23 | 1:AP:188:PRO:CB   | 2.28                     | 0.62              |
| 1:AY:120:GLN:HG3  | 1:AY:129:ARG:HG2  | 1.82                     | 0.62              |
| 1:AS:120:GLN:HG3  | 1:AS:129:ARG:HG2  | 1.82                     | 0.62              |
| 2:BT:226:LEU:HD23 | 3:CQ:126:PRO:HG2  | 1.80                     | 0.62              |
| 2:BP:226:LEU:HD23 | 3:CS:126:PRO:HG2  | 114.52                   | 0.62              |
| 2:BQ:114:VAL:HG22 | 2:BQ:209:VAL:CG1  | 2.29                     | 0.62              |
| 2:BR:114:VAL:HG22 | 2:BR:209:VAL:CG1  | 2.29                     | 0.62              |
| 2:B6:226:LEU:HD23 | 3:C6:126:PRO:HG2  | 1.80                     | 0.62              |
| 2:B9:226:LEU:HD23 | 3:C9:126:PRO:HG2  | 1.80                     | 0.62              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A4:115:THR:HG23 | 1:A4:132:GLN:HB3 | 1.82                     | 0.62              |
| 1:AI:74:THR:O     | 1:AI:74:THR:HG22 | 2.00                     | 0.62              |
| 1:A3:74:THR:HG22  | 1:A3:74:THR:O    | 2.00                     | 0.62              |
| 1:AQ:120:GLN:HG3  | 1:AQ:129:ARG:HG2 | 1.82                     | 0.62              |
| 2:BH:226:LEU:HD23 | 3:CJ:126:PRO:HG2 | 1.80                     | 0.62              |
| 2:BP:226:LEU:HD23 | 3:CT:126:PRO:HG2 | 1.80                     | 0.62              |
| 2:BS:226:LEU:HD23 | 3:CW:126:PRO:HG2 | 292.81                   | 0.62              |
| 2:BB:226:LEU:HD23 | 3:DB:126:PRO:HG2 | 256.22                   | 0.62              |
| 1:DJ:146:ILE:O    | 1:DJ:147:ALA:HB2 | 1.99                     | 0.62              |
| 1:DK:146:ILE:O    | 1:DK:147:ALA:HB2 | 1.99                     | 0.62              |
| 1:DD:146:ILE:O    | 1:DD:147:ALA:HB2 | 1.99                     | 0.62              |
| 1:AR:146:ILE:O    | 1:AR:147:ALA:HB2 | 1.99                     | 0.62              |
| 1:AJ:115:THR:HG23 | 1:AJ:132:GLN:HB3 | 1.82                     | 0.62              |
| 1:DG:115:THR:HG23 | 1:DG:132:GLN:HB3 | 1.82                     | 0.62              |
| 1:AK:74:THR:O     | 1:AK:74:THR:HG22 | 1.99                     | 0.62              |
| 1:DH:74:THR:HG22  | 1:DH:74:THR:O    | 2.00                     | 0.62              |
| 1:DE:74:THR:O     | 1:DE:74:THR:HG22 | 1.99                     | 0.62              |
| 1:DF:74:THR:HG22  | 1:DF:74:THR:O    | 2.00                     | 0.62              |
| 1:A8:120:GLN:HG3  | 1:A8:129:ARG:HG2 | 1.82                     | 0.62              |
| 1:AL:120:GLN:HG3  | 1:AL:129:ARG:HG2 | 1.82                     | 0.62              |
| 1:AO:120:GLN:HG3  | 1:AO:129:ARG:HG2 | 1.82                     | 0.62              |
| 1:AH:120:GLN:HG3  | 1:AH:129:ARG:HG2 | 1.82                     | 0.62              |
| 1:A6:120:GLN:HG3  | 1:A6:129:ARG:HG2 | 1.82                     | 0.62              |
| 1:DC:120:GLN:HG3  | 1:DC:129:ARG:HG2 | 1.82                     | 0.62              |
| 2:B3:226:LEU:HD23 | 3:C0:126:PRO:HG2 | 1.80                     | 0.62              |
| 1:AY:146:ILE:O    | 1:AY:147:ALA:HB2 | 1.99                     | 0.62              |
| 2:B0:226:LEU:HD23 | 3:CZ:126:PRO:HG2 | 1.80                     | 0.62              |
| 2:B2:114:VAL:HG22 | 2:B2:209:VAL:CG1 | 2.29                     | 0.62              |
| 1:AK:115:THR:HG23 | 1:AK:132:GLN:HB3 | 1.82                     | 0.62              |
| 1:AT:115:THR:HG23 | 1:AT:132:GLN:HB3 | 1.82                     | 0.62              |
| 1:A1:115:THR:HG23 | 1:A1:132:GLN:HB3 | 1.82                     | 0.62              |
| 1:AK:120:GLN:HG3  | 1:AK:129:ARG:HG2 | 1.82                     | 0.62              |
| 1:A7:120:GLN:HG3  | 1:A7:129:ARG:HG2 | 1.82                     | 0.62              |
| 2:BL:226:LEU:HD23 | 3:CK:126:PRO:HG2 | 1.80                     | 0.62              |
| 2:BO:226:LEU:HD23 | 3:CO:126:PRO:HG2 | 243.86                   | 0.62              |
| 2:B5:114:VAL:HG22 | 2:B5:209:VAL:CG1 | 2.29                     | 0.62              |
| 2:B4:226:LEU:HD23 | 3:C7:126:PRO:HG2 | 1.80                     | 0.62              |
| 2:B1:226:LEU:HD23 | 3:C3:126:PRO:HG2 | 1.80                     | 0.62              |
| 1:DI:115:THR:HG23 | 1:DI:132:GLN:HB3 | 1.82                     | 0.62              |
| 1:A0:115:THR:HG23 | 1:A0:132:GLN:HB3 | 1.82                     | 0.62              |
| 1:A3:115:THR:HG23 | 1:A3:132:GLN:HB3 | 1.82                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:DD:115:THR:HG23 | 1:DD:132:GLN:HB3  | 1.82                     | 0.62              |
| 1:AH:188:PRO:CB   | 1:DK:243:ILE:HG23 | 2.28                     | 0.62              |
| 1:AP:243:ILE:HG23 | 1:AS:188:PRO:CB   | 2.28                     | 0.62              |
| 1:DJ:74:THR:HG22  | 1:DJ:74:THR:O     | 1.99                     | 0.62              |
| 1:AV:74:THR:O     | 1:AV:74:THR:HG22  | 2.00                     | 0.62              |
| 1:AC:120:GLN:HG3  | 1:AC:129:ARG:HG2  | 1.82                     | 0.62              |
| 1:DH:120:GLN:HG3  | 1:DH:129:ARG:HG2  | 1.82                     | 0.62              |
| 1:DJ:120:GLN:HG3  | 1:DJ:129:ARG:HG2  | 1.82                     | 0.62              |
| 2:BR:226:LEU:HD23 | 3:CL:126:PRO:HG2  | 1.80                     | 0.62              |
| 1:A0:146:ILE:O    | 1:A0:147:ALA:HB2  | 1.99                     | 0.62              |
| 2:B8:149:ALA:HA   | 2:B8:152:TYR:CE2  | 2.33                     | 0.62              |
| 1:A5:115:THR:HG23 | 1:A5:132:GLN:HB3  | 1.82                     | 0.62              |
| 1:DH:115:THR:HG23 | 1:DH:132:GLN:HB3  | 1.82                     | 0.62              |
| 1:AD:74:THR:O     | 1:AD:74:THR:HG22  | 1.99                     | 0.62              |
| 1:A7:74:THR:O     | 1:A7:74:THR:HG22  | 1.99                     | 0.62              |
| 1:AT:74:THR:HG22  | 1:AT:74:THR:O     | 2.00                     | 0.62              |
| 1:A0:74:THR:HG22  | 1:A0:74:THR:O     | 2.00                     | 0.62              |
| 1:AA:120:GLN:HG3  | 1:AA:129:ARG:HG2  | 1.82                     | 0.62              |
| 1:AD:120:GLN:HG3  | 1:AD:129:ARG:HG2  | 1.82                     | 0.62              |
| 1:AB:120:GLN:HG3  | 1:AB:129:ARG:HG2  | 1.82                     | 0.62              |
| 1:DG:120:GLN:HG3  | 1:DG:129:ARG:HG2  | 1.82                     | 0.62              |
| 2:BG:226:LEU:HD23 | 3:CF:126:PRO:HG2  | 1.80                     | 0.62              |
| 2:BQ:226:LEU:HD23 | 3:CR:126:PRO:HG2  | 1.80                     | 0.62              |
| 1:AO:146:ILE:O    | 1:AO:147:ALA:HB2  | 1.99                     | 0.62              |
| 1:AA:115:THR:HG23 | 1:AA:132:GLN:HB3  | 1.82                     | 0.62              |
| 1:A7:115:THR:HG23 | 1:A7:132:GLN:HB3  | 1.82                     | 0.62              |
| 1:AR:115:THR:HG23 | 1:AR:132:GLN:HB3  | 1.82                     | 0.62              |
| 1:AM:115:THR:HG23 | 1:AM:132:GLN:HB3  | 1.82                     | 0.62              |
| 1:DF:115:THR:HG23 | 1:DF:132:GLN:HB3  | 1.82                     | 0.62              |
| 1:AG:74:THR:HG22  | 1:AG:74:THR:O     | 1.99                     | 0.62              |
| 1:DI:74:THR:O     | 1:DI:74:THR:HG22  | 2.00                     | 0.62              |
| 1:AA:74:THR:O     | 1:AA:74:THR:HG22  | 2.00                     | 0.62              |
| 2:BH:226:LEU:HD23 | 3:CF:126:PRO:HG2  | 115.40                   | 0.62              |
| 1:AH:115:THR:HG22 | 1:AH:131:GLN:OE1  | 2.01                     | 0.61              |
| 1:DG:74:THR:O     | 1:DG:74:THR:HG22  | 1.99                     | 0.61              |
| 1:AE:120:GLN:HG3  | 1:AE:129:ARG:HG2  | 1.82                     | 0.61              |
| 1:AI:120:GLN:HG3  | 1:AI:129:ARG:HG2  | 1.82                     | 0.61              |
| 2:BG:226:LEU:HD23 | 3:CG:126:PRO:HG2  | 69.91                    | 0.61              |
| 2:BV:226:LEU:HD23 | 3:CV:126:PRO:HG2  | 69.91                    | 0.61              |
| 2:BZ:114:VAL:HG22 | 2:BZ:209:VAL:CG1  | 2.29                     | 0.61              |
| 1:AN:115:THR:HG22 | 1:AN:131:GLN:OE1  | 2.01                     | 0.61              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:AW:115:THR:HG22 | 1:AW:131:GLN:OE1 | 2.00                     | 0.61              |
| 1:AO:115:THR:HG23 | 1:AO:132:GLN:HB3 | 1.82                     | 0.61              |
| 1:AC:115:THR:HG23 | 1:AC:132:GLN:HB3 | 1.82                     | 0.61              |
| 1:AL:115:THR:HG23 | 1:AL:132:GLN:HB3 | 1.82                     | 0.61              |
| 1:AZ:115:THR:HG23 | 1:AZ:132:GLN:HB3 | 1.82                     | 0.61              |
| 1:AE:74:THR:HG22  | 1:AE:74:THR:O    | 1.99                     | 0.61              |
| 1:AF:74:THR:HG22  | 1:AF:74:THR:O    | 2.00                     | 0.61              |
| 1:AU:74:THR:O     | 1:AU:74:THR:HG22 | 1.99                     | 0.61              |
| 1:AN:74:THR:O     | 1:AN:74:THR:HG22 | 1.99                     | 0.61              |
| 1:A8:74:THR:HG22  | 1:A8:74:THR:O    | 2.00                     | 0.61              |
| 1:DI:120:GLN:HG3  | 1:DI:129:ARG:HG2 | 1.82                     | 0.61              |
| 1:A3:120:GLN:HG3  | 1:A3:129:ARG:HG2 | 1.82                     | 0.61              |
| 1:A5:146:ILE:O    | 1:A5:147:ALA:HB2 | 1.99                     | 0.61              |
| 1:A2:146:ILE:O    | 1:A2:147:ALA:HB2 | 1.99                     | 0.61              |
| 1:AF:115:THR:HG23 | 1:AF:132:GLN:HB3 | 1.82                     | 0.61              |
| 1:AA:115:THR:HG22 | 1:AA:131:GLN:OE1 | 2.01                     | 0.61              |
| 1:A7:115:THR:HG22 | 1:A7:131:GLN:OE1 | 2.01                     | 0.61              |
| 1:AR:115:THR:HG22 | 1:AR:131:GLN:OE1 | 2.01                     | 0.61              |
| 1:AY:115:THR:HG23 | 1:AY:132:GLN:HB3 | 1.82                     | 0.61              |
| 1:DK:115:THR:HG23 | 1:DK:132:GLN:HB3 | 1.82                     | 0.61              |
| 1:AC:115:THR:HG22 | 1:AC:131:GLN:OE1 | 2.01                     | 0.61              |
| 1:AG:115:THR:HG23 | 1:AG:132:GLN:HB3 | 1.82                     | 0.61              |
| 1:AB:115:THR:HG22 | 1:AB:131:GLN:OE1 | 2.00                     | 0.61              |
| 1:AU:115:THR:HG22 | 1:AU:131:GLN:OE1 | 2.00                     | 0.61              |
| 1:A4:115:THR:HG22 | 1:A4:131:GLN:OE1 | 2.01                     | 0.61              |
| 1:AS:115:THR:HG22 | 1:AS:131:GLN:OE1 | 2.00                     | 0.61              |
| 1:AI:115:THR:HG23 | 1:AI:132:GLN:HB3 | 1.82                     | 0.61              |
| 1:AL:74:THR:O     | 1:AL:74:THR:HG22 | 2.00                     | 0.61              |
| 1:AM:74:THR:HG22  | 1:AM:74:THR:O    | 1.99                     | 0.61              |
| 1:DD:74:THR:O     | 1:DD:74:THR:HG22 | 2.00                     | 0.61              |
| 1:AM:120:GLN:HG3  | 1:AM:129:ARG:HG2 | 1.82                     | 0.61              |
| 1:AT:120:GLN:HG3  | 1:AT:129:ARG:HG2 | 1.82                     | 0.61              |
| 1:AN:115:THR:HG23 | 1:AN:132:GLN:HB3 | 1.82                     | 0.61              |
| 1:AD:115:THR:HG23 | 1:AD:132:GLN:HB3 | 1.82                     | 0.61              |
| 1:DF:115:THR:HG22 | 1:DF:131:GLN:OE1 | 2.01                     | 0.61              |
| 1:AL:115:THR:HG22 | 1:AL:131:GLN:OE1 | 2.01                     | 0.61              |
| 1:AJ:115:THR:HG22 | 1:AJ:131:GLN:OE1 | 2.01                     | 0.61              |
| 1:AQ:115:THR:HG22 | 1:AQ:131:GLN:OE1 | 2.01                     | 0.61              |
| 1:AI:115:THR:HG22 | 1:AI:131:GLN:OE1 | 2.00                     | 0.61              |
| 1:DG:115:THR:HG22 | 1:DG:131:GLN:OE1 | 2.01                     | 0.61              |
| 1:AB:74:THR:O     | 1:AB:74:THR:HG22 | 2.00                     | 0.61              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A2:74:THR:HG22  | 1:A2:74:THR:O    | 1.99                     | 0.61              |
| 1:A9:74:THR:HG22  | 1:A9:74:THR:O    | 1.99                     | 0.61              |
| 1:AQ:74:THR:HG22  | 1:AQ:74:THR:O    | 2.00                     | 0.61              |
| 1:AF:120:GLN:HG3  | 1:AF:129:ARG:HG2 | 1.82                     | 0.61              |
| 1:DE:120:GLN:HG3  | 1:DE:129:ARG:HG2 | 1.82                     | 0.61              |
| 1:A9:120:GLN:HG3  | 1:A9:129:ARG:HG2 | 1.82                     | 0.61              |
| 1:AG:120:GLN:HG3  | 1:AG:129:ARG:HG2 | 1.82                     | 0.61              |
| 1:AX:120:GLN:HG3  | 1:AX:129:ARG:HG2 | 1.82                     | 0.61              |
| 2:BJ:226:LEU:HD23 | 3:CJ:126:PRO:HG2 | 69.91                    | 0.61              |
| 2:BE:226:LEU:HD23 | 3:CE:126:PRO:HG2 | 69.91                    | 0.61              |
| 1:AW:115:THR:HG23 | 1:AW:132:GLN:HB3 | 1.82                     | 0.61              |
| 1:AO:115:THR:HG22 | 1:AO:131:GLN:OE1 | 2.01                     | 0.61              |
| 1:AM:115:THR:HG22 | 1:AM:131:GLN:OE1 | 2.00                     | 0.61              |
| 1:DD:115:THR:HG22 | 1:DD:131:GLN:OE1 | 2.00                     | 0.61              |
| 1:DE:115:THR:HG22 | 1:DE:131:GLN:OE1 | 2.01                     | 0.61              |
| 1:DK:74:THR:HG22  | 1:DK:74:THR:O    | 2.00                     | 0.61              |
| 1:AX:74:THR:HG22  | 1:AX:74:THR:O    | 2.00                     | 0.61              |
| 1:DD:120:GLN:HG3  | 1:DD:129:ARG:HG2 | 1.82                     | 0.61              |
| 2:BD:226:LEU:HD23 | 3:CC:126:PRO:HG2 | 1.80                     | 0.61              |
| 1:AZ:146:ILE:O    | 1:AZ:147:ALA:HB2 | 1.99                     | 0.61              |
| 1:DG:146:ILE:O    | 1:DG:147:ALA:HB2 | 1.99                     | 0.61              |
| 1:AE:115:THR:HG23 | 1:AE:132:GLN:HB3 | 1.82                     | 0.61              |
| 1:AS:115:THR:HG23 | 1:AS:132:GLN:HB3 | 1.82                     | 0.61              |
| 1:DH:115:THR:HG22 | 1:DH:131:GLN:OE1 | 2.00                     | 0.61              |
| 1:AO:74:THR:O     | 1:AO:74:THR:HG22 | 1.99                     | 0.61              |
| 1:AR:120:GLN:HG3  | 1:AR:129:ARG:HG2 | 1.82                     | 0.61              |
| 1:AJ:120:GLN:HG3  | 1:AJ:129:ARG:HG2 | 1.82                     | 0.61              |
| 2:BL:226:LEU:HD23 | 3:CL:126:PRO:HG2 | 69.91                    | 0.61              |
| 1:AF:115:THR:HG22 | 1:AF:131:GLN:OE1 | 2.01                     | 0.61              |
| 1:AV:115:THR:HG23 | 1:AV:132:GLN:HB3 | 1.82                     | 0.61              |
| 1:AD:115:THR:HG22 | 1:AD:131:GLN:OE1 | 2.01                     | 0.61              |
| 1:A2:115:THR:HG22 | 1:A2:131:GLN:OE1 | 2.00                     | 0.61              |
| 1:AG:115:THR:HG22 | 1:AG:131:GLN:OE1 | 2.00                     | 0.61              |
| 1:A9:115:THR:HG22 | 1:A9:131:GLN:OE1 | 2.00                     | 0.61              |
| 1:DI:163:MET:CE   | 1:DI:189:GLY:HA3 | 2.31                     | 0.61              |
| 1:AY:163:MET:CE   | 1:AY:189:GLY:HA3 | 2.31                     | 0.61              |
| 1:AQ:163:MET:CE   | 1:AQ:189:GLY:HA3 | 2.31                     | 0.61              |
| 1:AA:163:MET:CE   | 1:AA:189:GLY:HA3 | 2.31                     | 0.61              |
| 1:AK:163:MET:CE   | 1:AK:189:GLY:HA3 | 2.31                     | 0.61              |
| 1:A9:115:THR:HG23 | 1:A9:132:GLN:HB3 | 1.82                     | 0.61              |
| 2:BP:137:GLU:CB   | 1:DC:181:LYS:HE3 | 253.37                   | 0.61              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:AA:181:LYS:HE3  | 2:BA:137:GLU:CB  | 2.31                     | 0.61              |
| 1:AI:181:LYS:HE3  | 2:BI:137:GLU:CB  | 2.31                     | 0.61              |
| 1:AK:181:LYS:HE3  | 2:BK:137:GLU:CB  | 65.66                    | 0.61              |
| 1:AR:181:LYS:HE3  | 2:BQ:137:GLU:CB  | 2.31                     | 0.61              |
| 1:AB:163:MET:CE   | 1:AB:189:GLY:HA3 | 2.31                     | 0.61              |
| 1:AD:163:MET:CE   | 1:AD:189:GLY:HA3 | 2.31                     | 0.61              |
| 1:AE:163:MET:CE   | 1:AE:189:GLY:HA3 | 2.31                     | 0.61              |
| 1:DJ:163:MET:CE   | 1:DJ:189:GLY:HA3 | 2.31                     | 0.61              |
| 1:AO:163:MET:CE   | 1:AO:189:GLY:HA3 | 2.31                     | 0.61              |
| 1:AH:163:MET:CE   | 1:AH:189:GLY:HA3 | 2.31                     | 0.61              |
| 1:AZ:163:MET:CE   | 1:AZ:189:GLY:HA3 | 2.31                     | 0.61              |
| 1:A5:163:MET:CE   | 1:A5:189:GLY:HA3 | 2.31                     | 0.61              |
| 1:A8:115:THR:HG22 | 1:A8:131:GLN:OE1 | 2.01                     | 0.61              |
| 1:AT:115:THR:HG22 | 1:AT:131:GLN:OE1 | 2.01                     | 0.61              |
| 1:AF:181:LYS:HE3  | 2:BF:137:GLU:CB  | 2.31                     | 0.61              |
| 2:BS:137:GLU:CB   | 1:DF:181:LYS:HE3 | 271.75                   | 0.61              |
| 1:A9:181:LYS:HE3  | 2:B9:137:GLU:CB  | 2.31                     | 0.61              |
| 1:A4:120:GLN:HG3  | 1:A4:129:ARG:HG2 | 1.82                     | 0.61              |
| 1:DH:163:MET:CE   | 1:DH:189:GLY:HA3 | 2.31                     | 0.61              |
| 1:A8:146:ILE:O    | 1:A8:147:ALA:HB2 | 1.99                     | 0.61              |
| 1:A7:163:MET:CE   | 1:A7:189:GLY:HA3 | 2.31                     | 0.61              |
| 1:A1:146:ILE:O    | 1:A1:147:ALA:HB2 | 1.99                     | 0.61              |
| 1:AV:115:THR:HG22 | 1:AV:131:GLN:OE1 | 2.01                     | 0.61              |
| 1:AK:115:THR:HG22 | 1:AK:131:GLN:OE1 | 2.01                     | 0.61              |
| 1:DJ:115:THR:HG23 | 1:DJ:132:GLN:HB3 | 1.82                     | 0.61              |
| 1:A5:115:THR:HG22 | 1:A5:131:GLN:OE1 | 2.01                     | 0.61              |
| 1:DK:115:THR:HG22 | 1:DK:131:GLN:OE1 | 2.01                     | 0.61              |
| 1:AE:115:THR:HG22 | 1:AE:131:GLN:OE1 | 2.00                     | 0.61              |
| 1:A1:115:THR:HG22 | 1:A1:131:GLN:OE1 | 2.01                     | 0.61              |
| 1:AN:181:LYS:HE3  | 2:BN:137:GLU:CB  | 105.72                   | 0.61              |
| 2:BU:137:GLU:CB   | 1:DH:181:LYS:HE3 | 288.27                   | 0.61              |
| 1:AS:181:LYS:HE3  | 2:BT:137:GLU:CB  | 2.31                     | 0.61              |
| 2:B1:137:GLU:C    | 2:B1:139:ALA:N   | 2.54                     | 0.61              |
| 1:AC:74:THR:O     | 1:AC:74:THR:HG22 | 2.00                     | 0.61              |
| 1:AN:120:GLN:HG3  | 1:AN:129:ARG:HG2 | 1.82                     | 0.61              |
| 1:A5:120:GLN:HG3  | 1:A5:129:ARG:HG2 | 1.82                     | 0.61              |
| 1:A1:120:GLN:HG3  | 1:A1:129:ARG:HG2 | 1.82                     | 0.61              |
| 1:AF:163:MET:CE   | 1:AF:189:GLY:HA3 | 2.31                     | 0.61              |
| 1:AD:181:LYS:HE3  | 2:BD:137:GLU:CB  | 2.31                     | 0.60              |
| 1:AM:181:LYS:HE3  | 2:BN:137:GLU:CB  | 2.31                     | 0.60              |
| 1:AT:181:LYS:HE3  | 2:BU:137:GLU:CB  | 2.31                     | 0.60              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:AB:181:LYS:HE3  | 2:BB:137:GLU:CB  | 2.31                     | 0.60              |
| 1:DC:74:THR:HG22  | 1:DC:74:THR:O    | 2.00                     | 0.60              |
| 1:AP:120:GLN:HG3  | 1:AP:129:ARG:HG2 | 1.82                     | 0.60              |
| 1:A0:120:GLN:HG3  | 1:A0:129:ARG:HG2 | 1.82                     | 0.60              |
| 1:DF:120:GLN:HG3  | 1:DF:129:ARG:HG2 | 1.82                     | 0.60              |
| 1:AV:120:GLN:HG3  | 1:AV:129:ARG:HG2 | 1.82                     | 0.60              |
| 1:AM:163:MET:CE   | 1:AM:189:GLY:HA3 | 2.31                     | 0.60              |
| 1:AN:163:MET:CE   | 1:AN:189:GLY:HA3 | 2.31                     | 0.60              |
| 1:AP:163:MET:CE   | 1:AP:189:GLY:HA3 | 2.31                     | 0.60              |
| 1:DD:163:MET:CE   | 1:DD:189:GLY:HA3 | 2.31                     | 0.60              |
| 1:AI:163:MET:CE   | 1:AI:189:GLY:HA3 | 2.31                     | 0.60              |
| 1:AX:115:THR:HG23 | 1:AX:132:GLN:HB3 | 1.82                     | 0.60              |
| 1:DE:115:THR:HG23 | 1:DE:132:GLN:HB3 | 1.82                     | 0.60              |
| 1:A6:181:LYS:O    | 1:A6:182:ALA:HB2 | 2.01                     | 0.60              |
| 1:AI:181:LYS:O    | 1:AI:182:ALA:HB2 | 2.01                     | 0.60              |
| 1:AW:181:LYS:HE3  | 2:BX:137:GLU:CB  | 2.31                     | 0.60              |
| 1:AW:181:LYS:O    | 1:AW:182:ALA:HB2 | 2.02                     | 0.60              |
| 2:BB:137:GLU:C    | 2:BB:139:ALA:N   | 2.55                     | 0.60              |
| 1:A3:181:LYS:O    | 1:A3:182:ALA:HB2 | 2.01                     | 0.60              |
| 1:A0:181:LYS:HE3  | 2:B1:137:GLU:CB  | 2.31                     | 0.60              |
| 1:A1:74:THR:HG22  | 1:A1:74:THR:O    | 1.99                     | 0.60              |
| 1:AU:120:GLN:HG3  | 1:AU:129:ARG:HG2 | 1.82                     | 0.60              |
| 1:A2:163:MET:CE   | 1:A2:189:GLY:HA3 | 2.31                     | 0.60              |
| 1:AC:163:MET:CE   | 1:AC:189:GLY:HA3 | 2.31                     | 0.60              |
| 1:AJ:201:ALA:O    | 1:AJ:203:ASP:N   | 2.34                     | 0.60              |
| 3:CT:29:VAL:HG21  | 1:DF:159:PRO:HB2 | 252.80                   | 0.60              |
| 1:DJ:201:ALA:O    | 1:DJ:203:ASP:N   | 2.35                     | 0.60              |
| 1:A5:201:ALA:O    | 1:A5:203:ASP:N   | 2.34                     | 0.60              |
| 1:AJ:163:MET:CE   | 1:AJ:189:GLY:HA3 | 2.31                     | 0.60              |
| 1:AL:163:MET:CE   | 1:AL:189:GLY:HA3 | 2.31                     | 0.60              |
| 1:AU:115:THR:HG23 | 1:AU:132:GLN:HB3 | 1.82                     | 0.60              |
| 1:AZ:115:THR:HG22 | 1:AZ:131:GLN:OE1 | 2.01                     | 0.60              |
| 1:AH:115:THR:HG23 | 1:AH:132:GLN:HB3 | 1.82                     | 0.60              |
| 1:AU:181:LYS:HE3  | 2:BV:137:GLU:CB  | 2.31                     | 0.60              |
| 2:BV:137:GLU:CB   | 1:DI:181:LYS:HE3 | 291.33                   | 0.60              |
| 1:DC:181:LYS:O    | 1:DC:182:ALA:HB2 | 2.02                     | 0.60              |
| 1:AE:181:LYS:HE3  | 2:BE:137:GLU:CB  | 2.31                     | 0.60              |
| 2:BR:137:GLU:C    | 2:BR:139:ALA:N   | 2.55                     | 0.60              |
| 1:DH:181:LYS:O    | 1:DH:182:ALA:HB2 | 2.02                     | 0.60              |
| 1:A2:181:LYS:O    | 1:A2:182:ALA:HB2 | 2.01                     | 0.60              |
| 2:BW:137:GLU:CB   | 1:DJ:181:LYS:HE3 | 290.34                   | 0.60              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:AS:181:LYS:O    | 1:AS:182:ALA:HB2 | 2.01                     | 0.60              |
| 1:AY:74:THR:HG22  | 1:AY:74:THR:O    | 2.00                     | 0.60              |
| 1:AZ:120:GLN:HG3  | 1:AZ:129:ARG:HG2 | 1.82                     | 0.60              |
| 1:A1:201:ALA:O    | 1:A1:203:ASP:N   | 2.34                     | 0.60              |
| 1:AU:163:MET:CE   | 1:AU:189:GLY:HA3 | 2.31                     | 0.60              |
| 1:DI:115:THR:HG22 | 1:DI:131:GLN:OE1 | 2.01                     | 0.60              |
| 1:AB:115:THR:HG23 | 1:AB:132:GLN:HB3 | 1.82                     | 0.60              |
| 1:DC:115:THR:HG22 | 1:DC:131:GLN:OE1 | 2.01                     | 0.60              |
| 1:AU:181:LYS:O    | 1:AU:182:ALA:HB2 | 2.02                     | 0.60              |
| 2:BJ:137:GLU:CB   | 1:DK:181:LYS:HE3 | 2.31                     | 0.60              |
| 1:DK:181:LYS:O    | 1:DK:182:ALA:HB2 | 2.02                     | 0.60              |
| 1:AR:181:LYS:O    | 1:AR:182:ALA:HB2 | 2.01                     | 0.60              |
| 1:AV:181:LYS:HE3  | 2:BW:137:GLU:CB  | 2.31                     | 0.60              |
| 1:A7:181:LYS:O    | 1:A7:182:ALA:HB2 | 2.01                     | 0.60              |
| 1:AG:181:LYS:HE3  | 2:BG:137:GLU:CB  | 2.31                     | 0.60              |
| 1:AS:74:THR:HG22  | 1:AS:74:THR:O    | 2.00                     | 0.60              |
| 1:DK:120:GLN:HG3  | 1:DK:129:ARG:HG2 | 1.82                     | 0.60              |
| 1:AZ:201:ALA:O    | 1:AZ:203:ASP:N   | 2.34                     | 0.60              |
| 1:DE:163:MET:CE   | 1:DE:189:GLY:HA3 | 2.31                     | 0.60              |
| 1:AD:159:PRO:HB2  | 3:CE:29:VAL:HG21 | 53.35                    | 0.60              |
| 1:AV:201:ALA:O    | 1:AV:203:ASP:N   | 2.34                     | 0.60              |
| 1:A4:201:ALA:O    | 1:A4:203:ASP:N   | 2.34                     | 0.60              |
| 1:AY:201:ALA:O    | 1:AY:203:ASP:N   | 2.35                     | 0.60              |
| 1:DC:201:ALA:O    | 1:DC:203:ASP:N   | 2.35                     | 0.60              |
| 1:A2:115:THR:HG23 | 1:A2:132:GLN:HB3 | 1.82                     | 0.60              |
| 1:A6:115:THR:HG22 | 1:A6:131:GLN:OE1 | 2.01                     | 0.60              |
| 1:DI:181:LYS:O    | 1:DI:182:ALA:HB2 | 2.01                     | 0.60              |
| 1:A6:181:LYS:HE3  | 2:B6:137:GLU:CB  | 2.31                     | 0.60              |
| 1:AD:181:LYS:O    | 1:AD:182:ALA:HB2 | 2.02                     | 0.60              |
| 1:AJ:181:LYS:O    | 1:AJ:182:ALA:HB2 | 2.01                     | 0.60              |
| 1:AK:181:LYS:HE3  | 2:BL:137:GLU:CB  | 2.31                     | 0.60              |
| 1:AL:181:LYS:HE3  | 2:BL:137:GLU:CB  | 105.90                   | 0.60              |
| 1:AC:181:LYS:HE3  | 2:BC:137:GLU:CB  | 2.31                     | 0.60              |
| 1:A4:181:LYS:O    | 1:A4:182:ALA:HB2 | 2.02                     | 0.60              |
| 1:AT:181:LYS:O    | 1:AT:182:ALA:HB2 | 2.02                     | 0.60              |
| 1:AX:181:LYS:HE3  | 2:BY:137:GLU:CB  | 2.31                     | 0.60              |
| 1:A5:181:LYS:O    | 1:A5:182:ALA:HB2 | 2.01                     | 0.60              |
| 1:AW:74:THR:O     | 1:AW:74:THR:HG22 | 1.99                     | 0.60              |
| 1:AH:159:PRO:HB2  | 3:CH:29:VAL:HG21 | 1.84                     | 0.60              |
| 1:AT:163:MET:CE   | 1:AT:189:GLY:HA3 | 2.31                     | 0.60              |
| 1:AJ:159:PRO:HB2  | 3:CK:29:VAL:HG21 | 1.84                     | 0.60              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A4:163:MET:CE   | 1:A4:189:GLY:HA3 | 2.31                     | 0.60              |
| 1:AT:201:ALA:O    | 1:AT:203:ASP:N   | 2.35                     | 0.60              |
| 1:DH:201:ALA:O    | 1:DH:203:ASP:N   | 2.35                     | 0.60              |
| 1:A0:159:PRO:HB2  | 3:C1:29:VAL:HG21 | 1.84                     | 0.60              |
| 1:AP:115:THR:HG22 | 1:AP:131:GLN:OE1 | 2.01                     | 0.60              |
| 1:A0:115:THR:HG22 | 1:A0:131:GLN:OE1 | 2.01                     | 0.60              |
| 1:AX:115:THR:HG22 | 1:AX:131:GLN:OE1 | 2.01                     | 0.60              |
| 1:AA:181:LYS:O    | 1:AA:182:ALA:HB2 | 2.01                     | 0.60              |
| 1:AE:181:LYS:O    | 1:AE:182:ALA:HB2 | 2.01                     | 0.60              |
| 1:AJ:181:LYS:HE3  | 2:BJ:137:GLU:CB  | 259.83                   | 0.60              |
| 1:AK:181:LYS:O    | 1:AK:182:ALA:HB2 | 2.01                     | 0.60              |
| 1:AM:181:LYS:O    | 1:AM:182:ALA:HB2 | 2.01                     | 0.60              |
| 1:AN:181:LYS:O    | 1:AN:182:ALA:HB2 | 2.02                     | 0.60              |
| 1:AO:181:LYS:O    | 1:AO:182:ALA:HB2 | 2.01                     | 0.60              |
| 2:BJ:137:GLU:C    | 2:BJ:139:ALA:N   | 2.55                     | 0.60              |
| 1:AM:181:LYS:HE3  | 2:BM:137:GLU:CB  | 65.66                    | 0.60              |
| 1:DF:181:LYS:O    | 1:DF:182:ALA:HB2 | 2.02                     | 0.60              |
| 2:BC:137:GLU:C    | 2:BC:139:ALA:N   | 2.54                     | 0.60              |
| 1:AZ:181:LYS:O    | 1:AZ:182:ALA:HB2 | 2.02                     | 0.60              |
| 1:AX:181:LYS:O    | 1:AX:182:ALA:HB2 | 2.02                     | 0.60              |
| 1:DJ:181:LYS:O    | 1:DJ:182:ALA:HB2 | 2.01                     | 0.60              |
| 1:A7:181:LYS:HE3  | 2:B7:137:GLU:CB  | 2.31                     | 0.60              |
| 1:A1:181:LYS:HE3  | 2:B2:137:GLU:CB  | 2.31                     | 0.60              |
| 1:A2:120:GLN:HG3  | 1:A2:129:ARG:HG2 | 1.82                     | 0.60              |
| 1:AE:159:PRO:HB2  | 3:CF:29:VAL:HG21 | 119.49                   | 0.60              |
| 1:A8:159:PRO:HB2  | 3:C9:29:VAL:HG21 | 1.84                     | 0.60              |
| 1:AL:201:ALA:O    | 1:AL:203:ASP:N   | 2.35                     | 0.60              |
| 1:AS:163:MET:CE   | 1:AS:189:GLY:HA3 | 2.31                     | 0.60              |
| 1:AF:201:ALA:O    | 1:AF:203:ASP:N   | 2.35                     | 0.60              |
| 1:A8:163:MET:CE   | 1:A8:189:GLY:HA3 | 2.31                     | 0.60              |
| 1:DJ:115:THR:HG22 | 1:DJ:131:GLN:OE1 | 2.01                     | 0.60              |
| 1:AY:115:THR:HG22 | 1:AY:131:GLN:OE1 | 2.00                     | 0.60              |
| 1:AF:181:LYS:O    | 1:AF:182:ALA:HB2 | 2.01                     | 0.60              |
| 1:AL:181:LYS:HE3  | 2:BM:137:GLU:CB  | 2.31                     | 0.60              |
| 1:AN:181:LYS:HE3  | 2:BR:137:GLU:CB  | 2.31                     | 0.60              |
| 2:BH:137:GLU:C    | 2:BH:139:ALA:N   | 2.54                     | 0.60              |
| 1:AY:181:LYS:O    | 1:AY:182:ALA:HB2 | 2.01                     | 0.60              |
| 1:A9:181:LYS:O    | 1:A9:182:ALA:HB2 | 2.01                     | 0.60              |
| 2:BG:137:GLU:C    | 2:BG:139:ALA:N   | 2.55                     | 0.60              |
| 1:A6:159:PRO:HB2  | 3:C7:29:VAL:HG21 | 1.84                     | 0.60              |
| 1:AR:159:PRO:HB2  | 3:CS:29:VAL:HG21 | 1.84                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AS:201:ALA:O    | 1:AS:203:ASP:N    | 2.34                     | 0.60              |
| 1:DK:163:MET:CE   | 1:DK:189:GLY:HA3  | 2.31                     | 0.60              |
| 1:AD:201:ALA:O    | 1:AD:203:ASP:N    | 2.34                     | 0.60              |
| 1:DF:163:MET:CE   | 1:DF:189:GLY:HA3  | 2.31                     | 0.60              |
| 1:AP:115:THR:HG23 | 1:AP:132:GLN:HB3  | 1.82                     | 0.60              |
| 1:DC:115:THR:HG23 | 1:DC:132:GLN:HB3  | 1.82                     | 0.60              |
| 2:BM:137:GLU:C    | 2:BM:139:ALA:N    | 2.54                     | 0.60              |
| 2:B2:85:SER:HB2   | 2:B2:190:ASN:HD21 | 1.67                     | 0.60              |
| 1:AH:159:PRO:HB2  | 3:CI:29:VAL:HG21  | 31.33                    | 0.60              |
| 3:CX:29:VAL:HG21  | 1:DJ:159:PRO:HB2  | 245.80                   | 0.60              |
| 1:A4:159:PRO:HB2  | 3:C5:29:VAL:HG21  | 1.84                     | 0.60              |
| 1:AK:201:ALA:O    | 1:AK:203:ASP:N    | 2.34                     | 0.60              |
| 1:AW:163:MET:CE   | 1:AW:189:GLY:HA3  | 2.31                     | 0.60              |
| 1:DC:163:MET:CE   | 1:DC:189:GLY:HA3  | 2.31                     | 0.60              |
| 1:AN:201:ALA:O    | 1:AN:203:ASP:N    | 2.34                     | 0.60              |
| 1:A3:115:THR:HG22 | 1:A3:131:GLN:OE1  | 2.01                     | 0.60              |
| 1:AQ:115:THR:HG23 | 1:AQ:132:GLN:HB3  | 1.82                     | 0.60              |
| 1:AP:181:LYS:HE3  | 2:BS:137:GLU:CB   | 2.31                     | 0.60              |
| 2:BN:137:GLU:C    | 2:BN:139:ALA:N    | 2.55                     | 0.60              |
| 1:AH:181:LYS:O    | 1:AH:182:ALA:HB2  | 2.02                     | 0.60              |
| 1:DD:181:LYS:O    | 1:DD:182:ALA:HB2  | 2.01                     | 0.60              |
| 1:A2:181:LYS:HE3  | 2:B3:137:GLU:CB   | 2.31                     | 0.60              |
| 1:AB:181:LYS:O    | 1:AB:182:ALA:HB2  | 2.01                     | 0.60              |
| 1:AG:181:LYS:O    | 1:AG:182:ALA:HB2  | 2.02                     | 0.60              |
| 2:BS:85:SER:HB2   | 2:BS:190:ASN:HD21 | 1.67                     | 0.60              |
| 1:AC:159:PRO:HB2  | 3:CD:29:VAL:HG21  | 31.33                    | 0.60              |
| 3:CS:29:VAL:HG21  | 1:DE:159:PRO:HB2  | 267.89                   | 0.60              |
| 1:DE:201:ALA:O    | 1:DE:203:ASP:N    | 2.35                     | 0.60              |
| 1:A0:201:ALA:O    | 1:A0:203:ASP:N    | 2.34                     | 0.60              |
| 1:A7:159:PRO:HB2  | 3:C8:29:VAL:HG21  | 1.84                     | 0.60              |
| 1:AX:159:PRO:HB2  | 3:CY:29:VAL:HG21  | 1.84                     | 0.60              |
| 1:A1:163:MET:CE   | 1:A1:189:GLY:HA3  | 2.31                     | 0.60              |
| 1:AM:159:PRO:HB2  | 3:CN:29:VAL:HG21  | 1.84                     | 0.60              |
| 1:A6:115:THR:HG23 | 1:A6:132:GLN:HB3  | 1.82                     | 0.60              |
| 1:AL:181:LYS:O    | 1:AL:182:ALA:HB2  | 2.02                     | 0.60              |
| 2:BE:137:GLU:C    | 2:BE:139:ALA:N    | 2.55                     | 0.60              |
| 1:AH:181:LYS:HE3  | 2:BH:137:GLU:CB   | 2.31                     | 0.60              |
| 2:BQ:137:GLU:CB   | 1:DD:181:LYS:HE3  | 285.99                   | 0.60              |
| 1:AV:181:LYS:O    | 1:AV:182:ALA:HB2  | 2.02                     | 0.60              |
| 2:BT:137:GLU:CB   | 1:DG:181:LYS:HE3  | 253.35                   | 0.60              |
| 2:BM:85:SER:HB2   | 2:BM:190:ASN:HD21 | 1.67                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BO:85:SER:HB2   | 2:BO:190:ASN:HD21 | 1.67                     | 0.60              |
| 2:BP:85:SER:HB2   | 2:BP:190:ASN:HD21 | 1.67                     | 0.60              |
| 2:BG:85:SER:HB2   | 2:BG:190:ASN:HD21 | 1.67                     | 0.60              |
| 2:B4:85:SER:HB2   | 2:B4:190:ASN:HD21 | 1.67                     | 0.60              |
| 1:AO:163:MET:HE1  | 1:AO:189:GLY:HA3  | 1.88                     | 0.60              |
| 1:AI:201:ALA:O    | 1:AI:203:ASP:N    | 2.34                     | 0.60              |
| 1:AV:5:GLY:HA3    | 1:AV:15:PRO:HD3   | 1.84                     | 0.60              |
| 1:AY:159:PRO:HB2  | 3:CZ:29:VAL:HG21  | 1.84                     | 0.60              |
| 1:AB:201:ALA:O    | 1:AB:203:ASP:N    | 2.34                     | 0.60              |
| 1:AU:201:ALA:O    | 1:AU:203:ASP:N    | 2.35                     | 0.60              |
| 1:A2:201:ALA:O    | 1:A2:203:ASP:N    | 2.34                     | 0.60              |
| 3:CC:42:ASN:HD22  | 3:CC:44:ILE:H     | 1.50                     | 0.60              |
| 1:A6:163:MET:CE   | 1:A6:189:GLY:HA3  | 2.31                     | 0.60              |
| 1:AW:201:ALA:O    | 1:AW:203:ASP:N    | 2.34                     | 0.60              |
| 1:AO:201:ALA:O    | 1:AO:203:ASP:N    | 2.35                     | 0.60              |
| 1:AX:201:ALA:O    | 1:AX:203:ASP:N    | 2.35                     | 0.60              |
| 1:AW:5:GLY:HA3    | 1:AW:15:PRO:HD3   | 1.84                     | 0.60              |
| 1:AL:159:PRO:HB2  | 3:CM:29:VAL:HG21  | 1.84                     | 0.60              |
| 3:DB:42:ASN:HD22  | 3:DB:44:ILE:H     | 1.50                     | 0.60              |
| 1:AP:159:PRO:HB2  | 3:CQ:29:VAL:HG21  | 1.84                     | 0.60              |
| 1:A8:115:THR:HG23 | 1:A8:132:GLN:HB3  | 1.82                     | 0.59              |
| 2:BV:137:GLU:C    | 2:BV:139:ALA:N    | 2.55                     | 0.59              |
| 1:A8:181:LYS:O    | 1:A8:182:ALA:HB2  | 2.01                     | 0.59              |
| 1:AO:181:LYS:HE3  | 2:BO:137:GLU:CB   | 2.31                     | 0.59              |
| 2:BI:137:GLU:C    | 2:BI:139:ALA:N    | 2.55                     | 0.59              |
| 1:AZ:181:LYS:HE3  | 2:B0:137:GLU:CB   | 2.31                     | 0.59              |
| 1:A5:181:LYS:HE3  | 2:B5:137:GLU:CB   | 2.31                     | 0.59              |
| 2:BQ:85:SER:HB2   | 2:BQ:190:ASN:HD21 | 1.67                     | 0.59              |
| 1:AF:159:PRO:HB2  | 3:CG:29:VAL:HG21  | 31.33                    | 0.59              |
| 1:AC:159:PRO:HB2  | 3:CC:29:VAL:HG21  | 1.84                     | 0.59              |
| 3:CJ:29:VAL:HG21  | 1:DK:159:PRO:HB2  | 1.84                     | 0.59              |
| 3:CQ:42:ASN:HD22  | 3:CQ:44:ILE:H     | 1.50                     | 0.59              |
| 1:AJ:5:GLY:HA3    | 1:AJ:15:PRO:HD3   | 1.85                     | 0.59              |
| 1:AK:5:GLY:HA3    | 1:AK:15:PRO:HD3   | 1.84                     | 0.59              |
| 3:CA:42:ASN:HD22  | 3:CA:44:ILE:H     | 1.50                     | 0.59              |
| 1:A9:201:ALA:O    | 1:A9:203:ASP:N    | 2.34                     | 0.59              |
| 3:CK:42:ASN:HD22  | 3:CK:44:ILE:H     | 1.50                     | 0.59              |
| 1:AM:201:ALA:O    | 1:AM:203:ASP:N    | 2.34                     | 0.59              |
| 1:DK:201:ALA:O    | 1:DK:203:ASP:N    | 2.35                     | 0.59              |
| 1:AF:5:GLY:HA3    | 1:AF:15:PRO:HD3   | 1.84                     | 0.59              |
| 1:A4:181:LYS:HE3  | 2:BX:137:GLU:CB   | 292.12                   | 0.59              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A3:181:LYS:HE3 | 2:B4:137:GLU:CB   | 2.31                     | 0.59              |
| 2:BE:85:SER:HB2  | 2:BE:190:ASN:HD21 | 1.67                     | 0.59              |
| 2:BJ:85:SER:HB2  | 2:BJ:190:ASN:HD21 | 1.67                     | 0.59              |
| 2:BN:85:SER:HB2  | 2:BN:190:ASN:HD21 | 1.67                     | 0.59              |
| 1:AM:159:PRO:CB  | 3:CN:29:VAL:HG21  | 2.33                     | 0.59              |
| 1:AN:5:GLY:HA3   | 1:AN:15:PRO:HD3   | 1.85                     | 0.59              |
| 1:AH:201:ALA:O   | 1:AH:203:ASP:N    | 2.35                     | 0.59              |
| 1:AA:201:ALA:O   | 1:AA:203:ASP:N    | 2.35                     | 0.59              |
| 3:CJ:42:ASN:HD22 | 3:CJ:44:ILE:H     | 1.50                     | 0.59              |
| 3:C2:42:ASN:HD22 | 3:C2:44:ILE:H     | 1.51                     | 0.59              |
| 3:CD:42:ASN:HD22 | 3:CD:44:ILE:H     | 1.50                     | 0.59              |
| 1:AB:5:GLY:HA3   | 1:AB:15:PRO:HD3   | 1.84                     | 0.59              |
| 3:C1:42:ASN:HD22 | 3:C1:44:ILE:H     | 1.50                     | 0.59              |
| 3:CE:42:ASN:HD22 | 3:CE:44:ILE:H     | 1.50                     | 0.59              |
| 1:A1:159:PRO:HB2 | 3:C2:29:VAL:HG21  | 1.84                     | 0.59              |
| 1:AG:201:ALA:O   | 1:AG:203:ASP:N    | 2.35                     | 0.59              |
| 1:AP:201:ALA:O   | 1:AP:203:ASP:N    | 2.34                     | 0.59              |
| 3:C5:42:ASN:HD22 | 3:C5:44:ILE:H     | 1.51                     | 0.59              |
| 1:DE:181:LYS:O   | 1:DE:182:ALA:HB2  | 2.02                     | 0.59              |
| 2:BX:137:GLU:C   | 2:BX:139:ALA:N    | 2.55                     | 0.59              |
| 1:AY:181:LYS:HE3 | 2:BZ:137:GLU:CB   | 2.31                     | 0.59              |
| 2:BT:137:GLU:C   | 2:BT:139:ALA:N    | 2.55                     | 0.59              |
| 2:BY:85:SER:HB2  | 2:BY:190:ASN:HD21 | 1.67                     | 0.59              |
| 2:BK:85:SER:HB2  | 2:BK:190:ASN:HD21 | 1.67                     | 0.59              |
| 2:BB:85:SER:HB2  | 2:BB:190:ASN:HD21 | 1.67                     | 0.59              |
| 2:BD:85:SER:HB2  | 2:BD:190:ASN:HD21 | 1.67                     | 0.59              |
| 1:AJ:163:MET:HE1 | 1:AJ:189:GLY:HA3  | 1.93                     | 0.59              |
| 1:AI:159:PRO:CB  | 3:CJ:29:VAL:HG21  | 52.61                    | 0.59              |
| 1:A8:159:PRO:CB  | 3:C9:29:VAL:HG21  | 2.33                     | 0.59              |
| 1:AR:159:PRO:CB  | 3:CS:29:VAL:HG21  | 2.33                     | 0.59              |
| 1:AO:5:GLY:HA3   | 1:AO:15:PRO:HD3   | 1.84                     | 0.59              |
| 1:AD:5:GLY:HA3   | 1:AD:15:PRO:HD3   | 1.85                     | 0.59              |
| 1:A3:159:PRO:CB  | 3:C4:29:VAL:HG21  | 2.33                     | 0.59              |
| 1:A3:163:MET:CE  | 1:A3:189:GLY:HA3  | 2.31                     | 0.59              |
| 1:AE:5:GLY:HA3   | 1:AE:15:PRO:HD3   | 1.85                     | 0.59              |
| 1:AV:163:MET:CE  | 1:AV:189:GLY:HA3  | 2.31                     | 0.59              |
| 1:DF:201:ALA:O   | 1:DF:203:ASP:N    | 2.35                     | 0.59              |
| 1:AX:163:MET:CE  | 1:AX:189:GLY:HA3  | 2.31                     | 0.59              |
| 3:CS:42:ASN:HD22 | 3:CS:44:ILE:H     | 1.50                     | 0.59              |
| 3:C9:42:ASN:HD22 | 3:C9:44:ILE:H     | 1.50                     | 0.59              |
| 1:AQ:5:GLY:HA3   | 1:AQ:15:PRO:HD3   | 1.85                     | 0.59              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:AM:5:GLY:HA3   | 1:AM:15:PRO:HD3   | 1.84                     | 0.59              |
| 1:AE:201:ALA:O   | 1:AE:203:ASP:N    | 2.34                     | 0.59              |
| 1:A9:163:MET:CE  | 1:A9:189:GLY:HA3  | 2.31                     | 0.59              |
| 1:AX:5:GLY:HA3   | 1:AX:15:PRO:HD3   | 1.85                     | 0.59              |
| 3:CW:29:VAL:HG21 | 1:DI:159:PRO:CB   | 243.50                   | 0.59              |
| 1:AQ:181:LYS:HE3 | 2:BP:137:GLU:CB   | 2.31                     | 0.59              |
| 1:AQ:181:LYS:O   | 1:AQ:182:ALA:HB2  | 2.02                     | 0.59              |
| 2:BL:137:GLU:C   | 2:BL:139:ALA:N    | 2.55                     | 0.59              |
| 2:BW:85:SER:HB2  | 2:BW:190:ASN:HD21 | 1.67                     | 0.59              |
| 2:B1:85:SER:HB2  | 2:B1:190:ASN:HD21 | 1.67                     | 0.59              |
| 2:BH:85:SER:HB2  | 2:BH:190:ASN:HD21 | 1.67                     | 0.59              |
| 1:AW:120:GLN:HG3 | 1:AW:129:ARG:HG2  | 1.82                     | 0.59              |
| 1:AC:159:PRO:CB  | 3:CC:29:VAL:HG21  | 2.33                     | 0.59              |
| 1:AH:159:PRO:CB  | 3:CH:29:VAL:HG21  | 2.33                     | 0.59              |
| 1:AF:159:PRO:HB2 | 3:CF:29:VAL:HG21  | 1.84                     | 0.59              |
| 1:A4:163:MET:HE1 | 1:A4:189:GLY:HA3  | 1.84                     | 0.59              |
| 1:A7:159:PRO:CB  | 3:C8:29:VAL:HG21  | 2.33                     | 0.59              |
| 1:DJ:5:GLY:HA3   | 1:DJ:15:PRO:HD3   | 1.85                     | 0.59              |
| 1:AR:5:GLY:HA3   | 1:AR:15:PRO:HD3   | 1.84                     | 0.59              |
| 1:AI:5:GLY:HA3   | 1:AI:15:PRO:HD3   | 1.84                     | 0.59              |
| 1:DD:201:ALA:O   | 1:DD:203:ASP:N    | 2.34                     | 0.59              |
| 1:A7:201:ALA:O   | 1:A7:203:ASP:N    | 2.34                     | 0.59              |
| 1:AA:159:PRO:CB  | 3:DB:29:VAL:HG21  | 271.05                   | 0.59              |
| 3:CR:42:ASN:HD22 | 3:CR:44:ILE:H     | 1.50                     | 0.59              |
| 3:CU:42:ASN:HD22 | 3:CU:44:ILE:H     | 1.50                     | 0.59              |
| 1:AA:5:GLY:HA3   | 1:AA:15:PRO:HD3   | 1.84                     | 0.59              |
| 1:AU:159:PRO:CB  | 3:CV:29:VAL:HG21  | 2.33                     | 0.59              |
| 1:AU:159:PRO:HB2 | 3:CV:29:VAL:HG21  | 1.84                     | 0.59              |
| 1:A2:159:PRO:CB  | 3:C3:29:VAL:HG21  | 2.33                     | 0.59              |
| 1:AR:163:MET:CE  | 1:AR:189:GLY:HA3  | 2.31                     | 0.59              |
| 1:A6:201:ALA:O   | 1:A6:203:ASP:N    | 2.34                     | 0.59              |
| 1:A0:163:MET:CE  | 1:A0:189:GLY:HA3  | 2.31                     | 0.59              |
| 2:BU:137:GLU:C   | 2:BU:139:ALA:N    | 2.54                     | 0.59              |
| 1:A1:181:LYS:O   | 1:A1:182:ALA:HB2  | 2.01                     | 0.59              |
| 2:BF:85:SER:HB2  | 2:BF:190:ASN:HD21 | 1.67                     | 0.59              |
| 2:B3:85:SER:HB2  | 2:B3:190:ASN:HD21 | 1.67                     | 0.59              |
| 3:CT:29:VAL:HG21 | 1:DF:159:PRO:CB   | 252.93                   | 0.59              |
| 1:AG:159:PRO:HB2 | 3:CH:29:VAL:HG21  | 52.33                    | 0.59              |
| 1:AI:159:PRO:HB2 | 3:CI:29:VAL:HG21  | 1.84                     | 0.59              |
| 1:AC:159:PRO:CB  | 3:CD:29:VAL:HG21  | 31.00                    | 0.59              |
| 1:AX:159:PRO:CB  | 3:CY:29:VAL:HG21  | 2.33                     | 0.59              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:DI:5:GLY:HA3   | 1:DI:15:PRO:HD3   | 1.85                     | 0.59              |
| 1:AA:159:PRO:HB2 | 3:CA:29:VAL:HG21  | 1.84                     | 0.59              |
| 1:AP:5:GLY:HA3   | 1:AP:15:PRO:HD3   | 1.85                     | 0.59              |
| 1:AZ:159:PRO:CB  | 3:C0:29:VAL:HG21  | 2.33                     | 0.59              |
| 1:AK:159:PRO:HB2 | 3:CL:29:VAL:HG21  | 1.84                     | 0.59              |
| 1:A3:201:ALA:O   | 1:A3:203:ASP:N    | 2.35                     | 0.59              |
| 1:AC:201:ALA:O   | 1:AC:203:ASP:N    | 2.34                     | 0.59              |
| 3:CX:42:ASN:HD22 | 3:CX:44:ILE:H     | 1.50                     | 0.59              |
| 1:DI:201:ALA:O   | 1:DI:203:ASP:N    | 2.35                     | 0.59              |
| 1:AG:163:MET:CE  | 1:AG:189:GLY:HA3  | 2.31                     | 0.59              |
| 3:CP:42:ASN:HD22 | 3:CP:44:ILE:H     | 1.50                     | 0.59              |
| 1:AP:181:LYS:O   | 1:AP:182:ALA:HB2  | 2.02                     | 0.59              |
| 2:BA:85:SER:HB2  | 2:BA:190:ASN:HD21 | 1.67                     | 0.59              |
| 2:B9:85:SER:HB2  | 2:B9:190:ASN:HD21 | 1.67                     | 0.59              |
| 2:B6:85:SER:HB2  | 2:B6:190:ASN:HD21 | 1.67                     | 0.59              |
| 1:AS:159:PRO:HB2 | 3:CT:29:VAL:HG21  | 1.84                     | 0.59              |
| 1:AE:159:PRO:CB  | 3:CE:29:VAL:HG21  | 2.33                     | 0.59              |
| 1:AE:159:PRO:CB  | 3:CF:29:VAL:HG21  | 120.21                   | 0.59              |
| 1:AF:159:PRO:CB  | 3:CG:29:VAL:HG21  | 31.00                    | 0.59              |
| 1:AC:5:GLY:HA3   | 1:AC:15:PRO:HD3   | 1.85                     | 0.59              |
| 1:AG:5:GLY:HA3   | 1:AG:15:PRO:HD3   | 1.85                     | 0.59              |
| 1:A9:5:GLY:HA3   | 1:A9:15:PRO:HD3   | 1.85                     | 0.59              |
| 1:AV:159:PRO:HB2 | 3:CW:29:VAL:HG21  | 1.84                     | 0.59              |
| 1:AA:159:PRO:HB2 | 3:DB:29:VAL:HG21  | 270.90                   | 0.59              |
| 1:DF:5:GLY:HA3   | 1:DF:15:PRO:HD3   | 1.85                     | 0.59              |
| 1:AS:5:GLY:HA3   | 1:AS:15:PRO:HD3   | 1.85                     | 0.59              |
| 1:DE:5:GLY:HA3   | 1:DE:15:PRO:HD3   | 1.85                     | 0.59              |
| 1:AN:159:PRO:CB  | 3:CO:29:VAL:HG21  | 2.33                     | 0.59              |
| 1:AN:159:PRO:HB2 | 3:CO:29:VAL:HG21  | 1.84                     | 0.59              |
| 1:AR:201:ALA:O   | 1:AR:203:ASP:N    | 2.34                     | 0.59              |
| 1:A0:5:GLY:HA3   | 1:A0:15:PRO:HD3   | 1.85                     | 0.59              |
| 1:A8:201:ALA:O   | 1:A8:203:ASP:N    | 2.35                     | 0.59              |
| 1:A4:5:GLY:HA3   | 1:A4:15:PRO:HD3   | 1.84                     | 0.59              |
| 1:AT:159:PRO:HB2 | 3:CU:29:VAL:HG21  | 1.84                     | 0.59              |
| 1:AQ:159:PRO:CB  | 3:CR:29:VAL:HG21  | 2.33                     | 0.59              |
| 1:A9:159:PRO:HB2 | 3:DA:29:VAL:HG21  | 1.84                     | 0.59              |
| 3:CN:42:ASN:HD22 | 3:CN:44:ILE:H     | 1.51                     | 0.59              |
| 2:B8:137:GLU:C   | 2:B8:139:ALA:N    | 2.54                     | 0.59              |
| 1:A8:181:LYS:HE3 | 2:B8:137:GLU:CB   | 2.31                     | 0.59              |
| 1:AC:181:LYS:O   | 1:AC:182:ALA:HB2  | 2.01                     | 0.59              |
| 2:BY:137:GLU:C   | 2:BY:139:ALA:N    | 2.55                     | 0.59              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:DG:181:LYS:O   | 1:DG:182:ALA:HB2  | 2.01                     | 0.59              |
| 1:A0:181:LYS:O   | 1:A0:182:ALA:HB2  | 2.02                     | 0.59              |
| 2:BU:85:SER:HB2  | 2:BU:190:ASN:HD21 | 1.67                     | 0.59              |
| 2:BT:85:SER:HB2  | 2:BT:190:ASN:HD21 | 1.67                     | 0.59              |
| 1:AL:159:PRO:CB  | 3:CM:29:VAL:HG21  | 2.33                     | 0.59              |
| 1:AH:5:GLY:HA3   | 1:AH:15:PRO:HD3   | 1.85                     | 0.59              |
| 1:AL:5:GLY:HA3   | 1:AL:15:PRO:HD3   | 1.85                     | 0.59              |
| 1:AA:159:PRO:CB  | 3:CA:29:VAL:HG21  | 2.33                     | 0.59              |
| 1:A9:159:PRO:CB  | 3:DA:29:VAL:HG21  | 2.33                     | 0.59              |
| 3:C7:42:ASN:HD22 | 3:C7:44:ILE:H     | 1.50                     | 0.59              |
| 1:AU:5:GLY:HA3   | 1:AU:15:PRO:HD3   | 1.85                     | 0.59              |
| 1:DG:201:ALA:O   | 1:DG:203:ASP:N    | 2.35                     | 0.59              |
| 2:BA:137:GLU:C   | 2:BA:139:ALA:N    | 2.54                     | 0.59              |
| 2:BD:137:GLU:C   | 2:BD:139:ALA:N    | 2.55                     | 0.59              |
| 2:BR:137:GLU:CB  | 1:DE:181:LYS:HE3  | 273.33                   | 0.59              |
| 2:B0:137:GLU:C   | 2:B0:139:ALA:N    | 2.55                     | 0.59              |
| 2:B4:137:GLU:C   | 2:B4:139:ALA:N    | 2.55                     | 0.59              |
| 2:B9:137:GLU:C   | 2:B9:139:ALA:N    | 2.55                     | 0.59              |
| 2:BR:85:SER:HB2  | 2:BR:190:ASN:HD21 | 1.67                     | 0.59              |
| 2:B7:85:SER:HB2  | 2:B7:190:ASN:HD21 | 1.67                     | 0.59              |
| 2:BZ:85:SER:HB2  | 2:BZ:190:ASN:HD21 | 1.67                     | 0.59              |
| 1:AD:159:PRO:CB  | 3:CE:29:VAL:HG21  | 52.61                    | 0.59              |
| 1:AE:159:PRO:HB2 | 3:CE:29:VAL:HG21  | 1.84                     | 0.59              |
| 1:AG:159:PRO:CB  | 3:CH:29:VAL:HG21  | 51.66                    | 0.59              |
| 1:AK:159:PRO:CB  | 3:CL:29:VAL:HG21  | 2.33                     | 0.59              |
| 3:CU:29:VAL:HG21 | 1:DG:159:PRO:HB2  | 240.21                   | 0.59              |
| 1:A2:5:GLY:HA3   | 1:A2:15:PRO:HD3   | 1.85                     | 0.59              |
| 3:C8:42:ASN:HD22 | 3:C8:44:ILE:H     | 1.50                     | 0.59              |
| 1:AY:5:GLY:HA3   | 1:AY:15:PRO:HD3   | 1.85                     | 0.59              |
| 3:CB:42:ASN:HD22 | 3:CB:44:ILE:H     | 1.50                     | 0.59              |
| 3:CV:42:ASN:HD22 | 3:CV:44:ILE:H     | 1.50                     | 0.59              |
| 1:A7:5:GLY:HA3   | 1:A7:15:PRO:HD3   | 1.85                     | 0.59              |
| 2:BP:137:GLU:C   | 2:BP:139:ALA:N    | 2.54                     | 0.59              |
| 2:B5:137:GLU:C   | 2:B5:139:ALA:N    | 2.54                     | 0.59              |
| 2:BL:85:SER:HB2  | 2:BL:190:ASN:HD21 | 1.67                     | 0.59              |
| 2:BX:85:SER:HB2  | 2:BX:190:ASN:HD21 | 1.67                     | 0.59              |
| 1:AZ:163:MET:HE1 | 1:AZ:189:GLY:HA3  | 1.85                     | 0.59              |
| 1:AH:159:PRO:CB  | 3:CI:29:VAL:HG21  | 31.00                    | 0.59              |
| 1:AJ:159:PRO:CB  | 3:CK:29:VAL:HG21  | 2.33                     | 0.59              |
| 1:A4:159:PRO:CB  | 3:C5:29:VAL:HG21  | 2.33                     | 0.59              |
| 1:A1:159:PRO:CB  | 3:C2:29:VAL:HG21  | 2.33                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:DK:5:GLY:HA3    | 1:DK:15:PRO:HD3   | 1.85                     | 0.59              |
| 3:CV:29:VAL:HG21  | 1:DH:159:PRO:CB   | 268.09                   | 0.59              |
| 1:AZ:159:PRO:HB2  | 3:C0:29:VAL:HG21  | 1.84                     | 0.59              |
| 1:A5:5:GLY:HA3    | 1:A5:15:PRO:HD3   | 1.85                     | 0.59              |
| 3:CO:42:ASN:HD22  | 3:CO:44:ILE:H     | 1.50                     | 0.59              |
| 1:AT:5:GLY:HA3    | 1:AT:15:PRO:HD3   | 1.85                     | 0.59              |
| 1:AJ:181:LYS:HE3  | 2:BK:137:GLU:CB   | 2.31                     | 0.59              |
| 1:AC:163:MET:HE1  | 1:AC:189:GLY:HA3  | 1.92                     | 0.59              |
| 1:AF:159:PRO:CB   | 3:CF:29:VAL:HG21  | 2.33                     | 0.59              |
| 1:AI:159:PRO:HB2  | 3:CJ:29:VAL:HG21  | 53.35                    | 0.59              |
| 1:AB:159:PRO:HB2  | 3:CB:29:VAL:HG21  | 1.84                     | 0.59              |
| 1:AB:159:PRO:CB   | 3:CC:29:VAL:HG21  | 51.66                    | 0.59              |
| 3:CX:29:VAL:HG21  | 1:DJ:159:PRO:CB   | 245.79                   | 0.59              |
| 1:AP:159:PRO:CB   | 3:CQ:29:VAL:HG21  | 2.33                     | 0.59              |
| 3:CW:29:VAL:HG21  | 1:DI:159:PRO:HB2  | 243.01                   | 0.59              |
| 1:DG:163:MET:CE   | 1:DG:189:GLY:HA3  | 2.31                     | 0.59              |
| 2:B3:137:GLU:C    | 2:B3:139:ALA:N    | 2.54                     | 0.58              |
| 2:BI:85:SER:HB2   | 2:BI:190:ASN:HD21 | 1.67                     | 0.58              |
| 1:AG:159:PRO:CB   | 3:CG:29:VAL:HG21  | 2.33                     | 0.58              |
| 3:CS:29:VAL:HG21  | 1:DE:159:PRO:CB   | 268.10                   | 0.58              |
| 1:AQ:159:PRO:HB2  | 3:CR:29:VAL:HG21  | 1.84                     | 0.58              |
| 3:CZ:42:ASN:HD22  | 3:CZ:44:ILE:H     | 1.50                     | 0.58              |
| 2:BD:126:VAL:HG13 | 2:BD:171:VAL:HG21 | 1.85                     | 0.58              |
| 3:CT:42:ASN:HD22  | 3:CT:44:ILE:H     | 1.50                     | 0.58              |
| 3:DA:42:ASN:HD22  | 3:DA:44:ILE:H     | 1.50                     | 0.58              |
| 3:CM:42:ASN:HD22  | 3:CM:44:ILE:H     | 1.50                     | 0.58              |
| 3:CL:42:ASN:HD22  | 3:CL:44:ILE:H     | 1.50                     | 0.58              |
| 1:A8:5:GLY:HA3    | 1:A8:15:PRO:HD3   | 1.84                     | 0.58              |
| 2:B6:126:VAL:HG13 | 2:B6:171:VAL:HG21 | 1.85                     | 0.58              |
| 1:A5:159:PRO:CB   | 3:C6:29:VAL:HG21  | 2.33                     | 0.58              |
| 3:CG:42:ASN:HD22  | 3:CG:44:ILE:H     | 1.50                     | 0.58              |
| 2:BK:137:GLU:C    | 2:BK:139:ALA:N    | 2.55                     | 0.58              |
| 2:BQ:137:GLU:C    | 2:BQ:139:ALA:N    | 2.55                     | 0.58              |
| 2:B8:85:SER:HB2   | 2:B8:190:ASN:HD21 | 1.67                     | 0.58              |
| 2:B5:85:SER:HB2   | 2:B5:190:ASN:HD21 | 1.67                     | 0.58              |
| 1:AS:159:PRO:CB   | 3:CT:29:VAL:HG21  | 2.33                     | 0.58              |
| 1:AG:159:PRO:HB2  | 3:CG:29:VAL:HG21  | 1.84                     | 0.58              |
| 1:AW:159:PRO:CB   | 3:CX:29:VAL:HG21  | 2.33                     | 0.58              |
| 1:A3:5:GLY:HA3    | 1:A3:15:PRO:HD3   | 1.84                     | 0.58              |
| 1:AV:159:PRO:CB   | 3:CW:29:VAL:HG21  | 2.33                     | 0.58              |
| 1:AT:159:PRO:CB   | 3:CU:29:VAL:HG21  | 2.33                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A5:159:PRO:HB2  | 3:C6:29:VAL:HG21  | 1.84                     | 0.58              |
| 3:CH:42:ASN:HD22  | 3:CH:44:ILE:H     | 1.50                     | 0.58              |
| 2:B8:126:VAL:HG13 | 2:B8:171:VAL:HG21 | 1.85                     | 0.58              |
| 3:C4:42:ASN:HD22  | 3:C4:44:ILE:H     | 1.50                     | 0.58              |
| 3:CF:42:ASN:HD22  | 3:CF:44:ILE:H     | 1.50                     | 0.58              |
| 1:AD:87:GLN:NE2   | 1:AD:210:ARG:HH12 | 2.02                     | 0.58              |
| 1:A7:163:MET:HE1  | 1:A7:189:GLY:HA3  | 1.84                     | 0.58              |
| 1:AD:159:PRO:CB   | 3:CD:29:VAL:HG21  | 2.33                     | 0.58              |
| 1:A2:159:PRO:HB2  | 3:C3:29:VAL:HG21  | 1.84                     | 0.58              |
| 3:CR:29:VAL:HG21  | 1:DD:159:PRO:HB2  | 226.62                   | 0.58              |
| 3:CY:42:ASN:HD22  | 3:CY:44:ILE:H     | 1.50                     | 0.58              |
| 2:BY:126:VAL:HG13 | 2:BY:171:VAL:HG21 | 1.86                     | 0.58              |
| 2:BC:126:VAL:HG13 | 2:BC:171:VAL:HG21 | 1.86                     | 0.58              |
| 2:B3:126:VAL:HG13 | 2:B3:171:VAL:HG21 | 1.86                     | 0.58              |
| 2:BL:126:VAL:HG13 | 2:BL:171:VAL:HG21 | 1.86                     | 0.58              |
| 2:BQ:126:VAL:HG13 | 2:BQ:171:VAL:HG21 | 1.85                     | 0.58              |
| 2:BZ:126:VAL:HG13 | 2:BZ:171:VAL:HG21 | 1.85                     | 0.58              |
| 2:BF:137:GLU:C    | 2:BF:139:ALA:N    | 2.54                     | 0.58              |
| 1:AN:87:GLN:NE2   | 1:AN:210:ARG:HH12 | 2.02                     | 0.58              |
| 3:CR:29:VAL:HG21  | 1:DD:159:PRO:CB   | 227.49                   | 0.58              |
| 2:BL:49:ASP:OD2   | 3:CL:161:SER:OG   | 62.83                    | 0.58              |
| 2:BN:49:ASP:OD2   | 3:CM:161:SER:OG   | 2.22                     | 0.58              |
| 2:BT:126:VAL:HG13 | 2:BT:171:VAL:HG21 | 1.86                     | 0.58              |
| 2:BO:126:VAL:HG13 | 2:BO:171:VAL:HG21 | 1.86                     | 0.58              |
| 2:BV:126:VAL:HG13 | 2:BV:171:VAL:HG21 | 1.86                     | 0.58              |
| 1:A1:5:GLY:HA3    | 1:A1:15:PRO:HD3   | 1.85                     | 0.58              |
| 2:BQ:134:HIS:O    | 2:BQ:136:HIS:N    | 2.37                     | 0.58              |
| 2:B7:137:GLU:C    | 2:B7:139:ALA:N    | 2.55                     | 0.58              |
| 1:AC:87:GLN:NE2   | 1:AC:210:ARG:HH12 | 2.02                     | 0.58              |
| 1:A5:87:GLN:NE2   | 1:A5:210:ARG:HH12 | 2.02                     | 0.58              |
| 1:AB:159:PRO:HB2  | 3:CC:29:VAL:HG21  | 52.33                    | 0.58              |
| 1:AD:159:PRO:HB2  | 3:CD:29:VAL:HG21  | 1.84                     | 0.58              |
| 1:A6:159:PRO:CB   | 3:C7:29:VAL:HG21  | 2.33                     | 0.58              |
| 1:DD:5:GLY:HA3    | 1:DD:15:PRO:HD3   | 1.84                     | 0.58              |
| 2:BN:49:ASP:OD2   | 3:CR:161:SER:OG   | 241.62                   | 0.58              |
| 1:AQ:201:ALA:O    | 1:AQ:203:ASP:N    | 2.35                     | 0.58              |
| 2:BK:126:VAL:HG13 | 2:BK:171:VAL:HG21 | 1.86                     | 0.58              |
| 2:BG:126:VAL:HG13 | 2:BG:171:VAL:HG21 | 1.86                     | 0.58              |
| 2:BN:126:VAL:HG13 | 2:BN:171:VAL:HG21 | 1.85                     | 0.58              |
| 1:AO:159:PRO:HB2  | 3:CP:29:VAL:HG21  | 1.84                     | 0.58              |
| 1:AO:159:PRO:CB   | 3:CP:29:VAL:HG21  | 2.33                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BW:134:HIS:O    | 2:BW:136:HIS:N    | 2.36                     | 0.58              |
| 1:AU:87:GLN:NE2   | 1:AU:210:ARG:HH12 | 2.02                     | 0.58              |
| 1:AH:87:GLN:NE2   | 1:AH:210:ARG:HH12 | 2.02                     | 0.58              |
| 1:AO:87:GLN:NE2   | 1:AO:210:ARG:HH12 | 2.02                     | 0.58              |
| 1:DH:87:GLN:NE2   | 1:DH:210:ARG:HH12 | 2.02                     | 0.58              |
| 1:A7:87:GLN:NE2   | 1:A7:210:ARG:HH12 | 2.02                     | 0.58              |
| 2:BC:85:SER:HB2   | 2:BC:190:ASN:HD21 | 1.67                     | 0.58              |
| 1:AY:87:GLN:NE2   | 1:AY:210:ARG:HH12 | 2.02                     | 0.58              |
| 1:AT:87:GLN:NE2   | 1:AT:210:ARG:HH12 | 2.02                     | 0.58              |
| 1:AB:159:PRO:CB   | 3:CB:29:VAL:HG21  | 2.33                     | 0.58              |
| 3:CQ:29:VAL:HG21  | 1:DC:159:PRO:CB   | 243.51                   | 0.58              |
| 1:A3:159:PRO:HB2  | 3:C4:29:VAL:HG21  | 1.84                     | 0.58              |
| 1:DC:5:GLY:HA3    | 1:DC:15:PRO:HD3   | 1.84                     | 0.58              |
| 1:DG:5:GLY:HA3    | 1:DG:15:PRO:HD3   | 1.84                     | 0.58              |
| 2:BR:126:VAL:HG13 | 2:BR:171:VAL:HG21 | 1.86                     | 0.58              |
| 2:B2:126:VAL:HG13 | 2:B2:171:VAL:HG21 | 1.86                     | 0.58              |
| 2:BJ:126:VAL:HG13 | 2:BJ:171:VAL:HG21 | 1.86                     | 0.58              |
| 2:B6:137:GLU:C    | 2:B6:139:ALA:N    | 2.54                     | 0.58              |
| 1:AL:87:GLN:NE2   | 1:AL:210:ARG:HH12 | 2.02                     | 0.58              |
| 1:AI:159:PRO:CB   | 3:CI:29:VAL:HG21  | 2.33                     | 0.58              |
| 3:CJ:29:VAL:HG21  | 1:DK:159:PRO:CB   | 2.33                     | 0.58              |
| 1:A0:159:PRO:CB   | 3:C1:29:VAL:HG21  | 2.33                     | 0.58              |
| 3:CQ:29:VAL:HG21  | 1:DC:159:PRO:HB2  | 243.02                   | 0.58              |
| 1:DH:5:GLY:HA3    | 1:DH:15:PRO:HD3   | 1.84                     | 0.58              |
| 2:BR:49:ASP:OD2   | 3:CL:161:SER:OG   | 2.22                     | 0.58              |
| 2:B7:49:ASP:OD2   | 3:C5:161:SER:OG   | 2.22                     | 0.58              |
| 2:B0:126:VAL:HG13 | 2:B0:171:VAL:HG21 | 1.86                     | 0.58              |
| 2:B0:49:ASP:OD2   | 3:CZ:161:SER:OG   | 2.22                     | 0.58              |
| 2:BF:126:VAL:HG13 | 2:BF:171:VAL:HG21 | 1.86                     | 0.58              |
| 2:B6:134:HIS:O    | 2:B6:136:HIS:N    | 2.36                     | 0.58              |
| 2:BO:137:GLU:C    | 2:BO:139:ALA:N    | 2.54                     | 0.58              |
| 2:BS:137:GLU:C    | 2:BS:139:ALA:N    | 2.55                     | 0.58              |
| 1:AM:87:GLN:NE2   | 1:AM:210:ARG:HH12 | 2.02                     | 0.58              |
| 1:A8:87:GLN:NE2   | 1:A8:210:ARG:HH12 | 2.02                     | 0.58              |
| 1:AE:87:GLN:NE2   | 1:AE:210:ARG:HH12 | 2.02                     | 0.58              |
| 2:BK:132:TYR:HB3  | 2:BK:193:THR:CG2  | 2.34                     | 0.58              |
| 1:AP:87:GLN:NE2   | 1:AP:210:ARG:HH12 | 2.02                     | 0.58              |
| 2:BE:114:VAL:HG22 | 2:BE:209:VAL:HG12 | 1.86                     | 0.58              |
| 2:BO:114:VAL:HG22 | 2:BO:209:VAL:HG12 | 1.86                     | 0.58              |
| 1:AA:163:MET:HE1  | 1:AA:189:GLY:HA3  | 1.92                     | 0.58              |
| 1:AY:159:PRO:CB   | 3:CZ:29:VAL:HG21  | 2.33                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:CU:29:VAL:HG21  | 1:DG:159:PRO:CB   | 240.63                   | 0.58              |
| 2:BR:49:ASP:OD2   | 3:CP:161:SER:OG   | 239.86                   | 0.58              |
| 2:BC:49:ASP:OD2   | 3:DA:161:SER:OG   | 261.04                   | 0.58              |
| 2:BF:134:HIS:O    | 2:BF:136:HIS:N    | 2.36                     | 0.58              |
| 2:B2:134:HIS:O    | 2:B2:136:HIS:N    | 2.36                     | 0.58              |
| 1:AG:87:GLN:NE2   | 1:AG:210:ARG:HH12 | 2.02                     | 0.58              |
| 1:DD:87:GLN:NE2   | 1:DD:210:ARG:HH12 | 2.02                     | 0.58              |
| 1:AZ:87:GLN:NE2   | 1:AZ:210:ARG:HH12 | 2.02                     | 0.58              |
| 1:DJ:87:GLN:NE2   | 1:DJ:210:ARG:HH12 | 2.02                     | 0.58              |
| 2:BL:132:TYR:HB3  | 2:BL:193:THR:CG2  | 2.34                     | 0.58              |
| 2:BE:132:TYR:HB3  | 2:BE:193:THR:CG2  | 2.34                     | 0.58              |
| 2:BX:132:TYR:HB3  | 2:BX:193:THR:CG2  | 2.34                     | 0.58              |
| 2:BV:132:TYR:HB3  | 2:BV:193:THR:CG2  | 2.34                     | 0.58              |
| 2:BV:85:SER:HB2   | 2:BV:190:ASN:HD21 | 1.67                     | 0.58              |
| 2:B5:132:TYR:HB3  | 2:B5:193:THR:CG2  | 2.34                     | 0.58              |
| 2:B2:132:TYR:HB3  | 2:B2:193:THR:CG2  | 2.34                     | 0.58              |
| 3:CV:29:VAL:HG21  | 1:DH:159:PRO:HB2  | 267.88                   | 0.58              |
| 2:BI:49:ASP:OD2   | 3:CH:161:SER:OG   | 2.22                     | 0.58              |
| 2:BM:49:ASP:OD2   | 3:CO:161:SER:OG   | 2.22                     | 0.58              |
| 2:BC:49:ASP:OD2   | 3:CE:161:SER:OG   | 2.22                     | 0.58              |
| 2:BB:49:ASP:OD2   | 3:CA:161:SER:OG   | 2.22                     | 0.58              |
| 2:BB:49:ASP:OD2   | 3:DB:161:SER:OG   | 244.63                   | 0.58              |
| 2:BA:49:ASP:OD2   | 3:CD:161:SER:OG   | 2.22                     | 0.58              |
| 2:BP:126:VAL:HG13 | 2:BP:171:VAL:HG21 | 1.86                     | 0.58              |
| 2:BS:126:VAL:HG13 | 2:BS:171:VAL:HG21 | 1.86                     | 0.58              |
| 1:AA:87:GLN:NE2   | 1:AA:210:ARG:HH12 | 2.02                     | 0.58              |
| 1:AS:87:GLN:NE2   | 1:AS:210:ARG:HH12 | 2.02                     | 0.58              |
| 1:AF:87:GLN:NE2   | 1:AF:210:ARG:HH12 | 2.02                     | 0.58              |
| 1:A2:87:GLN:NE2   | 1:A2:210:ARG:HH12 | 2.02                     | 0.58              |
| 1:A1:87:GLN:NE2   | 1:A1:210:ARG:HH12 | 2.02                     | 0.58              |
| 2:B0:85:SER:HB2   | 2:B0:190:ASN:HD21 | 1.68                     | 0.58              |
| 2:BA:132:TYR:HB3  | 2:BA:193:THR:CG2  | 2.34                     | 0.58              |
| 2:BJ:132:TYR:HB3  | 2:BJ:193:THR:CG2  | 2.34                     | 0.58              |
| 2:BN:132:TYR:HB3  | 2:BN:193:THR:CG2  | 2.34                     | 0.58              |
| 2:B1:132:TYR:HB3  | 2:B1:193:THR:CG2  | 2.34                     | 0.58              |
| 2:BS:114:VAL:HG22 | 2:BS:209:VAL:HG12 | 1.86                     | 0.58              |
| 1:A9:163:MET:HE1  | 1:A9:189:GLY:HA3  | 1.86                     | 0.58              |
| 2:B8:49:ASP:OD2   | 3:CC:161:SER:OG   | 239.86                   | 0.58              |
| 2:BI:97:VAL:O     | 2:BI:101:HIS:HD2  | 1.87                     | 0.58              |
| 2:BF:97:VAL:O     | 2:BF:101:HIS:HD2  | 1.87                     | 0.58              |
| 3:CI:42:ASN:HD22  | 3:CI:44:ILE:H     | 1.51                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BY:97:VAL:O     | 2:BY:101:HIS:HD2  | 1.87                     | 0.58              |
| 2:BQ:97:VAL:O     | 2:BQ:101:HIS:HD2  | 1.87                     | 0.58              |
| 2:BV:49:ASP:OD2   | 3:CU:161:SER:OG   | 2.22                     | 0.58              |
| 2:BC:97:VAL:O     | 2:BC:101:HIS:HD2  | 1.87                     | 0.58              |
| 2:BU:97:VAL:O     | 2:BU:101:HIS:HD2  | 1.87                     | 0.58              |
| 2:BK:97:VAL:O     | 2:BK:101:HIS:HD2  | 1.87                     | 0.58              |
| 2:B5:49:ASP:OD2   | 3:C8:161:SER:OG   | 2.22                     | 0.58              |
| 2:B2:97:VAL:O     | 2:B2:101:HIS:HD2  | 1.87                     | 0.58              |
| 2:BM:97:VAL:O     | 2:BM:101:HIS:HD2  | 1.87                     | 0.58              |
| 2:BP:97:VAL:O     | 2:BP:101:HIS:HD2  | 1.87                     | 0.58              |
| 1:AI:87:GLN:NE2   | 1:AI:210:ARG:HH12 | 2.02                     | 0.57              |
| 1:AK:87:GLN:NE2   | 1:AK:210:ARG:HH12 | 2.02                     | 0.57              |
| 1:AR:87:GLN:NE2   | 1:AR:210:ARG:HH12 | 2.02                     | 0.57              |
| 1:A3:87:GLN:NE2   | 1:A3:210:ARG:HH12 | 2.02                     | 0.57              |
| 2:B0:132:TYR:HB3  | 2:B0:193:THR:CG2  | 2.34                     | 0.57              |
| 1:AX:87:GLN:NE2   | 1:AX:210:ARG:HH12 | 2.02                     | 0.57              |
| 2:B7:132:TYR:HB3  | 2:B7:193:THR:CG2  | 2.34                     | 0.57              |
| 2:BS:132:TYR:HB3  | 2:BS:193:THR:CG2  | 2.34                     | 0.57              |
| 2:B4:132:TYR:HB3  | 2:B4:193:THR:CG2  | 2.34                     | 0.57              |
| 2:B6:132:TYR:HB3  | 2:B6:193:THR:CG2  | 2.34                     | 0.57              |
| 2:BZ:132:TYR:HB3  | 2:BZ:193:THR:CG2  | 2.34                     | 0.57              |
| 1:A0:163:MET:HE1  | 1:A0:189:GLY:HA3  | 1.86                     | 0.57              |
| 2:BP:49:ASP:OD2   | 3:CT:161:SER:OG   | 2.22                     | 0.57              |
| 2:BI:49:ASP:OD2   | 3:CM:161:SER:OG   | 122.36                   | 0.57              |
| 2:B5:126:VAL:HG13 | 2:B5:171:VAL:HG21 | 1.85                     | 0.57              |
| 2:B4:97:VAL:O     | 2:B4:101:HIS:HD2  | 1.87                     | 0.57              |
| 2:BZ:97:VAL:O     | 2:BZ:101:HIS:HD2  | 1.87                     | 0.57              |
| 2:BI:126:VAL:HG13 | 2:BI:171:VAL:HG21 | 1.85                     | 0.57              |
| 2:BU:49:ASP:OD2   | 3:CX:161:SER:OG   | 2.22                     | 0.57              |
| 2:BW:126:VAL:HG13 | 2:BW:171:VAL:HG21 | 1.85                     | 0.57              |
| 2:B7:97:VAL:O     | 2:B7:101:HIS:HD2  | 1.87                     | 0.57              |
| 2:BJ:97:VAL:O     | 2:BJ:101:HIS:HD2  | 1.87                     | 0.57              |
| 2:BH:49:ASP:OD2   | 3:CF:161:SER:OG   | 101.79                   | 0.57              |
| 3:C3:42:ASN:HD22  | 3:C3:44:ILE:H     | 1.50                     | 0.57              |
| 2:BM:134:HIS:O    | 2:BM:136:HIS:N    | 2.36                     | 0.57              |
| 1:AU:87:GLN:NE2   | 1:AU:210:ARG:HH22 | 2.02                     | 0.57              |
| 1:AD:87:GLN:NE2   | 1:AD:210:ARG:HH22 | 2.02                     | 0.57              |
| 1:AL:87:GLN:NE2   | 1:AL:210:ARG:HH22 | 2.02                     | 0.57              |
| 1:AW:87:GLN:NE2   | 1:AW:210:ARG:HH12 | 2.02                     | 0.57              |
| 1:A3:87:GLN:NE2   | 1:A3:210:ARG:HH22 | 2.03                     | 0.57              |
| 1:A2:87:GLN:NE2   | 1:A2:210:ARG:HH22 | 2.03                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:DE:87:GLN:NE2   | 1:DE:210:ARG:HH12 | 2.02                     | 0.57              |
| 2:BB:132:TYR:HB3  | 2:BB:193:THR:CG2  | 2.34                     | 0.57              |
| 2:BM:132:TYR:HB3  | 2:BM:193:THR:CG2  | 2.34                     | 0.57              |
| 2:BO:132:TYR:HB3  | 2:BO:193:THR:CG2  | 2.34                     | 0.57              |
| 2:BG:132:TYR:HB3  | 2:BG:193:THR:CG2  | 2.34                     | 0.57              |
| 2:B3:132:TYR:HB3  | 2:B3:193:THR:CG2  | 2.34                     | 0.57              |
| 2:BG:114:VAL:HG22 | 2:BG:209:VAL:HG12 | 1.86                     | 0.57              |
| 2:BT:114:VAL:HG22 | 2:BT:209:VAL:HG12 | 1.86                     | 0.57              |
| 2:BD:114:VAL:HG22 | 2:BD:209:VAL:HG12 | 1.86                     | 0.57              |
| 2:B9:114:VAL:HG22 | 2:B9:209:VAL:HG12 | 1.86                     | 0.57              |
| 2:BK:114:VAL:HG22 | 2:BK:209:VAL:HG12 | 1.86                     | 0.57              |
| 2:BQ:114:VAL:HG22 | 2:BQ:209:VAL:HG12 | 1.86                     | 0.57              |
| 1:AB:163:MET:HE1  | 1:AB:189:GLY:HA3  | 1.86                     | 0.57              |
| 3:CC:44:ILE:O     | 3:CC:48:LYS:HG3   | 2.05                     | 0.57              |
| 3:DB:44:ILE:O     | 3:DB:48:LYS:HG3   | 2.05                     | 0.57              |
| 3:CE:44:ILE:O     | 3:CE:48:LYS:HG3   | 2.04                     | 0.57              |
| 3:CO:44:ILE:O     | 3:CO:48:LYS:HG3   | 2.05                     | 0.57              |
| 2:BW:49:ASP:OD2   | 3:CU:161:SER:OG   | 101.79                   | 0.57              |
| 2:BJ:49:ASP:OD2   | 3:CJ:161:SER:OG   | 62.83                    | 0.57              |
| 2:BA:97:VAL:O     | 2:BA:101:HIS:HD2  | 1.87                     | 0.57              |
| 2:BM:126:VAL:HG13 | 2:BM:171:VAL:HG21 | 1.85                     | 0.57              |
| 2:BV:97:VAL:O     | 2:BV:101:HIS:HD2  | 1.87                     | 0.57              |
| 2:BB:97:VAL:O     | 2:BB:101:HIS:HD2  | 1.87                     | 0.57              |
| 2:B4:49:ASP:OD2   | 3:C7:161:SER:OG   | 2.22                     | 0.57              |
| 3:CW:42:ASN:HD22  | 3:CW:44:ILE:H     | 1.50                     | 0.57              |
| 2:B1:97:VAL:O     | 2:B1:101:HIS:HD2  | 1.87                     | 0.57              |
| 1:AV:87:GLN:NE2   | 1:AV:210:ARG:HH12 | 2.02                     | 0.57              |
| 1:A4:87:GLN:NE2   | 1:A4:210:ARG:HH22 | 2.03                     | 0.57              |
| 1:A9:87:GLN:NE2   | 1:A9:210:ARG:HH12 | 2.02                     | 0.57              |
| 1:DI:87:GLN:NE2   | 1:DI:210:ARG:HH12 | 2.02                     | 0.57              |
| 1:DG:87:GLN:NE2   | 1:DG:210:ARG:HH12 | 2.02                     | 0.57              |
| 2:BT:132:TYR:HB3  | 2:BT:193:THR:CG2  | 2.34                     | 0.57              |
| 1:DC:87:GLN:NE2   | 1:DC:210:ARG:HH12 | 2.02                     | 0.57              |
| 2:BH:132:TYR:HB3  | 2:BH:193:THR:CG2  | 2.34                     | 0.57              |
| 1:AW:159:PRO:HB2  | 3:CX:29:VAL:HG21  | 1.84                     | 0.57              |
| 3:CR:44:ILE:O     | 3:CR:48:LYS:HG3   | 2.05                     | 0.57              |
| 2:B6:97:VAL:O     | 2:B6:101:HIS:HD2  | 1.87                     | 0.57              |
| 2:B9:126:VAL:HG13 | 2:B9:171:VAL:HG21 | 1.86                     | 0.57              |
| 3:C6:42:ASN:HD22  | 3:C6:44:ILE:H     | 1.50                     | 0.57              |
| 2:BU:126:VAL:HG13 | 2:BU:171:VAL:HG21 | 1.86                     | 0.57              |
| 3:C0:42:ASN:HD22  | 3:C0:44:ILE:H     | 1.51                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BH:97:VAL:O     | 2:BH:101:HIS:HD2  | 1.87                     | 0.57              |
| 2:BS:97:VAL:O     | 2:BS:101:HIS:HD2  | 1.87                     | 0.57              |
| 2:BL:97:VAL:O     | 2:BL:101:HIS:HD2  | 1.87                     | 0.57              |
| 2:B5:97:VAL:O     | 2:B5:101:HIS:HD2  | 1.87                     | 0.57              |
| 2:BA:134:HIS:O    | 2:BA:136:HIS:N    | 2.36                     | 0.57              |
| 2:BH:134:HIS:O    | 2:BH:136:HIS:N    | 2.36                     | 0.57              |
| 2:BK:134:HIS:O    | 2:BK:136:HIS:N    | 2.36                     | 0.57              |
| 2:BZ:137:GLU:C    | 2:BZ:139:ALA:N    | 2.54                     | 0.57              |
| 1:AC:87:GLN:NE2   | 1:AC:210:ARG:HH22 | 2.02                     | 0.57              |
| 1:AM:87:GLN:NE2   | 1:AM:210:ARG:HH22 | 2.02                     | 0.57              |
| 1:AV:87:GLN:NE2   | 1:AV:210:ARG:HH22 | 2.02                     | 0.57              |
| 1:A6:87:GLN:NE2   | 1:A6:210:ARG:HH12 | 2.02                     | 0.57              |
| 1:DG:87:GLN:NE2   | 1:DG:210:ARG:HH22 | 2.03                     | 0.57              |
| 2:BR:132:TYR:HB3  | 2:BR:193:THR:CG2  | 2.34                     | 0.57              |
| 2:BQ:132:TYR:HB3  | 2:BQ:193:THR:CG2  | 2.34                     | 0.57              |
| 3:CH:44:ILE:O     | 3:CH:48:LYS:HG3   | 2.04                     | 0.57              |
| 2:BQ:49:ASP:OD2   | 3:CR:161:SER:OG   | 2.22                     | 0.57              |
| 3:CW:44:ILE:O     | 3:CW:48:LYS:HG3   | 2.04                     | 0.57              |
| 2:BO:97:VAL:O     | 2:BO:101:HIS:HD2  | 1.87                     | 0.57              |
| 2:BG:134:HIS:O    | 2:BG:136:HIS:N    | 2.36                     | 0.57              |
| 2:BW:137:GLU:C    | 2:BW:139:ALA:N    | 2.55                     | 0.57              |
| 1:AH:87:GLN:NE2   | 1:AH:210:ARG:HH22 | 2.03                     | 0.57              |
| 1:AJ:87:GLN:NE2   | 1:AJ:210:ARG:HH22 | 2.02                     | 0.57              |
| 1:A4:87:GLN:NE2   | 1:A4:210:ARG:HH12 | 2.02                     | 0.57              |
| 1:AF:87:GLN:NE2   | 1:AF:210:ARG:HH22 | 2.03                     | 0.57              |
| 1:AQ:87:GLN:NE2   | 1:AQ:210:ARG:HH22 | 2.03                     | 0.57              |
| 2:BL:114:VAL:HG22 | 2:BL:209:VAL:HG12 | 1.86                     | 0.57              |
| 2:BH:114:VAL:HG22 | 2:BH:209:VAL:HG12 | 1.86                     | 0.57              |
| 3:CJ:44:ILE:O     | 3:CJ:48:LYS:HG3   | 2.05                     | 0.57              |
| 3:CB:44:ILE:O     | 3:CB:48:LYS:HG3   | 2.05                     | 0.57              |
| 2:BM:49:ASP:OD2   | 3:CK:161:SER:OG   | 101.79                   | 0.57              |
| 2:BQ:49:ASP:OD2   | 3:CQ:161:SER:OG   | 101.79                   | 0.57              |
| 2:BY:49:ASP:OD2   | 3:CV:161:SER:OG   | 2.22                     | 0.57              |
| 2:BO:54:LEU:HD21  | 2:BO:97:VAL:HG11  | 1.87                     | 0.57              |
| 2:BB:126:VAL:HG13 | 2:BB:171:VAL:HG21 | 1.86                     | 0.57              |
| 2:BK:49:ASP:OD2   | 3:CN:161:SER:OG   | 2.22                     | 0.57              |
| 2:B1:49:ASP:OD2   | 3:C3:161:SER:OG   | 2.22                     | 0.57              |
| 2:BX:126:VAL:HG13 | 2:BX:171:VAL:HG21 | 1.86                     | 0.57              |
| 2:BN:97:VAL:O     | 2:BN:101:HIS:HD2  | 1.87                     | 0.57              |
| 2:BF:49:ASP:OD2   | 3:CI:161:SER:OG   | 2.22                     | 0.57              |
| 2:BY:134:HIS:O    | 2:BY:136:HIS:N    | 2.36                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A1:87:GLN:NE2   | 1:A1:210:ARG:HH22 | 2.02                     | 0.57              |
| 2:BW:132:TYR:HB3  | 2:BW:193:THR:CG2  | 2.34                     | 0.57              |
| 1:AQ:87:GLN:NE2   | 1:AQ:210:ARG:HH12 | 2.02                     | 0.57              |
| 2:BF:132:TYR:HB3  | 2:BF:193:THR:CG2  | 2.34                     | 0.57              |
| 1:AT:87:GLN:NE2   | 1:AT:210:ARG:HH22 | 2.03                     | 0.57              |
| 2:BD:132:TYR:HB3  | 2:BD:193:THR:CG2  | 2.34                     | 0.57              |
| 2:BB:114:VAL:HG22 | 2:BB:209:VAL:HG12 | 1.86                     | 0.57              |
| 2:BJ:114:VAL:HG22 | 2:BJ:209:VAL:HG12 | 1.86                     | 0.57              |
| 3:CS:44:ILE:O     | 3:CS:48:LYS:HG3   | 2.04                     | 0.57              |
| 3:CM:44:ILE:O     | 3:CM:48:LYS:HG3   | 2.05                     | 0.57              |
| 2:BD:49:ASP:OD2   | 3:CH:161:SER:OG   | 171.74                   | 0.57              |
| 2:BS:49:ASP:OD2   | 3:CP:161:SER:OG   | 2.22                     | 0.57              |
| 2:BF:54:LEU:HD21  | 2:BF:97:VAL:HG11  | 1.87                     | 0.57              |
| 2:BQ:54:LEU:HD21  | 2:BQ:97:VAL:HG11  | 1.87                     | 0.57              |
| 2:BK:54:LEU:HD21  | 2:BK:97:VAL:HG11  | 1.87                     | 0.57              |
| 2:BM:54:LEU:HD21  | 2:BM:97:VAL:HG11  | 1.87                     | 0.57              |
| 2:BZ:54:LEU:HD21  | 2:BZ:97:VAL:HG11  | 1.87                     | 0.57              |
| 2:BJ:54:LEU:HD21  | 2:BJ:97:VAL:HG11  | 1.87                     | 0.57              |
| 2:BL:54:LEU:HD21  | 2:BL:97:VAL:HG11  | 1.87                     | 0.57              |
| 2:BR:97:VAL:O     | 2:BR:101:HIS:HD2  | 1.87                     | 0.57              |
| 2:BX:97:VAL:O     | 2:BX:101:HIS:HD2  | 1.87                     | 0.57              |
| 2:B9:49:ASP:OD2   | 3:C9:161:SER:OG   | 2.22                     | 0.57              |
| 2:BL:134:HIS:O    | 2:BL:136:HIS:N    | 2.36                     | 0.57              |
| 2:B2:137:GLU:C    | 2:B2:139:ALA:N    | 2.55                     | 0.57              |
| 1:AG:87:GLN:NE2   | 1:AG:210:ARG:HH22 | 2.03                     | 0.57              |
| 2:BU:132:TYR:HB3  | 2:BU:193:THR:CG2  | 2.34                     | 0.57              |
| 2:BC:132:TYR:HB3  | 2:BC:193:THR:CG2  | 2.34                     | 0.57              |
| 2:BF:114:VAL:HG22 | 2:BF:209:VAL:HG12 | 1.86                     | 0.57              |
| 2:B0:114:VAL:HG22 | 2:B0:209:VAL:HG12 | 1.86                     | 0.57              |
| 1:AN:163:MET:HE1  | 1:AN:189:GLY:HA3  | 1.86                     | 0.57              |
| 3:CQ:44:ILE:O     | 3:CQ:48:LYS:HG3   | 2.05                     | 0.57              |
| 3:CA:44:ILE:O     | 3:CA:48:LYS:HG3   | 2.05                     | 0.57              |
| 3:C5:44:ILE:O     | 3:C5:48:LYS:HG3   | 2.04                     | 0.57              |
| 3:CX:44:ILE:O     | 3:CX:48:LYS:HG3   | 2.04                     | 0.57              |
| 3:CP:44:ILE:O     | 3:CP:48:LYS:HG3   | 2.05                     | 0.57              |
| 3:CF:44:ILE:O     | 3:CF:48:LYS:HG3   | 2.05                     | 0.57              |
| 2:BX:49:ASP:OD2   | 3:C4:161:SER:OG   | 267.35                   | 0.57              |
| 2:BX:49:ASP:OD2   | 3:CW:161:SER:OG   | 2.22                     | 0.57              |
| 2:BP:49:ASP:OD2   | 3:CS:161:SER:OG   | 101.72                   | 0.57              |
| 2:BE:49:ASP:OD2   | 3:CB:161:SER:OG   | 2.22                     | 0.57              |
| 3:CI:44:ILE:O     | 3:CI:48:LYS:HG3   | 2.04                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BG:49:ASP:OD2   | 3:CG:161:SER:OG   | 62.83                    | 0.57              |
| 2:BB:54:LEU:HD21  | 2:BB:97:VAL:HG11  | 1.87                     | 0.57              |
| 3:C6:44:ILE:O     | 3:C6:48:LYS:HG3   | 2.04                     | 0.57              |
| 2:BX:54:LEU:HD21  | 2:BX:97:VAL:HG11  | 1.87                     | 0.57              |
| 1:AZ:5:GLY:HA3    | 1:AZ:15:PRO:HD3   | 1.85                     | 0.57              |
| 2:B9:97:VAL:O     | 2:B9:101:HIS:HD2  | 1.87                     | 0.57              |
| 2:B6:49:ASP:OD2   | 3:C6:161:SER:OG   | 2.22                     | 0.57              |
| 2:B3:49:ASP:OD2   | 3:C0:161:SER:OG   | 2.22                     | 0.57              |
| 2:BU:134:HIS:O    | 2:BU:136:HIS:N    | 2.37                     | 0.57              |
| 2:B0:134:HIS:O    | 2:B0:136:HIS:N    | 2.36                     | 0.57              |
| 1:AB:87:GLN:NE2   | 1:AB:210:ARG:HH12 | 2.02                     | 0.57              |
| 1:DI:87:GLN:NE2   | 1:DI:210:ARG:HH22 | 2.02                     | 0.57              |
| 1:AX:87:GLN:NE2   | 1:AX:210:ARG:HH22 | 2.03                     | 0.57              |
| 2:BI:132:TYR:HB3  | 2:BI:193:THR:CG2  | 2.34                     | 0.57              |
| 2:BP:132:TYR:HB3  | 2:BP:193:THR:CG2  | 2.34                     | 0.57              |
| 2:B9:132:TYR:HB3  | 2:B9:193:THR:CG2  | 2.34                     | 0.57              |
| 3:CD:44:ILE:O     | 3:CD:48:LYS:HG3   | 2.04                     | 0.57              |
| 3:CL:44:ILE:O     | 3:CL:48:LYS:HG3   | 2.05                     | 0.57              |
| 2:BT:49:ASP:OD2   | 3:CT:161:SER:OG   | 62.83                    | 0.57              |
| 2:BU:54:LEU:HD21  | 2:BU:97:VAL:HG11  | 1.87                     | 0.57              |
| 3:C0:44:ILE:O     | 3:C0:48:LYS:HG3   | 2.05                     | 0.57              |
| 2:BW:54:LEU:HD21  | 2:BW:97:VAL:HG11  | 1.87                     | 0.57              |
| 1:A6:5:GLY:HA3    | 1:A6:15:PRO:HD3   | 1.84                     | 0.57              |
| 2:BT:97:VAL:O     | 2:BT:101:HIS:HD2  | 1.87                     | 0.57              |
| 2:BV:134:HIS:O    | 2:BV:136:HIS:N    | 2.36                     | 0.57              |
| 2:BN:134:HIS:O    | 2:BN:136:HIS:N    | 2.36                     | 0.57              |
| 1:AJ:87:GLN:NE2   | 1:AJ:210:ARG:HH12 | 2.02                     | 0.57              |
| 2:BY:132:TYR:HB3  | 2:BY:193:THR:CG2  | 2.34                     | 0.57              |
| 1:DF:87:GLN:NE2   | 1:DF:210:ARG:HH12 | 2.02                     | 0.57              |
| 2:B8:132:TYR:HB3  | 2:B8:193:THR:CG2  | 2.34                     | 0.57              |
| 2:B6:114:VAL:HG22 | 2:B6:209:VAL:HG12 | 1.86                     | 0.57              |
| 3:CN:44:ILE:O     | 3:CN:48:LYS:HG3   | 2.05                     | 0.57              |
| 2:BD:49:ASP:OD2   | 3:CC:161:SER:OG   | 2.22                     | 0.57              |
| 2:BC:54:LEU:HD21  | 2:BC:97:VAL:HG11  | 1.87                     | 0.57              |
| 2:BJ:49:ASP:OD2   | 3:CG:161:SER:OG   | 2.22                     | 0.57              |
| 2:BS:54:LEU:HD21  | 2:BS:97:VAL:HG11  | 1.87                     | 0.57              |
| 2:B5:54:LEU:HD21  | 2:B5:97:VAL:HG11  | 1.87                     | 0.57              |
| 2:BG:54:LEU:HD21  | 2:BG:97:VAL:HG11  | 1.87                     | 0.57              |
| 2:BH:126:VAL:HG13 | 2:BH:171:VAL:HG21 | 1.86                     | 0.57              |
| 2:B7:126:VAL:HG13 | 2:B7:171:VAL:HG21 | 1.86                     | 0.57              |
| 2:BC:134:HIS:O    | 2:BC:136:HIS:N    | 2.36                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:87:GLN:NE2   | 1:AA:210:ARG:HH22 | 2.03                     | 0.57              |
| 1:DK:87:GLN:NE2   | 1:DK:210:ARG:HH22 | 2.03                     | 0.57              |
| 1:DK:87:GLN:NE2   | 1:DK:210:ARG:HH12 | 2.02                     | 0.57              |
| 1:A7:87:GLN:NE2   | 1:A7:210:ARG:HH22 | 2.03                     | 0.57              |
| 1:DC:87:GLN:NE2   | 1:DC:210:ARG:HH22 | 2.02                     | 0.57              |
| 2:B4:114:VAL:HG22 | 2:B4:209:VAL:HG12 | 1.86                     | 0.57              |
| 2:BA:114:VAL:HG22 | 2:BA:209:VAL:HG12 | 1.86                     | 0.57              |
| 2:BR:114:VAL:HG22 | 2:BR:209:VAL:HG12 | 1.86                     | 0.57              |
| 3:C7:44:ILE:O     | 3:C7:48:LYS:HG3   | 2.04                     | 0.57              |
| 3:CY:44:ILE:O     | 3:CY:48:LYS:HG3   | 2.04                     | 0.57              |
| 2:BT:49:ASP:OD2   | 3:CQ:161:SER:OG   | 2.22                     | 0.57              |
| 2:BP:54:LEU:HD21  | 2:BP:97:VAL:HG11  | 1.87                     | 0.57              |
| 2:BH:49:ASP:OD2   | 3:CJ:161:SER:OG   | 2.22                     | 0.57              |
| 2:BV:54:LEU:HD21  | 2:BV:97:VAL:HG11  | 1.87                     | 0.57              |
| 2:B6:54:LEU:HD21  | 2:B6:97:VAL:HG11  | 1.87                     | 0.57              |
| 2:BZ:49:ASP:OD2   | 3:C2:161:SER:OG   | 2.22                     | 0.57              |
| 2:BD:54:LEU:HD21  | 2:BD:97:VAL:HG11  | 1.87                     | 0.57              |
| 2:BD:97:VAL:O     | 2:BD:101:HIS:HD2  | 1.87                     | 0.57              |
| 2:BE:126:VAL:HG13 | 2:BE:171:VAL:HG21 | 1.86                     | 0.57              |
| 2:BD:134:HIS:O    | 2:BD:136:HIS:N    | 2.36                     | 0.56              |
| 2:BX:134:HIS:O    | 2:BX:136:HIS:N    | 2.36                     | 0.56              |
| 1:AR:87:GLN:NE2   | 1:AR:210:ARG:HH22 | 2.02                     | 0.56              |
| 1:A0:87:GLN:NE2   | 1:A0:210:ARG:HH12 | 2.02                     | 0.56              |
| 2:BU:114:VAL:HG22 | 2:BU:209:VAL:HG12 | 1.86                     | 0.56              |
| 2:BI:114:VAL:HG22 | 2:BI:209:VAL:HG12 | 1.86                     | 0.56              |
| 2:BW:49:ASP:OD2   | 3:CY:161:SER:OG   | 2.22                     | 0.56              |
| 2:BW:97:VAL:O     | 2:BW:101:HIS:HD2  | 1.87                     | 0.56              |
| 2:B2:49:ASP:OD2   | 3:C1:161:SER:OG   | 2.22                     | 0.56              |
| 2:B8:97:VAL:O     | 2:B8:101:HIS:HD2  | 1.87                     | 0.56              |
| 2:BE:97:VAL:O     | 2:BE:101:HIS:HD2  | 1.87                     | 0.56              |
| 2:B9:134:HIS:O    | 2:B9:136:HIS:N    | 2.36                     | 0.56              |
| 1:DD:87:GLN:NE2   | 1:DD:210:ARG:HH22 | 2.02                     | 0.56              |
| 1:AO:87:GLN:NE2   | 1:AO:210:ARG:HH22 | 2.03                     | 0.56              |
| 1:AY:87:GLN:NE2   | 1:AY:210:ARG:HH22 | 2.03                     | 0.56              |
| 2:BW:114:VAL:HG22 | 2:BW:209:VAL:HG12 | 1.86                     | 0.56              |
| 2:BX:114:VAL:HG22 | 2:BX:209:VAL:HG12 | 1.86                     | 0.56              |
| 2:BY:114:VAL:HG22 | 2:BY:209:VAL:HG12 | 1.86                     | 0.56              |
| 3:C2:44:ILE:O     | 3:C2:48:LYS:HG3   | 2.05                     | 0.56              |
| 2:BW:50:PRO:HD3   | 1:DG:15:PRO:O     | 241.12                   | 0.56              |
| 2:BL:49:ASP:OD2   | 3:CK:161:SER:OG   | 2.22                     | 0.56              |
| 2:BV:49:ASP:OD2   | 3:CV:161:SER:OG   | 62.83                    | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BC:113:GLN:HB2  | 2:BC:212:THR:HG22 | 1.88                     | 0.56              |
| 2:BA:126:VAL:HG13 | 2:BA:171:VAL:HG21 | 1.86                     | 0.56              |
| 2:BP:134:HIS:O    | 2:BP:136:HIS:N    | 2.37                     | 0.56              |
| 1:AK:87:GLN:NE2   | 1:AK:210:ARG:HH22 | 2.03                     | 0.56              |
| 1:AS:87:GLN:NE2   | 1:AS:210:ARG:HH22 | 2.02                     | 0.56              |
| 1:DJ:87:GLN:NE2   | 1:DJ:210:ARG:HH22 | 2.03                     | 0.56              |
| 1:AP:87:GLN:NE2   | 1:AP:210:ARG:HH22 | 2.03                     | 0.56              |
| 2:BN:114:VAL:HG22 | 2:BN:209:VAL:HG12 | 1.86                     | 0.56              |
| 2:B8:114:VAL:HG22 | 2:B8:209:VAL:HG12 | 1.86                     | 0.56              |
| 1:DF:163:MET:HE1  | 1:DF:189:GLY:HA3  | 1.87                     | 0.56              |
| 1:AW:163:MET:HE1  | 1:AW:189:GLY:HA3  | 1.87                     | 0.56              |
| 1:A3:15:PRO:O     | 2:BX:50:PRO:HD3   | 261.27                   | 0.56              |
| 2:BS:50:PRO:HD3   | 1:DI:15:PRO:O     | 239.44                   | 0.56              |
| 3:CK:44:ILE:O     | 3:CK:48:LYS:HG3   | 2.05                     | 0.56              |
| 1:AE:15:PRO:O     | 2:BH:50:PRO:HD3   | 154.73                   | 0.56              |
| 1:AE:15:PRO:O     | 2:BC:50:PRO:HD3   | 2.06                     | 0.56              |
| 1:AM:15:PRO:O     | 2:BK:50:PRO:HD3   | 2.06                     | 0.56              |
| 3:CU:44:ILE:O     | 3:CU:48:LYS:HG3   | 2.05                     | 0.56              |
| 3:C8:44:ILE:O     | 3:C8:48:LYS:HG3   | 2.05                     | 0.56              |
| 3:CV:44:ILE:O     | 3:CV:48:LYS:HG3   | 2.05                     | 0.56              |
| 3:CZ:44:ILE:O     | 3:CZ:48:LYS:HG3   | 2.05                     | 0.56              |
| 3:C4:44:ILE:O     | 3:C4:48:LYS:HG3   | 2.04                     | 0.56              |
| 2:BO:49:ASP:OD2   | 3:CO:161:SER:OG   | 231.09                   | 0.56              |
| 2:BE:49:ASP:OD2   | 3:CE:161:SER:OG   | 62.83                    | 0.56              |
| 2:BG:49:ASP:OD2   | 3:CF:161:SER:OG   | 2.22                     | 0.56              |
| 3:C3:44:ILE:O     | 3:C3:48:LYS:HG3   | 2.04                     | 0.56              |
| 2:B1:54:LEU:HD21  | 2:B1:97:VAL:HG11  | 1.87                     | 0.56              |
| 2:BN:54:LEU:HD21  | 2:BN:97:VAL:HG11  | 1.87                     | 0.56              |
| 2:BG:97:VAL:O     | 2:BG:101:HIS:HD2  | 1.87                     | 0.56              |
| 2:B8:54:LEU:HD21  | 2:B8:97:VAL:HG11  | 1.87                     | 0.56              |
| 2:B3:97:VAL:O     | 2:B3:101:HIS:HD2  | 1.87                     | 0.56              |
| 2:BP:113:GLN:HB2  | 2:BP:212:THR:HG22 | 1.88                     | 0.56              |
| 2:B1:126:VAL:HG13 | 2:B1:171:VAL:HG21 | 1.85                     | 0.56              |
| 2:BR:113:GLN:HB2  | 2:BR:212:THR:HG22 | 1.88                     | 0.56              |
| 2:BI:134:HIS:O    | 2:BI:136:HIS:N    | 2.36                     | 0.56              |
| 2:BB:134:HIS:O    | 2:BB:136:HIS:N    | 2.36                     | 0.56              |
| 1:AI:87:GLN:NE2   | 1:AI:210:ARG:HH22 | 2.03                     | 0.56              |
| 1:A6:87:GLN:NE2   | 1:A6:210:ARG:HH22 | 2.03                     | 0.56              |
| 1:DE:87:GLN:NE2   | 1:DE:210:ARG:HH22 | 2.03                     | 0.56              |
| 2:BC:114:VAL:HG22 | 2:BC:209:VAL:HG12 | 1.86                     | 0.56              |
| 2:BP:114:VAL:HG22 | 2:BP:209:VAL:HG12 | 1.86                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AW:15:PRO:O     | 2:BU:50:PRO:HD3   | 2.06                     | 0.56              |
| 1:AC:15:PRO:O     | 2:BD:50:PRO:HD3   | 2.06                     | 0.56              |
| 1:AG:15:PRO:O     | 2:BD:50:PRO:HD3   | 186.28                   | 0.56              |
| 1:AQ:15:PRO:O     | 2:BQ:50:PRO:HD3   | 2.06                     | 0.56              |
| 3:CG:44:ILE:O     | 3:CG:48:LYS:HG3   | 2.04                     | 0.56              |
| 2:BH:54:LEU:HD21  | 2:BH:97:VAL:HG11  | 1.87                     | 0.56              |
| 2:B9:54:LEU:HD21  | 2:B9:97:VAL:HG11  | 1.87                     | 0.56              |
| 2:BL:113:GLN:HB2  | 2:BL:212:THR:HG22 | 1.88                     | 0.56              |
| 2:BE:113:GLN:HB2  | 2:BE:212:THR:HG22 | 1.88                     | 0.56              |
| 2:BW:113:GLN:HB2  | 2:BW:212:THR:HG22 | 1.88                     | 0.56              |
| 2:B7:114:VAL:HG22 | 2:B7:209:VAL:HG12 | 1.86                     | 0.56              |
| 2:B5:114:VAL:HG22 | 2:B5:209:VAL:HG12 | 1.86                     | 0.56              |
| 1:AB:15:PRO:O     | 2:BE:50:PRO:HD3   | 2.06                     | 0.56              |
| 1:A8:15:PRO:O     | 2:B9:50:PRO:HD3   | 2.06                     | 0.56              |
| 2:BH:113:GLN:HB2  | 2:BH:212:THR:HG22 | 1.88                     | 0.56              |
| 2:BA:113:GLN:HB2  | 2:BA:212:THR:HG22 | 1.88                     | 0.56              |
| 2:B4:126:VAL:HG13 | 2:B4:171:VAL:HG21 | 1.85                     | 0.56              |
| 2:BD:113:GLN:HB2  | 2:BD:212:THR:HG22 | 1.88                     | 0.56              |
| 2:BV:113:GLN:HB2  | 2:BV:212:THR:HG22 | 1.88                     | 0.56              |
| 2:BF:113:GLN:HB2  | 2:BF:212:THR:HG22 | 1.88                     | 0.56              |
| 2:BR:134:HIS:O    | 2:BR:136:HIS:N    | 2.36                     | 0.56              |
| 1:AW:191:HIS:CD2  | 1:AW:193:GLY:H    | 2.21                     | 0.56              |
| 1:AB:87:GLN:NE2   | 1:AB:210:ARG:HH22 | 2.03                     | 0.56              |
| 1:A8:87:GLN:NE2   | 1:A8:210:ARG:HH22 | 2.03                     | 0.56              |
| 1:A5:87:GLN:NE2   | 1:A5:210:ARG:HH22 | 2.02                     | 0.56              |
| 1:DF:87:GLN:NE2   | 1:DF:210:ARG:HH22 | 2.03                     | 0.56              |
| 1:AP:163:MET:HE1  | 1:AP:189:GLY:HA3  | 1.87                     | 0.56              |
| 1:AV:15:PRO:O     | 2:BX:50:PRO:HD3   | 2.06                     | 0.56              |
| 1:A6:163:MET:HE1  | 1:A6:189:GLY:HA3  | 1.88                     | 0.56              |
| 1:AO:15:PRO:O     | 2:BS:50:PRO:HD3   | 2.06                     | 0.56              |
| 1:AF:15:PRO:O     | 2:BG:50:PRO:HD3   | 2.06                     | 0.56              |
| 1:AH:15:PRO:O     | 2:BI:50:PRO:HD3   | 2.06                     | 0.56              |
| 3:C9:44:ILE:O     | 3:C9:48:LYS:HG3   | 2.04                     | 0.56              |
| 1:AA:15:PRO:O     | 2:BB:50:PRO:HD3   | 2.06                     | 0.56              |
| 1:A2:15:PRO:O     | 2:B1:50:PRO:HD3   | 2.06                     | 0.56              |
| 3:CT:44:ILE:O     | 3:CT:48:LYS:HG3   | 2.04                     | 0.56              |
| 2:B7:54:LEU:HD21  | 2:B7:97:VAL:HG11  | 1.87                     | 0.56              |
| 2:BE:54:LEU:HD21  | 2:BE:97:VAL:HG11  | 1.87                     | 0.56              |
| 2:B3:54:LEU:HD21  | 2:B3:97:VAL:HG11  | 1.87                     | 0.56              |
| 2:B0:54:LEU:HD21  | 2:B0:97:VAL:HG11  | 1.87                     | 0.56              |
| 2:B4:134:HIS:O    | 2:B4:136:HIS:N    | 2.36                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BM:114:VAL:HG22 | 2:BM:209:VAL:HG12 | 1.86                     | 0.56              |
| 1:AB:15:PRO:O     | 2:B8:50:PRO:HD3   | 165.34                   | 0.56              |
| 1:AL:15:PRO:O     | 2:BN:50:PRO:HD3   | 2.06                     | 0.56              |
| 3:C1:44:ILE:O     | 3:C1:48:LYS:HG3   | 2.04                     | 0.56              |
| 1:A9:15:PRO:O     | 2:BC:50:PRO:HD3   | 251.53                   | 0.56              |
| 1:AS:15:PRO:O     | 2:BP:50:PRO:HD3   | 2.06                     | 0.56              |
| 2:BO:49:ASP:OD2   | 3:CS:161:SER:OG   | 2.22                     | 0.56              |
| 2:BJ:113:GLN:HB2  | 2:BJ:212:THR:HG22 | 1.88                     | 0.56              |
| 2:BX:113:GLN:HB2  | 2:BX:212:THR:HG22 | 1.88                     | 0.56              |
| 2:BV:114:VAL:HG22 | 2:BV:209:VAL:HG12 | 1.86                     | 0.56              |
| 2:B1:114:VAL:HG22 | 2:B1:209:VAL:HG12 | 1.86                     | 0.56              |
| 1:AU:163:MET:HE1  | 1:AU:189:GLY:HA3  | 1.88                     | 0.56              |
| 1:AR:15:PRO:O     | 2:BO:50:PRO:HD3   | 2.06                     | 0.56              |
| 3:DA:44:ILE:O     | 3:DA:48:LYS:HG3   | 2.05                     | 0.56              |
| 2:B2:54:LEU:HD21  | 2:B2:97:VAL:HG11  | 1.87                     | 0.56              |
| 2:BR:54:LEU:HD21  | 2:BR:97:VAL:HG11  | 1.87                     | 0.56              |
| 1:A6:15:PRO:O     | 2:B4:50:PRO:HD3   | 2.06                     | 0.56              |
| 2:BQ:113:GLN:HB2  | 2:BQ:212:THR:HG22 | 1.88                     | 0.56              |
| 2:BK:113:GLN:HB2  | 2:BK:212:THR:HG22 | 1.88                     | 0.56              |
| 2:BJ:134:HIS:O    | 2:BJ:136:HIS:N    | 2.36                     | 0.56              |
| 1:AR:191:HIS:CD2  | 1:AR:193:GLY:H    | 2.21                     | 0.56              |
| 1:A0:87:GLN:NE2   | 1:A0:210:ARG:HH22 | 2.03                     | 0.56              |
| 1:AG:15:PRO:O     | 2:BJ:50:PRO:HD3   | 2.06                     | 0.56              |
| 2:BN:50:PRO:HD3   | 1:DD:15:PRO:O     | 239.48                   | 0.56              |
| 1:AT:15:PRO:O     | 2:BV:50:PRO:HD3   | 2.06                     | 0.56              |
| 2:BG:113:GLN:HB2  | 2:BG:212:THR:HG22 | 1.88                     | 0.56              |
| 2:B7:113:GLN:HB2  | 2:B7:212:THR:HG22 | 1.88                     | 0.56              |
| 2:BI:113:GLN:HB2  | 2:BI:212:THR:HG22 | 1.88                     | 0.56              |
| 2:B1:113:GLN:HB2  | 2:B1:212:THR:HG22 | 1.88                     | 0.56              |
| 1:AN:87:GLN:NE2   | 1:AN:210:ARG:HH22 | 2.02                     | 0.56              |
| 1:DH:87:GLN:NE2   | 1:DH:210:ARG:HH22 | 2.02                     | 0.56              |
| 1:AN:15:PRO:O     | 2:BO:50:PRO:HD3   | 217.64                   | 0.56              |
| 1:AD:15:PRO:O     | 2:BA:50:PRO:HD3   | 2.06                     | 0.56              |
| 1:AI:15:PRO:O     | 2:BJ:50:PRO:HD3   | 106.56                   | 0.56              |
| 1:AY:15:PRO:O     | 2:B0:50:PRO:HD3   | 2.06                     | 0.56              |
| 2:BS:49:ASP:OD2   | 3:CW:161:SER:OG   | 278.05                   | 0.56              |
| 2:BO:113:GLN:HB2  | 2:BO:212:THR:HG22 | 1.88                     | 0.56              |
| 1:AJ:191:HIS:CD2  | 1:AJ:193:GLY:H    | 2.21                     | 0.55              |
| 2:B3:114:VAL:HG22 | 2:B3:209:VAL:HG12 | 1.86                     | 0.55              |
| 2:B2:114:VAL:HG22 | 2:B2:209:VAL:HG12 | 1.86                     | 0.55              |
| 1:AH:15:PRO:O     | 2:BF:50:PRO:HD3   | 66.92                    | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AL:15:PRO:O     | 2:BI:50:PRO:HD3   | 113.30                   | 0.55              |
| 2:BV:50:PRO:HD3   | 1:DH:15:PRO:O     | 242.55                   | 0.55              |
| 2:BI:54:LEU:HD21  | 2:BI:97:VAL:HG11  | 1.87                     | 0.55              |
| 2:B4:54:LEU:HD21  | 2:B4:97:VAL:HG11  | 1.87                     | 0.55              |
| 2:B5:113:GLN:HB2  | 2:B5:212:THR:HG22 | 1.88                     | 0.55              |
| 2:BZ:113:GLN:HB2  | 2:BZ:212:THR:HG22 | 1.88                     | 0.55              |
| 2:BS:113:GLN:HB2  | 2:BS:212:THR:HG22 | 1.88                     | 0.55              |
| 2:BB:113:GLN:HB2  | 2:BB:212:THR:HG22 | 1.88                     | 0.55              |
| 2:B3:113:GLN:HB2  | 2:B3:212:THR:HG22 | 1.88                     | 0.55              |
| 2:BE:134:HIS:O    | 2:BE:136:HIS:N    | 2.36                     | 0.55              |
| 2:BZ:114:VAL:HG22 | 2:BZ:209:VAL:HG12 | 1.86                     | 0.55              |
| 1:AN:15:PRO:O     | 2:BM:50:PRO:HD3   | 2.06                     | 0.55              |
| 1:AP:15:PRO:O     | 2:BT:50:PRO:HD3   | 2.06                     | 0.55              |
| 2:BP:50:PRO:HD3   | 1:DE:15:PRO:O     | 205.60                   | 0.55              |
| 1:AU:15:PRO:O     | 2:BY:50:PRO:HD3   | 2.06                     | 0.55              |
| 1:A5:15:PRO:O     | 2:B6:50:PRO:HD3   | 2.06                     | 0.55              |
| 2:BY:54:LEU:HD21  | 2:BY:97:VAL:HG11  | 1.87                     | 0.55              |
| 2:B0:97:VAL:O     | 2:B0:101:HIS:HD2  | 1.87                     | 0.55              |
| 2:BO:134:HIS:O    | 2:BO:136:HIS:N    | 2.36                     | 0.55              |
| 2:BS:134:HIS:O    | 2:BS:136:HIS:N    | 2.36                     | 0.55              |
| 1:AM:191:HIS:CD2  | 1:AM:193:GLY:H    | 2.21                     | 0.55              |
| 1:AE:87:GLN:NE2   | 1:AE:210:ARG:HH22 | 2.02                     | 0.55              |
| 2:BQ:50:PRO:HD3   | 1:DC:15:PRO:O     | 229.91                   | 0.55              |
| 2:BT:54:LEU:HD21  | 2:BT:97:VAL:HG11  | 1.87                     | 0.55              |
| 3:CL:139:MET:HG2  | 3:CL:139:MET:O    | 2.07                     | 0.55              |
| 1:AY:191:HIS:CD2  | 1:AY:193:GLY:H    | 2.21                     | 0.55              |
| 1:A0:15:PRO:O     | 2:B2:50:PRO:HD3   | 2.06                     | 0.55              |
| 1:A1:15:PRO:O     | 2:BZ:50:PRO:HD3   | 2.06                     | 0.55              |
| 2:BU:113:GLN:HB2  | 2:BU:212:THR:HG22 | 1.88                     | 0.55              |
| 1:AZ:87:GLN:NE2   | 1:AZ:210:ARG:HH22 | 2.03                     | 0.55              |
| 1:AS:163:MET:HE1  | 1:AS:189:GLY:HA3  | 1.89                     | 0.55              |
| 1:AJ:15:PRO:O     | 2:BL:50:PRO:HD3   | 2.06                     | 0.55              |
| 1:AJ:15:PRO:O     | 2:BM:50:PRO:HD3   | 106.56                   | 0.55              |
| 1:A4:15:PRO:O     | 2:B7:50:PRO:HD3   | 2.06                     | 0.55              |
| 2:B0:113:GLN:HB2  | 2:B0:212:THR:HG22 | 1.88                     | 0.55              |
| 2:BT:113:GLN:HB2  | 2:BT:212:THR:HG22 | 1.88                     | 0.55              |
| 3:CI:139:MET:HG2  | 3:CI:139:MET:O    | 2.07                     | 0.55              |
| 3:CS:139:MET:HG2  | 3:CS:139:MET:O    | 2.07                     | 0.55              |
| 3:CE:139:MET:O    | 3:CE:139:MET:HG2  | 2.07                     | 0.55              |
| 3:CW:139:MET:O    | 3:CW:139:MET:HG2  | 2.07                     | 0.55              |
| 3:CH:139:MET:HG2  | 3:CH:139:MET:O    | 2.07                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A8:163:MET:HE1  | 1:A8:189:GLY:HA3  | 1.88                     | 0.55              |
| 1:AK:15:PRO:O     | 2:BL:50:PRO:HD3   | 64.15                    | 0.55              |
| 1:AI:15:PRO:O     | 2:BF:50:PRO:HD3   | 2.06                     | 0.55              |
| 2:BT:50:PRO:HD3   | 1:DF:15:PRO:O     | 205.58                   | 0.55              |
| 2:BA:54:LEU:HD21  | 2:BA:97:VAL:HG11  | 1.87                     | 0.55              |
| 2:B4:126:VAL:HG22 | 2:B4:171:VAL:HG11 | 1.89                     | 0.55              |
| 3:CB:139:MET:HG2  | 3:CB:139:MET:O    | 2.07                     | 0.55              |
| 3:CK:139:MET:O    | 3:CK:139:MET:HG2  | 2.07                     | 0.55              |
| 3:DA:139:MET:O    | 3:DA:139:MET:HG2  | 2.07                     | 0.55              |
| 3:CD:139:MET:HG2  | 3:CD:139:MET:O    | 2.07                     | 0.55              |
| 2:BN:113:GLN:HB2  | 2:BN:212:THR:HG22 | 1.88                     | 0.55              |
| 2:B8:134:HIS:O    | 2:B8:136:HIS:N    | 2.36                     | 0.55              |
| 1:DE:191:HIS:CD2  | 1:DE:193:GLY:H    | 2.21                     | 0.55              |
| 1:A9:87:GLN:NE2   | 1:A9:210:ARG:HH22 | 2.03                     | 0.55              |
| 2:BU:50:PRO:HD3   | 1:DJ:15:PRO:O     | 245.20                   | 0.55              |
| 1:AX:15:PRO:O     | 2:BW:50:PRO:HD3   | 2.05                     | 0.55              |
| 1:AG:163:MET:HE1  | 1:AG:189:GLY:HA3  | 1.89                     | 0.55              |
| 2:BE:126:VAL:HG22 | 2:BE:171:VAL:HG11 | 1.89                     | 0.55              |
| 3:CR:139:MET:HG2  | 3:CR:139:MET:O    | 2.07                     | 0.55              |
| 2:B1:134:HIS:O    | 2:B1:136:HIS:N    | 2.36                     | 0.55              |
| 1:AM:163:MET:HE1  | 1:AM:189:GLY:HA3  | 1.88                     | 0.55              |
| 1:DC:163:MET:HE1  | 1:DC:189:GLY:HA3  | 1.87                     | 0.55              |
| 1:AO:15:PRO:O     | 2:BR:50:PRO:HD3   | 229.41                   | 0.55              |
| 1:AD:15:PRO:O     | 2:BE:50:PRO:HD3   | 106.56                   | 0.55              |
| 2:BT:126:VAL:HG22 | 2:BT:171:VAL:HG11 | 1.89                     | 0.55              |
| 2:BI:126:VAL:HG22 | 2:BI:171:VAL:HG11 | 1.89                     | 0.55              |
| 2:BB:126:VAL:HG22 | 2:BB:171:VAL:HG11 | 1.89                     | 0.55              |
| 1:AZ:15:PRO:O     | 2:B3:50:PRO:HD3   | 2.06                     | 0.55              |
| 2:BY:113:GLN:HB2  | 2:BY:212:THR:HG22 | 1.88                     | 0.55              |
| 2:B9:113:GLN:HB2  | 2:B9:212:THR:HG22 | 1.88                     | 0.55              |
| 3:CV:139:MET:HG2  | 3:CV:139:MET:O    | 2.07                     | 0.55              |
| 3:CN:139:MET:O    | 3:CN:139:MET:HG2  | 2.07                     | 0.55              |
| 3:CQ:139:MET:HG2  | 3:CQ:139:MET:O    | 2.07                     | 0.55              |
| 1:AI:163:MET:HE1  | 1:AI:189:GLY:HA3  | 1.90                     | 0.55              |
| 2:B3:126:VAL:HG22 | 2:B3:171:VAL:HG11 | 1.89                     | 0.55              |
| 2:BH:126:VAL:HG22 | 2:BH:171:VAL:HG11 | 1.89                     | 0.55              |
| 3:CT:139:MET:O    | 3:CT:139:MET:HG2  | 2.07                     | 0.55              |
| 3:C2:139:MET:O    | 3:C2:139:MET:HG2  | 2.07                     | 0.55              |
| 3:CX:139:MET:O    | 3:CX:139:MET:HG2  | 2.07                     | 0.55              |
| 3:C5:139:MET:O    | 3:C5:139:MET:HG2  | 2.07                     | 0.55              |
| 1:AO:191:HIS:CD2  | 1:AO:193:GLY:H    | 2.21                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AK:15:PRO:O     | 2:BR:50:PRO:HD3   | 2.06                     | 0.55              |
| 1:AX:163:MET:HE1  | 1:AX:189:GLY:HA3  | 1.89                     | 0.55              |
| 2:BK:126:VAL:HG22 | 2:BK:171:VAL:HG11 | 1.89                     | 0.55              |
| 2:BN:126:VAL:HG22 | 2:BN:171:VAL:HG11 | 1.89                     | 0.55              |
| 2:B5:126:VAL:HG22 | 2:B5:171:VAL:HG11 | 1.89                     | 0.55              |
| 2:BM:126:VAL:HG22 | 2:BM:171:VAL:HG11 | 1.89                     | 0.55              |
| 2:B9:126:VAL:HG22 | 2:B9:171:VAL:HG11 | 1.89                     | 0.55              |
| 3:CA:139:MET:HG2  | 3:CA:139:MET:O    | 2.07                     | 0.55              |
| 3:CF:139:MET:O    | 3:CF:139:MET:HG2  | 2.07                     | 0.55              |
| 2:BM:113:GLN:HB2  | 2:BM:212:THR:HG22 | 1.88                     | 0.55              |
| 2:BT:134:HIS:O    | 2:BT:136:HIS:N    | 2.36                     | 0.54              |
| 1:AB:191:HIS:CD2  | 1:AB:193:GLY:H    | 2.21                     | 0.54              |
| 1:A7:15:PRO:O     | 2:B5:50:PRO:HD3   | 2.06                     | 0.54              |
| 2:BV:126:VAL:HG22 | 2:BV:171:VAL:HG11 | 1.89                     | 0.54              |
| 2:BA:126:VAL:HG22 | 2:BA:171:VAL:HG11 | 1.89                     | 0.54              |
| 3:CJ:139:MET:O    | 3:CJ:139:MET:HG2  | 2.07                     | 0.54              |
| 1:AN:191:HIS:CD2  | 1:AN:193:GLY:H    | 2.21                     | 0.54              |
| 1:AC:15:PRO:O     | 2:BA:50:PRO:HD3   | 66.92                    | 0.54              |
| 2:BH:50:PRO:HD3   | 1:DK:15:PRO:O     | 2.06                     | 0.54              |
| 2:BY:126:VAL:HG22 | 2:BY:171:VAL:HG11 | 1.89                     | 0.54              |
| 2:BO:126:VAL:HG22 | 2:BO:171:VAL:HG11 | 1.89                     | 0.54              |
| 2:BR:126:VAL:HG22 | 2:BR:171:VAL:HG11 | 1.89                     | 0.54              |
| 2:B7:126:VAL:HG22 | 2:B7:171:VAL:HG11 | 1.89                     | 0.54              |
| 3:CN:56:ILE:HD12  | 3:CN:74:PHE:CE1   | 2.43                     | 0.54              |
| 3:CP:139:MET:HG2  | 3:CP:139:MET:O    | 2.07                     | 0.54              |
| 1:AW:87:GLN:NE2   | 1:AW:210:ARG:HH22 | 2.02                     | 0.54              |
| 1:AS:159:PRO:CG   | 3:CT:29:VAL:HG21  | 2.38                     | 0.54              |
| 2:BS:126:VAL:HG22 | 2:BS:171:VAL:HG11 | 1.89                     | 0.54              |
| 3:CO:56:ILE:HD12  | 3:CO:74:PHE:CE1   | 2.43                     | 0.54              |
| 1:AN:33:LEU:O     | 1:AN:36:ARG:HD2   | 2.08                     | 0.54              |
| 2:B8:113:GLN:HB2  | 2:B8:212:THR:HG22 | 1.88                     | 0.54              |
| 3:CC:139:MET:O    | 3:CC:139:MET:HG2  | 2.07                     | 0.54              |
| 3:CO:139:MET:O    | 3:CO:139:MET:HG2  | 2.07                     | 0.54              |
| 3:C6:139:MET:O    | 3:C6:139:MET:HG2  | 2.07                     | 0.54              |
| 3:CX:56:ILE:HD12  | 3:CX:74:PHE:CE1   | 2.43                     | 0.54              |
| 2:B2:113:GLN:HB2  | 2:B2:212:THR:HG22 | 1.88                     | 0.54              |
| 3:CM:56:ILE:HD12  | 3:CM:74:PHE:CE1   | 2.43                     | 0.54              |
| 1:AF:191:HIS:CD2  | 1:AF:193:GLY:H    | 2.21                     | 0.54              |
| 1:DD:163:MET:HE1  | 1:DD:189:GLY:HA3  | 1.90                     | 0.54              |
| 1:AB:159:PRO:CG   | 3:CC:29:VAL:HG21  | 52.17                    | 0.54              |
| 2:BQ:126:VAL:HG22 | 2:BQ:171:VAL:HG11 | 1.89                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:CQ:56:ILE:HD12  | 3:CQ:74:PHE:CE1   | 2.43                     | 0.54              |
| 1:DD:45:LEU:HB2   | 1:DD:202:HIS:HA   | 1.90                     | 0.54              |
| 3:C7:56:ILE:HD12  | 3:C7:74:PHE:CE1   | 2.43                     | 0.54              |
| 3:CT:56:ILE:HD12  | 3:CT:74:PHE:CE1   | 2.43                     | 0.54              |
| 3:CD:56:ILE:HD12  | 3:CD:74:PHE:CE1   | 2.43                     | 0.54              |
| 1:AO:45:LEU:HB2   | 1:AO:202:HIS:HA   | 1.90                     | 0.54              |
| 3:CU:139:MET:HG2  | 3:CU:139:MET:O    | 2.07                     | 0.54              |
| 3:CM:139:MET:HG2  | 3:CM:139:MET:O    | 2.07                     | 0.54              |
| 1:AA:33:LEU:O     | 1:AA:36:ARG:HD2   | 2.08                     | 0.54              |
| 3:C8:56:ILE:HD12  | 3:C8:74:PHE:CE1   | 2.43                     | 0.54              |
| 3:CR:29:VAL:HG21  | 1:DD:159:PRO:CG   | 228.04                   | 0.54              |
| 1:A9:159:PRO:CG   | 3:DA:29:VAL:HG21  | 2.38                     | 0.54              |
| 2:BU:126:VAL:HG22 | 2:BU:171:VAL:HG11 | 1.89                     | 0.54              |
| 2:BX:126:VAL:HG22 | 2:BX:171:VAL:HG11 | 1.89                     | 0.54              |
| 1:AU:33:LEU:O     | 1:AU:36:ARG:HD2   | 2.08                     | 0.54              |
| 1:AR:45:LEU:HB2   | 1:AR:202:HIS:HA   | 1.90                     | 0.54              |
| 2:B4:113:GLN:HB2  | 2:B4:212:THR:HG22 | 1.88                     | 0.54              |
| 1:DI:45:LEU:HB2   | 1:DI:202:HIS:HA   | 1.90                     | 0.54              |
| 1:AE:191:HIS:CD2  | 1:AE:193:GLY:H    | 2.21                     | 0.54              |
| 1:AI:159:PRO:CG   | 3:CJ:29:VAL:HG21  | 52.35                    | 0.54              |
| 1:AI:159:PRO:CG   | 3:CI:29:VAL:HG21  | 2.38                     | 0.54              |
| 1:AL:159:PRO:CG   | 3:CM:29:VAL:HG21  | 2.38                     | 0.54              |
| 1:A3:159:PRO:CG   | 3:C4:29:VAL:HG21  | 2.38                     | 0.54              |
| 1:A5:159:PRO:CG   | 3:C6:29:VAL:HG21  | 2.38                     | 0.54              |
| 2:B0:126:VAL:HG22 | 2:B0:171:VAL:HG11 | 1.89                     | 0.54              |
| 1:AJ:45:LEU:HB2   | 1:AJ:202:HIS:HA   | 1.90                     | 0.54              |
| 1:AB:33:LEU:O     | 1:AB:36:ARG:HD2   | 2.08                     | 0.54              |
| 1:AK:33:LEU:O     | 1:AK:36:ARG:HD2   | 2.08                     | 0.54              |
| 1:AT:33:LEU:O     | 1:AT:36:ARG:HD2   | 2.08                     | 0.54              |
| 1:AL:33:LEU:O     | 1:AL:36:ARG:HD2   | 2.08                     | 0.54              |
| 1:DG:45:LEU:HB2   | 1:DG:202:HIS:HA   | 1.90                     | 0.54              |
| 1:AD:33:LEU:O     | 1:AD:36:ARG:HD2   | 2.08                     | 0.54              |
| 1:AM:33:LEU:O     | 1:AM:36:ARG:HD2   | 2.08                     | 0.54              |
| 1:A3:33:LEU:O     | 1:A3:36:ARG:HD2   | 2.08                     | 0.54              |
| 1:AL:45:LEU:HB2   | 1:AL:202:HIS:HA   | 1.90                     | 0.54              |
| 3:C0:139:MET:HG2  | 3:C0:139:MET:O    | 2.07                     | 0.54              |
| 3:CY:139:MET:O    | 3:CY:139:MET:HG2  | 2.07                     | 0.54              |
| 3:C2:56:ILE:HD12  | 3:C2:74:PHE:CE1   | 2.43                     | 0.54              |
| 1:DF:33:LEU:O     | 1:DF:36:ARG:HD2   | 2.08                     | 0.54              |
| 2:B5:134:HIS:O    | 2:B5:136:HIS:N    | 2.36                     | 0.54              |
| 1:AE:159:PRO:CG   | 3:CF:29:VAL:HG21  | 121.49                   | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AH:159:PRO:CG   | 3:CI:29:VAL:HG21  | 32.12                    | 0.54              |
| 2:BC:126:VAL:HG22 | 2:BC:171:VAL:HG11 | 1.89                     | 0.54              |
| 3:CA:56:ILE:HD12  | 3:CA:74:PHE:CE1   | 2.43                     | 0.54              |
| 2:B6:113:GLN:HB2  | 2:B6:212:THR:HG22 | 1.88                     | 0.54              |
| 1:AW:33:LEU:O     | 1:AW:36:ARG:HD2   | 2.08                     | 0.54              |
| 1:AC:45:LEU:HB2   | 1:AC:202:HIS:HA   | 1.90                     | 0.54              |
| 3:CU:56:ILE:HD12  | 3:CU:74:PHE:CE1   | 2.43                     | 0.54              |
| 1:A2:45:LEU:HB2   | 1:A2:202:HIS:HA   | 1.90                     | 0.54              |
| 1:AD:45:LEU:HB2   | 1:AD:202:HIS:HA   | 1.90                     | 0.54              |
| 3:C9:139:MET:O    | 3:C9:139:MET:HG2  | 2.07                     | 0.54              |
| 3:CW:56:ILE:HD12  | 3:CW:74:PHE:CE1   | 2.43                     | 0.54              |
| 1:AG:45:LEU:HB2   | 1:AG:202:HIS:HA   | 1.90                     | 0.54              |
| 1:DE:45:LEU:HB2   | 1:DE:202:HIS:HA   | 1.90                     | 0.54              |
| 3:CV:56:ILE:HD12  | 3:CV:74:PHE:CE1   | 2.43                     | 0.54              |
| 1:A8:45:LEU:HB2   | 1:A8:202:HIS:HA   | 1.90                     | 0.54              |
| 2:BZ:134:HIS:O    | 2:BZ:136:HIS:N    | 2.37                     | 0.54              |
| 1:AA:183:THR:HA   | 1:AC:246:GLN:HE22 | 56.61                    | 0.54              |
| 1:AI:246:GLN:HE22 | 1:AJ:183:THR:HA   | 184.21                   | 0.54              |
| 1:AJ:183:THR:HA   | 1:AM:246:GLN:HE22 | 1.73                     | 0.54              |
| 1:AJ:159:PRO:CG   | 3:CK:29:VAL:HG21  | 2.38                     | 0.54              |
| 1:A0:159:PRO:CG   | 3:C1:29:VAL:HG21  | 2.38                     | 0.54              |
| 1:AV:163:MET:HE1  | 1:AV:189:GLY:HA3  | 1.89                     | 0.54              |
| 1:AA:159:PRO:CG   | 3:DB:29:VAL:HG21  | 272.01                   | 0.54              |
| 3:CV:29:VAL:HG21  | 1:DH:159:PRO:CG   | 269.18                   | 0.54              |
| 2:BG:126:VAL:HG22 | 2:BG:171:VAL:HG11 | 1.89                     | 0.54              |
| 3:CP:56:ILE:HD12  | 3:CP:74:PHE:CE1   | 2.43                     | 0.54              |
| 3:CH:56:ILE:HD12  | 3:CH:74:PHE:CE1   | 2.43                     | 0.54              |
| 1:A1:45:LEU:HB2   | 1:A1:202:HIS:HA   | 1.90                     | 0.54              |
| 3:CK:56:ILE:HD12  | 3:CK:74:PHE:CE1   | 2.43                     | 0.54              |
| 3:C4:139:MET:O    | 3:C4:139:MET:HG2  | 2.07                     | 0.54              |
| 1:AH:33:LEU:O     | 1:AH:36:ARG:HD2   | 2.08                     | 0.54              |
| 3:CB:56:ILE:HD12  | 3:CB:74:PHE:CE1   | 2.43                     | 0.54              |
| 1:DE:33:LEU:O     | 1:DE:36:ARG:HD2   | 2.08                     | 0.54              |
| 1:AJ:33:LEU:O     | 1:AJ:36:ARG:HD2   | 2.08                     | 0.54              |
| 1:A6:45:LEU:HB2   | 1:A6:202:HIS:HA   | 1.90                     | 0.54              |
| 1:AO:246:GLN:HE22 | 1:AP:183:THR:HA   | 1.73                     | 0.54              |
| 2:BA:137:GLU:O    | 2:BA:139:ALA:N    | 2.41                     | 0.54              |
| 1:AY:246:GLN:HE22 | 1:AZ:183:THR:HA   | 1.73                     | 0.54              |
| 1:AA:246:GLN:HE22 | 1:AB:183:THR:HA   | 1.73                     | 0.54              |
| 1:A5:163:MET:HE1  | 1:A5:189:GLY:HA3  | 1.88                     | 0.54              |
| 3:CT:29:VAL:HG21  | 1:DF:159:PRO:CG   | 254.07                   | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:159:PRO:CG   | 3:CA:29:VAL:HG21  | 2.38                     | 0.54              |
| 2:B1:126:VAL:HG22 | 2:B1:171:VAL:HG11 | 1.89                     | 0.54              |
| 1:AZ:45:LEU:HB2   | 1:AZ:202:HIS:HA   | 1.90                     | 0.54              |
| 3:C1:56:ILE:HD12  | 3:C1:74:PHE:CE1   | 2.43                     | 0.54              |
| 3:CG:56:ILE:HD12  | 3:CG:74:PHE:CE1   | 2.43                     | 0.54              |
| 3:CC:56:ILE:HD12  | 3:CC:74:PHE:CE1   | 2.43                     | 0.54              |
| 3:C9:193:SER:HB3  | 3:C9:196:ILE:HD12 | 1.90                     | 0.54              |
| 1:AM:45:LEU:HB2   | 1:AM:202:HIS:HA   | 1.90                     | 0.54              |
| 1:AX:45:LEU:HB2   | 1:AX:202:HIS:HA   | 1.90                     | 0.54              |
| 1:AY:45:LEU:HB2   | 1:AY:202:HIS:HA   | 1.90                     | 0.54              |
| 1:DK:45:LEU:HB2   | 1:DK:202:HIS:HA   | 1.90                     | 0.54              |
| 3:CK:220:VAL:HG12 | 3:CK:221:ASP:N    | 2.24                     | 0.54              |
| 3:CN:220:VAL:HG12 | 3:CN:221:ASP:N    | 2.23                     | 0.54              |
| 3:CL:220:VAL:HG12 | 3:CL:221:ASP:N    | 2.24                     | 0.54              |
| 3:C6:220:VAL:HG12 | 3:C6:221:ASP:N    | 2.23                     | 0.54              |
| 2:B7:134:HIS:O    | 2:B7:136:HIS:N    | 2.36                     | 0.54              |
| 1:A5:246:GLN:HE22 | 1:A6:183:THR:HA   | 1.73                     | 0.54              |
| 1:AA:183:THR:HA   | 1:AD:246:GLN:HE22 | 1.73                     | 0.54              |
| 1:AK:246:GLN:HE22 | 1:AN:183:THR:HA   | 1.73                     | 0.54              |
| 1:AK:183:THR:HA   | 1:AM:246:GLN:HE22 | 56.61                    | 0.54              |
| 1:AC:183:THR:HA   | 1:A9:246:GLN:HE22 | 295.91                   | 0.54              |
| 1:AE:246:GLN:HE22 | 1:AH:183:THR:HA   | 184.21                   | 0.54              |
| 1:AF:163:MET:HE1  | 1:AF:189:GLY:HA3  | 1.89                     | 0.54              |
| 1:AB:159:PRO:CG   | 3:CB:29:VAL:HG21  | 2.38                     | 0.54              |
| 1:AM:159:PRO:CG   | 3:CN:29:VAL:HG21  | 2.38                     | 0.54              |
| 1:A2:159:PRO:CG   | 3:C3:29:VAL:HG21  | 2.38                     | 0.54              |
| 1:AR:163:MET:HE1  | 1:AR:189:GLY:HA3  | 1.90                     | 0.54              |
| 1:AN:159:PRO:CG   | 3:CO:29:VAL:HG21  | 2.38                     | 0.54              |
| 2:BP:126:VAL:HG22 | 2:BP:171:VAL:HG11 | 1.89                     | 0.54              |
| 3:C3:56:ILE:HD12  | 3:C3:74:PHE:CE1   | 2.43                     | 0.54              |
| 1:DF:45:LEU:HB2   | 1:DF:202:HIS:HA   | 1.90                     | 0.54              |
| 1:A9:45:LEU:HB2   | 1:A9:202:HIS:HA   | 1.90                     | 0.54              |
| 1:DJ:33:LEU:O     | 1:DJ:36:ARG:HD2   | 2.08                     | 0.54              |
| 3:CK:193:SER:HB3  | 3:CK:196:ILE:HD12 | 1.90                     | 0.54              |
| 1:A4:33:LEU:O     | 1:A4:36:ARG:HD2   | 2.08                     | 0.54              |
| 1:AO:33:LEU:O     | 1:AO:36:ARG:HD2   | 2.08                     | 0.54              |
| 3:C9:56:ILE:HD12  | 3:C9:74:PHE:CE1   | 2.43                     | 0.54              |
| 3:C1:139:MET:O    | 3:C1:139:MET:HG2  | 2.07                     | 0.54              |
| 3:CG:139:MET:O    | 3:CG:139:MET:HG2  | 2.07                     | 0.54              |
| 3:CL:56:ILE:HD12  | 3:CL:74:PHE:CE1   | 2.43                     | 0.54              |
| 3:C5:193:SER:HB3  | 3:C5:196:ILE:HD12 | 1.90                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:CG:220:VAL:HG12 | 3:CG:221:ASP:N    | 2.24                     | 0.53              |
| 3:CE:220:VAL:HG12 | 3:CE:221:ASP:N    | 2.24                     | 0.53              |
| 3:C2:220:VAL:HG12 | 3:C2:221:ASP:N    | 2.23                     | 0.53              |
| 1:AT:246:GLN:HE22 | 1:AU:183:THR:HA   | 1.73                     | 0.53              |
| 1:AL:183:THR:HA   | 1:AN:246:GLN:HE22 | 1.73                     | 0.53              |
| 2:BJ:137:GLU:O    | 2:BJ:139:ALA:N    | 2.41                     | 0.53              |
| 2:BR:137:GLU:O    | 2:BR:139:ALA:N    | 2.42                     | 0.53              |
| 1:AT:183:THR:HA   | 1:AW:246:GLN:HE22 | 1.73                     | 0.53              |
| 1:AU:246:GLN:HE22 | 1:AX:183:THR:HA   | 1.73                     | 0.53              |
| 1:AP:246:GLN:HE22 | 1:AS:183:THR:HA   | 1.74                     | 0.53              |
| 2:BM:83:LEU:HD11  | 2:BM:194:ILE:HD12 | 1.91                     | 0.53              |
| 1:AC:159:PRO:CG   | 3:CC:29:VAL:HG21  | 2.38                     | 0.53              |
| 1:AD:159:PRO:CG   | 3:CD:29:VAL:HG21  | 2.38                     | 0.53              |
| 1:A7:159:PRO:CG   | 3:C8:29:VAL:HG21  | 2.38                     | 0.53              |
| 2:B8:126:VAL:HG22 | 2:B8:171:VAL:HG11 | 1.89                     | 0.53              |
| 1:DC:33:LEU:O     | 1:DC:36:ARG:HD2   | 2.08                     | 0.53              |
| 1:AC:33:LEU:O     | 1:AC:36:ARG:HD2   | 2.08                     | 0.53              |
| 1:DI:33:LEU:O     | 1:DI:36:ARG:HD2   | 2.08                     | 0.53              |
| 3:CA:193:SER:HB3  | 3:CA:196:ILE:HD12 | 1.90                     | 0.53              |
| 1:AE:33:LEU:O     | 1:AE:36:ARG:HD2   | 2.08                     | 0.53              |
| 3:C5:135:ARG:HB3  | 3:C5:186:TYR:CG   | 2.44                     | 0.53              |
| 3:CB:193:SER:HB3  | 3:CB:196:ILE:HD12 | 1.90                     | 0.53              |
| 1:AN:45:LEU:HB2   | 1:AN:202:HIS:HA   | 1.90                     | 0.53              |
| 1:DK:33:LEU:O     | 1:DK:36:ARG:HD2   | 2.08                     | 0.53              |
| 1:DD:33:LEU:O     | 1:DD:36:ARG:HD2   | 2.08                     | 0.53              |
| 1:AP:33:LEU:O     | 1:AP:36:ARG:HD2   | 2.08                     | 0.53              |
| 3:CW:193:SER:HB3  | 3:CW:196:ILE:HD12 | 1.90                     | 0.53              |
| 1:AF:45:LEU:HB2   | 1:AF:202:HIS:HA   | 1.90                     | 0.53              |
| 1:A7:33:LEU:O     | 1:A7:36:ARG:HD2   | 2.08                     | 0.53              |
| 1:AI:33:LEU:O     | 1:AI:36:ARG:HD2   | 2.08                     | 0.53              |
| 3:CT:135:ARG:HB3  | 3:CT:186:TYR:CG   | 2.44                     | 0.53              |
| 3:DB:56:ILE:HD12  | 3:DB:74:PHE:CE1   | 2.43                     | 0.53              |
| 3:CJ:220:VAL:HG12 | 3:CJ:221:ASP:N    | 2.23                     | 0.53              |
| 3:CO:220:VAL:HG12 | 3:CO:221:ASP:N    | 2.24                     | 0.53              |
| 3:CV:220:VAL:HG12 | 3:CV:221:ASP:N    | 2.24                     | 0.53              |
| 3:CP:220:VAL:HG12 | 3:CP:221:ASP:N    | 2.23                     | 0.53              |
| 3:CQ:220:VAL:HG12 | 3:CQ:221:ASP:N    | 2.24                     | 0.53              |
| 3:DB:220:VAL:HG12 | 3:DB:221:ASP:N    | 2.24                     | 0.53              |
| 1:AB:246:GLN:HE22 | 1:AE:183:THR:HA   | 1.74                     | 0.53              |
| 1:AC:183:THR:HA   | 1:AE:246:GLN:HE22 | 1.73                     | 0.53              |
| 1:AV:183:THR:HA   | 1:AX:246:GLN:HE22 | 1.73                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A8:191:HIS:CD2  | 1:A8:193:GLY:H    | 2.21                     | 0.53              |
| 2:BA:83:LEU:HD11  | 2:BA:194:ILE:HD12 | 1.91                     | 0.53              |
| 2:BB:83:LEU:HD11  | 2:BB:194:ILE:HD12 | 1.91                     | 0.53              |
| 2:BU:83:LEU:HD11  | 2:BU:194:ILE:HD12 | 1.91                     | 0.53              |
| 2:B9:83:LEU:HD11  | 2:B9:194:ILE:HD12 | 1.91                     | 0.53              |
| 1:A4:159:PRO:CG   | 3:C5:29:VAL:HG21  | 2.38                     | 0.53              |
| 1:AX:159:PRO:CG   | 3:CY:29:VAL:HG21  | 2.38                     | 0.53              |
| 1:A1:163:MET:HE1  | 1:A1:189:GLY:HA3  | 1.90                     | 0.53              |
| 1:AT:159:PRO:CG   | 3:CU:29:VAL:HG21  | 2.38                     | 0.53              |
| 2:BL:126:VAL:HG22 | 2:BL:171:VAL:HG11 | 1.89                     | 0.53              |
| 1:AQ:45:LEU:HB2   | 1:AQ:202:HIS:HA   | 1.90                     | 0.53              |
| 3:C4:56:ILE:HD12  | 3:C4:74:PHE:CE1   | 2.43                     | 0.53              |
| 3:C5:56:ILE:HD12  | 3:C5:74:PHE:CE1   | 2.43                     | 0.53              |
| 3:CI:56:ILE:HD12  | 3:CI:74:PHE:CE1   | 2.43                     | 0.53              |
| 3:DA:135:ARG:HB3  | 3:DA:186:TYR:CG   | 2.44                     | 0.53              |
| 3:CG:135:ARG:HB3  | 3:CG:186:TYR:CG   | 2.44                     | 0.53              |
| 3:CD:193:SER:HB3  | 3:CD:196:ILE:HD12 | 1.90                     | 0.53              |
| 3:C1:135:ARG:HB3  | 3:C1:186:TYR:CG   | 2.44                     | 0.53              |
| 1:AF:33:LEU:O     | 1:AF:36:ARG:HD2   | 2.08                     | 0.53              |
| 3:C1:193:SER:HB3  | 3:C1:196:ILE:HD12 | 1.90                     | 0.53              |
| 3:C8:139:MET:O    | 3:C8:139:MET:HG2  | 2.07                     | 0.53              |
| 1:AQ:33:LEU:O     | 1:AQ:36:ARG:HD2   | 2.08                     | 0.53              |
| 3:CN:193:SER:HB3  | 3:CN:196:ILE:HD12 | 1.90                     | 0.53              |
| 3:CO:135:ARG:HB3  | 3:CO:186:TYR:CG   | 2.44                     | 0.53              |
| 3:CO:193:SER:HB3  | 3:CO:196:ILE:HD12 | 1.90                     | 0.53              |
| 3:CF:56:ILE:HD12  | 3:CF:74:PHE:CE1   | 2.43                     | 0.53              |
| 3:CU:220:VAL:HG12 | 3:CU:221:ASP:N    | 2.24                     | 0.53              |
| 3:CS:220:VAL:HG12 | 3:CS:221:ASP:N    | 2.24                     | 0.53              |
| 1:DH:246:GLN:HE22 | 1:DI:183:THR:HA   | 1.73                     | 0.53              |
| 1:AD:183:THR:HA   | 1:AG:246:GLN:HE22 | 217.58                   | 0.53              |
| 1:DF:183:THR:HA   | 1:DI:246:GLN:HE22 | 1.74                     | 0.53              |
| 1:AG:246:GLN:HE22 | 1:DK:183:THR:HA   | 1.73                     | 0.53              |
| 1:A3:246:GLN:HE22 | 1:A4:183:THR:HA   | 1.73                     | 0.53              |
| 1:AV:246:GLN:HE22 | 1:AW:183:THR:HA   | 1.73                     | 0.53              |
| 2:BX:137:GLU:O    | 2:BX:139:ALA:N    | 2.41                     | 0.53              |
| 2:BQ:137:GLU:O    | 2:BQ:139:ALA:N    | 2.41                     | 0.53              |
| 1:DI:191:HIS:CD2  | 1:DI:193:GLY:H    | 2.21                     | 0.53              |
| 2:BE:83:LEU:HD11  | 2:BE:194:ILE:HD12 | 1.91                     | 0.53              |
| 2:BF:83:LEU:HD11  | 2:BF:194:ILE:HD12 | 1.91                     | 0.53              |
| 2:BJ:83:LEU:HD11  | 2:BJ:194:ILE:HD12 | 1.91                     | 0.53              |
| 2:BC:83:LEU:HD11  | 2:BC:194:ILE:HD12 | 1.91                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BO:83:LEU:HD11  | 2:BO:194:ILE:HD12 | 1.91                     | 0.53              |
| 2:BP:83:LEU:HD11  | 2:BP:194:ILE:HD12 | 1.91                     | 0.53              |
| 1:AG:159:PRO:CG   | 3:CH:29:VAL:HG21  | 52.17                    | 0.53              |
| 1:A8:159:PRO:CG   | 3:C9:29:VAL:HG21  | 2.38                     | 0.53              |
| 1:A6:159:PRO:CG   | 3:C7:29:VAL:HG21  | 2.38                     | 0.53              |
| 1:AR:159:PRO:CG   | 3:CS:29:VAL:HG21  | 2.38                     | 0.53              |
| 1:AP:159:PRO:CG   | 3:CQ:29:VAL:HG21  | 2.38                     | 0.53              |
| 3:CW:29:VAL:HG21  | 1:DI:159:PRO:CG   | 244.86                   | 0.53              |
| 1:AU:159:PRO:CG   | 3:CV:29:VAL:HG21  | 2.38                     | 0.53              |
| 1:AK:159:PRO:CG   | 3:CL:29:VAL:HG21  | 2.38                     | 0.53              |
| 1:AQ:159:PRO:CG   | 3:CR:29:VAL:HG21  | 2.38                     | 0.53              |
| 2:BF:126:VAL:HG22 | 2:BF:171:VAL:HG11 | 1.89                     | 0.53              |
| 3:CE:56:ILE:HD12  | 3:CE:74:PHE:CE1   | 2.43                     | 0.53              |
| 1:DG:33:LEU:O     | 1:DG:36:ARG:HD2   | 2.08                     | 0.53              |
| 3:CI:135:ARG:HB3  | 3:CI:186:TYR:CG   | 2.44                     | 0.53              |
| 3:CR:135:ARG:HB3  | 3:CR:186:TYR:CG   | 2.44                     | 0.53              |
| 3:C3:135:ARG:HB3  | 3:C3:186:TYR:CG   | 2.44                     | 0.53              |
| 3:CG:148:VAL:HG12 | 3:CG:149:GLY:N    | 2.24                     | 0.53              |
| 3:CQ:148:VAL:HG12 | 3:CQ:149:GLY:N    | 2.24                     | 0.53              |
| 3:CK:135:ARG:HB3  | 3:CK:186:TYR:CG   | 2.44                     | 0.53              |
| 1:AG:33:LEU:O     | 1:AG:36:ARG:HD2   | 2.08                     | 0.53              |
| 3:CJ:56:ILE:HD12  | 3:CJ:74:PHE:CE1   | 2.43                     | 0.53              |
| 1:AW:45:LEU:HB2   | 1:AW:202:HIS:HA   | 1.90                     | 0.53              |
| 1:DJ:45:LEU:HB2   | 1:DJ:202:HIS:HA   | 1.90                     | 0.53              |
| 3:CH:135:ARG:HB3  | 3:CH:186:TYR:CG   | 2.44                     | 0.53              |
| 3:CD:135:ARG:HB3  | 3:CD:186:TYR:CG   | 2.44                     | 0.53              |
| 3:CN:135:ARG:HB3  | 3:CN:186:TYR:CG   | 2.44                     | 0.53              |
| 3:CE:193:SER:HB3  | 3:CE:196:ILE:HD12 | 1.90                     | 0.53              |
| 3:CV:135:ARG:HB3  | 3:CV:186:TYR:CG   | 2.44                     | 0.53              |
| 1:A8:33:LEU:O     | 1:A8:36:ARG:HD2   | 2.08                     | 0.53              |
| 3:CG:193:SER:HB3  | 3:CG:196:ILE:HD12 | 1.90                     | 0.53              |
| 1:AK:115:THR:HG22 | 1:AK:116:THR:N    | 2.24                     | 0.53              |
| 3:CC:220:VAL:HG12 | 3:CC:221:ASP:N    | 2.24                     | 0.53              |
| 3:CM:220:VAL:HG12 | 3:CM:221:ASP:N    | 2.23                     | 0.53              |
| 3:CT:220:VAL:HG12 | 3:CT:221:ASP:N    | 2.24                     | 0.53              |
| 3:CB:220:VAL:HG12 | 3:CB:221:ASP:N    | 2.24                     | 0.53              |
| 3:CD:220:VAL:HG12 | 3:CD:221:ASP:N    | 2.24                     | 0.53              |
| 1:AC:246:GLN:HE22 | 1:AD:183:THR:HA   | 1.73                     | 0.53              |
| 1:AL:246:GLN:HE22 | 1:AM:183:THR:HA   | 1.73                     | 0.53              |
| 2:BS:137:GLU:O    | 2:BS:139:ALA:N    | 2.41                     | 0.53              |
| 1:AH:159:PRO:CG   | 3:CH:29:VAL:HG21  | 2.38                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B6:126:VAL:HG22 | 2:B6:171:VAL:HG11 | 1.89                     | 0.53              |
| 2:BW:126:VAL:HG22 | 2:BW:171:VAL:HG11 | 1.89                     | 0.53              |
| 1:A0:33:LEU:O     | 1:A0:36:ARG:HD2   | 2.08                     | 0.53              |
| 3:CM:135:ARG:HB3  | 3:CM:186:TYR:CG   | 2.44                     | 0.53              |
| 1:AU:45:LEU:HB2   | 1:AU:202:HIS:HA   | 1.90                     | 0.53              |
| 3:C0:135:ARG:HB3  | 3:C0:186:TYR:CG   | 2.44                     | 0.53              |
| 1:DH:45:LEU:HB2   | 1:DH:202:HIS:HA   | 1.90                     | 0.53              |
| 3:DB:135:ARG:HB3  | 3:DB:186:TYR:CG   | 2.44                     | 0.53              |
| 3:CR:56:ILE:HD12  | 3:CR:74:PHE:CE1   | 2.43                     | 0.53              |
| 3:CZ:135:ARG:HB3  | 3:CZ:186:TYR:CG   | 2.43                     | 0.53              |
| 3:C7:139:MET:O    | 3:C7:139:MET:HG2  | 2.07                     | 0.53              |
| 3:CZ:139:MET:O    | 3:CZ:139:MET:HG2  | 2.07                     | 0.53              |
| 3:CJ:148:VAL:HG12 | 3:CJ:149:GLY:N    | 2.24                     | 0.53              |
| 3:CF:220:VAL:HG12 | 3:CF:221:ASP:N    | 2.23                     | 0.53              |
| 2:B3:134:HIS:O    | 2:B3:136:HIS:N    | 2.36                     | 0.53              |
| 3:CZ:220:VAL:HG12 | 3:CZ:221:ASP:N    | 2.24                     | 0.53              |
| 1:DC:183:THR:HA   | 1:DE:246:GLN:HE22 | 1.73                     | 0.53              |
| 1:AB:246:GLN:HE22 | 1:A8:183:THR:HA   | 217.58                   | 0.53              |
| 1:AH:183:THR:HA   | 1:DK:246:GLN:HE22 | 1.73                     | 0.53              |
| 1:AY:183:THR:HA   | 1:A1:246:GLN:HE22 | 1.73                     | 0.53              |
| 1:A5:183:THR:HA   | 1:A7:246:GLN:HE22 | 1.73                     | 0.53              |
| 1:A2:191:HIS:CD2  | 1:A2:193:GLY:H    | 2.21                     | 0.53              |
| 2:BW:83:LEU:HD11  | 2:BW:194:ILE:HD12 | 1.91                     | 0.53              |
| 2:B7:83:LEU:HD11  | 2:B7:194:ILE:HD12 | 1.91                     | 0.53              |
| 2:BH:83:LEU:HD11  | 2:BH:194:ILE:HD12 | 1.91                     | 0.53              |
| 2:B5:83:LEU:HD11  | 2:B5:194:ILE:HD12 | 1.91                     | 0.53              |
| 1:AG:159:PRO:CG   | 3:CG:29:VAL:HG21  | 2.38                     | 0.53              |
| 3:CW:148:VAL:HG12 | 3:CW:149:GLY:N    | 2.24                     | 0.53              |
| 1:A9:33:LEU:O     | 1:A9:36:ARG:HD2   | 2.08                     | 0.53              |
| 3:CH:193:SER:HB3  | 3:CH:196:ILE:HD12 | 1.90                     | 0.53              |
| 3:CS:56:ILE:HD12  | 3:CS:74:PHE:CE1   | 2.43                     | 0.53              |
| 3:CJ:135:ARG:HB3  | 3:CJ:186:TYR:CG   | 2.44                     | 0.53              |
| 1:AV:33:LEU:O     | 1:AV:36:ARG:HD2   | 2.08                     | 0.53              |
| 3:CP:135:ARG:HB3  | 3:CP:186:TYR:CG   | 2.44                     | 0.53              |
| 3:CU:135:ARG:HB3  | 3:CU:186:TYR:CG   | 2.43                     | 0.53              |
| 1:A5:33:LEU:O     | 1:A5:36:ARG:HD2   | 2.08                     | 0.53              |
| 1:AR:33:LEU:O     | 1:AR:36:ARG:HD2   | 2.08                     | 0.53              |
| 1:AZ:115:THR:HG22 | 1:AZ:116:THR:N    | 2.24                     | 0.53              |
| 1:A6:115:THR:HG22 | 1:A6:116:THR:N    | 2.24                     | 0.53              |
| 1:DG:115:THR:HG22 | 1:DG:116:THR:N    | 2.24                     | 0.53              |
| 1:DE:115:THR:HG22 | 1:DE:116:THR:N    | 2.24                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C3:220:VAL:HG12 | 3:C3:221:ASP:N    | 2.24                     | 0.53              |
| 3:CX:220:VAL:HG12 | 3:CX:221:ASP:N    | 2.23                     | 0.53              |
| 3:C5:220:VAL:HG12 | 3:C5:221:ASP:N    | 2.24                     | 0.53              |
| 3:C0:220:VAL:HG12 | 3:C0:221:ASP:N    | 2.24                     | 0.53              |
| 1:AH:246:GLN:HE22 | 1:AI:183:THR:HA   | 1.73                     | 0.53              |
| 1:AI:191:HIS:CD2  | 1:AI:193:GLY:H    | 2.21                     | 0.53              |
| 1:AA:191:HIS:CD2  | 1:AA:193:GLY:H    | 2.21                     | 0.53              |
| 1:A4:246:GLN:HE22 | 1:A7:183:THR:HA   | 1.73                     | 0.53              |
| 1:A8:246:GLN:HE22 | 1:A9:183:THR:HA   | 1.73                     | 0.53              |
| 1:AH:191:HIS:CD2  | 1:AH:193:GLY:H    | 2.21                     | 0.53              |
| 2:BI:83:LEU:HD11  | 2:BI:194:ILE:HD12 | 1.91                     | 0.53              |
| 2:BD:83:LEU:HD11  | 2:BD:194:ILE:HD12 | 1.91                     | 0.53              |
| 3:CS:29:VAL:HG21  | 1:DE:159:PRO:CG   | 269.19                   | 0.53              |
| 3:CQ:29:VAL:HG21  | 1:DC:159:PRO:CG   | 244.87                   | 0.53              |
| 1:AV:159:PRO:CG   | 3:CW:29:VAL:HG21  | 2.38                     | 0.53              |
| 3:CH:148:VAL:HG12 | 3:CH:149:GLY:N    | 2.24                     | 0.53              |
| 3:C2:135:ARG:HB3  | 3:C2:186:TYR:CG   | 2.44                     | 0.53              |
| 3:C7:135:ARG:HB3  | 3:C7:186:TYR:CG   | 2.44                     | 0.53              |
| 3:CQ:193:SER:HB3  | 3:CQ:196:ILE:HD12 | 1.90                     | 0.53              |
| 1:A1:33:LEU:O     | 1:A1:36:ARG:HD2   | 2.08                     | 0.53              |
| 1:DH:33:LEU:O     | 1:DH:36:ARG:HD2   | 2.08                     | 0.53              |
| 3:C6:56:ILE:HD12  | 3:C6:74:PHE:CE1   | 2.43                     | 0.53              |
| 3:CA:135:ARG:HB3  | 3:CA:186:TYR:CG   | 2.44                     | 0.53              |
| 3:C9:135:ARG:HB3  | 3:C9:186:TYR:CG   | 2.44                     | 0.53              |
| 1:AK:45:LEU:HB2   | 1:AK:202:HIS:HA   | 1.90                     | 0.53              |
| 3:CZ:56:ILE:HD12  | 3:CZ:74:PHE:CE1   | 2.43                     | 0.53              |
| 3:CT:193:SER:HB3  | 3:CT:196:ILE:HD12 | 1.90                     | 0.53              |
| 3:C0:56:ILE:HD12  | 3:C0:74:PHE:CE1   | 2.43                     | 0.53              |
| 1:AI:45:LEU:HB2   | 1:AI:202:HIS:HA   | 1.90                     | 0.53              |
| 1:AS:33:LEU:O     | 1:AS:36:ARG:HD2   | 2.08                     | 0.53              |
| 3:CL:135:ARG:HB3  | 3:CL:186:TYR:CG   | 2.44                     | 0.53              |
| 1:AF:115:THR:HG22 | 1:AF:116:THR:N    | 2.24                     | 0.53              |
| 1:A7:115:THR:HG22 | 1:A7:116:THR:N    | 2.24                     | 0.53              |
| 1:AR:115:THR:HG22 | 1:AR:116:THR:N    | 2.24                     | 0.53              |
| 1:A3:115:THR:HG22 | 1:A3:116:THR:N    | 2.24                     | 0.53              |
| 1:AJ:115:THR:HG22 | 1:AJ:116:THR:N    | 2.24                     | 0.53              |
| 3:DA:220:VAL:HG12 | 3:DA:221:ASP:N    | 2.24                     | 0.53              |
| 3:C9:220:VAL:HG12 | 3:C9:221:ASP:N    | 2.24                     | 0.53              |
| 1:AK:246:GLN:HE22 | 1:AL:183:THR:HA   | 56.61                    | 0.53              |
| 1:AO:246:GLN:HE22 | 1:DE:183:THR:HA   | 290.20                   | 0.53              |
| 1:AZ:246:GLN:HE22 | 1:A2:183:THR:HA   | 1.73                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AT:191:HIS:CD2  | 1:AT:193:GLY:H    | 2.21                     | 0.53              |
| 2:BR:83:LEU:HD11  | 2:BR:194:ILE:HD12 | 1.91                     | 0.53              |
| 2:BK:83:LEU:HD11  | 2:BK:194:ILE:HD12 | 1.91                     | 0.53              |
| 2:BQ:83:LEU:HD11  | 2:BQ:194:ILE:HD12 | 1.91                     | 0.53              |
| 1:AE:163:MET:HE1  | 1:AE:189:GLY:HA3  | 1.95                     | 0.53              |
| 1:AE:159:PRO:CG   | 3:CE:29:VAL:HG21  | 2.38                     | 0.53              |
| 1:AF:159:PRO:CG   | 3:CF:29:VAL:HG21  | 2.38                     | 0.53              |
| 1:AZ:159:PRO:CG   | 3:C0:29:VAL:HG21  | 2.38                     | 0.53              |
| 2:BZ:126:VAL:HG22 | 2:BZ:171:VAL:HG11 | 1.89                     | 0.53              |
| 2:B2:126:VAL:HG22 | 2:B2:171:VAL:HG11 | 1.89                     | 0.53              |
| 3:CT:148:VAL:HG12 | 3:CT:149:GLY:N    | 2.24                     | 0.53              |
| 3:C7:193:SER:HB3  | 3:C7:196:ILE:HD12 | 1.90                     | 0.53              |
| 3:CR:193:SER:HB3  | 3:CR:196:ILE:HD12 | 1.90                     | 0.53              |
| 3:CY:56:ILE:HD12  | 3:CY:74:PHE:CE1   | 2.43                     | 0.53              |
| 3:CV:193:SER:HB3  | 3:CV:196:ILE:HD12 | 1.90                     | 0.53              |
| 3:C3:139:MET:O    | 3:C3:139:MET:HG2  | 2.07                     | 0.53              |
| 3:CW:135:ARG:HB3  | 3:CW:186:TYR:CG   | 2.44                     | 0.53              |
| 1:AY:33:LEU:O     | 1:AY:36:ARG:HD2   | 2.08                     | 0.53              |
| 3:CF:193:SER:HB3  | 3:CF:196:ILE:HD12 | 1.90                     | 0.53              |
| 3:CX:193:SER:HB3  | 3:CX:196:ILE:HD12 | 1.90                     | 0.53              |
| 1:AP:45:LEU:HB2   | 1:AP:202:HIS:HA   | 1.90                     | 0.53              |
| 1:AL:115:THR:HG22 | 1:AL:116:THR:N    | 2.24                     | 0.53              |
| 1:DC:115:THR:HG22 | 1:DC:116:THR:N    | 2.24                     | 0.53              |
| 3:CR:220:VAL:HG12 | 3:CR:221:ASP:N    | 2.23                     | 0.53              |
| 3:CW:220:VAL:HG12 | 3:CW:221:ASP:N    | 2.24                     | 0.53              |
| 1:AN:183:THR:HA   | 1:DD:246:GLN:HE22 | 311.47                   | 0.53              |
| 1:AP:191:HIS:CD2  | 1:AP:193:GLY:H    | 2.21                     | 0.53              |
| 2:BL:83:LEU:HD11  | 2:BL:194:ILE:HD12 | 1.91                     | 0.53              |
| 2:BT:83:LEU:HD11  | 2:BT:194:ILE:HD12 | 1.91                     | 0.53              |
| 2:BX:83:LEU:HD11  | 2:BX:194:ILE:HD12 | 1.91                     | 0.53              |
| 2:B4:83:LEU:HD11  | 2:B4:194:ILE:HD12 | 1.91                     | 0.53              |
| 2:B2:83:LEU:HD11  | 2:B2:194:ILE:HD12 | 1.91                     | 0.53              |
| 1:AH:163:MET:HE1  | 1:AH:189:GLY:HA3  | 1.91                     | 0.53              |
| 1:AF:159:PRO:CG   | 3:CG:29:VAL:HG21  | 32.12                    | 0.53              |
| 1:AY:159:PRO:CG   | 3:CZ:29:VAL:HG21  | 2.38                     | 0.53              |
| 1:AO:159:PRO:CG   | 3:CP:29:VAL:HG21  | 2.38                     | 0.53              |
| 3:CF:148:VAL:HG12 | 3:CF:149:GLY:N    | 2.24                     | 0.53              |
| 3:CI:148:VAL:HG12 | 3:CI:149:GLY:N    | 2.24                     | 0.53              |
| 3:CI:193:SER:HB3  | 3:CI:196:ILE:HD12 | 1.90                     | 0.53              |
| 3:CB:135:ARG:HB3  | 3:CB:186:TYR:CG   | 2.44                     | 0.53              |
| 1:AX:33:LEU:O     | 1:AX:36:ARG:HD2   | 2.08                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:DB:139:MET:HG2  | 3:DB:139:MET:O    | 2.07                     | 0.53              |
| 1:A6:33:LEU:O     | 1:A6:36:ARG:HD2   | 2.08                     | 0.53              |
| 3:CS:135:ARG:HB3  | 3:CS:186:TYR:CG   | 2.44                     | 0.53              |
| 3:CP:193:SER:HB3  | 3:CP:196:ILE:HD12 | 1.90                     | 0.53              |
| 1:A2:115:THR:HG22 | 1:A2:116:THR:N    | 2.24                     | 0.53              |
| 1:DK:115:THR:HG22 | 1:DK:116:THR:N    | 2.24                     | 0.53              |
| 3:C1:220:VAL:HG12 | 3:C1:221:ASP:N    | 2.24                     | 0.53              |
| 3:C4:220:VAL:HG12 | 3:C4:221:ASP:N    | 2.24                     | 0.53              |
| 3:C8:220:VAL:HG12 | 3:C8:221:ASP:N    | 2.23                     | 0.53              |
| 3:CA:220:VAL:HG12 | 3:CA:221:ASP:N    | 2.23                     | 0.53              |
| 3:CY:220:VAL:HG12 | 3:CY:221:ASP:N    | 2.24                     | 0.53              |
| 1:AF:183:THR:HA   | 1:AH:246:GLN:HE22 | 56.61                    | 0.53              |
| 1:DH:183:THR:HA   | 1:DJ:246:GLN:HE22 | 1.73                     | 0.53              |
| 2:BT:137:GLU:O    | 2:BT:139:ALA:N    | 2.41                     | 0.53              |
| 2:BV:83:LEU:HD11  | 2:BV:194:ILE:HD12 | 1.91                     | 0.53              |
| 1:AC:159:PRO:CG   | 3:CD:29:VAL:HG21  | 32.12                    | 0.53              |
| 1:AW:159:PRO:CG   | 3:CX:29:VAL:HG21  | 2.38                     | 0.53              |
| 2:BD:126:VAL:HG22 | 2:BD:171:VAL:HG11 | 1.89                     | 0.53              |
| 2:BJ:126:VAL:HG22 | 2:BJ:171:VAL:HG11 | 1.89                     | 0.53              |
| 3:C8:135:ARG:HB3  | 3:C8:186:TYR:CG   | 2.44                     | 0.53              |
| 1:AS:45:LEU:HB2   | 1:AS:202:HIS:HA   | 1.90                     | 0.53              |
| 3:CJ:193:SER:HB3  | 3:CJ:196:ILE:HD12 | 1.90                     | 0.53              |
| 1:AT:45:LEU:HB2   | 1:AT:202:HIS:HA   | 1.90                     | 0.53              |
| 1:AE:45:LEU:HB2   | 1:AE:202:HIS:HA   | 1.90                     | 0.53              |
| 3:CL:193:SER:HB3  | 3:CL:196:ILE:HD12 | 1.90                     | 0.53              |
| 1:DC:45:LEU:HB2   | 1:DC:202:HIS:HA   | 1.90                     | 0.53              |
| 3:DA:56:ILE:HD12  | 3:DA:74:PHE:CE1   | 2.43                     | 0.53              |
| 3:C3:193:SER:HB3  | 3:C3:196:ILE:HD12 | 1.90                     | 0.53              |
| 3:CF:135:ARG:HB3  | 3:CF:186:TYR:CG   | 2.44                     | 0.53              |
| 1:AH:45:LEU:HB2   | 1:AH:202:HIS:HA   | 1.90                     | 0.53              |
| 1:AN:115:THR:HG22 | 1:AN:116:THR:N    | 2.24                     | 0.53              |
| 1:AA:115:THR:HG22 | 1:AA:116:THR:N    | 2.24                     | 0.53              |
| 1:A1:115:THR:HG22 | 1:A1:116:THR:N    | 2.24                     | 0.53              |
| 1:A4:115:THR:HG22 | 1:A4:116:THR:N    | 2.24                     | 0.53              |
| 1:AQ:183:THR:HA   | 1:AS:246:GLN:HE22 | 1.73                     | 0.53              |
| 2:BW:137:GLU:O    | 2:BW:139:ALA:N    | 2.41                     | 0.53              |
| 1:A3:183:THR:HA   | 1:A6:246:GLN:HE22 | 1.73                     | 0.53              |
| 2:BN:83:LEU:HD11  | 2:BN:194:ILE:HD12 | 1.91                     | 0.53              |
| 3:CQ:135:ARG:HB3  | 3:CQ:186:TYR:CG   | 2.44                     | 0.53              |
| 1:A7:45:LEU:HB2   | 1:A7:202:HIS:HA   | 1.90                     | 0.53              |
| 3:C0:193:SER:HB3  | 3:C0:196:ILE:HD12 | 1.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:CY:135:ARG:HB3  | 3:CY:186:TYR:CG   | 2.44                     | 0.53              |
| 3:CR:148:VAL:HG12 | 3:CR:149:GLY:N    | 2.24                     | 0.53              |
| 1:AY:115:THR:HG22 | 1:AY:116:THR:N    | 2.24                     | 0.52              |
| 1:AW:115:THR:HG22 | 1:AW:116:THR:N    | 2.24                     | 0.52              |
| 1:AM:115:THR:HG22 | 1:AM:116:THR:N    | 2.24                     | 0.52              |
| 2:BC:137:GLU:O    | 2:BC:139:ALA:N    | 2.41                     | 0.52              |
| 1:DC:246:GLN:HE22 | 1:DD:183:THR:HA   | 1.73                     | 0.52              |
| 1:DF:246:GLN:HE22 | 1:DG:183:THR:HA   | 1.73                     | 0.52              |
| 1:AQ:191:HIS:CD2  | 1:AQ:193:GLY:H    | 2.21                     | 0.52              |
| 2:BY:83:LEU:HD11  | 2:BY:194:ILE:HD12 | 1.91                     | 0.52              |
| 2:B0:83:LEU:HD11  | 2:B0:194:ILE:HD12 | 1.91                     | 0.52              |
| 3:CJ:29:VAL:HG21  | 1:DK:159:PRO:CG   | 2.38                     | 0.52              |
| 3:CM:148:VAL:HG12 | 3:CM:149:GLY:N    | 2.24                     | 0.52              |
| 3:CS:148:VAL:HG12 | 3:CS:149:GLY:N    | 2.24                     | 0.52              |
| 1:A0:45:LEU:HB2   | 1:A0:202:HIS:HA   | 1.90                     | 0.52              |
| 3:C8:193:SER:HB3  | 3:C8:196:ILE:HD12 | 1.90                     | 0.52              |
| 3:CO:148:VAL:HG12 | 3:CO:149:GLY:N    | 2.24                     | 0.52              |
| 1:A3:45:LEU:HB2   | 1:A3:202:HIS:HA   | 1.90                     | 0.52              |
| 2:BL:73:GLN:NE2   | 2:BL:73:GLN:HA    | 2.25                     | 0.52              |
| 1:DD:115:THR:HG22 | 1:DD:116:THR:N    | 2.24                     | 0.52              |
| 1:AX:115:THR:HG22 | 1:AX:116:THR:N    | 2.24                     | 0.52              |
| 3:CH:220:VAL:HG12 | 3:CH:221:ASP:N    | 2.24                     | 0.52              |
| 3:CI:220:VAL:HG12 | 3:CI:221:ASP:N    | 2.23                     | 0.52              |
| 1:AF:183:THR:HA   | 1:AI:246:GLN:HE22 | 1.73                     | 0.52              |
| 2:BK:137:GLU:O    | 2:BK:139:ALA:N    | 2.41                     | 0.52              |
| 2:BU:137:GLU:O    | 2:BU:139:ALA:N    | 2.41                     | 0.52              |
| 1:A1:207:CYS:O    | 1:A1:208:TYR:CB   | 2.58                     | 0.52              |
| 1:AO:207:CYS:O    | 1:AO:208:TYR:CB   | 2.57                     | 0.52              |
| 2:B5:137:GLU:O    | 2:B5:139:ALA:N    | 2.41                     | 0.52              |
| 2:B4:137:GLU:O    | 2:B4:139:ALA:N    | 2.41                     | 0.52              |
| 1:AK:163:MET:HE1  | 1:AK:189:GLY:HA3  | 1.90                     | 0.52              |
| 3:CU:148:VAL:HG12 | 3:CU:149:GLY:N    | 2.24                     | 0.52              |
| 3:CV:148:VAL:HG12 | 3:CV:149:GLY:N    | 2.24                     | 0.52              |
| 2:B5:73:GLN:HA    | 2:B5:73:GLN:NE2   | 2.25                     | 0.52              |
| 3:CX:148:VAL:HG12 | 3:CX:149:GLY:N    | 2.24                     | 0.52              |
| 2:BI:73:GLN:NE2   | 2:BI:73:GLN:HA    | 2.25                     | 0.52              |
| 1:DG:104:VAL:HG22 | 1:DG:197:LEU:HD23 | 1.92                     | 0.52              |
| 2:B7:73:GLN:NE2   | 2:B7:73:GLN:HA    | 2.25                     | 0.52              |
| 3:C0:148:VAL:HG12 | 3:C0:149:GLY:N    | 2.24                     | 0.52              |
| 2:BJ:73:GLN:NE2   | 2:BJ:73:GLN:HA    | 2.25                     | 0.52              |
| 3:C4:135:ARG:HB3  | 3:C4:186:TYR:CG   | 2.44                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AV:115:THR:HG22 | 1:AV:116:THR:N    | 2.24                     | 0.52              |
| 1:AD:115:THR:HG22 | 1:AD:116:THR:N    | 2.24                     | 0.52              |
| 1:AC:115:THR:HG22 | 1:AC:116:THR:N    | 2.24                     | 0.52              |
| 1:DF:115:THR:HG22 | 1:DF:116:THR:N    | 2.24                     | 0.52              |
| 1:AG:115:THR:HG22 | 1:AG:116:THR:N    | 2.24                     | 0.52              |
| 1:AI:115:THR:HG22 | 1:AI:116:THR:N    | 2.24                     | 0.52              |
| 1:A5:246:GLN:NE2  | 1:A6:182:ALA:O    | 2.43                     | 0.52              |
| 1:AA:182:ALA:O    | 1:AD:246:GLN:NE2  | 2.43                     | 0.52              |
| 1:AA:182:ALA:O    | 1:AC:246:GLN:NE2  | 57.04                    | 0.52              |
| 1:AJ:246:GLN:HE22 | 1:AK:183:THR:HA   | 1.73                     | 0.52              |
| 1:AN:246:GLN:HE22 | 1:AO:183:THR:HA   | 274.15                   | 0.52              |
| 1:AO:183:THR:HA   | 1:AR:246:GLN:HE22 | 1.73                     | 0.52              |
| 2:BD:137:GLU:O    | 2:BD:139:ALA:N    | 2.41                     | 0.52              |
| 1:A0:191:HIS:CD2  | 1:A0:193:GLY:H    | 2.21                     | 0.52              |
| 2:BH:157:VAL:HG23 | 3:CH:50:THR:CG2   | 2.39                     | 0.52              |
| 1:AA:246:GLN:NE2  | 1:AB:182:ALA:O    | 2.43                     | 0.52              |
| 2:BB:137:GLU:O    | 2:BB:139:ALA:N    | 2.41                     | 0.52              |
| 1:A0:183:THR:HA   | 1:A2:246:GLN:HE22 | 1.73                     | 0.52              |
| 1:DC:191:HIS:CD2  | 1:DC:193:GLY:H    | 2.21                     | 0.52              |
| 2:BS:83:LEU:HD11  | 2:BS:194:ILE:HD12 | 1.91                     | 0.52              |
| 3:CU:29:VAL:HG21  | 1:DG:159:PRO:CG   | 240.61                   | 0.52              |
| 3:CD:148:VAL:HG12 | 3:CD:149:GLY:N    | 2.24                     | 0.52              |
| 3:CE:148:VAL:HG12 | 3:CE:149:GLY:N    | 2.24                     | 0.52              |
| 3:CY:193:SER:HB3  | 3:CY:196:ILE:HD12 | 1.91                     | 0.52              |
| 3:CC:148:VAL:HG12 | 3:CC:149:GLY:N    | 2.24                     | 0.52              |
| 3:CZ:193:SER:HB3  | 3:CZ:196:ILE:HD12 | 1.90                     | 0.52              |
| 2:BP:73:GLN:HA    | 2:BP:73:GLN:NE2   | 2.25                     | 0.52              |
| 3:C2:148:VAL:HG12 | 3:C2:149:GLY:N    | 2.24                     | 0.52              |
| 1:A2:33:LEU:O     | 1:A2:36:ARG:HD2   | 2.08                     | 0.52              |
| 2:BH:73:GLN:NE2   | 2:BH:73:GLN:HA    | 2.25                     | 0.52              |
| 3:CZ:148:VAL:HG12 | 3:CZ:149:GLY:N    | 2.24                     | 0.52              |
| 2:BR:73:GLN:NE2   | 2:BR:73:GLN:HA    | 2.25                     | 0.52              |
| 1:A5:45:LEU:HB2   | 1:A5:202:HIS:HA   | 1.90                     | 0.52              |
| 3:CU:193:SER:HB3  | 3:CU:196:ILE:HD12 | 1.90                     | 0.52              |
| 3:CE:135:ARG:HB3  | 3:CE:186:TYR:CG   | 2.44                     | 0.52              |
| 1:AO:104:VAL:HG22 | 1:AO:197:LEU:HD23 | 1.92                     | 0.52              |
| 3:C1:148:VAL:HG12 | 3:C1:149:GLY:N    | 2.24                     | 0.52              |
| 3:CC:135:ARG:HB3  | 3:CC:186:TYR:CG   | 2.44                     | 0.52              |
| 1:AA:45:LEU:HB2   | 1:AA:202:HIS:HA   | 1.90                     | 0.52              |
| 1:AO:115:THR:HG22 | 1:AO:116:THR:N    | 2.24                     | 0.52              |
| 1:AH:115:THR:HG22 | 1:AH:116:THR:N    | 2.24                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AU:246:GLN:NE2  | 1:AX:182:ALA:O    | 2.43                     | 0.52              |
| 1:AZ:246:GLN:NE2  | 1:A2:182:ALA:O    | 2.43                     | 0.52              |
| 2:BN:157:VAL:HG23 | 3:CO:50:THR:CG2   | 91.70                    | 0.52              |
| 1:DJ:207:CYS:O    | 1:DJ:208:TYR:CB   | 2.57                     | 0.52              |
| 1:AD:191:HIS:CD2  | 1:AD:193:GLY:H    | 2.21                     | 0.52              |
| 2:B1:137:GLU:O    | 2:B1:139:ALA:N    | 2.41                     | 0.52              |
| 1:AF:246:GLN:HE22 | 1:AG:183:THR:HA   | 1.73                     | 0.52              |
| 1:AF:246:GLN:NE2  | 1:AG:182:ALA:O    | 2.43                     | 0.52              |
| 1:AD:159:PRO:CG   | 3:CE:29:VAL:HG21  | 52.35                    | 0.52              |
| 3:CX:29:VAL:HG21  | 1:DJ:159:PRO:CG   | 245.99                   | 0.52              |
| 1:A1:159:PRO:CG   | 3:C2:29:VAL:HG21  | 2.38                     | 0.52              |
| 3:C5:148:VAL:HG12 | 3:C5:149:GLY:N    | 2.24                     | 0.52              |
| 3:CB:148:VAL:HG12 | 3:CB:149:GLY:N    | 2.24                     | 0.52              |
| 3:CL:148:VAL:HG12 | 3:CL:149:GLY:N    | 2.24                     | 0.52              |
| 2:BO:73:GLN:NE2   | 2:BO:73:GLN:HA    | 2.25                     | 0.52              |
| 1:A8:104:VAL:HG22 | 1:A8:197:LEU:HD23 | 1.92                     | 0.52              |
| 2:BY:73:GLN:HA    | 2:BY:73:GLN:NE2   | 2.25                     | 0.52              |
| 2:BQ:73:GLN:HA    | 2:BQ:73:GLN:NE2   | 2.25                     | 0.52              |
| 1:A0:104:VAL:HG22 | 1:A0:197:LEU:HD23 | 1.92                     | 0.52              |
| 1:AU:104:VAL:HG22 | 1:AU:197:LEU:HD23 | 1.92                     | 0.52              |
| 1:AM:104:VAL:HG22 | 1:AM:197:LEU:HD23 | 1.92                     | 0.52              |
| 1:A1:104:VAL:HG22 | 1:A1:197:LEU:HD23 | 1.92                     | 0.52              |
| 3:C9:148:VAL:HG12 | 3:C9:149:GLY:N    | 2.24                     | 0.52              |
| 3:CM:193:SER:HB3  | 3:CM:196:ILE:HD12 | 1.90                     | 0.52              |
| 3:DA:148:VAL:HG12 | 3:DA:149:GLY:N    | 2.24                     | 0.52              |
| 1:AH:104:VAL:HG22 | 1:AH:197:LEU:HD23 | 1.92                     | 0.52              |
| 3:CX:135:ARG:HB3  | 3:CX:186:TYR:CG   | 2.44                     | 0.52              |
| 1:DH:246:GLN:NE2  | 1:DI:182:ALA:O    | 2.43                     | 0.52              |
| 1:AD:246:GLN:HE22 | 1:AE:183:THR:HA   | 91.40                    | 0.52              |
| 1:AK:246:GLN:NE2  | 1:AN:182:ALA:O    | 2.43                     | 0.52              |
| 1:AI:183:THR:HA   | 1:AL:246:GLN:HE22 | 150.46                   | 0.52              |
| 1:AL:246:GLN:NE2  | 1:AM:182:ALA:O    | 2.43                     | 0.52              |
| 1:AO:246:GLN:NE2  | 1:DE:182:ALA:O    | 291.04                   | 0.52              |
| 1:AK:207:CYS:O    | 1:AK:208:TYR:CB   | 2.57                     | 0.52              |
| 2:BJ:157:VAL:HG23 | 3:CJ:50:THR:CG2   | 2.39                     | 0.52              |
| 1:DF:246:GLN:NE2  | 1:DG:182:ALA:O    | 2.43                     | 0.52              |
| 2:B9:157:VAL:HG23 | 3:DA:50:THR:CG2   | 2.40                     | 0.52              |
| 1:A6:191:HIS:CD2  | 1:A6:193:GLY:H    | 2.21                     | 0.52              |
| 2:B1:83:LEU:HD11  | 2:B1:194:ILE:HD12 | 1.91                     | 0.52              |
| 2:B3:83:LEU:HD11  | 2:B3:194:ILE:HD12 | 1.90                     | 0.52              |
| 2:BZ:83:LEU:HD11  | 2:BZ:194:ILE:HD12 | 1.91                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A0:237:HIS:HB3  | 1:A0:239:PHE:CE1  | 2.45                     | 0.52              |
| 3:C6:193:SER:HB3  | 3:C6:196:ILE:HD12 | 1.90                     | 0.52              |
| 2:BG:73:GLN:NE2   | 2:BG:73:GLN:HA    | 2.25                     | 0.52              |
| 1:AC:104:VAL:HG22 | 1:AC:197:LEU:HD23 | 1.91                     | 0.52              |
| 3:C2:193:SER:HB3  | 3:C2:196:ILE:HD12 | 1.90                     | 0.52              |
| 2:BS:73:GLN:HA    | 2:BS:73:GLN:NE2   | 2.25                     | 0.52              |
| 3:C6:135:ARG:HB3  | 3:C6:186:TYR:CG   | 2.44                     | 0.52              |
| 1:A4:45:LEU:HB2   | 1:A4:202:HIS:HA   | 1.90                     | 0.52              |
| 2:BU:73:GLN:NE2   | 2:BU:73:GLN:HA    | 2.25                     | 0.52              |
| 1:A6:104:VAL:HG22 | 1:A6:197:LEU:HD23 | 1.91                     | 0.52              |
| 1:DD:104:VAL:HG22 | 1:DD:197:LEU:HD23 | 1.92                     | 0.52              |
| 1:DC:104:VAL:HG22 | 1:DC:197:LEU:HD23 | 1.92                     | 0.52              |
| 3:CA:148:VAL:HG12 | 3:CA:149:GLY:N    | 2.24                     | 0.52              |
| 1:AU:115:THR:HG22 | 1:AU:116:THR:N    | 2.24                     | 0.52              |
| 1:AT:115:THR:HG22 | 1:AT:116:THR:N    | 2.24                     | 0.52              |
| 1:A9:115:THR:HG22 | 1:A9:116:THR:N    | 2.24                     | 0.52              |
| 1:AS:115:THR:HG22 | 1:AS:116:THR:N    | 2.24                     | 0.52              |
| 1:AT:246:GLN:NE2  | 1:AU:182:ALA:O    | 2.43                     | 0.52              |
| 1:AJ:246:GLN:NE2  | 1:AK:182:ALA:O    | 2.43                     | 0.52              |
| 1:AN:246:GLN:NE2  | 1:AO:182:ALA:O    | 276.45                   | 0.52              |
| 2:BM:137:GLU:O    | 2:BM:139:ALA:N    | 2.41                     | 0.52              |
| 2:BN:137:GLU:O    | 2:BN:139:ALA:N    | 2.41                     | 0.52              |
| 1:AG:246:GLN:NE2  | 1:DK:182:ALA:O    | 2.43                     | 0.52              |
| 1:AE:246:GLN:NE2  | 1:AH:182:ALA:O    | 184.33                   | 0.52              |
| 1:AH:182:ALA:O    | 1:DK:246:GLN:NE2  | 2.43                     | 0.52              |
| 1:AY:182:ALA:O    | 1:A1:246:GLN:NE2  | 2.43                     | 0.52              |
| 1:AV:182:ALA:O    | 1:AX:246:GLN:NE2  | 2.43                     | 0.52              |
| 2:BE:157:VAL:HG23 | 3:CF:50:THR:CG2   | 65.65                    | 0.52              |
| 1:A4:246:GLN:NE2  | 1:A7:182:ALA:O    | 2.43                     | 0.52              |
| 1:AD:163:MET:HE1  | 1:AD:189:GLY:HA3  | 1.96                     | 0.52              |
| 2:BF:73:GLN:NE2   | 2:BF:73:GLN:HA    | 2.25                     | 0.52              |
| 1:AT:104:VAL:HG22 | 1:AT:197:LEU:HD23 | 1.92                     | 0.52              |
| 2:BZ:73:GLN:NE2   | 2:BZ:73:GLN:HA    | 2.25                     | 0.52              |
| 1:AY:237:HIS:HB3  | 1:AY:239:PHE:CE1  | 2.45                     | 0.52              |
| 1:DC:237:HIS:HB3  | 1:DC:239:PHE:CE1  | 2.45                     | 0.52              |
| 1:AH:237:HIS:HB3  | 1:AH:239:PHE:CE1  | 2.45                     | 0.52              |
| 1:AD:104:VAL:HG22 | 1:AD:197:LEU:HD23 | 1.92                     | 0.52              |
| 3:CS:193:SER:HB3  | 3:CS:196:ILE:HD12 | 1.90                     | 0.52              |
| 2:BA:73:GLN:NE2   | 2:BA:73:GLN:HA    | 2.25                     | 0.52              |
| 3:DA:193:SER:HB3  | 3:DA:196:ILE:HD12 | 1.90                     | 0.52              |
| 1:AZ:33:LEU:O     | 1:AZ:36:ARG:HD2   | 2.08                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BV:73:GLN:HA    | 2:BV:73:GLN:NE2   | 2.25                     | 0.52              |
| 2:BM:73:GLN:NE2   | 2:BM:73:GLN:HA    | 2.25                     | 0.52              |
| 1:AQ:104:VAL:HG22 | 1:AQ:197:LEU:HD23 | 1.92                     | 0.52              |
| 1:AM:237:HIS:HB3  | 1:AM:239:PHE:CE1  | 2.45                     | 0.52              |
| 1:A3:237:HIS:HB3  | 1:A3:239:PHE:CE1  | 2.45                     | 0.52              |
| 1:AW:237:HIS:HB3  | 1:AW:239:PHE:CE1  | 2.45                     | 0.52              |
| 1:AP:115:THR:HG22 | 1:AP:116:THR:N    | 2.24                     | 0.52              |
| 1:A8:115:THR:HG22 | 1:A8:116:THR:N    | 2.24                     | 0.52              |
| 3:C7:220:VAL:HG12 | 3:C7:221:ASP:N    | 2.23                     | 0.52              |
| 1:AD:246:GLN:NE2  | 1:AE:182:ALA:O    | 90.51                    | 0.52              |
| 1:AI:246:GLN:NE2  | 1:AJ:182:ALA:O    | 184.34                   | 0.52              |
| 1:AI:182:ALA:O    | 1:AL:246:GLN:NE2  | 151.55                   | 0.52              |
| 1:AJ:182:ALA:O    | 1:AM:246:GLN:NE2  | 2.43                     | 0.52              |
| 2:BE:137:GLU:O    | 2:BE:139:ALA:N    | 2.42                     | 0.52              |
| 1:A3:246:GLN:NE2  | 1:A4:182:ALA:O    | 2.43                     | 0.52              |
| 2:BD:157:VAL:HG23 | 3:CE:50:THR:CG2   | 91.70                    | 0.52              |
| 2:BV:157:VAL:HG23 | 3:CV:50:THR:CG2   | 2.40                     | 0.52              |
| 1:A0:246:GLN:NE2  | 1:A1:182:ALA:O    | 2.43                     | 0.52              |
| 2:B8:83:LEU:HD11  | 2:B8:194:ILE:HD12 | 1.91                     | 0.52              |
| 2:BG:83:LEU:HD11  | 2:BG:194:ILE:HD12 | 1.91                     | 0.52              |
| 1:AL:163:MET:HE1  | 1:AL:189:GLY:HA3  | 1.90                     | 0.52              |
| 3:DB:148:VAL:HG12 | 3:DB:149:GLY:N    | 2.24                     | 0.52              |
| 1:AF:237:HIS:HB3  | 1:AF:239:PHE:CE1  | 2.45                     | 0.52              |
| 1:A5:237:HIS:HB3  | 1:A5:239:PHE:CE1  | 2.45                     | 0.52              |
| 1:AQ:237:HIS:HB3  | 1:AQ:239:PHE:CE1  | 2.45                     | 0.52              |
| 1:AR:237:HIS:HB3  | 1:AR:239:PHE:CE1  | 2.45                     | 0.52              |
| 1:AN:104:VAL:HG22 | 1:AN:197:LEU:HD23 | 1.92                     | 0.52              |
| 1:A8:237:HIS:HB3  | 1:A8:239:PHE:CE1  | 2.45                     | 0.52              |
| 3:C8:148:VAL:HG12 | 3:C8:149:GLY:N    | 2.24                     | 0.52              |
| 1:AC:237:HIS:HB3  | 1:AC:239:PHE:CE1  | 2.45                     | 0.52              |
| 1:AU:237:HIS:HB3  | 1:AU:239:PHE:CE1  | 2.45                     | 0.52              |
| 3:DB:193:SER:HB3  | 3:DB:196:ILE:HD12 | 1.90                     | 0.52              |
| 1:AD:237:HIS:HB3  | 1:AD:239:PHE:CE1  | 2.45                     | 0.52              |
| 1:AN:237:HIS:HB3  | 1:AN:239:PHE:CE1  | 2.45                     | 0.52              |
| 1:AB:115:THR:HG22 | 1:AB:116:THR:N    | 2.24                     | 0.52              |
| 1:AE:115:THR:HG22 | 1:AE:116:THR:N    | 2.24                     | 0.52              |
| 1:AQ:182:ALA:O    | 1:AS:246:GLN:NE2  | 2.43                     | 0.52              |
| 1:AK:182:ALA:O    | 1:AM:246:GLN:NE2  | 57.04                    | 0.52              |
| 1:DG:207:CYS:O    | 1:DG:208:TYR:CB   | 2.57                     | 0.52              |
| 1:A3:182:ALA:O    | 1:A6:246:GLN:NE2  | 2.43                     | 0.52              |
| 1:A0:246:GLN:HE22 | 1:A1:183:THR:HA   | 1.73                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A1:173:GLY:O    | 1:A1:184:TYR:O    | 2.28                     | 0.52              |
| 1:AE:207:CYS:O    | 1:AE:208:TYR:CB   | 2.57                     | 0.52              |
| 1:DK:191:HIS:CD2  | 1:DK:193:GLY:H    | 2.21                     | 0.52              |
| 1:AO:237:HIS:HB3  | 1:AO:239:PHE:CE1  | 2.45                     | 0.52              |
| 1:AB:45:LEU:HB2   | 1:AB:202:HIS:HA   | 1.90                     | 0.52              |
| 1:AB:237:HIS:HB3  | 1:AB:239:PHE:CE1  | 2.45                     | 0.52              |
| 1:A6:237:HIS:HB3  | 1:A6:239:PHE:CE1  | 2.45                     | 0.52              |
| 1:AV:45:LEU:HB2   | 1:AV:202:HIS:HA   | 1.90                     | 0.52              |
| 1:AL:104:VAL:HG22 | 1:AL:197:LEU:HD23 | 1.92                     | 0.52              |
| 1:A3:104:VAL:HG22 | 1:A3:197:LEU:HD23 | 1.92                     | 0.52              |
| 3:CP:148:VAL:HG12 | 3:CP:149:GLY:N    | 2.24                     | 0.52              |
| 1:A1:237:HIS:HB3  | 1:A1:239:PHE:CE1  | 2.45                     | 0.52              |
| 1:AW:104:VAL:HG22 | 1:AW:197:LEU:HD23 | 1.92                     | 0.52              |
| 2:BE:73:GLN:NE2   | 2:BE:73:GLN:HA    | 2.25                     | 0.52              |
| 1:DK:104:VAL:HG22 | 1:DK:197:LEU:HD23 | 1.92                     | 0.52              |
| 1:AE:237:HIS:HB3  | 1:AE:239:PHE:CE1  | 2.45                     | 0.52              |
| 1:A0:115:THR:HG22 | 1:A0:116:THR:N    | 2.24                     | 0.52              |
| 1:AL:182:ALA:O    | 1:AN:246:GLN:NE2  | 2.43                     | 0.52              |
| 1:AO:173:GLY:O    | 1:AO:184:TYR:O    | 2.28                     | 0.52              |
| 2:BI:137:GLU:O    | 2:BI:139:ALA:N    | 2.41                     | 0.52              |
| 1:DC:246:GLN:NE2  | 1:DD:182:ALA:O    | 2.43                     | 0.52              |
| 1:DG:246:GLN:HE22 | 1:DJ:183:THR:HA   | 1.73                     | 0.52              |
| 2:BP:157:VAL:HG23 | 3:CR:50:THR:CG2   | 2.39                     | 0.52              |
| 1:A5:182:ALA:O    | 1:A7:246:GLN:NE2  | 2.43                     | 0.52              |
| 1:AB:173:GLY:O    | 1:AB:184:TYR:O    | 2.28                     | 0.52              |
| 1:A0:182:ALA:O    | 1:A2:246:GLN:NE2  | 2.43                     | 0.52              |
| 1:AG:173:GLY:O    | 1:AG:184:TYR:O    | 2.28                     | 0.52              |
| 1:DK:163:MET:HE1  | 1:DK:189:GLY:HA3  | 1.92                     | 0.52              |
| 2:BY:101:HIS:CG   | 2:BY:222:VAL:CG1  | 2.93                     | 0.52              |
| 2:BP:101:HIS:CG   | 2:BP:222:VAL:CG1  | 2.93                     | 0.52              |
| 1:AI:104:VAL:HG22 | 1:AI:197:LEU:HD23 | 1.92                     | 0.52              |
| 3:C6:148:VAL:HG12 | 3:C6:149:GLY:N    | 2.24                     | 0.52              |
| 1:AX:237:HIS:HB3  | 1:AX:239:PHE:CE1  | 2.45                     | 0.52              |
| 1:A9:237:HIS:HB3  | 1:A9:239:PHE:CE1  | 2.45                     | 0.52              |
| 1:AG:237:HIS:HB3  | 1:AG:239:PHE:CE1  | 2.45                     | 0.52              |
| 2:B6:73:GLN:NE2   | 2:B6:73:GLN:HA    | 2.25                     | 0.52              |
| 3:CN:148:VAL:HG12 | 3:CN:149:GLY:N    | 2.24                     | 0.52              |
| 2:BE:167:THR:HB   | 2:BE:168:ASN:ND2  | 2.25                     | 0.52              |
| 2:BW:167:THR:HB   | 2:BW:168:ASN:ND2  | 2.25                     | 0.52              |
| 2:BG:167:THR:HB   | 2:BG:168:ASN:ND2  | 2.25                     | 0.52              |
| 3:CK:148:VAL:HG12 | 3:CK:149:GLY:N    | 2.24                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:104:VAL:HG22 | 1:AA:197:LEU:HD23 | 1.92                     | 0.52              |
| 1:DJ:115:THR:HG22 | 1:DJ:116:THR:N    | 2.24                     | 0.52              |
| 1:AD:182:ALA:O    | 1:AG:246:GLN:NE2  | 218.50                   | 0.52              |
| 1:AI:173:GLY:O    | 1:AI:184:TYR:O    | 2.28                     | 0.52              |
| 1:AK:173:GLY:O    | 1:AK:184:TYR:O    | 2.28                     | 0.52              |
| 1:AL:173:GLY:O    | 1:AL:184:TYR:O    | 2.28                     | 0.52              |
| 1:AV:246:GLN:NE2  | 1:AW:182:ALA:O    | 2.43                     | 0.52              |
| 1:AT:182:ALA:O    | 1:AW:246:GLN:NE2  | 2.43                     | 0.52              |
| 1:DH:182:ALA:O    | 1:DJ:246:GLN:NE2  | 2.43                     | 0.52              |
| 1:AQ:246:GLN:HE22 | 1:AR:183:THR:HA   | 1.73                     | 0.52              |
| 2:BN:157:VAL:HG23 | 3:CN:50:THR:CG2   | 2.39                     | 0.52              |
| 1:A8:246:GLN:NE2  | 1:A9:182:ALA:O    | 2.43                     | 0.52              |
| 1:A0:173:GLY:O    | 1:A0:184:TYR:O    | 2.28                     | 0.52              |
| 2:BM:101:HIS:CG   | 2:BM:222:VAL:CG1  | 2.93                     | 0.52              |
| 2:BJ:101:HIS:CG   | 2:BJ:222:VAL:CG1  | 2.93                     | 0.52              |
| 2:BB:101:HIS:CG   | 2:BB:222:VAL:CG1  | 2.93                     | 0.52              |
| 2:B6:101:HIS:CG   | 2:B6:222:VAL:CG1  | 2.94                     | 0.52              |
| 2:BX:101:HIS:CG   | 2:BX:222:VAL:CG1  | 2.94                     | 0.52              |
| 2:B8:101:HIS:CG   | 2:B8:222:VAL:CG1  | 2.93                     | 0.52              |
| 2:B0:101:HIS:CG   | 2:B0:222:VAL:CG1  | 2.93                     | 0.52              |
| 2:BX:73:GLN:NE2   | 2:BX:73:GLN:HA    | 2.25                     | 0.52              |
| 1:AK:237:HIS:HB3  | 1:AK:239:PHE:CE1  | 2.45                     | 0.52              |
| 2:B4:167:THR:HB   | 2:B4:168:ASN:ND2  | 2.25                     | 0.52              |
| 1:AJ:237:HIS:HB3  | 1:AJ:239:PHE:CE1  | 2.45                     | 0.52              |
| 2:BS:167:THR:HB   | 2:BS:168:ASN:ND2  | 2.25                     | 0.52              |
| 1:DI:237:HIS:HB3  | 1:DI:239:PHE:CE1  | 2.45                     | 0.52              |
| 2:B9:167:THR:HB   | 2:B9:168:ASN:ND2  | 2.25                     | 0.52              |
| 1:DC:182:ALA:O    | 1:DE:246:GLN:NE2  | 2.43                     | 0.51              |
| 1:AC:246:GLN:NE2  | 1:AD:182:ALA:O    | 2.43                     | 0.51              |
| 1:AJ:246:GLN:NE2  | 1:AM:182:ALA:O    | 89.43                    | 0.51              |
| 1:AO:246:GLN:NE2  | 1:AP:182:ALA:O    | 2.43                     | 0.51              |
| 1:DE:173:GLY:O    | 1:DE:184:TYR:O    | 2.28                     | 0.51              |
| 1:DF:173:GLY:O    | 1:DF:184:TYR:O    | 2.28                     | 0.51              |
| 1:AZ:207:CYS:O    | 1:AZ:208:TYR:CB   | 2.57                     | 0.51              |
| 1:DH:173:GLY:O    | 1:DH:184:TYR:O    | 2.28                     | 0.51              |
| 1:AQ:246:GLN:NE2  | 1:AR:182:ALA:O    | 2.43                     | 0.51              |
| 2:BB:157:VAL:HG23 | 3:CB:50:THR:CG2   | 2.40                     | 0.51              |
| 2:BT:157:VAL:HG23 | 3:CT:50:THR:CG2   | 2.39                     | 0.51              |
| 1:A5:173:GLY:O    | 1:A5:184:TYR:O    | 2.28                     | 0.51              |
| 1:A1:191:HIS:CD2  | 1:A1:193:GLY:H    | 2.21                     | 0.51              |
| 2:BF:101:HIS:CG   | 2:BF:222:VAL:CG1  | 2.93                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B1:101:HIS:CG   | 2:B1:222:VAL:CG1  | 2.93                     | 0.51              |
| 2:BS:101:HIS:CG   | 2:BS:222:VAL:CG1  | 2.94                     | 0.51              |
| 2:BL:101:HIS:CG   | 2:BL:222:VAL:CG1  | 2.93                     | 0.51              |
| 2:BO:101:HIS:CG   | 2:BO:222:VAL:CG1  | 2.93                     | 0.51              |
| 2:BN:101:HIS:CG   | 2:BN:222:VAL:CG1  | 2.94                     | 0.51              |
| 1:A4:237:HIS:HB3  | 1:A4:239:PHE:CE1  | 2.45                     | 0.51              |
| 2:B1:167:THR:HB   | 2:B1:168:ASN:ND2  | 2.25                     | 0.51              |
| 2:BM:167:THR:HB   | 2:BM:168:ASN:ND2  | 2.25                     | 0.51              |
| 1:AK:104:VAL:HG22 | 1:AK:197:LEU:HD23 | 1.92                     | 0.51              |
| 2:B3:167:THR:HB   | 2:B3:168:ASN:ND2  | 2.25                     | 0.51              |
| 2:B8:73:GLN:HA    | 2:B8:73:GLN:NE2   | 2.25                     | 0.51              |
| 1:DI:104:VAL:HG22 | 1:DI:197:LEU:HD23 | 1.91                     | 0.51              |
| 2:BP:167:THR:HB   | 2:BP:168:ASN:ND2  | 2.26                     | 0.51              |
| 2:BK:73:GLN:NE2   | 2:BK:73:GLN:HA    | 2.25                     | 0.51              |
| 2:BZ:167:THR:HB   | 2:BZ:168:ASN:ND2  | 2.25                     | 0.51              |
| 1:DG:237:HIS:HB3  | 1:DG:239:PHE:CE1  | 2.45                     | 0.51              |
| 1:A2:237:HIS:HB3  | 1:A2:239:PHE:CE1  | 2.45                     | 0.51              |
| 1:A5:115:THR:HG22 | 1:A5:116:THR:N    | 2.24                     | 0.51              |
| 1:AE:173:GLY:O    | 1:AE:184:TYR:O    | 2.28                     | 0.51              |
| 1:AF:182:ALA:O    | 1:AH:246:GLN:NE2  | 57.04                    | 0.51              |
| 2:BF:137:GLU:O    | 2:BF:139:ALA:N    | 2.41                     | 0.51              |
| 1:DF:182:ALA:O    | 1:DI:246:GLN:NE2  | 2.43                     | 0.51              |
| 1:A4:173:GLY:O    | 1:A4:184:TYR:O    | 2.28                     | 0.51              |
| 1:AW:173:GLY:O    | 1:AW:184:TYR:O    | 2.28                     | 0.51              |
| 1:AY:246:GLN:NE2  | 1:AZ:182:ALA:O    | 2.43                     | 0.51              |
| 1:AT:173:GLY:O    | 1:AT:184:TYR:O    | 2.28                     | 0.51              |
| 1:DG:246:GLN:NE2  | 1:DJ:182:ALA:O    | 2.43                     | 0.51              |
| 2:BU:157:VAL:HG23 | 3:CU:50:THR:CG2   | 2.40                     | 0.51              |
| 2:BK:157:VAL:HG23 | 3:CK:50:THR:CG2   | 2.40                     | 0.51              |
| 1:AV:191:HIS:CD2  | 1:AV:193:GLY:H    | 2.21                     | 0.51              |
| 2:BQ:101:HIS:CG   | 2:BQ:222:VAL:CG1  | 2.93                     | 0.51              |
| 2:BW:101:HIS:CG   | 2:BW:222:VAL:CG1  | 2.94                     | 0.51              |
| 2:BL:167:THR:HB   | 2:BL:168:ASN:ND2  | 2.25                     | 0.51              |
| 2:BU:167:THR:HB   | 2:BU:168:ASN:ND2  | 2.25                     | 0.51              |
| 1:DK:237:HIS:HB3  | 1:DK:239:PHE:CE1  | 2.45                     | 0.51              |
| 2:BV:167:THR:HB   | 2:BV:168:ASN:ND2  | 2.25                     | 0.51              |
| 1:AZ:237:HIS:HB3  | 1:AZ:239:PHE:CE1  | 2.45                     | 0.51              |
| 1:AI:237:HIS:HB3  | 1:AI:239:PHE:CE1  | 2.45                     | 0.51              |
| 3:CC:193:SER:HB3  | 3:CC:196:ILE:HD12 | 1.90                     | 0.51              |
| 2:BB:73:GLN:HA    | 2:BB:73:GLN:NE2   | 2.25                     | 0.51              |
| 1:AP:104:VAL:HG22 | 1:AP:197:LEU:HD23 | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BC:73:GLN:HA    | 2:BC:73:GLN:NE2   | 2.25                     | 0.51              |
| 1:AF:104:VAL:HG22 | 1:AF:197:LEU:HD23 | 1.91                     | 0.51              |
| 2:BI:167:THR:HB   | 2:BI:168:ASN:ND2  | 2.25                     | 0.51              |
| 2:BR:167:THR:HB   | 2:BR:168:ASN:ND2  | 2.25                     | 0.51              |
| 2:BK:167:THR:HB   | 2:BK:168:ASN:ND2  | 2.25                     | 0.51              |
| 1:AS:70:ARG:HH11  | 3:CT:222:LEU:HD21 | 1.76                     | 0.51              |
| 1:AO:70:ARG:HH11  | 3:CP:222:LEU:HD21 | 1.76                     | 0.51              |
| 1:AF:173:GLY:O    | 1:AF:184:TYR:O    | 2.28                     | 0.51              |
| 1:AJ:246:GLN:HE22 | 1:AM:183:THR:HA   | 91.28                    | 0.51              |
| 1:AH:173:GLY:O    | 1:AH:184:TYR:O    | 2.28                     | 0.51              |
| 2:BZ:137:GLU:O    | 2:BZ:139:ALA:N    | 2.41                     | 0.51              |
| 1:AV:173:GLY:O    | 1:AV:184:TYR:O    | 2.28                     | 0.51              |
| 1:DD:191:HIS:CD2  | 1:DD:193:GLY:H    | 2.21                     | 0.51              |
| 2:BI:101:HIS:CG   | 2:BI:222:VAL:CG1  | 2.93                     | 0.51              |
| 2:BC:101:HIS:CG   | 2:BC:222:VAL:CG1  | 2.93                     | 0.51              |
| 2:BU:101:HIS:CG   | 2:BU:222:VAL:CG1  | 2.94                     | 0.51              |
| 2:BK:101:HIS:CG   | 2:BK:222:VAL:CG1  | 2.94                     | 0.51              |
| 2:BZ:101:HIS:CG   | 2:BZ:222:VAL:CG1  | 2.93                     | 0.51              |
| 2:BG:101:HIS:CG   | 2:BG:222:VAL:CG1  | 2.93                     | 0.51              |
| 2:BD:101:HIS:CG   | 2:BD:222:VAL:CG1  | 2.94                     | 0.51              |
| 2:BC:167:THR:HB   | 2:BC:168:ASN:ND2  | 2.25                     | 0.51              |
| 2:BD:167:THR:HB   | 2:BD:168:ASN:ND2  | 2.25                     | 0.51              |
| 3:C3:148:VAL:HG12 | 3:C3:149:GLY:N    | 2.24                     | 0.51              |
| 1:DD:237:HIS:HB3  | 1:DD:239:PHE:CE1  | 2.45                     | 0.51              |
| 1:AA:237:HIS:HB3  | 1:AA:239:PHE:CE1  | 2.45                     | 0.51              |
| 1:AG:104:VAL:HG22 | 1:AG:197:LEU:HD23 | 1.92                     | 0.51              |
| 1:DF:237:HIS:HB3  | 1:DF:239:PHE:CE1  | 2.45                     | 0.51              |
| 1:AL:237:HIS:HB3  | 1:AL:239:PHE:CE1  | 2.45                     | 0.51              |
| 2:B3:73:GLN:NE2   | 2:B3:73:GLN:HA    | 2.25                     | 0.51              |
| 1:A5:104:VAL:HG22 | 1:A5:197:LEU:HD23 | 1.92                     | 0.51              |
| 1:AZ:104:VAL:HG22 | 1:AZ:197:LEU:HD23 | 1.92                     | 0.51              |
| 3:C4:193:SER:HB3  | 3:C4:196:ILE:HD12 | 1.90                     | 0.51              |
| 1:AE:70:ARG:HH11  | 3:CF:222:LEU:HD21 | 96.38                    | 0.51              |
| 1:AF:70:ARG:HH11  | 3:CG:222:LEU:HD21 | 46.80                    | 0.51              |
| 1:AH:70:ARG:HH11  | 3:CI:222:LEU:HD21 | 46.80                    | 0.51              |
| 1:AN:70:ARG:HH11  | 3:CO:222:LEU:HD21 | 1.76                     | 0.51              |
| 1:AQ:173:GLY:O    | 1:AQ:184:TYR:O    | 2.28                     | 0.51              |
| 1:AB:246:GLN:NE2  | 1:A8:182:ALA:O    | 220.41                   | 0.51              |
| 1:AH:246:GLN:NE2  | 1:AI:182:ALA:O    | 2.43                     | 0.51              |
| 1:AN:173:GLY:O    | 1:AN:184:TYR:O    | 2.28                     | 0.51              |
| 1:AN:182:ALA:O    | 1:DD:246:GLN:NE2  | 312.29                   | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AC:182:ALA:O    | 1:AE:246:GLN:NE2  | 2.43                     | 0.51              |
| 1:AZ:173:GLY:O    | 1:AZ:184:TYR:O    | 2.28                     | 0.51              |
| 1:AX:173:GLY:O    | 1:AX:184:TYR:O    | 2.28                     | 0.51              |
| 1:A3:191:HIS:CD2  | 1:A3:193:GLY:H    | 2.21                     | 0.51              |
| 2:BA:101:HIS:CG   | 2:BA:222:VAL:CG1  | 2.93                     | 0.51              |
| 2:B9:101:HIS:CG   | 2:B9:222:VAL:CG1  | 2.93                     | 0.51              |
| 1:AR:104:VAL:HG22 | 1:AR:197:LEU:HD23 | 1.92                     | 0.51              |
| 1:A2:104:VAL:HG22 | 1:A2:197:LEU:HD23 | 1.92                     | 0.51              |
| 2:BN:167:THR:HB   | 2:BN:168:ASN:ND2  | 2.26                     | 0.51              |
| 3:C7:148:VAL:HG12 | 3:C7:149:GLY:N    | 2.24                     | 0.51              |
| 1:DE:237:HIS:HB3  | 1:DE:239:PHE:CE1  | 2.45                     | 0.51              |
| 2:BT:73:GLN:HA    | 2:BT:73:GLN:NE2   | 2.25                     | 0.51              |
| 1:A7:104:VAL:HG22 | 1:A7:197:LEU:HD23 | 1.92                     | 0.51              |
| 2:BJ:167:THR:HB   | 2:BJ:168:ASN:ND2  | 2.25                     | 0.51              |
| 1:DE:104:VAL:HG22 | 1:DE:197:LEU:HD23 | 1.92                     | 0.51              |
| 1:DH:115:THR:HG22 | 1:DH:116:THR:N    | 2.24                     | 0.51              |
| 3:CS:222:LEU:HD21 | 1:DE:70:ARG:HH11  | 291.40                   | 0.51              |
| 3:CV:222:LEU:HD21 | 1:DH:70:ARG:HH11  | 291.38                   | 0.51              |
| 1:AK:246:GLN:NE2  | 1:AL:182:ALA:O    | 57.04                    | 0.51              |
| 1:AO:182:ALA:O    | 1:AR:246:GLN:NE2  | 2.43                     | 0.51              |
| 2:BO:137:GLU:O    | 2:BO:139:ALA:N    | 2.41                     | 0.51              |
| 1:DK:173:GLY:O    | 1:DK:184:TYR:O    | 2.28                     | 0.51              |
| 1:AC:182:ALA:O    | 1:A9:246:GLN:NE2  | 297.90                   | 0.51              |
| 2:B0:137:GLU:O    | 2:B0:139:ALA:N    | 2.42                     | 0.51              |
| 1:AC:191:HIS:CD2  | 1:AC:193:GLY:H    | 2.21                     | 0.51              |
| 1:DG:173:GLY:O    | 1:DG:184:TYR:O    | 2.28                     | 0.51              |
| 2:B9:137:GLU:O    | 2:B9:139:ALA:N    | 2.41                     | 0.51              |
| 2:BA:157:VAL:HG23 | 3:DB:50:THR:CG2   | 270.98                   | 0.51              |
| 1:AT:163:MET:HE1  | 1:AT:189:GLY:HA3  | 1.92                     | 0.51              |
| 2:BV:101:HIS:CG   | 2:BV:222:VAL:CG1  | 2.93                     | 0.51              |
| 2:BE:101:HIS:CG   | 2:BE:222:VAL:CG1  | 2.94                     | 0.51              |
| 2:B3:101:HIS:CG   | 2:B3:222:VAL:CG1  | 2.93                     | 0.51              |
| 1:DJ:237:HIS:HB3  | 1:DJ:239:PHE:CE1  | 2.45                     | 0.51              |
| 2:B2:167:THR:HB   | 2:B2:168:ASN:ND2  | 2.25                     | 0.51              |
| 3:C4:148:VAL:HG12 | 3:C4:149:GLY:N    | 2.24                     | 0.51              |
| 2:BO:167:THR:HB   | 2:BO:168:ASN:ND2  | 2.25                     | 0.51              |
| 1:AV:104:VAL:HG22 | 1:AV:197:LEU:HD23 | 1.92                     | 0.51              |
| 1:AE:104:VAL:HG22 | 1:AE:197:LEU:HD23 | 1.92                     | 0.51              |
| 2:BA:167:THR:HB   | 2:BA:168:ASN:ND2  | 2.25                     | 0.51              |
| 1:DI:115:THR:HG22 | 1:DI:116:THR:N    | 2.24                     | 0.51              |
| 2:BV:137:GLU:O    | 2:BV:139:ALA:N    | 2.41                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AB:246:GLN:NE2  | 1:AE:182:ALA:O    | 2.43                     | 0.51              |
| 1:AF:182:ALA:O    | 1:AI:246:GLN:NE2  | 2.43                     | 0.51              |
| 1:AC:173:GLY:O    | 1:AC:184:TYR:O    | 2.28                     | 0.51              |
| 2:BC:157:VAL:HG23 | 3:CC:50:THR:CG2   | 2.39                     | 0.51              |
| 1:DE:207:CYS:O    | 1:DE:208:TYR:CB   | 2.57                     | 0.51              |
| 2:B7:84:PRO:CG    | 2:B7:85:SER:H     | 2.24                     | 0.51              |
| 2:BU:84:PRO:CG    | 2:BU:85:SER:H     | 2.24                     | 0.51              |
| 2:B2:101:HIS:CG   | 2:B2:222:VAL:CG1  | 2.94                     | 0.51              |
| 2:B4:101:HIS:CG   | 2:B4:222:VAL:CG1  | 2.94                     | 0.51              |
| 2:BH:101:HIS:CG   | 2:BH:222:VAL:CG1  | 2.93                     | 0.51              |
| 3:C2:132:PRO:HG2  | 3:C2:184:GLN:HE22 | 1.76                     | 0.51              |
| 1:AJ:104:VAL:HG22 | 1:AJ:197:LEU:HD23 | 1.92                     | 0.51              |
| 1:AP:237:HIS:HB3  | 1:AP:239:PHE:CE1  | 2.45                     | 0.51              |
| 1:A9:104:VAL:HG22 | 1:A9:197:LEU:HD23 | 1.92                     | 0.51              |
| 2:BH:167:THR:HB   | 2:BH:168:ASN:ND2  | 2.25                     | 0.51              |
| 1:DJ:104:VAL:HG22 | 1:DJ:197:LEU:HD23 | 1.92                     | 0.51              |
| 2:BQ:167:THR:HB   | 2:BQ:168:ASN:ND2  | 2.26                     | 0.51              |
| 1:AS:237:HIS:HB3  | 1:AS:239:PHE:CE1  | 2.45                     | 0.51              |
| 3:CY:148:VAL:HG12 | 3:CY:149:GLY:N    | 2.24                     | 0.51              |
| 2:B2:73:GLN:HA    | 2:B2:73:GLN:NE2   | 2.25                     | 0.51              |
| 3:CS:132:PRO:HG2  | 3:CS:184:GLN:HE22 | 1.76                     | 0.51              |
| 1:DH:237:HIS:HB3  | 1:DH:239:PHE:CE1  | 2.45                     | 0.51              |
| 2:BN:73:GLN:NE2   | 2:BN:73:GLN:HA    | 2.25                     | 0.51              |
| 2:BT:167:THR:HB   | 2:BT:168:ASN:ND2  | 2.25                     | 0.51              |
| 1:AQ:115:THR:HG22 | 1:AQ:116:THR:N    | 2.24                     | 0.51              |
| 3:CQ:222:LEU:HD21 | 1:DC:70:ARG:HH11  | 230.15                   | 0.51              |
| 1:AD:70:ARG:HH11  | 3:CD:222:LEU:HD21 | 1.76                     | 0.51              |
| 1:AH:70:ARG:HH11  | 3:CH:222:LEU:HD21 | 1.76                     | 0.51              |
| 1:AK:70:ARG:HH11  | 3:CL:222:LEU:HD21 | 1.76                     | 0.51              |
| 3:CX:222:LEU:HD21 | 1:DJ:70:ARG:HH11  | 275.46                   | 0.51              |
| 3:CR:222:LEU:HD21 | 1:DD:70:ARG:HH11  | 265.31                   | 0.51              |
| 1:AJ:70:ARG:HH11  | 3:CK:222:LEU:HD21 | 1.76                     | 0.51              |
| 1:AC:207:CYS:O    | 1:AC:208:TYR:CB   | 2.57                     | 0.51              |
| 2:BV:157:VAL:HG23 | 3:CW:50:THR:CG2   | 92.72                    | 0.51              |
| 2:BU:157:VAL:HG23 | 3:CV:50:THR:CG2   | 58.34                    | 0.51              |
| 1:A7:173:GLY:O    | 1:A7:184:TYR:O    | 2.28                     | 0.51              |
| 2:BG:137:GLU:O    | 2:BG:139:ALA:N    | 2.41                     | 0.51              |
| 2:BF:84:PRO:CG    | 2:BF:85:SER:H     | 2.24                     | 0.51              |
| 2:BB:84:PRO:CG    | 2:BB:85:SER:H     | 2.24                     | 0.51              |
| 2:BM:84:PRO:CG    | 2:BM:85:SER:H     | 2.24                     | 0.51              |
| 2:BI:84:PRO:CG    | 2:BI:85:SER:H     | 2.24                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BX:84:PRO:CG    | 2:BX:85:SER:H     | 2.24                     | 0.51              |
| 2:BH:84:PRO:CG    | 2:BH:85:SER:H     | 2.24                     | 0.51              |
| 2:B6:83:LEU:HD11  | 2:B6:194:ILE:HD12 | 1.91                     | 0.51              |
| 2:BE:102:HIS:CE1  | 3:CE:127:PRO:HG2  | 62.85                    | 0.51              |
| 1:DF:104:VAL:HG22 | 1:DF:197:LEU:HD23 | 1.92                     | 0.51              |
| 3:CN:132:PRO:HG2  | 3:CN:184:GLN:HE22 | 1.76                     | 0.51              |
| 1:A7:237:HIS:HB3  | 1:A7:239:PHE:CE1  | 2.45                     | 0.51              |
| 3:CC:132:PRO:HG2  | 3:CC:184:GLN:HE22 | 1.76                     | 0.51              |
| 2:B0:73:GLN:HA    | 2:B0:73:GLN:NE2   | 2.25                     | 0.51              |
| 2:BY:167:THR:HB   | 2:BY:168:ASN:ND2  | 2.25                     | 0.51              |
| 2:BN:102:HIS:CE1  | 3:CR:127:PRO:HG2  | 254.32                   | 0.51              |
| 2:BS:102:HIS:CE1  | 3:CW:127:PRO:HG2  | 290.74                   | 0.51              |
| 2:BT:102:HIS:CE1  | 3:CQ:127:PRO:HG2  | 2.46                     | 0.51              |
| 2:BR:102:HIS:CE1  | 3:CP:127:PRO:HG2  | 253.62                   | 0.51              |
| 2:BA:102:HIS:CE1  | 3:CD:127:PRO:HG2  | 2.46                     | 0.51              |
| 1:AL:70:ARG:HH11  | 3:CM:222:LEU:HD21 | 1.76                     | 0.51              |
| 1:AM:70:ARG:HH11  | 3:CN:222:LEU:HD21 | 1.76                     | 0.51              |
| 1:AJ:173:GLY:O    | 1:AJ:184:TYR:O    | 2.28                     | 0.51              |
| 1:AR:173:GLY:O    | 1:AR:184:TYR:O    | 2.28                     | 0.51              |
| 1:AL:191:HIS:CD2  | 1:AL:193:GLY:H    | 2.21                     | 0.51              |
| 2:B8:157:VAL:HG23 | 3:C9:50:THR:CG2   | 2.39                     | 0.51              |
| 1:A3:207:CYS:O    | 1:A3:208:TYR:CB   | 2.57                     | 0.51              |
| 2:BK:84:PRO:CG    | 2:BK:85:SER:H     | 2.24                     | 0.51              |
| 2:B9:84:PRO:CG    | 2:B9:85:SER:H     | 2.24                     | 0.51              |
| 1:DH:163:MET:HE1  | 1:DH:189:GLY:HA3  | 1.93                     | 0.51              |
| 2:BT:101:HIS:CG   | 2:BT:222:VAL:CG1  | 2.94                     | 0.51              |
| 2:BC:102:HIS:CE1  | 3:CE:127:PRO:HG2  | 2.46                     | 0.51              |
| 2:BM:102:HIS:CE1  | 3:CK:127:PRO:HG2  | 104.43                   | 0.51              |
| 2:BQ:102:HIS:CE1  | 3:CQ:127:PRO:HG2  | 104.43                   | 0.51              |
| 2:BD:102:HIS:CE1  | 3:CH:127:PRO:HG2  | 181.33                   | 0.51              |
| 2:BQ:102:HIS:CE1  | 3:CR:127:PRO:HG2  | 2.46                     | 0.51              |
| 3:CI:132:PRO:HG2  | 3:CI:184:GLN:HE22 | 1.76                     | 0.51              |
| 2:BF:167:THR:HB   | 2:BF:168:ASN:ND2  | 2.25                     | 0.51              |
| 2:BD:73:GLN:HA    | 2:BD:73:GLN:NE2   | 2.25                     | 0.51              |
| 2:BH:102:HIS:CE1  | 3:CF:127:PRO:HG2  | 104.43                   | 0.51              |
| 2:BJ:102:HIS:CE1  | 3:CG:127:PRO:HG2  | 2.46                     | 0.51              |
| 2:BW:73:GLN:NE2   | 2:BW:73:GLN:HA    | 2.25                     | 0.51              |
| 3:DA:132:PRO:HG2  | 3:DA:184:GLN:HE22 | 1.76                     | 0.51              |
| 1:AY:70:ARG:HH11  | 3:CZ:222:LEU:HD21 | 1.76                     | 0.51              |
| 1:AG:191:HIS:CD2  | 1:AG:193:GLY:H    | 2.21                     | 0.51              |
| 2:BX:157:VAL:HG23 | 3:CX:50:THR:CG2   | 2.40                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AP:246:GLN:NE2  | 1:AS:182:ALA:O    | 2.43                     | 0.51              |
| 1:A3:173:GLY:O    | 1:A3:184:TYR:O    | 2.28                     | 0.51              |
| 1:AS:191:HIS:CD2  | 1:AS:193:GLY:H    | 2.21                     | 0.51              |
| 2:BE:84:PRO:CG    | 2:BE:85:SER:H     | 2.24                     | 0.51              |
| 2:BA:84:PRO:CG    | 2:BA:85:SER:H     | 2.24                     | 0.51              |
| 2:BT:84:PRO:CG    | 2:BT:85:SER:H     | 2.24                     | 0.51              |
| 2:BG:84:PRO:CG    | 2:BG:85:SER:H     | 2.24                     | 0.51              |
| 1:AQ:163:MET:HE1  | 1:AQ:189:GLY:HA3  | 1.92                     | 0.51              |
| 2:B7:101:HIS:CG   | 2:B7:222:VAL:CG1  | 2.93                     | 0.51              |
| 1:AT:237:HIS:HB3  | 1:AT:239:PHE:CE1  | 2.45                     | 0.51              |
| 1:DH:104:VAL:HG22 | 1:DH:197:LEU:HD23 | 1.92                     | 0.51              |
| 2:BX:167:THR:HB   | 2:BX:168:ASN:ND2  | 2.26                     | 0.51              |
| 2:B7:167:THR:HB   | 2:B7:168:ASN:ND2  | 2.25                     | 0.51              |
| 1:AV:237:HIS:HB3  | 1:AV:239:PHE:CE1  | 2.45                     | 0.51              |
| 2:BB:167:THR:HB   | 2:BB:168:ASN:ND2  | 2.25                     | 0.51              |
| 1:AI:70:ARG:HH11  | 3:CI:222:LEU:HD21 | 1.76                     | 0.51              |
| 3:CT:222:LEU:HD21 | 1:DF:70:ARG:HH11  | 275.58                   | 0.51              |
| 1:AZ:70:ARG:HH11  | 3:C0:222:LEU:HD21 | 1.76                     | 0.51              |
| 1:AX:70:ARG:HH11  | 3:CY:222:LEU:HD21 | 1.76                     | 0.51              |
| 1:AU:173:GLY:O    | 1:AU:184:TYR:O    | 2.28                     | 0.51              |
| 1:DC:173:GLY:O    | 1:DC:184:TYR:O    | 2.28                     | 0.51              |
| 1:A2:173:GLY:O    | 1:A2:184:TYR:O    | 2.28                     | 0.51              |
| 2:BY:157:VAL:HG23 | 3:CY:50:THR:CG2   | 2.40                     | 0.51              |
| 1:A8:188:PRO:HG3  | 3:CC:175:THR:HG23 | 264.23                   | 0.51              |
| 1:AE:188:PRO:HG3  | 3:CB:175:THR:HG23 | 1.93                     | 0.51              |
| 1:AI:188:PRO:HG3  | 3:CM:175:THR:HG23 | 142.34                   | 0.51              |
| 1:AQ:188:PRO:HG3  | 3:CT:175:THR:HG23 | 1.93                     | 0.51              |
| 1:A2:188:PRO:HG3  | 3:C0:175:THR:HG23 | 1.93                     | 0.51              |
| 1:AS:188:PRO:HG3  | 3:CQ:175:THR:HG23 | 1.93                     | 0.51              |
| 1:AH:38:PHE:O     | 1:AH:210:ARG:HA   | 2.12                     | 0.51              |
| 1:AM:38:PHE:O     | 1:AM:210:ARG:HA   | 2.12                     | 0.51              |
| 1:AS:38:PHE:O     | 1:AS:210:ARG:HA   | 2.11                     | 0.51              |
| 1:DE:38:PHE:O     | 1:DE:210:ARG:HA   | 2.12                     | 0.51              |
| 2:BY:84:PRO:CG    | 2:BY:85:SER:H     | 2.24                     | 0.51              |
| 2:BJ:84:PRO:CG    | 2:BJ:85:SER:H     | 2.24                     | 0.51              |
| 2:BS:84:PRO:CG    | 2:BS:85:SER:H     | 2.24                     | 0.51              |
| 2:BN:84:PRO:CG    | 2:BN:85:SER:H     | 2.24                     | 0.51              |
| 2:B2:84:PRO:CG    | 2:B2:85:SER:H     | 2.24                     | 0.51              |
| 2:BZ:84:PRO:CG    | 2:BZ:85:SER:H     | 2.24                     | 0.51              |
| 2:BR:101:HIS:CG   | 2:BR:222:VAL:CG1  | 2.94                     | 0.51              |
| 2:BE:102:HIS:CE1  | 3:CB:127:PRO:HG2  | 2.46                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BP:102:HIS:CE1  | 3:CS:127:PRO:HG2  | 103.38                   | 0.51              |
| 2:BG:102:HIS:CE1  | 3:CG:127:PRO:HG2  | 62.85                    | 0.51              |
| 2:BH:102:HIS:CE1  | 3:CJ:127:PRO:HG2  | 2.46                     | 0.51              |
| 3:CD:132:PRO:HG2  | 3:CD:184:GLN:HE22 | 1.76                     | 0.51              |
| 3:CE:132:PRO:HG2  | 3:CE:184:GLN:HE22 | 1.76                     | 0.51              |
| 3:CX:132:PRO:HG2  | 3:CX:184:GLN:HE22 | 1.76                     | 0.51              |
| 2:B1:73:GLN:HA    | 2:B1:73:GLN:NE2   | 2.25                     | 0.51              |
| 2:B2:102:HIS:CE1  | 3:C1:127:PRO:HG2  | 2.46                     | 0.51              |
| 3:CH:132:PRO:HG2  | 3:CH:184:GLN:HE22 | 1.76                     | 0.51              |
| 2:BU:102:HIS:CE1  | 3:CX:127:PRO:HG2  | 2.46                     | 0.51              |
| 1:AY:104:VAL:HG22 | 1:AY:197:LEU:HD23 | 1.92                     | 0.51              |
| 3:CK:132:PRO:HG2  | 3:CK:184:GLN:HE22 | 1.76                     | 0.51              |
| 3:C6:132:PRO:HG2  | 3:C6:184:GLN:HE22 | 1.76                     | 0.51              |
| 1:AF:70:ARG:HH11  | 3:CF:222:LEU:HD21 | 1.76                     | 0.50              |
| 1:AG:70:ARG:HH11  | 3:CG:222:LEU:HD21 | 1.76                     | 0.50              |
| 1:AD:70:ARG:HH11  | 3:CE:222:LEU:HD21 | 74.03                    | 0.50              |
| 1:AV:70:ARG:HH11  | 3:CW:222:LEU:HD21 | 1.76                     | 0.50              |
| 2:BW:157:VAL:HG23 | 3:CW:50:THR:CG2   | 2.39                     | 0.50              |
| 1:AH:188:PRO:HG3  | 3:CF:175:THR:HG23 | 88.85                    | 0.50              |
| 1:AC:188:PRO:HG3  | 3:CE:175:THR:HG23 | 1.93                     | 0.50              |
| 1:AO:188:PRO:HG3  | 3:CO:175:THR:HG23 | 257.21                   | 0.50              |
| 3:CS:175:THR:HG23 | 1:DC:188:PRO:HG3  | 283.20                   | 0.50              |
| 2:B7:157:VAL:HG23 | 3:C8:50:THR:CG2   | 2.39                     | 0.50              |
| 3:CP:175:THR:HG23 | 1:DE:188:PRO:HG3  | 283.03                   | 0.50              |
| 3:CX:175:THR:HG23 | 1:DH:188:PRO:HG3  | 273.08                   | 0.50              |
| 1:A0:188:PRO:HG3  | 3:C3:175:THR:HG23 | 1.93                     | 0.50              |
| 1:AB:188:PRO:HG3  | 3:CA:175:THR:HG23 | 1.93                     | 0.50              |
| 2:BR:84:PRO:CG    | 2:BR:85:SER:H     | 2.24                     | 0.50              |
| 2:BC:84:PRO:CG    | 2:BC:85:SER:H     | 2.24                     | 0.50              |
| 2:BP:102:HIS:CE1  | 3:CT:127:PRO:HG2  | 2.46                     | 0.50              |
| 2:BI:102:HIS:CE1  | 3:CH:127:PRO:HG2  | 2.46                     | 0.50              |
| 2:BL:102:HIS:CE1  | 3:CL:127:PRO:HG2  | 62.85                    | 0.50              |
| 2:BI:102:HIS:CE1  | 3:CM:127:PRO:HG2  | 130.45                   | 0.50              |
| 1:AS:104:VAL:HG22 | 1:AS:197:LEU:HD23 | 1.92                     | 0.50              |
| 1:AB:104:VAL:HG22 | 1:AB:197:LEU:HD23 | 1.92                     | 0.50              |
| 3:CF:132:PRO:HG2  | 3:CF:184:GLN:HE22 | 1.76                     | 0.50              |
| 3:CB:132:PRO:HG2  | 3:CB:184:GLN:HE22 | 1.76                     | 0.50              |
| 3:CO:132:PRO:HG2  | 3:CO:184:GLN:HE22 | 1.76                     | 0.50              |
| 2:B4:102:HIS:CE1  | 3:C7:127:PRO:HG2  | 2.46                     | 0.50              |
| 2:B0:167:THR:HB   | 2:B0:168:ASN:ND2  | 2.25                     | 0.50              |
| 3:CL:132:PRO:HG2  | 3:CL:184:GLN:HE22 | 1.76                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AC:70:ARG:HH11  | 3:CC:222:LEU:HD21 | 1.76                     | 0.50              |
| 3:CW:222:LEU:HD21 | 1:DI:70:ARG:HH11  | 230.14                   | 0.50              |
| 1:A5:70:ARG:HH11  | 3:C6:222:LEU:HD21 | 1.76                     | 0.50              |
| 1:A3:70:ARG:HH11  | 3:C4:222:LEU:HD21 | 1.76                     | 0.50              |
| 1:DJ:173:GLY:O    | 1:DJ:184:TYR:O    | 2.28                     | 0.50              |
| 2:BB:157:VAL:HG23 | 3:CC:50:THR:CG2   | 92.72                    | 0.50              |
| 2:BL:157:VAL:HG23 | 3:CL:50:THR:CG2   | 2.39                     | 0.50              |
| 2:BR:157:VAL:HG23 | 3:CO:50:THR:CG2   | 2.40                     | 0.50              |
| 2:BT:157:VAL:HG23 | 3:CU:50:THR:CG2   | 242.73                   | 0.50              |
| 2:BW:157:VAL:HG23 | 3:CX:50:THR:CG2   | 58.34                    | 0.50              |
| 2:BO:157:VAL:HG23 | 3:CP:50:THR:CG2   | 2.39                     | 0.50              |
| 1:AD:188:PRO:HG3  | 3:CC:175:THR:HG23 | 1.93                     | 0.50              |
| 1:AX:188:PRO:HG3  | 3:CV:175:THR:HG23 | 1.93                     | 0.50              |
| 1:AZ:188:PRO:HG3  | 3:CZ:175:THR:HG23 | 1.93                     | 0.50              |
| 1:AY:188:PRO:HG3  | 3:C2:175:THR:HG23 | 1.93                     | 0.50              |
| 1:AE:38:PHE:O     | 1:AE:210:ARG:HA   | 2.12                     | 0.50              |
| 2:BQ:84:PRO:CG    | 2:BQ:85:SER:H     | 2.24                     | 0.50              |
| 2:BP:84:PRO:CG    | 2:BP:85:SER:H     | 2.24                     | 0.50              |
| 2:B5:101:HIS:CG   | 2:B5:222:VAL:CG1  | 2.94                     | 0.50              |
| 3:C3:132:PRO:HG2  | 3:C3:184:GLN:HE22 | 1.76                     | 0.50              |
| 2:B9:102:HIS:CE1  | 3:C9:127:PRO:HG2  | 2.46                     | 0.50              |
| 3:C5:132:PRO:HG2  | 3:C5:184:GLN:HE22 | 1.76                     | 0.50              |
| 2:B6:102:HIS:CE1  | 3:C6:127:PRO:HG2  | 2.46                     | 0.50              |
| 2:B1:102:HIS:CE1  | 3:C3:127:PRO:HG2  | 2.46                     | 0.50              |
| 2:B9:73:GLN:NE2   | 2:B9:73:GLN:HA    | 2.25                     | 0.50              |
| 2:BB:102:HIS:CE1  | 3:CA:127:PRO:HG2  | 2.46                     | 0.50              |
| 1:A1:70:ARG:HH11  | 3:C2:222:LEU:HD21 | 1.76                     | 0.50              |
| 1:A4:70:ARG:HH11  | 3:C5:222:LEU:HD21 | 1.76                     | 0.50              |
| 1:A0:70:ARG:HH11  | 3:C1:222:LEU:HD21 | 1.76                     | 0.50              |
| 1:DI:173:GLY:O    | 1:DI:184:TYR:O    | 2.28                     | 0.50              |
| 1:AA:173:GLY:O    | 1:AA:184:TYR:O    | 2.28                     | 0.50              |
| 1:AM:173:GLY:O    | 1:AM:184:TYR:O    | 2.28                     | 0.50              |
| 2:BS:157:VAL:HG23 | 3:CQ:50:THR:CG2   | 2.39                     | 0.50              |
| 1:A9:173:GLY:O    | 1:A9:184:TYR:O    | 2.28                     | 0.50              |
| 1:AJ:188:PRO:HG3  | 3:CJ:175:THR:HG23 | 217.02                   | 0.50              |
| 1:AI:188:PRO:HG3  | 3:CH:175:THR:HG23 | 1.94                     | 0.50              |
| 1:A6:188:PRO:HG3  | 3:C6:175:THR:HG23 | 1.93                     | 0.50              |
| 1:A7:188:PRO:HG3  | 3:C5:175:THR:HG23 | 1.93                     | 0.50              |
| 1:AL:188:PRO:HG3  | 3:CL:175:THR:HG23 | 55.88                    | 0.50              |
| 1:AD:38:PHE:O     | 1:AD:210:ARG:HA   | 2.12                     | 0.50              |
| 1:AG:38:PHE:O     | 1:AG:210:ARG:HA   | 2.12                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AR:38:PHE:O     | 1:AR:210:ARG:HA   | 2.12                     | 0.50              |
| 1:A6:38:PHE:O     | 1:A6:210:ARG:HA   | 2.12                     | 0.50              |
| 1:AF:38:PHE:O     | 1:AF:210:ARG:HA   | 2.12                     | 0.50              |
| 1:A2:38:PHE:O     | 1:A2:210:ARG:HA   | 2.11                     | 0.50              |
| 2:B3:84:PRO:CG    | 2:B3:85:SER:H     | 2.24                     | 0.50              |
| 1:DI:163:MET:HE1  | 1:DI:189:GLY:HA3  | 1.92                     | 0.50              |
| 2:BS:102:HIS:CE1  | 3:CP:127:PRO:HG2  | 2.46                     | 0.50              |
| 2:BG:102:HIS:CE1  | 3:CF:127:PRO:HG2  | 2.46                     | 0.50              |
| 3:CV:132:PRO:HG2  | 3:CV:184:GLN:HE22 | 1.76                     | 0.50              |
| 3:CR:132:PRO:HG2  | 3:CR:184:GLN:HE22 | 1.76                     | 0.50              |
| 3:CQ:132:PRO:HG2  | 3:CQ:184:GLN:HE22 | 1.76                     | 0.50              |
| 2:B3:102:HIS:CE1  | 3:C0:127:PRO:HG2  | 2.46                     | 0.50              |
| 2:BV:102:HIS:CE1  | 3:CU:127:PRO:HG2  | 2.46                     | 0.50              |
| 3:CT:132:PRO:HG2  | 3:CT:184:GLN:HE22 | 1.76                     | 0.50              |
| 2:B7:102:HIS:CE1  | 3:C5:127:PRO:HG2  | 2.46                     | 0.50              |
| 1:AI:70:ARG:HH11  | 3:CJ:222:LEU:HD21 | 74.03                    | 0.50              |
| 1:AG:70:ARG:HH11  | 3:CH:222:LEU:HD21 | 74.67                    | 0.50              |
| 1:AR:70:ARG:HH11  | 3:CS:222:LEU:HD21 | 1.76                     | 0.50              |
| 1:AU:70:ARG:HH11  | 3:CV:222:LEU:HD21 | 1.76                     | 0.50              |
| 1:AQ:70:ARG:HH11  | 3:CR:222:LEU:HD21 | 1.76                     | 0.50              |
| 1:A8:173:GLY:O    | 1:A8:184:TYR:O    | 2.28                     | 0.50              |
| 1:AD:173:GLY:O    | 1:AD:184:TYR:O    | 2.28                     | 0.50              |
| 2:BZ:157:VAL:HG23 | 3:CZ:50:THR:CG2   | 2.39                     | 0.50              |
| 1:AS:173:GLY:O    | 1:AS:184:TYR:O    | 2.28                     | 0.50              |
| 1:A9:191:HIS:CD2  | 1:A9:193:GLY:H    | 2.21                     | 0.50              |
| 1:AJ:188:PRO:HG3  | 3:CN:175:THR:HG23 | 1.93                     | 0.50              |
| 1:AE:188:PRO:HG3  | 3:CE:175:THR:HG23 | 53.38                    | 0.50              |
| 1:A9:188:PRO:HG3  | 3:C9:175:THR:HG23 | 1.93                     | 0.50              |
| 1:DJ:38:PHE:O     | 1:DJ:210:ARG:HA   | 2.12                     | 0.50              |
| 1:AX:38:PHE:O     | 1:AX:210:ARG:HA   | 2.12                     | 0.50              |
| 1:DJ:163:MET:HE1  | 1:DJ:189:GLY:HA3  | 1.93                     | 0.50              |
| 2:BD:102:HIS:CE1  | 3:CC:127:PRO:HG2  | 2.46                     | 0.50              |
| 2:BX:102:HIS:CE1  | 3:CW:127:PRO:HG2  | 2.46                     | 0.50              |
| 3:C0:132:PRO:HG2  | 3:C0:184:GLN:HE22 | 1.76                     | 0.50              |
| 2:BK:102:HIS:CE1  | 3:CN:127:PRO:HG2  | 2.46                     | 0.50              |
| 2:B0:102:HIS:CE1  | 3:CZ:127:PRO:HG2  | 2.46                     | 0.50              |
| 2:B4:73:GLN:NE2   | 2:B4:73:GLN:HA    | 2.24                     | 0.50              |
| 1:AP:70:ARG:HH11  | 3:CQ:222:LEU:HD21 | 1.76                     | 0.50              |
| 3:CJ:222:LEU:HD21 | 1:DK:70:ARG:HH11  | 1.76                     | 0.50              |
| 3:CU:222:LEU:HD21 | 1:DG:70:ARG:HH11  | 288.15                   | 0.50              |
| 1:AW:70:ARG:HH11  | 3:CX:222:LEU:HD21 | 1.76                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A7:70:ARG:HH11  | 3:C8:222:LEU:HD21 | 1.76                     | 0.50              |
| 1:AP:173:GLY:O    | 1:AP:184:TYR:O    | 2.28                     | 0.50              |
| 1:AY:173:GLY:O    | 1:AY:184:TYR:O    | 2.28                     | 0.50              |
| 1:A8:207:CYS:O    | 1:A8:208:TYR:CB   | 2.57                     | 0.50              |
| 2:BF:157:VAL:HG23 | 3:CF:50:THR:CG2   | 2.39                     | 0.50              |
| 2:BR:157:VAL:HG23 | 3:CS:50:THR:CG2   | 207.12                   | 0.50              |
| 2:B6:157:VAL:HG23 | 3:C7:50:THR:CG2   | 2.39                     | 0.50              |
| 1:AK:188:PRO:HG3  | 3:CN:175:THR:HG23 | 55.88                    | 0.50              |
| 3:CU:175:THR:HG23 | 1:DJ:188:PRO:HG3  | 301.89                   | 0.50              |
| 3:CV:175:THR:HG23 | 1:DI:188:PRO:HG3  | 283.18                   | 0.50              |
| 3:CW:175:THR:HG23 | 1:DF:188:PRO:HG3  | 208.81                   | 0.50              |
| 1:AK:38:PHE:O     | 1:AK:210:ARG:HA   | 2.12                     | 0.50              |
| 1:A8:38:PHE:O     | 1:A8:210:ARG:HA   | 2.12                     | 0.50              |
| 1:A1:38:PHE:O     | 1:A1:210:ARG:HA   | 2.12                     | 0.50              |
| 2:BL:84:PRO:CG    | 2:BL:85:SER:H     | 2.24                     | 0.50              |
| 2:BD:84:PRO:CG    | 2:BD:85:SER:H     | 2.24                     | 0.50              |
| 2:B4:84:PRO:CG    | 2:B4:85:SER:H     | 2.24                     | 0.50              |
| 2:B8:102:HIS:CE1  | 3:CC:127:PRO:HG2  | 253.61                   | 0.50              |
| 2:BT:102:HIS:CE1  | 3:CT:127:PRO:HG2  | 62.85                    | 0.50              |
| 2:BJ:102:HIS:CE1  | 3:CJ:127:PRO:HG2  | 62.85                    | 0.50              |
| 3:CZ:132:PRO:HG2  | 3:CZ:184:GLN:HE22 | 1.76                     | 0.50              |
| 1:A4:104:VAL:HG22 | 1:A4:197:LEU:HD23 | 1.92                     | 0.50              |
| 2:BF:102:HIS:CE1  | 3:CI:127:PRO:HG2  | 2.46                     | 0.50              |
| 3:CA:132:PRO:HG2  | 3:CA:184:GLN:HE22 | 1.76                     | 0.50              |
| 3:CJ:132:PRO:HG2  | 3:CJ:184:GLN:HE22 | 1.76                     | 0.50              |
| 3:CP:132:PRO:HG2  | 3:CP:184:GLN:HE22 | 1.76                     | 0.50              |
| 1:AB:70:ARG:HH11  | 3:CC:222:LEU:HD21 | 74.67                    | 0.50              |
| 1:AA:70:ARG:HH11  | 3:DB:222:LEU:HD21 | 281.52                   | 0.50              |
| 1:A6:70:ARG:HH11  | 3:C7:222:LEU:HD21 | 1.76                     | 0.50              |
| 1:A9:70:ARG:HH11  | 3:DA:222:LEU:HD21 | 1.76                     | 0.50              |
| 2:BH:137:GLU:O    | 2:BH:139:ALA:N    | 2.41                     | 0.50              |
| 1:AA:188:PRO:HG3  | 3:CD:175:THR:HG23 | 1.93                     | 0.50              |
| 1:AM:188:PRO:HG3  | 3:CM:175:THR:HG23 | 1.93                     | 0.50              |
| 1:A3:188:PRO:HG3  | 3:C7:175:THR:HG23 | 1.93                     | 0.50              |
| 1:AC:38:PHE:O     | 1:AC:210:ARG:HA   | 2.12                     | 0.50              |
| 1:A9:38:PHE:O     | 1:A9:210:ARG:HA   | 2.12                     | 0.50              |
| 1:DG:38:PHE:O     | 1:DG:210:ARG:HA   | 2.11                     | 0.50              |
| 2:BO:102:HIS:CE1  | 3:CO:127:PRO:HG2  | 245.60                   | 0.50              |
| 3:CY:132:PRO:HG2  | 3:CY:184:GLN:HE22 | 1.76                     | 0.50              |
| 2:B5:167:THR:HB   | 2:B5:168:ASN:ND2  | 2.25                     | 0.50              |
| 3:C1:132:PRO:HG2  | 3:C1:184:GLN:HE22 | 1.76                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:CU:132:PRO:HG2  | 3:CU:184:GLN:HE22 | 1.76                     | 0.50              |
| 1:AK:191:HIS:CD2  | 1:AK:193:GLY:H    | 2.21                     | 0.50              |
| 2:BM:157:VAL:HG23 | 3:CM:50:THR:CG2   | 2.39                     | 0.50              |
| 2:BP:157:VAL:HG23 | 3:CQ:50:THR:CG2   | 91.70                    | 0.50              |
| 2:BC:157:VAL:HG23 | 3:CD:50:THR:CG2   | 58.34                    | 0.50              |
| 2:B2:137:GLU:O    | 2:B2:139:ALA:N    | 2.41                     | 0.50              |
| 1:DH:207:CYS:O    | 1:DH:208:TYR:CB   | 2.57                     | 0.50              |
| 2:B5:157:VAL:HG23 | 3:C6:50:THR:CG2   | 2.39                     | 0.50              |
| 1:AP:188:PRO:HG3  | 3:CP:175:THR:HG23 | 1.93                     | 0.50              |
| 3:CT:175:THR:HG23 | 1:DG:188:PRO:HG3  | 273.58                   | 0.50              |
| 1:A4:188:PRO:HG3  | 3:C4:175:THR:HG23 | 1.93                     | 0.50              |
| 1:A5:188:PRO:HG3  | 3:C8:175:THR:HG23 | 1.93                     | 0.50              |
| 1:AU:38:PHE:O     | 1:AU:210:ARG:HA   | 2.12                     | 0.50              |
| 1:AB:38:PHE:O     | 1:AB:210:ARG:HA   | 2.12                     | 0.50              |
| 1:AJ:38:PHE:O     | 1:AJ:210:ARG:HA   | 2.12                     | 0.50              |
| 1:AL:38:PHE:O     | 1:AL:210:ARG:HA   | 2.12                     | 0.50              |
| 1:AN:38:PHE:O     | 1:AN:210:ARG:HA   | 2.12                     | 0.50              |
| 1:DH:38:PHE:O     | 1:DH:210:ARG:HA   | 2.12                     | 0.50              |
| 2:BO:84:PRO:CG    | 2:BO:85:SER:H     | 2.24                     | 0.50              |
| 2:B8:84:PRO:CG    | 2:B8:85:SER:H     | 2.24                     | 0.50              |
| 2:BM:102:HIS:CE1  | 3:CO:127:PRO:HG2  | 2.46                     | 0.50              |
| 2:BV:102:HIS:CE1  | 3:CV:127:PRO:HG2  | 62.85                    | 0.50              |
| 2:B5:102:HIS:CE1  | 3:C8:127:PRO:HG2  | 2.46                     | 0.50              |
| 3:CG:132:PRO:HG2  | 3:CG:184:GLN:HE22 | 1.76                     | 0.50              |
| 3:C8:132:PRO:HG2  | 3:C8:184:GLN:HE22 | 1.76                     | 0.50              |
| 3:C9:132:PRO:HG2  | 3:C9:184:GLN:HE22 | 1.76                     | 0.50              |
| 1:A8:70:ARG:HH11  | 3:C9:222:LEU:HD21 | 1.76                     | 0.50              |
| 1:DD:173:GLY:O    | 1:DD:184:TYR:O    | 2.28                     | 0.50              |
| 2:BX:157:VAL:HG23 | 3:C5:50:THR:CG2   | 242.74                   | 0.50              |
| 1:AU:188:PRO:HG3  | 3:CU:175:THR:HG23 | 1.93                     | 0.50              |
| 1:AN:188:PRO:HG3  | 3:CR:175:THR:HG23 | 208.78                   | 0.50              |
| 1:A9:207:CYS:O    | 1:A9:208:TYR:CB   | 2.57                     | 0.50              |
| 1:A1:188:PRO:HG3  | 3:C1:175:THR:HG23 | 1.94                     | 0.50              |
| 1:DI:38:PHE:O     | 1:DI:210:ARG:HA   | 2.12                     | 0.50              |
| 2:BX:102:HIS:CE1  | 3:C4:127:PRO:HG2  | 278.88                   | 0.50              |
| 2:BY:102:HIS:CE1  | 3:CV:127:PRO:HG2  | 2.46                     | 0.50              |
| 3:CM:132:PRO:HG2  | 3:CM:184:GLN:HE22 | 1.76                     | 0.50              |
| 1:AY:236:ARG:NH1  | 3:CZ:172:ALA:O    | 2.45                     | 0.50              |
| 3:C4:132:PRO:HG2  | 3:C4:184:GLN:HE22 | 1.76                     | 0.50              |
| 1:AR:236:ARG:NH1  | 3:CS:172:ALA:O    | 2.45                     | 0.50              |
| 1:AU:236:ARG:NH1  | 3:CV:172:ALA:O    | 2.45                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AX:104:VAL:HG22 | 1:AX:197:LEU:HD23 | 1.92                     | 0.50              |
| 1:AO:236:ARG:NH1  | 3:CP:172:ALA:O    | 2.45                     | 0.50              |
| 1:AF:236:ARG:NH1  | 3:CF:172:ALA:O    | 2.45                     | 0.50              |
| 1:AB:236:ARG:NH1  | 3:CB:172:ALA:O    | 2.45                     | 0.50              |
| 1:AE:236:ARG:NH1  | 3:CF:172:ALA:O    | 97.20                    | 0.50              |
| 1:AP:236:ARG:NH1  | 3:CQ:172:ALA:O    | 2.45                     | 0.50              |
| 3:CX:172:ALA:O    | 1:DJ:236:ARG:NH1  | 283.93                   | 0.50              |
| 2:B0:157:VAL:HG23 | 3:C0:50:THR:CG2   | 2.39                     | 0.50              |
| 1:AD:188:PRO:HG3  | 3:CH:175:THR:HG23 | 184.88                   | 0.50              |
| 1:AH:188:PRO:HG3  | 3:CJ:175:THR:HG23 | 1.94                     | 0.50              |
| 3:CQ:175:THR:HG23 | 1:DD:188:PRO:HG3  | 208.81                   | 0.50              |
| 1:A7:38:PHE:O     | 1:A7:210:ARG:HA   | 2.12                     | 0.50              |
| 2:BW:84:PRO:CG    | 2:BW:85:SER:H     | 2.24                     | 0.50              |
| 2:B0:84:PRO:CG    | 2:B0:85:SER:H     | 2.24                     | 0.50              |
| 1:AQ:38:PHE:O     | 1:AQ:210:ARG:HA   | 2.12                     | 0.50              |
| 2:BA:82:PRO:HB2   | 2:BA:190:ASN:HD22 | 1.77                     | 0.50              |
| 1:DC:38:PHE:O     | 1:DC:210:ARG:HA   | 2.12                     | 0.50              |
| 2:BV:84:PRO:CG    | 2:BV:85:SER:H     | 2.24                     | 0.50              |
| 2:B5:84:PRO:CG    | 2:B5:85:SER:H     | 2.24                     | 0.50              |
| 2:BC:102:HIS:CE1  | 3:DA:127:PRO:HG2  | 275.52                   | 0.50              |
| 2:BO:102:HIS:CE1  | 3:CS:127:PRO:HG2  | 2.46                     | 0.50              |
| 1:AF:236:ARG:NH1  | 3:CG:172:ALA:O    | 60.22                    | 0.50              |
| 1:AG:236:ARG:NH1  | 3:CH:172:ALA:O    | 96.58                    | 0.50              |
| 1:AH:236:ARG:NH1  | 3:CH:172:ALA:O    | 2.45                     | 0.50              |
| 2:BZ:102:HIS:CE1  | 3:C2:127:PRO:HG2  | 2.46                     | 0.50              |
| 1:AK:236:ARG:NH1  | 3:CL:172:ALA:O    | 2.45                     | 0.50              |
| 2:B6:167:THR:HB   | 2:B6:168:ASN:ND2  | 2.25                     | 0.50              |
| 1:AV:236:ARG:NH1  | 3:CW:172:ALA:O    | 2.45                     | 0.50              |
| 1:AI:38:PHE:O     | 1:AI:210:ARG:HA   | 2.12                     | 0.49              |
| 2:BL:82:PRO:HB2   | 2:BL:190:ASN:HD22 | 1.77                     | 0.49              |
| 2:BQ:82:PRO:HB2   | 2:BQ:190:ASN:HD22 | 1.77                     | 0.49              |
| 2:BZ:82:PRO:HB2   | 2:BZ:190:ASN:HD22 | 1.77                     | 0.49              |
| 2:BL:102:HIS:CE1  | 3:CK:127:PRO:HG2  | 2.46                     | 0.49              |
| 2:BN:102:HIS:CE1  | 3:CM:127:PRO:HG2  | 2.46                     | 0.49              |
| 2:BR:102:HIS:CE1  | 3:CL:127:PRO:HG2  | 2.46                     | 0.49              |
| 2:BW:102:HIS:CE1  | 3:CY:127:PRO:HG2  | 2.46                     | 0.49              |
| 1:AH:236:ARG:NH1  | 3:CI:172:ALA:O    | 60.22                    | 0.49              |
| 1:AI:236:ARG:NH1  | 3:CI:172:ALA:O    | 2.45                     | 0.49              |
| 1:AE:236:ARG:NH1  | 3:CE:172:ALA:O    | 2.45                     | 0.49              |
| 3:CT:172:ALA:O    | 1:DF:236:ARG:NH1  | 281.68                   | 0.49              |
| 3:CU:172:ALA:O    | 1:DG:236:ARG:NH1  | 310.15                   | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AN:236:ARG:NH1  | 3:CO:172:ALA:O    | 2.45                     | 0.49              |
| 1:AL:236:ARG:NH1  | 3:CM:172:ALA:O    | 2.45                     | 0.49              |
| 2:B8:167:THR:HB   | 2:B8:168:ASN:ND2  | 2.25                     | 0.49              |
| 1:A2:70:ARG:HH11  | 3:C3:222:LEU:HD21 | 1.76                     | 0.49              |
| 1:AA:70:ARG:HH11  | 3:CA:222:LEU:HD21 | 1.76                     | 0.49              |
| 2:BL:157:VAL:HG23 | 3:CM:50:THR:CG2   | 92.72                    | 0.49              |
| 1:AR:188:PRO:HG3  | 3:CR:175:THR:HG23 | 1.94                     | 0.49              |
| 1:A5:191:HIS:CD2  | 1:A5:193:GLY:H    | 2.21                     | 0.49              |
| 1:A5:38:PHE:O     | 1:A5:210:ARG:HA   | 2.12                     | 0.49              |
| 1:AO:38:PHE:O     | 1:AO:210:ARG:HA   | 2.12                     | 0.49              |
| 1:A4:38:PHE:O     | 1:A4:210:ARG:HA   | 2.12                     | 0.49              |
| 2:BR:82:PRO:HB2   | 2:BR:190:ASN:HD22 | 1.78                     | 0.49              |
| 2:B0:82:PRO:HB2   | 2:B0:190:ASN:HD22 | 1.77                     | 0.49              |
| 2:BO:82:PRO:HB2   | 2:BO:190:ASN:HD22 | 1.77                     | 0.49              |
| 1:AP:38:PHE:O     | 1:AP:210:ARG:HA   | 2.12                     | 0.49              |
| 2:BX:82:PRO:HB2   | 2:BX:190:ASN:HD22 | 1.77                     | 0.49              |
| 1:AY:163:MET:HE1  | 1:AY:189:GLY:HA3  | 1.94                     | 0.49              |
| 2:BB:102:HIS:CE1  | 3:DB:127:PRO:HG2  | 253.70                   | 0.49              |
| 1:AG:236:ARG:NH1  | 3:CG:172:ALA:O    | 2.45                     | 0.49              |
| 3:CQ:172:ALA:O    | 1:DC:236:ARG:NH1  | 212.52                   | 0.49              |
| 1:AT:236:ARG:NH1  | 3:CU:172:ALA:O    | 2.45                     | 0.49              |
| 3:DB:132:PRO:HG2  | 3:DB:184:GLN:HE22 | 1.76                     | 0.49              |
| 1:DE:88:PHE:HA    | 1:DE:206:GLY:O    | 2.13                     | 0.49              |
| 1:AQ:88:PHE:HA    | 1:AQ:206:GLY:O    | 2.12                     | 0.49              |
| 1:AZ:236:ARG:NH1  | 3:C0:172:ALA:O    | 2.45                     | 0.49              |
| 1:A7:236:ARG:NH1  | 3:C8:172:ALA:O    | 2.45                     | 0.49              |
| 1:A3:88:PHE:HA    | 1:A3:206:GLY:O    | 2.13                     | 0.49              |
| 1:A1:236:ARG:NH1  | 3:C2:172:ALA:O    | 2.45                     | 0.49              |
| 1:AM:236:ARG:NH1  | 3:CN:172:ALA:O    | 2.45                     | 0.49              |
| 1:A0:236:ARG:NH1  | 3:C1:172:ALA:O    | 2.45                     | 0.49              |
| 1:AB:70:ARG:HH11  | 3:CB:222:LEU:HD21 | 1.76                     | 0.49              |
| 1:AP:207:CYS:O    | 1:AP:208:TYR:CB   | 2.57                     | 0.49              |
| 1:AV:207:CYS:O    | 1:AV:208:TYR:CB   | 2.57                     | 0.49              |
| 2:B3:157:VAL:HG23 | 3:C3:50:THR:CG2   | 2.40                     | 0.49              |
| 1:A0:38:PHE:O     | 1:A0:210:ARG:HA   | 2.12                     | 0.49              |
| 2:B7:82:PRO:HB2   | 2:B7:190:ASN:HD22 | 1.77                     | 0.49              |
| 2:BS:82:PRO:HB2   | 2:BS:190:ASN:HD22 | 1.78                     | 0.49              |
| 2:BG:82:PRO:HB2   | 2:BG:190:ASN:HD22 | 1.77                     | 0.49              |
| 2:B1:84:PRO:CG    | 2:B1:85:SER:H     | 2.24                     | 0.49              |
| 1:AT:87:GLN:O     | 1:AT:152:GLN:O    | 2.31                     | 0.49              |
| 1:AT:38:PHE:O     | 1:AT:210:ARG:HA   | 2.12                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B2:82:PRO:HB2   | 2:B2:190:ASN:HD22 | 1.77                     | 0.49              |
| 2:BW:102:HIS:CE1  | 3:CU:127:PRO:HG2  | 104.43                   | 0.49              |
| 1:AD:236:ARG:NH1  | 3:CD:172:ALA:O    | 2.45                     | 0.49              |
| 1:AH:88:PHE:HA    | 1:AH:206:GLY:O    | 2.12                     | 0.49              |
| 1:AI:88:PHE:HA    | 1:AI:206:GLY:O    | 2.13                     | 0.49              |
| 1:AN:88:PHE:HA    | 1:AN:206:GLY:O    | 2.12                     | 0.49              |
| 1:A6:88:PHE:HA    | 1:A6:206:GLY:O    | 2.13                     | 0.49              |
| 1:AE:70:ARG:HH11  | 3:CE:222:LEU:HD21 | 1.76                     | 0.49              |
| 1:A6:173:GLY:O    | 1:A6:184:TYR:O    | 2.28                     | 0.49              |
| 2:B6:137:GLU:O    | 2:B6:139:ALA:N    | 2.41                     | 0.49              |
| 2:BG:157:VAL:HG23 | 3:CG:50:THR:CG2   | 2.40                     | 0.49              |
| 2:BJ:157:VAL:HG23 | 3:CK:50:THR:CG2   | 221.81                   | 0.49              |
| 1:AD:87:GLN:O     | 1:AD:152:GLN:O    | 2.31                     | 0.49              |
| 1:DK:38:PHE:O     | 1:DK:210:ARG:HA   | 2.12                     | 0.49              |
| 1:DF:38:PHE:O     | 1:DF:210:ARG:HA   | 2.12                     | 0.49              |
| 2:BF:82:PRO:HB2   | 2:BF:190:ASN:HD22 | 1.77                     | 0.49              |
| 2:BT:82:PRO:HB2   | 2:BT:190:ASN:HD22 | 1.78                     | 0.49              |
| 2:BN:82:PRO:HB2   | 2:BN:190:ASN:HD22 | 1.77                     | 0.49              |
| 1:AC:236:ARG:NH1  | 3:CC:172:ALA:O    | 2.45                     | 0.49              |
| 1:AD:236:ARG:NH1  | 3:CE:172:ALA:O    | 96.08                    | 0.49              |
| 1:AS:236:ARG:NH1  | 3:CT:172:ALA:O    | 2.45                     | 0.49              |
| 1:A7:88:PHE:HA    | 1:A7:206:GLY:O    | 2.13                     | 0.49              |
| 1:AA:236:ARG:NH1  | 3:CA:172:ALA:O    | 2.45                     | 0.49              |
| 1:AW:88:PHE:HA    | 1:AW:206:GLY:O    | 2.12                     | 0.49              |
| 1:A1:88:PHE:HA    | 1:A1:206:GLY:O    | 2.12                     | 0.49              |
| 1:AG:88:PHE:HA    | 1:AG:206:GLY:O    | 2.13                     | 0.49              |
| 2:BF:157:VAL:HG23 | 3:CG:50:THR:CG2   | 58.34                    | 0.49              |
| 2:BM:157:VAL:HG23 | 3:CN:50:THR:CG2   | 58.34                    | 0.49              |
| 1:AF:188:PRO:HG3  | 3:CI:175:THR:HG23 | 1.93                     | 0.49              |
| 1:AV:188:PRO:HG3  | 3:CY:175:THR:HG23 | 1.94                     | 0.49              |
| 1:AU:87:GLN:O     | 1:AU:152:GLN:O    | 2.31                     | 0.49              |
| 1:AB:87:GLN:O     | 1:AB:152:GLN:O    | 2.31                     | 0.49              |
| 1:AG:87:GLN:O     | 1:AG:152:GLN:O    | 2.31                     | 0.49              |
| 1:AJ:87:GLN:O     | 1:AJ:152:GLN:O    | 2.31                     | 0.49              |
| 1:AM:87:GLN:O     | 1:AM:152:GLN:O    | 2.31                     | 0.49              |
| 1:AK:87:GLN:O     | 1:AK:152:GLN:O    | 2.31                     | 0.49              |
| 1:AN:87:GLN:O     | 1:AN:152:GLN:O    | 2.31                     | 0.49              |
| 1:DK:87:GLN:O     | 1:DK:152:GLN:O    | 2.31                     | 0.49              |
| 1:DJ:87:GLN:O     | 1:DJ:152:GLN:O    | 2.31                     | 0.49              |
| 2:BU:82:PRO:HB2   | 2:BU:190:ASN:HD22 | 1.77                     | 0.49              |
| 1:AP:87:GLN:O     | 1:AP:152:GLN:O    | 2.31                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BD:82:PRO:HB2   | 2:BD:190:ASN:HD22 | 1.77                     | 0.49              |
| 3:CS:172:ALA:O    | 1:DE:236:ARG:NH1  | 296.43                   | 0.49              |
| 3:CV:172:ALA:O    | 1:DH:236:ARG:NH1  | 296.41                   | 0.49              |
| 1:DI:88:PHE:HA    | 1:DI:206:GLY:O    | 2.12                     | 0.49              |
| 1:AL:88:PHE:HA    | 1:AL:206:GLY:O    | 2.13                     | 0.49              |
| 1:AR:88:PHE:HA    | 1:AR:206:GLY:O    | 2.12                     | 0.49              |
| 1:A9:88:PHE:HA    | 1:A9:206:GLY:O    | 2.13                     | 0.49              |
| 1:AX:88:PHE:HA    | 1:AX:206:GLY:O    | 2.12                     | 0.49              |
| 1:AT:70:ARG:HH11  | 3:CU:222:LEU:HD21 | 1.76                     | 0.49              |
| 1:AD:243:ILE:HG22 | 1:AD:244:ASN:N    | 2.28                     | 0.49              |
| 1:AG:188:PRO:HG3  | 3:CF:175:THR:HG23 | 1.93                     | 0.49              |
| 1:AM:188:PRO:HG3  | 3:CK:175:THR:HG23 | 87.90                    | 0.49              |
| 1:AL:188:PRO:HG3  | 3:CO:175:THR:HG23 | 1.93                     | 0.49              |
| 1:AO:188:PRO:HG3  | 3:CS:175:THR:HG23 | 1.93                     | 0.49              |
| 1:AX:243:ILE:HG22 | 1:AX:244:ASN:N    | 2.28                     | 0.49              |
| 1:AH:87:GLN:O     | 1:AH:152:GLN:O    | 2.31                     | 0.49              |
| 1:AI:87:GLN:O     | 1:AI:152:GLN:O    | 2.31                     | 0.49              |
| 1:AP:242:ASN:HD22 | 1:AS:110:GLY:N    | 2.10                     | 0.49              |
| 2:BP:82:PRO:HB2   | 2:BP:190:ASN:HD22 | 1.77                     | 0.49              |
| 2:B1:82:PRO:HB2   | 2:B1:190:ASN:HD22 | 1.78                     | 0.49              |
| 1:AI:236:ARG:NH1  | 3:CJ:172:ALA:O    | 96.08                    | 0.49              |
| 1:AA:236:ARG:NH1  | 3:DB:172:ALA:O    | 275.45                   | 0.49              |
| 1:AS:88:PHE:HA    | 1:AS:206:GLY:O    | 2.13                     | 0.49              |
| 1:AQ:236:ARG:NH1  | 3:CR:172:ALA:O    | 2.45                     | 0.49              |
| 1:A8:88:PHE:HA    | 1:A8:206:GLY:O    | 2.12                     | 0.49              |
| 1:AA:88:PHE:HA    | 1:AA:206:GLY:O    | 2.13                     | 0.49              |
| 1:AJ:236:ARG:NH1  | 3:CK:172:ALA:O    | 2.45                     | 0.49              |
| 1:AM:88:PHE:HA    | 1:AM:206:GLY:O    | 2.13                     | 0.49              |
| 1:AD:88:PHE:HA    | 1:AD:206:GLY:O    | 2.13                     | 0.49              |
| 1:DK:88:PHE:HA    | 1:DK:206:GLY:O    | 2.13                     | 0.49              |
| 1:AC:70:ARG:HH11  | 3:CD:222:LEU:HD21 | 46.80                    | 0.49              |
| 1:AX:191:HIS:CD2  | 1:AX:193:GLY:H    | 2.21                     | 0.49              |
| 1:AC:188:PRO:HG3  | 3:DA:175:THR:HG23 | 282.64                   | 0.49              |
| 1:AK:188:PRO:HG3  | 3:CK:175:THR:HG23 | 1.93                     | 0.49              |
| 1:DI:243:ILE:HG22 | 1:DI:244:ASN:N    | 2.28                     | 0.49              |
| 1:AV:38:PHE:O     | 1:AV:210:ARG:HA   | 2.12                     | 0.49              |
| 1:AA:38:PHE:O     | 1:AA:210:ARG:HA   | 2.12                     | 0.49              |
| 1:A8:87:GLN:O     | 1:A8:152:GLN:O    | 2.31                     | 0.49              |
| 1:AO:87:GLN:O     | 1:AO:152:GLN:O    | 2.31                     | 0.49              |
| 1:A9:87:GLN:O     | 1:A9:152:GLN:O    | 2.31                     | 0.49              |
| 1:A3:38:PHE:O     | 1:A3:210:ARG:HA   | 2.12                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AX:87:GLN:O     | 1:AX:152:GLN:O    | 2.31                     | 0.49              |
| 2:B8:82:PRO:HB2   | 2:B8:190:ASN:HD22 | 1.77                     | 0.49              |
| 1:AY:38:PHE:O     | 1:AY:210:ARG:HA   | 2.12                     | 0.49              |
| 1:AW:236:ARG:NH1  | 3:CX:172:ALA:O    | 2.45                     | 0.49              |
| 1:DG:88:PHE:HA    | 1:DG:206:GLY:O    | 2.13                     | 0.49              |
| 3:CY:130:ALA:O    | 3:CY:131:ALA:HB3  | 2.13                     | 0.49              |
| 1:AC:88:PHE:HA    | 1:AC:206:GLY:O    | 2.13                     | 0.49              |
| 3:C8:130:ALA:O    | 3:C8:131:ALA:HB3  | 2.13                     | 0.49              |
| 1:AE:88:PHE:HA    | 1:AE:206:GLY:O    | 2.13                     | 0.49              |
| 3:C0:130:ALA:O    | 3:C0:131:ALA:HB3  | 2.13                     | 0.49              |
| 1:A5:236:ARG:NH1  | 3:C6:172:ALA:O    | 2.45                     | 0.49              |
| 1:AG:188:PRO:HG3  | 3:CG:175:THR:HG23 | 53.38                    | 0.49              |
| 1:AN:188:PRO:HG3  | 3:CL:175:THR:HG23 | 1.93                     | 0.49              |
| 1:DC:243:ILE:HG22 | 1:DC:244:ASN:N    | 2.28                     | 0.49              |
| 1:AB:188:PRO:HG3  | 3:DB:175:THR:HG23 | 259.06                   | 0.49              |
| 1:AL:87:GLN:O     | 1:AL:152:GLN:O    | 2.31                     | 0.49              |
| 1:AV:87:GLN:O     | 1:AV:152:GLN:O    | 2.31                     | 0.49              |
| 1:DD:38:PHE:O     | 1:DD:210:ARG:HA   | 2.12                     | 0.49              |
| 1:AW:38:PHE:O     | 1:AW:210:ARG:HA   | 2.12                     | 0.49              |
| 1:AZ:38:PHE:O     | 1:AZ:210:ARG:HA   | 2.12                     | 0.49              |
| 1:DH:110:GLY:N    | 1:DJ:242:ASN:HD22 | 2.10                     | 0.49              |
| 2:BV:82:PRO:HB2   | 2:BV:190:ASN:HD22 | 1.77                     | 0.49              |
| 2:BH:82:PRO:HB2   | 2:BH:190:ASN:HD22 | 1.78                     | 0.49              |
| 2:B6:84:PRO:CG    | 2:B6:85:SER:H     | 2.24                     | 0.49              |
| 1:AB:236:ARG:NH1  | 3:CC:172:ALA:O    | 96.58                    | 0.49              |
| 1:AX:236:ARG:NH1  | 3:CY:172:ALA:O    | 2.45                     | 0.49              |
| 3:CW:130:ALA:O    | 3:CW:131:ALA:HB3  | 2.13                     | 0.49              |
| 1:AT:88:PHE:HA    | 1:AT:206:GLY:O    | 2.12                     | 0.49              |
| 1:AK:88:PHE:HA    | 1:AK:206:GLY:O    | 2.13                     | 0.49              |
| 1:AU:191:HIS:CD2  | 1:AU:193:GLY:H    | 2.21                     | 0.49              |
| 1:AH:207:CYS:O    | 1:AH:208:TYR:CB   | 2.57                     | 0.49              |
| 1:AC:243:ILE:HG22 | 1:AC:244:ASN:N    | 2.28                     | 0.49              |
| 1:AN:243:ILE:HG22 | 1:AN:244:ASN:N    | 2.28                     | 0.49              |
| 1:A3:243:ILE:HG22 | 1:A3:244:ASN:N    | 2.28                     | 0.49              |
| 1:AA:87:GLN:O     | 1:AA:152:GLN:O    | 2.31                     | 0.49              |
| 3:CW:132:PRO:HG2  | 3:CW:184:GLN:HE22 | 1.76                     | 0.49              |
| 1:A8:236:ARG:NH1  | 3:C9:172:ALA:O    | 2.45                     | 0.49              |
| 3:CX:130:ALA:O    | 3:CX:131:ALA:HB3  | 2.13                     | 0.49              |
| 3:CR:130:ALA:O    | 3:CR:131:ALA:HB3  | 2.13                     | 0.49              |
| 3:CG:130:ALA:O    | 3:CG:131:ALA:HB3  | 2.13                     | 0.49              |
| 1:DH:88:PHE:HA    | 1:DH:206:GLY:O    | 2.13                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:CA:130:ALA:O    | 3:CA:131:ALA:HB3  | 2.13                     | 0.49              |
| 1:A4:236:ARG:NH1  | 3:C5:172:ALA:O    | 2.45                     | 0.49              |
| 1:A2:236:ARG:NH1  | 3:C3:172:ALA:O    | 2.45                     | 0.49              |
| 1:DF:191:HIS:CD2  | 1:DF:193:GLY:H    | 2.21                     | 0.49              |
| 2:B2:157:VAL:HG23 | 3:C2:50:THR:CG2   | 2.39                     | 0.49              |
| 1:AT:207:CYS:O    | 1:AT:208:TYR:CB   | 2.57                     | 0.49              |
| 1:AL:243:ILE:HG22 | 1:AL:244:ASN:N    | 2.28                     | 0.49              |
| 1:AW:188:PRO:HG3  | 3:CW:175:THR:HG23 | 1.93                     | 0.49              |
| 1:DJ:243:ILE:HG22 | 1:DJ:244:ASN:N    | 2.28                     | 0.49              |
| 1:AH:110:GLY:N    | 1:DK:242:ASN:HD22 | 2.10                     | 0.49              |
| 1:AO:110:GLY:N    | 1:AR:242:ASN:HD22 | 2.10                     | 0.49              |
| 1:A6:87:GLN:O     | 1:A6:152:GLN:O    | 2.31                     | 0.49              |
| 2:BW:82:PRO:HB2   | 2:BW:190:ASN:HD22 | 1.78                     | 0.49              |
| 2:BK:82:PRO:HB2   | 2:BK:190:ASN:HD22 | 1.77                     | 0.49              |
| 2:BB:82:PRO:HB2   | 2:BB:190:ASN:HD22 | 1.77                     | 0.49              |
| 1:AY:87:GLN:O     | 1:AY:152:GLN:O    | 2.31                     | 0.49              |
| 2:B4:82:PRO:HB2   | 2:B4:190:ASN:HD22 | 1.77                     | 0.49              |
| 2:B6:82:PRO:HB2   | 2:B6:190:ASN:HD22 | 1.77                     | 0.49              |
| 1:AC:236:ARG:NH1  | 3:CD:172:ALA:O    | 60.22                    | 0.49              |
| 3:CJ:172:ALA:O    | 1:DK:236:ARG:NH1  | 2.45                     | 0.49              |
| 3:CR:172:ALA:O    | 1:DD:236:ARG:NH1  | 286.20                   | 0.49              |
| 3:CM:130:ALA:O    | 3:CM:131:ALA:HB3  | 2.13                     | 0.49              |
| 1:DC:88:PHE:HA    | 1:DC:206:GLY:O    | 2.12                     | 0.49              |
| 1:AV:88:PHE:HA    | 1:AV:206:GLY:O    | 2.13                     | 0.49              |
| 1:AJ:88:PHE:HA    | 1:AJ:206:GLY:O    | 2.13                     | 0.49              |
| 3:CF:130:ALA:O    | 3:CF:131:ALA:HB3  | 2.13                     | 0.49              |
| 3:CH:130:ALA:O    | 3:CH:131:ALA:HB3  | 2.13                     | 0.49              |
| 1:A4:88:PHE:HA    | 1:A4:206:GLY:O    | 2.13                     | 0.49              |
| 1:AD:181:LYS:O    | 1:AD:182:ALA:CB   | 2.62                     | 0.48              |
| 1:A5:181:LYS:O    | 1:A5:182:ALA:CB   | 2.61                     | 0.48              |
| 1:AY:207:CYS:O    | 1:AY:208:TYR:CB   | 2.57                     | 0.48              |
| 1:A5:207:CYS:O    | 1:A5:208:TYR:CB   | 2.57                     | 0.48              |
| 1:A3:191:HIS:HD2  | 1:A3:193:GLY:N    | 2.08                     | 0.48              |
| 3:CG:175:THR:HG23 | 1:DK:188:PRO:HG3  | 1.93                     | 0.48              |
| 1:AT:243:ILE:HG22 | 1:AT:244:ASN:N    | 2.28                     | 0.48              |
| 1:A4:243:ILE:HG22 | 1:A4:244:ASN:N    | 2.28                     | 0.48              |
| 1:AQ:243:ILE:HG22 | 1:AQ:244:ASN:N    | 2.28                     | 0.48              |
| 1:AY:243:ILE:HG22 | 1:AY:244:ASN:N    | 2.28                     | 0.48              |
| 1:AF:242:ASN:HD22 | 1:AG:110:GLY:N    | 2.10                     | 0.48              |
| 2:BM:82:PRO:HB2   | 2:BM:190:ASN:HD22 | 1.78                     | 0.48              |
| 2:BC:82:PRO:HB2   | 2:BC:190:ASN:HD22 | 1.77                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:CS:42:ASN:ND2   | 3:CS:44:ILE:H     | 2.12                     | 0.48              |
| 3:DB:130:ALA:O    | 3:DB:131:ALA:HB3  | 2.13                     | 0.48              |
| 1:AZ:88:PHE:HA    | 1:AZ:206:GLY:O    | 2.13                     | 0.48              |
| 3:C7:132:PRO:HG2  | 3:C7:184:GLN:HE22 | 1.76                     | 0.48              |
| 3:CI:130:ALA:O    | 3:CI:131:ALA:HB3  | 2.13                     | 0.48              |
| 1:AO:89:LYS:HE3   | 1:AP:128:VAL:HG21 | 1.96                     | 0.48              |
| 1:AP:88:PHE:HA    | 1:AP:206:GLY:O    | 2.13                     | 0.48              |
| 1:AM:181:LYS:O    | 1:AM:182:ALA:CB   | 2.61                     | 0.48              |
| 1:AW:181:LYS:O    | 1:AW:182:ALA:CB   | 2.62                     | 0.48              |
| 2:B3:137:GLU:O    | 2:B3:139:ALA:N    | 2.42                     | 0.48              |
| 2:BI:157:VAL:HG23 | 3:CI:50:THR:CG2   | 2.39                     | 0.48              |
| 2:BK:157:VAL:HG23 | 3:CL:50:THR:CG2   | 58.34                    | 0.48              |
| 2:BL:157:VAL:CG2  | 3:CL:50:THR:HG21  | 2.43                     | 0.48              |
| 2:BW:157:VAL:CG2  | 3:CW:50:THR:HG21  | 2.42                     | 0.48              |
| 2:B7:137:GLU:O    | 2:B7:139:ALA:N    | 2.42                     | 0.48              |
| 1:AB:181:LYS:O    | 1:AB:182:ALA:CB   | 2.61                     | 0.48              |
| 2:B1:157:VAL:HG23 | 3:C1:50:THR:CG2   | 2.39                     | 0.48              |
| 1:A6:243:ILE:HG22 | 1:A6:244:ASN:N    | 2.28                     | 0.48              |
| 1:AF:110:GLY:N    | 1:AI:242:ASN:HD22 | 2.10                     | 0.48              |
| 1:DH:242:ASN:HD22 | 1:DI:110:GLY:N    | 2.10                     | 0.48              |
| 1:AW:87:GLN:O     | 1:AW:152:GLN:O    | 2.31                     | 0.48              |
| 1:AY:242:ASN:HD22 | 1:AZ:110:GLY:N    | 2.10                     | 0.48              |
| 1:AQ:87:GLN:O     | 1:AQ:152:GLN:O    | 2.31                     | 0.48              |
| 1:DC:87:GLN:O     | 1:DC:152:GLN:O    | 2.31                     | 0.48              |
| 3:CF:42:ASN:ND2   | 3:CF:44:ILE:H     | 2.12                     | 0.48              |
| 3:C2:130:ALA:O    | 3:C2:131:ALA:HB3  | 2.13                     | 0.48              |
| 1:A9:236:ARG:NH1  | 3:DA:172:ALA:O    | 2.45                     | 0.48              |
| 3:CD:130:ALA:O    | 3:CD:131:ALA:HB3  | 2.13                     | 0.48              |
| 3:C7:130:ALA:O    | 3:C7:131:ALA:HB3  | 2.13                     | 0.48              |
| 3:CP:130:ALA:O    | 3:CP:131:ALA:HB3  | 2.13                     | 0.48              |
| 1:A0:88:PHE:HA    | 1:A0:206:GLY:O    | 2.13                     | 0.48              |
| 1:AB:88:PHE:HA    | 1:AB:206:GLY:O    | 2.13                     | 0.48              |
| 3:CX:36:VAL:HA    | 3:CX:37:PRO:HD3   | 1.64                     | 0.48              |
| 1:AF:181:LYS:O    | 1:AF:182:ALA:CB   | 2.61                     | 0.48              |
| 1:DE:181:LYS:O    | 1:DE:182:ALA:CB   | 2.61                     | 0.48              |
| 1:DF:181:LYS:O    | 1:DF:182:ALA:CB   | 2.62                     | 0.48              |
| 1:DD:181:LYS:O    | 1:DD:182:ALA:CB   | 2.61                     | 0.48              |
| 2:BD:157:VAL:HG23 | 3:CD:50:THR:CG2   | 2.40                     | 0.48              |
| 2:BG:157:VAL:HG23 | 3:CH:50:THR:CG2   | 92.72                    | 0.48              |
| 2:BQ:157:VAL:HG23 | 3:CS:50:THR:CG2   | 2.39                     | 0.48              |
| 1:AG:243:ILE:HG22 | 1:AG:244:ASN:N    | 2.28                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AI:243:ILE:HG22 | 1:AI:244:ASN:N    | 2.28                     | 0.48              |
| 1:AR:243:ILE:HG22 | 1:AR:244:ASN:N    | 2.28                     | 0.48              |
| 1:AG:181:LYS:O    | 1:AG:182:ALA:CB   | 2.62                     | 0.48              |
| 1:AT:188:PRO:HG3  | 3:CX:175:THR:HG23 | 1.93                     | 0.48              |
| 1:AP:243:ILE:HG22 | 1:AP:244:ASN:N    | 2.28                     | 0.48              |
| 1:A0:87:GLN:O     | 1:A0:152:GLN:O    | 2.31                     | 0.48              |
| 2:BI:82:PRO:HB2   | 2:BI:190:ASN:HD22 | 1.77                     | 0.48              |
| 3:CC:42:ASN:ND2   | 3:CC:44:ILE:H     | 2.12                     | 0.48              |
| 3:CE:42:ASN:ND2   | 3:CE:44:ILE:H     | 2.12                     | 0.48              |
| 3:CZ:42:ASN:ND2   | 3:CZ:44:ILE:H     | 2.12                     | 0.48              |
| 3:CM:42:ASN:ND2   | 3:CM:44:ILE:H     | 2.11                     | 0.48              |
| 3:C6:42:ASN:ND2   | 3:C6:44:ILE:H     | 2.12                     | 0.48              |
| 3:CM:76:MET:HB2   | 3:CM:84:GLU:HG2   | 1.96                     | 0.48              |
| 1:AC:128:VAL:HG21 | 1:AE:89:LYS:HE3   | 1.96                     | 0.48              |
| 3:CE:130:ALA:O    | 3:CE:131:ALA:HB3  | 2.13                     | 0.48              |
| 1:AL:128:VAL:HG21 | 1:AN:89:LYS:HE3   | 1.96                     | 0.48              |
| 1:AV:128:VAL:HG21 | 1:AX:89:LYS:HE3   | 1.96                     | 0.48              |
| 1:AJ:89:LYS:HE3   | 1:AK:128:VAL:HG21 | 1.96                     | 0.48              |
| 3:C9:130:ALA:O    | 3:C9:131:ALA:HB3  | 2.13                     | 0.48              |
| 1:AO:88:PHE:HA    | 1:AO:206:GLY:O    | 2.13                     | 0.48              |
| 1:AU:181:LYS:O    | 1:AU:182:ALA:CB   | 2.62                     | 0.48              |
| 1:AQ:181:LYS:O    | 1:AQ:182:ALA:CB   | 2.62                     | 0.48              |
| 1:AN:181:LYS:O    | 1:AN:182:ALA:CB   | 2.61                     | 0.48              |
| 1:DH:191:HIS:CD2  | 1:DH:193:GLY:H    | 2.21                     | 0.48              |
| 1:AV:181:LYS:O    | 1:AV:182:ALA:CB   | 2.62                     | 0.48              |
| 2:BE:157:VAL:HG23 | 3:CE:50:THR:CG2   | 2.39                     | 0.48              |
| 2:BG:157:VAL:CG2  | 3:CH:50:THR:HG21  | 91.76                    | 0.48              |
| 1:AB:243:ILE:HG22 | 1:AB:244:ASN:N    | 2.28                     | 0.48              |
| 1:AW:243:ILE:HG22 | 1:AW:244:ASN:N    | 2.28                     | 0.48              |
| 1:DE:191:HIS:HD2  | 1:DE:193:GLY:N    | 2.09                     | 0.48              |
| 1:AH:242:ASN:HD22 | 1:AI:110:GLY:N    | 2.10                     | 0.48              |
| 1:A5:87:GLN:O     | 1:A5:152:GLN:O    | 2.31                     | 0.48              |
| 1:AE:87:GLN:O     | 1:AE:152:GLN:O    | 2.31                     | 0.48              |
| 1:DH:87:GLN:O     | 1:DH:152:GLN:O    | 2.31                     | 0.48              |
| 1:AZ:87:GLN:O     | 1:AZ:152:GLN:O    | 2.31                     | 0.48              |
| 2:BJ:82:PRO:HB2   | 2:BJ:190:ASN:HD22 | 1.78                     | 0.48              |
| 2:B3:82:PRO:HB2   | 2:B3:190:ASN:HD22 | 1.78                     | 0.48              |
| 3:CV:42:ASN:ND2   | 3:CV:44:ILE:H     | 2.12                     | 0.48              |
| 3:CH:42:ASN:ND2   | 3:CH:44:ILE:H     | 2.12                     | 0.48              |
| 3:C0:42:ASN:ND2   | 3:C0:44:ILE:H     | 2.12                     | 0.48              |
| 3:CA:76:MET:HB2   | 3:CA:84:GLU:HG2   | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A5:88:PHE:HA    | 1:A5:206:GLY:O    | 2.13                     | 0.48              |
| 1:AY:88:PHE:HA    | 1:AY:206:GLY:O    | 2.13                     | 0.48              |
| 3:CV:130:ALA:O    | 3:CV:131:ALA:HB3  | 2.13                     | 0.48              |
| 3:CN:130:ALA:O    | 3:CN:131:ALA:HB3  | 2.13                     | 0.48              |
| 1:DF:88:PHE:HA    | 1:DF:206:GLY:O    | 2.12                     | 0.48              |
| 3:C4:130:ALA:O    | 3:C4:131:ALA:HB3  | 2.13                     | 0.48              |
| 3:CO:130:ALA:O    | 3:CO:131:ALA:HB3  | 2.13                     | 0.48              |
| 1:AA:89:LYS:HE3   | 1:AB:128:VAL:HG21 | 1.96                     | 0.48              |
| 1:DF:225:PRO:HA   | 1:DF:226:PRO:HD3  | 1.78                     | 0.48              |
| 1:AD:128:VAL:HG21 | 1:AG:89:LYS:HE3   | 174.27                   | 0.48              |
| 1:DJ:88:PHE:HA    | 1:DJ:206:GLY:O    | 2.13                     | 0.48              |
| 3:CJ:130:ALA:O    | 3:CJ:131:ALA:HB3  | 2.13                     | 0.48              |
| 3:CS:130:ALA:O    | 3:CS:131:ALA:HB3  | 2.13                     | 0.48              |
| 2:BU:86:ASP:HB3   | 2:BU:141:LYS:HA   | 1.96                     | 0.48              |
| 3:CL:130:ALA:O    | 3:CL:131:ALA:HB3  | 2.13                     | 0.48              |
| 1:AM:191:HIS:HD2  | 1:AM:193:GLY:N    | 2.08                     | 0.48              |
| 1:DJ:181:LYS:O    | 1:DJ:182:ALA:CB   | 2.61                     | 0.48              |
| 2:BY:157:VAL:CG2  | 3:CY:50:THR:HG21  | 2.42                     | 0.48              |
| 2:BS:157:VAL:HG23 | 3:CT:50:THR:CG2   | 58.34                    | 0.48              |
| 2:BC:157:VAL:CG2  | 3:CD:50:THR:HG21  | 57.94                    | 0.48              |
| 1:A3:181:LYS:O    | 1:A3:182:ALA:CB   | 2.61                     | 0.48              |
| 1:A9:243:ILE:HG22 | 1:A9:244:ASN:N    | 2.28                     | 0.48              |
| 1:AJ:243:ILE:HG22 | 1:AJ:244:ASN:N    | 2.28                     | 0.48              |
| 1:AA:243:ILE:HG22 | 1:AA:244:ASN:N    | 2.28                     | 0.48              |
| 1:AK:110:GLY:N    | 1:AM:242:ASN:HD22 | 42.15                    | 0.48              |
| 1:AA:242:ASN:HD22 | 1:AB:110:GLY:N    | 2.10                     | 0.48              |
| 1:A4:87:GLN:O     | 1:A4:152:GLN:O    | 2.31                     | 0.48              |
| 1:DG:87:GLN:O     | 1:DG:152:GLN:O    | 2.31                     | 0.48              |
| 3:CQ:42:ASN:ND2   | 3:CQ:44:ILE:H     | 2.12                     | 0.48              |
| 3:CG:42:ASN:ND2   | 3:CG:44:ILE:H     | 2.12                     | 0.48              |
| 3:CW:172:ALA:O    | 1:DI:236:ARG:NH1  | 212.52                   | 0.48              |
| 1:AC:128:VAL:HG21 | 1:A9:89:LYS:HE3   | 289.80                   | 0.48              |
| 1:AF:128:VAL:HG21 | 1:AI:89:LYS:HE3   | 1.96                     | 0.48              |
| 1:AI:89:LYS:HE3   | 1:AJ:128:VAL:HG21 | 180.00                   | 0.48              |
| 1:AG:89:LYS:HE3   | 1:DK:128:VAL:HG21 | 1.96                     | 0.48              |
| 1:AY:128:VAL:HG21 | 1:A1:89:LYS:HE3   | 1.96                     | 0.48              |
| 3:CW:76:MET:HB2   | 3:CW:84:GLU:HG2   | 1.96                     | 0.48              |
| 1:DD:225:PRO:HA   | 1:DD:226:PRO:HD3  | 1.78                     | 0.48              |
| 1:A6:236:ARG:NH1  | 3:C7:172:ALA:O    | 2.45                     | 0.48              |
| 1:DF:89:LYS:HE3   | 1:DG:128:VAL:HG21 | 1.96                     | 0.48              |
| 3:CQ:130:ALA:O    | 3:CQ:131:ALA:HB3  | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A2:88:PHE:HA    | 1:A2:206:GLY:O    | 2.13                     | 0.48              |
| 3:C0:76:MET:HB2   | 3:C0:84:GLU:HG2   | 1.96                     | 0.48              |
| 1:AF:88:PHE:HA    | 1:AF:206:GLY:O    | 2.12                     | 0.48              |
| 3:CC:76:MET:HB2   | 3:CC:84:GLU:HG2   | 1.96                     | 0.48              |
| 3:CK:130:ALA:O    | 3:CK:131:ALA:HB3  | 2.13                     | 0.48              |
| 2:BD:86:ASP:HB3   | 2:BD:141:LYS:HA   | 1.96                     | 0.48              |
| 1:AI:181:LYS:O    | 1:AI:182:ALA:CB   | 2.61                     | 0.48              |
| 1:AH:181:LYS:O    | 1:AH:182:ALA:CB   | 2.62                     | 0.48              |
| 1:AN:191:HIS:HD2  | 1:AN:193:GLY:N    | 2.08                     | 0.48              |
| 1:DI:207:CYS:O    | 1:DI:208:TYR:CB   | 2.58                     | 0.48              |
| 2:BI:157:VAL:HG23 | 3:CJ:50:THR:CG2   | 91.70                    | 0.48              |
| 2:BU:157:VAL:CG2  | 3:CV:50:THR:HG21  | 57.94                    | 0.48              |
| 2:B9:157:VAL:CG2  | 3:DA:50:THR:HG21  | 2.43                     | 0.48              |
| 1:DC:191:HIS:HD2  | 1:DC:193:GLY:N    | 2.08                     | 0.48              |
| 1:AM:243:ILE:HG22 | 1:AM:244:ASN:N    | 2.28                     | 0.48              |
| 2:B4:157:VAL:HG23 | 3:C4:50:THR:CG2   | 2.39                     | 0.48              |
| 1:AC:87:GLN:O     | 1:AC:152:GLN:O    | 2.31                     | 0.48              |
| 1:A3:87:GLN:O     | 1:A3:152:GLN:O    | 2.31                     | 0.48              |
| 1:A7:87:GLN:O     | 1:A7:152:GLN:O    | 2.31                     | 0.48              |
| 1:DE:87:GLN:O     | 1:DE:152:GLN:O    | 2.31                     | 0.48              |
| 2:B5:82:PRO:HB2   | 2:B5:190:ASN:HD22 | 1.78                     | 0.48              |
| 3:CR:42:ASN:ND2   | 3:CR:44:ILE:H     | 2.12                     | 0.48              |
| 2:BX:86:ASP:HB3   | 2:BX:141:LYS:HA   | 1.96                     | 0.48              |
| 2:BE:86:ASP:HB3   | 2:BE:141:LYS:HA   | 1.96                     | 0.48              |
| 3:C3:130:ALA:O    | 3:C3:131:ALA:HB3  | 2.13                     | 0.48              |
| 2:BG:86:ASP:HB3   | 2:BG:141:LYS:HA   | 1.96                     | 0.48              |
| 2:BO:86:ASP:HB3   | 2:BO:141:LYS:HA   | 1.96                     | 0.48              |
| 3:C6:76:MET:HB2   | 3:C6:84:GLU:HG2   | 1.96                     | 0.48              |
| 2:BT:86:ASP:HB3   | 2:BT:141:LYS:HA   | 1.96                     | 0.48              |
| 3:CT:76:MET:HB2   | 3:CT:84:GLU:HG2   | 1.96                     | 0.48              |
| 1:A3:89:LYS:HE3   | 1:A4:128:VAL:HG21 | 1.96                     | 0.48              |
| 3:CV:76:MET:HB2   | 3:CV:84:GLU:HG2   | 1.96                     | 0.48              |
| 1:A5:128:VAL:HG21 | 1:A7:89:LYS:HE3   | 1.96                     | 0.48              |
| 1:DC:181:LYS:O    | 1:DC:182:ALA:CB   | 2.62                     | 0.48              |
| 1:AE:181:LYS:O    | 1:AE:182:ALA:CB   | 2.61                     | 0.48              |
| 1:AK:181:LYS:O    | 1:AK:182:ALA:CB   | 2.61                     | 0.48              |
| 1:A7:191:HIS:CD2  | 1:A7:193:GLY:H    | 2.21                     | 0.48              |
| 1:AR:174:TRP:CZ2  | 2:BQ:139:ALA:HB3  | 2.49                     | 0.48              |
| 2:BQ:157:VAL:HG23 | 3:CR:50:THR:CG2   | 55.67                    | 0.48              |
| 1:AF:207:CYS:O    | 1:AF:208:TYR:CB   | 2.57                     | 0.48              |
| 1:A9:181:LYS:O    | 1:A9:182:ALA:CB   | 2.61                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AV:243:ILE:HG22 | 1:AV:244:ASN:N    | 2.28                     | 0.48              |
| 1:A2:243:ILE:HG22 | 1:A2:244:ASN:N    | 2.28                     | 0.48              |
| 1:A7:243:ILE:HG22 | 1:A7:244:ASN:N    | 2.28                     | 0.48              |
| 1:AC:110:GLY:N    | 1:AE:242:ASN:HD22 | 2.10                     | 0.48              |
| 1:AT:110:GLY:N    | 1:AW:242:ASN:HD22 | 2.10                     | 0.48              |
| 1:DI:87:GLN:O     | 1:DI:152:GLN:O    | 2.31                     | 0.48              |
| 2:BR:83:LEU:HA    | 2:BR:84:PRO:HA    | 1.60                     | 0.48              |
| 3:CD:42:ASN:ND2   | 3:CD:44:ILE:H     | 2.12                     | 0.48              |
| 3:C5:42:ASN:ND2   | 3:C5:44:ILE:H     | 2.12                     | 0.48              |
| 3:CX:42:ASN:ND2   | 3:CX:44:ILE:H     | 2.12                     | 0.48              |
| 3:CT:42:ASN:ND2   | 3:CT:44:ILE:H     | 2.12                     | 0.48              |
| 1:AK:128:VAL:HG21 | 1:AM:89:LYS:HE3   | 23.97                    | 0.48              |
| 1:DC:128:VAL:HG21 | 1:DE:89:LYS:HE3   | 1.96                     | 0.48              |
| 2:BR:86:ASP:HB3   | 2:BR:141:LYS:HA   | 1.96                     | 0.48              |
| 1:DG:89:LYS:HE3   | 1:DJ:128:VAL:HG21 | 1.96                     | 0.48              |
| 3:CG:76:MET:HB2   | 3:CG:84:GLU:HG2   | 1.96                     | 0.48              |
| 1:A7:225:PRO:HA   | 1:A7:226:PRO:HD3  | 1.78                     | 0.48              |
| 2:BP:86:ASP:HB3   | 2:BP:141:LYS:HA   | 1.96                     | 0.48              |
| 1:A0:128:VAL:HG21 | 1:A2:89:LYS:HE3   | 1.96                     | 0.48              |
| 1:AU:88:PHE:HA    | 1:AU:206:GLY:O    | 2.13                     | 0.48              |
| 1:A0:89:LYS:HE3   | 1:A1:128:VAL:HG21 | 1.96                     | 0.48              |
| 2:BL:86:ASP:HB3   | 2:BL:141:LYS:HA   | 1.96                     | 0.48              |
| 3:CL:76:MET:HB2   | 3:CL:84:GLU:HG2   | 1.96                     | 0.48              |
| 2:BC:86:ASP:HB3   | 2:BC:141:LYS:HA   | 1.96                     | 0.48              |
| 1:A3:236:ARG:NH1  | 3:C4:172:ALA:O    | 2.45                     | 0.48              |
| 1:DI:181:LYS:O    | 1:DI:182:ALA:CB   | 2.61                     | 0.48              |
| 1:AJ:181:LYS:O    | 1:AJ:182:ALA:CB   | 2.61                     | 0.48              |
| 1:AR:181:LYS:O    | 1:AR:182:ALA:CB   | 2.61                     | 0.48              |
| 1:AB:174:TRP:CZ2  | 2:BB:139:ALA:HB3  | 2.49                     | 0.48              |
| 1:A0:181:LYS:O    | 1:A0:182:ALA:CB   | 2.62                     | 0.48              |
| 1:DE:243:ILE:HG22 | 1:DE:244:ASN:N    | 2.28                     | 0.48              |
| 1:AO:243:ILE:HG22 | 1:AO:244:ASN:N    | 2.28                     | 0.48              |
| 1:A8:243:ILE:HG22 | 1:A8:244:ASN:N    | 2.28                     | 0.48              |
| 1:DF:243:ILE:HG22 | 1:DF:244:ASN:N    | 2.28                     | 0.48              |
| 1:AD:110:GLY:N    | 1:AG:242:ASN:HD22 | 187.88                   | 0.48              |
| 1:AQ:242:ASN:HD22 | 1:AR:110:GLY:N    | 2.10                     | 0.48              |
| 1:DD:87:GLN:O     | 1:DD:152:GLN:O    | 2.31                     | 0.48              |
| 1:DF:87:GLN:O     | 1:DF:152:GLN:O    | 2.31                     | 0.48              |
| 3:CA:42:ASN:ND2   | 3:CA:44:ILE:H     | 2.12                     | 0.48              |
| 3:C9:42:ASN:ND2   | 3:C9:44:ILE:H     | 2.12                     | 0.48              |
| 3:CU:42:ASN:ND2   | 3:CU:44:ILE:H     | 2.12                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:CP:42:ASN:ND2   | 3:CP:44:ILE:H     | 2.12                     | 0.48              |
| 3:C7:42:ASN:ND2   | 3:C7:44:ILE:H     | 2.12                     | 0.48              |
| 3:CL:42:ASN:ND2   | 3:CL:44:ILE:H     | 2.12                     | 0.48              |
| 1:A0:104:VAL:HG22 | 1:A0:197:LEU:CD2  | 2.44                     | 0.48              |
| 1:AU:104:VAL:HG22 | 1:AU:197:LEU:CD2  | 2.44                     | 0.48              |
| 1:A1:104:VAL:HG22 | 1:A1:197:LEU:CD2  | 2.44                     | 0.48              |
| 1:DD:104:VAL:HG22 | 1:DD:197:LEU:CD2  | 2.44                     | 0.48              |
| 1:DC:104:VAL:HG22 | 1:DC:197:LEU:CD2  | 2.44                     | 0.48              |
| 1:AA:104:VAL:HG22 | 1:AA:197:LEU:CD2  | 2.44                     | 0.48              |
| 1:AK:104:VAL:HG22 | 1:AK:197:LEU:CD2  | 2.44                     | 0.48              |
| 1:A4:104:VAL:HG22 | 1:A4:197:LEU:CD2  | 2.44                     | 0.48              |
| 1:AH:128:VAL:HG21 | 1:DK:89:LYS:HE3   | 1.96                     | 0.48              |
| 1:AF:128:VAL:HG21 | 1:AH:89:LYS:HE3   | 23.97                    | 0.48              |
| 1:AD:89:LYS:HE3   | 1:AE:128:VAL:HG21 | 39.48                    | 0.48              |
| 1:DD:88:PHE:HA    | 1:DD:206:GLY:O    | 2.13                     | 0.48              |
| 3:CX:76:MET:HB2   | 3:CX:84:GLU:HG2   | 1.96                     | 0.48              |
| 2:B0:86:ASP:HB3   | 2:B0:141:LYS:HA   | 1.96                     | 0.48              |
| 3:CJ:76:MET:HB2   | 3:CJ:84:GLU:HG2   | 1.96                     | 0.48              |
| 2:BB:86:ASP:HB3   | 2:BB:141:LYS:HA   | 1.96                     | 0.48              |
| 3:CU:76:MET:HB2   | 3:CU:84:GLU:HG2   | 1.96                     | 0.48              |
| 1:AT:165:ARG:HG2  | 2:BU:180:PRO:O    | 2.14                     | 0.48              |
| 2:B2:86:ASP:HB3   | 2:B2:141:LYS:HA   | 1.96                     | 0.48              |
| 3:CW:75:GLN:HB3   | 1:DI:234:LYS:HD2  | 197.67                   | 0.48              |
| 3:CC:130:ALA:O    | 3:CC:131:ALA:HB3  | 2.13                     | 0.48              |
| 3:CU:130:ALA:O    | 3:CU:131:ALA:HB3  | 2.13                     | 0.48              |
| 2:BP:139:ALA:HB3  | 1:DC:174:TRP:CZ2  | 244.88                   | 0.48              |
| 1:A8:181:LYS:O    | 1:A8:182:ALA:CB   | 2.61                     | 0.48              |
| 1:AA:174:TRP:CZ2  | 2:BA:139:ALA:HB3  | 2.49                     | 0.48              |
| 1:AL:181:LYS:O    | 1:AL:182:ALA:CB   | 2.62                     | 0.48              |
| 2:BS:139:ALA:HB3  | 1:DF:174:TRP:CZ2  | 266.69                   | 0.48              |
| 1:AC:181:LYS:O    | 1:AC:182:ALA:CB   | 2.61                     | 0.48              |
| 1:A4:181:LYS:O    | 1:A4:182:ALA:CB   | 2.62                     | 0.48              |
| 1:A4:174:TRP:CZ2  | 2:BX:139:ALA:HB3  | 287.70                   | 0.48              |
| 1:A6:207:CYS:O    | 1:A6:208:TYR:CB   | 2.57                     | 0.48              |
| 2:BF:157:VAL:CG2  | 3:CF:50:THR:HG21  | 2.42                     | 0.48              |
| 1:A5:174:TRP:CZ2  | 2:B5:139:ALA:HB3  | 2.49                     | 0.48              |
| 2:BT:139:ALA:HB3  | 1:DG:174:TRP:CZ2  | 244.86                   | 0.48              |
| 1:DD:191:HIS:HD2  | 1:DD:193:GLY:N    | 2.08                     | 0.48              |
| 1:A0:174:TRP:CZ2  | 2:B1:139:ALA:HB3  | 2.49                     | 0.48              |
| 1:A5:243:ILE:HG22 | 1:A5:244:ASN:N    | 2.28                     | 0.48              |
| 1:AG:174:TRP:CZ2  | 2:BG:139:ALA:HB3  | 2.49                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AM:207:CYS:O    | 1:AM:208:TYR:CB   | 2.57                     | 0.48              |
| 1:AJ:242:ASN:HD22 | 1:AM:110:GLY:N    | 69.35                    | 0.48              |
| 1:AR:87:GLN:O     | 1:AR:152:GLN:O    | 2.31                     | 0.48              |
| 1:AS:87:GLN:O     | 1:AS:152:GLN:O    | 2.31                     | 0.48              |
| 1:AC:74:THR:HG21  | 3:CD:43:PHE:CE2   | 46.55                    | 0.48              |
| 3:DA:42:ASN:ND2   | 3:DA:44:ILE:H     | 2.12                     | 0.48              |
| 1:AH:104:VAL:HG22 | 1:AH:197:LEU:CD2  | 2.44                     | 0.48              |
| 1:AL:104:VAL:HG22 | 1:AL:197:LEU:CD2  | 2.44                     | 0.48              |
| 1:DI:104:VAL:HG22 | 1:DI:197:LEU:CD2  | 2.44                     | 0.48              |
| 1:AR:104:VAL:HG22 | 1:AR:197:LEU:CD2  | 2.44                     | 0.48              |
| 1:A2:104:VAL:HG22 | 1:A2:197:LEU:CD2  | 2.44                     | 0.48              |
| 1:AN:89:LYS:HE3   | 1:AO:128:VAL:HG21 | 276.48                   | 0.48              |
| 1:AK:165:ARG:HG2  | 2:BK:180:PRO:O    | 48.68                    | 0.48              |
| 1:AU:165:ARG:HG2  | 2:BV:180:PRO:O    | 2.14                     | 0.48              |
| 2:BW:180:PRO:O    | 1:DJ:165:ARG:HG2  | 253.04                   | 0.48              |
| 1:AA:165:ARG:HG2  | 2:BA:180:PRO:O    | 2.14                     | 0.48              |
| 3:CO:76:MET:HB2   | 3:CO:84:GLU:HG2   | 1.96                     | 0.48              |
| 1:AQ:89:LYS:HE3   | 1:AR:128:VAL:HG21 | 1.96                     | 0.48              |
| 3:CP:76:MET:HB2   | 3:CP:84:GLU:HG2   | 1.96                     | 0.48              |
| 1:AQ:234:LYS:HD2  | 3:CR:75:GLN:HB3   | 1.96                     | 0.48              |
| 3:CR:75:GLN:HB3   | 1:DD:234:LYS:HD2  | 284.04                   | 0.48              |
| 1:DF:128:VAL:HG21 | 1:DI:89:LYS:HE3   | 1.96                     | 0.48              |
| 3:CQ:76:MET:HB2   | 3:CQ:84:GLU:HG2   | 1.96                     | 0.48              |
| 1:A8:89:LYS:HE3   | 1:A9:128:VAL:HG21 | 1.96                     | 0.48              |
| 3:C7:76:MET:HB2   | 3:C7:84:GLU:HG2   | 1.96                     | 0.48              |
| 3:CR:76:MET:HB2   | 3:CR:84:GLU:HG2   | 1.96                     | 0.48              |
| 2:BS:86:ASP:HB3   | 2:BS:141:LYS:HA   | 1.96                     | 0.48              |
| 1:AT:128:VAL:HG21 | 1:AW:89:LYS:HE3   | 1.96                     | 0.48              |
| 1:AL:234:LYS:HD2  | 3:CM:75:GLN:HB3   | 1.96                     | 0.48              |
| 2:BP:137:GLU:O    | 2:BP:139:ALA:N    | 2.41                     | 0.48              |
| 1:AA:181:LYS:O    | 1:AA:182:ALA:CB   | 2.61                     | 0.48              |
| 1:AE:174:TRP:CZ2  | 2:BE:139:ALA:HB3  | 2.49                     | 0.48              |
| 1:AC:174:TRP:CZ2  | 2:BC:139:ALA:HB3  | 2.49                     | 0.48              |
| 1:AW:174:TRP:CZ2  | 2:BX:139:ALA:HB3  | 2.49                     | 0.48              |
| 1:DH:191:HIS:HD2  | 1:DH:193:GLY:N    | 2.08                     | 0.48              |
| 2:B2:157:VAL:CG2  | 3:C2:50:THR:HG21  | 2.43                     | 0.48              |
| 1:DG:191:HIS:CD2  | 1:DG:193:GLY:H    | 2.21                     | 0.48              |
| 1:AE:243:ILE:HG22 | 1:AE:244:ASN:N    | 2.28                     | 0.48              |
| 1:AH:243:ILE:HG22 | 1:AH:244:ASN:N    | 2.28                     | 0.48              |
| 1:DG:243:ILE:HG22 | 1:DG:244:ASN:N    | 2.28                     | 0.48              |
| 1:A2:87:GLN:O     | 1:A2:152:GLN:O    | 2.31                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:DG:242:ASN:HD22 | 1:DJ:110:GLY:N    | 2.10                     | 0.48              |
| 2:BE:82:PRO:HB2   | 2:BE:190:ASN:HD22 | 1.77                     | 0.48              |
| 1:DG:163:MET:HE1  | 1:DG:189:GLY:HA3  | 1.96                     | 0.48              |
| 1:AN:104:VAL:HG22 | 1:AN:197:LEU:CD2  | 2.44                     | 0.48              |
| 1:AF:104:VAL:HG22 | 1:AF:197:LEU:CD2  | 2.44                     | 0.48              |
| 1:AK:89:LYS:HE3   | 1:AL:128:VAL:HG21 | 23.97                    | 0.48              |
| 1:AE:165:ARG:HG2  | 2:BE:180:PRO:O    | 2.14                     | 0.48              |
| 2:BM:86:ASP:HB3   | 2:BM:141:LYS:HA   | 1.96                     | 0.48              |
| 3:CN:76:MET:HB2   | 3:CN:84:GLU:HG2   | 1.96                     | 0.48              |
| 1:A5:89:LYS:HE3   | 1:A6:128:VAL:HG21 | 1.96                     | 0.48              |
| 1:A6:165:ARG:HG2  | 2:B6:180:PRO:O    | 2.14                     | 0.48              |
| 3:CQ:75:GLN:HB3   | 1:DC:234:LYS:HD2  | 197.68                   | 0.48              |
| 1:AO:234:LYS:HD2  | 3:CP:75:GLN:HB3   | 1.96                     | 0.48              |
| 2:BH:86:ASP:HB3   | 2:BH:141:LYS:HA   | 1.96                     | 0.48              |
| 1:A5:234:LYS:HD2  | 3:C6:75:GLN:HB3   | 1.96                     | 0.48              |
| 1:AY:165:ARG:HG2  | 2:BZ:180:PRO:O    | 2.14                     | 0.48              |
| 1:AF:234:LYS:HD2  | 3:CG:75:GLN:HB3   | 74.02                    | 0.48              |
| 3:CH:76:MET:HB2   | 3:CH:84:GLU:HG2   | 1.96                     | 0.48              |
| 2:B7:86:ASP:HB3   | 2:B7:141:LYS:HA   | 1.96                     | 0.48              |
| 3:C6:130:ALA:O    | 3:C6:131:ALA:HB3  | 2.13                     | 0.48              |
| 3:CZ:130:ALA:O    | 3:CZ:131:ALA:HB3  | 2.13                     | 0.48              |
| 2:BJ:86:ASP:HB3   | 2:BJ:141:LYS:HA   | 1.96                     | 0.48              |
| 2:BA:86:ASP:HB3   | 2:BA:141:LYS:HA   | 1.96                     | 0.48              |
| 3:CK:76:MET:HB2   | 3:CK:84:GLU:HG2   | 1.96                     | 0.48              |
| 1:A7:165:ARG:HG2  | 2:B7:180:PRO:O    | 2.14                     | 0.48              |
| 3:C1:76:MET:HB2   | 3:C1:84:GLU:HG2   | 1.96                     | 0.48              |
| 1:AK:234:LYS:HD2  | 3:CL:75:GLN:HB3   | 1.96                     | 0.48              |
| 2:BV:86:ASP:HB3   | 2:BV:141:LYS:HA   | 1.96                     | 0.48              |
| 3:DA:130:ALA:O    | 3:DA:131:ALA:HB3  | 2.13                     | 0.48              |
| 1:AX:165:ARG:HG2  | 2:BY:180:PRO:O    | 2.14                     | 0.48              |
| 1:AD:174:TRP:CZ2  | 2:BD:139:ALA:HB3  | 2.49                     | 0.47              |
| 1:AF:174:TRP:CZ2  | 2:BF:139:ALA:HB3  | 2.49                     | 0.47              |
| 1:AJ:174:TRP:CZ2  | 2:BJ:139:ALA:HB3  | 257.94                   | 0.47              |
| 1:AN:174:TRP:CZ2  | 2:BN:139:ALA:HB3  | 109.64                   | 0.47              |
| 1:AP:181:LYS:O    | 1:AP:182:ALA:CB   | 2.62                     | 0.47              |
| 1:AL:184:TYR:CE1  | 2:BL:139:ALA:HB2  | 105.34                   | 0.47              |
| 1:AM:174:TRP:CZ2  | 2:BM:139:ALA:HB3  | 65.44                    | 0.47              |
| 1:AN:184:TYR:CE1  | 2:BR:139:ALA:HB2  | 2.49                     | 0.47              |
| 1:AT:174:TRP:CZ2  | 2:BU:139:ALA:HB3  | 2.49                     | 0.47              |
| 1:A2:207:CYS:O    | 1:A2:208:TYR:CB   | 2.57                     | 0.47              |
| 2:BD:157:VAL:CG2  | 3:CE:50:THR:HG21  | 90.55                    | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A1:181:LYS:O    | 1:A1:182:ALA:CB   | 2.61                     | 0.47              |
| 1:A1:243:ILE:HG22 | 1:A1:244:ASN:N    | 2.28                     | 0.47              |
| 1:AS:243:ILE:HG22 | 1:AS:244:ASN:N    | 2.28                     | 0.47              |
| 1:AK:242:ASN:HD22 | 1:AL:110:GLY:N    | 42.14                    | 0.47              |
| 1:A0:242:ASN:HD22 | 1:A1:110:GLY:N    | 2.10                     | 0.47              |
| 1:AF:87:GLN:O     | 1:AF:152:GLN:O    | 2.31                     | 0.47              |
| 3:CU:43:PHE:CE2   | 1:DG:74:THR:HG21  | 269.06                   | 0.47              |
| 3:CY:42:ASN:ND2   | 3:CY:44:ILE:H     | 2.12                     | 0.47              |
| 1:A8:104:VAL:HG22 | 1:A8:197:LEU:CD2  | 2.44                     | 0.47              |
| 1:AM:104:VAL:HG22 | 1:AM:197:LEU:CD2  | 2.44                     | 0.47              |
| 1:AZ:104:VAL:HG22 | 1:AZ:197:LEU:CD2  | 2.44                     | 0.47              |
| 1:A7:104:VAL:HG22 | 1:A7:197:LEU:CD2  | 2.44                     | 0.47              |
| 1:AO:89:LYS:HE3   | 1:DE:128:VAL:HG21 | 308.84                   | 0.47              |
| 1:AI:128:VAL:HG21 | 1:AL:89:LYS:HE3   | 171.01                   | 0.47              |
| 1:AB:165:ARG:HG2  | 2:BB:180:PRO:O    | 2.14                     | 0.47              |
| 1:AC:165:ARG:HG2  | 2:BC:180:PRO:O    | 2.14                     | 0.47              |
| 1:AF:165:ARG:HG2  | 2:BF:180:PRO:O    | 2.14                     | 0.47              |
| 1:AI:165:ARG:HG2  | 2:BI:180:PRO:O    | 2.14                     | 0.47              |
| 1:AJ:165:ARG:HG2  | 2:BK:180:PRO:O    | 2.14                     | 0.47              |
| 1:AS:165:ARG:HG2  | 2:BT:180:PRO:O    | 2.14                     | 0.47              |
| 2:BJ:180:PRO:O    | 1:DK:165:ARG:HG2  | 2.14                     | 0.47              |
| 3:CE:76:MET:HB2   | 3:CE:84:GLU:HG2   | 1.96                     | 0.47              |
| 1:AQ:128:VAL:HG21 | 1:AS:89:LYS:HE3   | 1.96                     | 0.47              |
| 3:C3:76:MET:HB2   | 3:C3:84:GLU:HG2   | 1.96                     | 0.47              |
| 3:CF:76:MET:HB2   | 3:CF:84:GLU:HG2   | 1.96                     | 0.47              |
| 1:AN:234:LYS:HD2  | 3:CO:75:GLN:HB3   | 1.97                     | 0.47              |
| 3:CS:76:MET:HB2   | 3:CS:84:GLU:HG2   | 1.96                     | 0.47              |
| 1:A0:165:ARG:HG2  | 2:B1:180:PRO:O    | 2.14                     | 0.47              |
| 1:A2:165:ARG:HG2  | 2:B3:180:PRO:O    | 2.14                     | 0.47              |
| 1:A8:234:LYS:HD2  | 3:C9:75:GLN:HB3   | 1.96                     | 0.47              |
| 2:B1:86:ASP:HB3   | 2:B1:141:LYS:HA   | 1.96                     | 0.47              |
| 1:A3:128:VAL:HG21 | 1:A6:89:LYS:HE3   | 1.96                     | 0.47              |
| 1:AM:234:LYS:HD2  | 3:CN:75:GLN:HB3   | 1.96                     | 0.47              |
| 1:A5:165:ARG:HG2  | 2:B5:180:PRO:O    | 2.14                     | 0.47              |
| 2:BV:139:ALA:HB3  | 1:DI:174:TRP:CZ2  | 284.40                   | 0.47              |
| 1:AL:174:TRP:CZ2  | 2:BM:139:ALA:HB3  | 2.49                     | 0.47              |
| 1:AO:184:TYR:CE1  | 2:BO:139:ALA:HB2  | 2.50                     | 0.47              |
| 1:AC:184:TYR:CE1  | 2:BC:139:ALA:HB2  | 2.50                     | 0.47              |
| 1:A7:191:HIS:HD2  | 1:A7:193:GLY:N    | 2.08                     | 0.47              |
| 1:AX:181:LYS:O    | 1:AX:182:ALA:CB   | 2.61                     | 0.47              |
| 2:BQ:139:ALA:HB2  | 1:DD:184:TYR:CE1  | 277.62                   | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A2:181:LYS:O    | 1:A2:182:ALA:CB   | 2.61                     | 0.47              |
| 2:BM:157:VAL:CG2  | 3:CN:50:THR:HG21  | 57.94                    | 0.47              |
| 1:AH:191:HIS:HD2  | 1:AH:193:GLY:N    | 2.08                     | 0.47              |
| 1:DD:243:ILE:HG22 | 1:DD:244:ASN:N    | 2.28                     | 0.47              |
| 1:AA:110:GLY:N    | 1:AC:242:ASN:HD22 | 42.15                    | 0.47              |
| 1:AN:242:ASN:HD22 | 1:AO:110:GLY:N    | 253.71                   | 0.47              |
| 2:BY:82:PRO:HB2   | 2:BY:190:ASN:HD22 | 1.78                     | 0.47              |
| 3:CO:42:ASN:ND2   | 3:CO:44:ILE:H     | 2.12                     | 0.47              |
| 1:DG:104:VAL:HG22 | 1:DG:197:LEU:CD2  | 2.44                     | 0.47              |
| 1:DE:104:VAL:HG22 | 1:DE:197:LEU:CD2  | 2.44                     | 0.47              |
| 1:A9:104:VAL:HG22 | 1:A9:197:LEU:CD2  | 2.44                     | 0.47              |
| 1:AG:165:ARG:HG2  | 2:BG:180:PRO:O    | 2.14                     | 0.47              |
| 1:AH:165:ARG:HG2  | 2:BH:180:PRO:O    | 2.14                     | 0.47              |
| 2:BR:180:PRO:O    | 1:DE:165:ARG:HG2  | 242.83                   | 0.47              |
| 1:AV:165:ARG:HG2  | 2:BW:180:PRO:O    | 2.14                     | 0.47              |
| 2:BT:180:PRO:O    | 1:DG:165:ARG:HG2  | 226.01                   | 0.47              |
| 2:BV:180:PRO:O    | 1:DI:165:ARG:HG2  | 254.36                   | 0.47              |
| 1:AG:234:LYS:HD2  | 3:CH:75:GLN:HB3   | 119.40                   | 0.47              |
| 2:BN:86:ASP:HB3   | 2:BN:141:LYS:HA   | 1.96                     | 0.47              |
| 2:BY:86:ASP:HB3   | 2:BY:141:LYS:HA   | 1.96                     | 0.47              |
| 1:AZ:234:LYS:HD2  | 3:C0:75:GLN:HB3   | 1.96                     | 0.47              |
| 3:C5:130:ALA:O    | 3:C5:131:ALA:HB3  | 2.13                     | 0.47              |
| 2:B6:86:ASP:HB3   | 2:B6:141:LYS:HA   | 1.96                     | 0.47              |
| 3:CI:76:MET:HB2   | 3:CI:84:GLU:HG2   | 1.96                     | 0.47              |
| 1:A9:225:PRO:HA   | 1:A9:226:PRO:HD3  | 1.78                     | 0.47              |
| 2:BI:86:ASP:HB3   | 2:BI:141:LYS:HA   | 1.96                     | 0.47              |
| 3:CB:150:LEU:HD12 | 3:CB:150:LEU:HA   | 1.79                     | 0.47              |
| 1:A8:165:ARG:HG2  | 2:B8:180:PRO:O    | 2.14                     | 0.47              |
| 3:C9:76:MET:HB2   | 3:C9:84:GLU:HG2   | 1.96                     | 0.47              |
| 1:AQ:174:TRP:CZ2  | 2:BP:139:ALA:HB3  | 2.49                     | 0.47              |
| 2:BP:139:ALA:HB2  | 1:DC:184:TYR:CE1  | 244.71                   | 0.47              |
| 1:A6:184:TYR:CE1  | 2:B6:139:ALA:HB2  | 2.49                     | 0.47              |
| 1:AK:174:TRP:CZ2  | 2:BK:139:ALA:HB3  | 65.45                    | 0.47              |
| 1:AD:184:TYR:CE1  | 2:BD:139:ALA:HB2  | 2.49                     | 0.47              |
| 1:AO:174:TRP:CZ2  | 2:BO:139:ALA:HB3  | 2.49                     | 0.47              |
| 1:AZ:174:TRP:CZ2  | 2:B0:139:ALA:HB3  | 2.49                     | 0.47              |
| 2:BU:139:ALA:HB3  | 1:DH:174:TRP:CZ2  | 282.04                   | 0.47              |
| 2:BB:157:VAL:CG2  | 3:CB:50:THR:HG21  | 2.43                     | 0.47              |
| 1:DJ:191:HIS:CD2  | 1:DJ:193:GLY:H    | 2.21                     | 0.47              |
| 1:AN:207:CYS:O    | 1:AN:208:TYR:CB   | 2.57                     | 0.47              |
| 1:DK:243:ILE:HG22 | 1:DK:244:ASN:N    | 2.28                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AK:243:ILE:HG22 | 1:AK:244:ASN:N    | 2.28                     | 0.47              |
| 1:AG:184:TYR:CE1  | 2:BG:139:ALA:HB2  | 2.50                     | 0.47              |
| 1:AZ:243:ILE:HG22 | 1:AZ:244:ASN:N    | 2.28                     | 0.47              |
| 1:AV:74:THR:HG21  | 3:CW:43:PHE:CE2   | 2.45                     | 0.47              |
| 1:A1:87:GLN:O     | 1:A1:152:GLN:O    | 2.31                     | 0.47              |
| 2:B9:82:PRO:HB2   | 2:B9:190:ASN:HD22 | 1.77                     | 0.47              |
| 1:AM:146:ILE:O    | 1:AM:147:ALA:CB   | 2.62                     | 0.47              |
| 3:CK:42:ASN:ND2   | 3:CK:44:ILE:H     | 2.11                     | 0.47              |
| 3:CN:42:ASN:ND2   | 3:CN:44:ILE:H     | 2.12                     | 0.47              |
| 3:CI:42:ASN:ND2   | 3:CI:44:ILE:H     | 2.12                     | 0.47              |
| 1:A5:104:VAL:HG22 | 1:A5:197:LEU:CD2  | 2.44                     | 0.47              |
| 1:AX:104:VAL:HG22 | 1:AX:197:LEU:CD2  | 2.44                     | 0.47              |
| 1:AL:165:ARG:HG2  | 2:BL:180:PRO:O    | 79.27                    | 0.47              |
| 1:AN:165:ARG:HG2  | 2:BR:180:PRO:O    | 2.14                     | 0.47              |
| 1:AD:165:ARG:HG2  | 2:BD:180:PRO:O    | 2.14                     | 0.47              |
| 2:BP:180:PRO:O    | 1:DC:165:ARG:HG2  | 226.02                   | 0.47              |
| 2:BU:180:PRO:O    | 1:DH:165:ARG:HG2  | 253.18                   | 0.47              |
| 1:A4:165:ARG:HG2  | 2:BX:180:PRO:O    | 257.41                   | 0.47              |
| 1:AB:234:LYS:HD2  | 3:CC:75:GLN:HB3   | 119.40                   | 0.47              |
| 2:BW:86:ASP:HB3   | 2:BW:141:LYS:HA   | 1.96                     | 0.47              |
| 3:C5:76:MET:HB2   | 3:C5:84:GLU:HG2   | 1.96                     | 0.47              |
| 1:AP:89:LYS:HE3   | 1:AS:128:VAL:HG21 | 1.96                     | 0.47              |
| 3:CT:36:VAL:HA    | 3:CT:37:PRO:HD3   | 1.64                     | 0.47              |
| 1:AA:225:PRO:HA   | 1:AA:226:PRO:HD3  | 1.78                     | 0.47              |
| 3:CZ:76:MET:HB2   | 3:CZ:84:GLU:HG2   | 1.96                     | 0.47              |
| 1:A1:165:ARG:HG2  | 2:B2:180:PRO:O    | 2.14                     | 0.47              |
| 1:AT:89:LYS:HE3   | 1:AU:128:VAL:HG21 | 1.96                     | 0.47              |
| 3:CJ:150:LEU:HA   | 3:CJ:150:LEU:HD12 | 1.79                     | 0.47              |
| 1:A3:165:ARG:HG2  | 2:B4:180:PRO:O    | 2.14                     | 0.47              |
| 3:CT:130:ALA:O    | 3:CT:131:ALA:HB3  | 2.13                     | 0.47              |
| 3:C1:130:ALA:O    | 3:C1:131:ALA:HB3  | 2.13                     | 0.47              |
| 3:CV:75:GLN:HB3   | 1:DH:234:LYS:HD2  | 304.10                   | 0.47              |
| 1:A6:181:LYS:O    | 1:A6:182:ALA:CB   | 2.62                     | 0.47              |
| 1:A6:174:TRP:CZ2  | 2:B6:139:ALA:HB3  | 2.49                     | 0.47              |
| 1:A8:184:TYR:CE1  | 2:B8:139:ALA:HB2  | 2.50                     | 0.47              |
| 1:AA:184:TYR:CE1  | 2:BA:139:ALA:HB2  | 2.50                     | 0.47              |
| 1:AI:184:TYR:CE1  | 2:BI:139:ALA:HB2  | 2.49                     | 0.47              |
| 1:AK:174:TRP:CZ2  | 2:BL:139:ALA:HB3  | 2.49                     | 0.47              |
| 1:AO:181:LYS:O    | 1:AO:182:ALA:CB   | 2.61                     | 0.47              |
| 1:AN:174:TRP:CZ2  | 2:BR:139:ALA:HB3  | 2.49                     | 0.47              |
| 2:BR:139:ALA:HB3  | 1:DE:174:TRP:CZ2  | 266.56                   | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BJ:139:ALA:HB2  | 1:DK:184:TYR:CE1  | 2.50                     | 0.47              |
| 1:AH:184:TYR:CE1  | 2:BH:139:ALA:HB2  | 2.50                     | 0.47              |
| 1:DH:181:LYS:O    | 1:DH:182:ALA:CB   | 2.62                     | 0.47              |
| 1:AY:181:LYS:O    | 1:AY:182:ALA:CB   | 2.61                     | 0.47              |
| 1:DK:207:CYS:O    | 1:DK:208:TYR:CB   | 2.57                     | 0.47              |
| 2:BX:157:VAL:CG2  | 3:C5:50:THR:HG21  | 243.75                   | 0.47              |
| 2:BI:157:VAL:CG2  | 3:CJ:50:THR:HG21  | 90.55                    | 0.47              |
| 1:AS:174:TRP:CZ2  | 2:BT:139:ALA:HB3  | 2.49                     | 0.47              |
| 1:A1:174:TRP:CZ2  | 2:B2:139:ALA:HB3  | 2.49                     | 0.47              |
| 1:AF:243:ILE:HG22 | 1:AF:244:ASN:N    | 2.28                     | 0.47              |
| 1:AU:243:ILE:HG22 | 1:AU:244:ASN:N    | 2.28                     | 0.47              |
| 1:DH:243:ILE:HG22 | 1:DH:244:ASN:N    | 2.28                     | 0.47              |
| 1:A0:243:ILE:HG22 | 1:A0:244:ASN:N    | 2.28                     | 0.47              |
| 1:AV:110:GLY:N    | 1:AX:242:ASN:HD22 | 2.10                     | 0.47              |
| 1:AO:104:VAL:HG22 | 1:AO:197:LEU:CD2  | 2.44                     | 0.47              |
| 1:AC:104:VAL:HG22 | 1:AC:197:LEU:CD2  | 2.44                     | 0.47              |
| 1:A6:104:VAL:HG22 | 1:A6:197:LEU:CD2  | 2.44                     | 0.47              |
| 1:AT:104:VAL:HG22 | 1:AT:197:LEU:CD2  | 2.44                     | 0.47              |
| 1:AG:104:VAL:HG22 | 1:AG:197:LEU:CD2  | 2.44                     | 0.47              |
| 1:AE:104:VAL:HG22 | 1:AE:197:LEU:CD2  | 2.44                     | 0.47              |
| 1:AS:104:VAL:HG22 | 1:AS:197:LEU:CD2  | 2.44                     | 0.47              |
| 1:AJ:165:ARG:HG2  | 2:BJ:180:PRO:O    | 218.42                   | 0.47              |
| 2:BS:180:PRO:O    | 1:DF:165:ARG:HG2  | 241.72                   | 0.47              |
| 1:AF:234:LYS:HD2  | 3:CF:75:GLN:HB3   | 1.96                     | 0.47              |
| 1:A2:234:LYS:HD2  | 3:C3:75:GLN:HB3   | 1.96                     | 0.47              |
| 3:CF:36:VAL:HA    | 3:CF:37:PRO:HD3   | 1.64                     | 0.47              |
| 1:AZ:165:ARG:HG2  | 2:B0:180:PRO:O    | 2.14                     | 0.47              |
| 3:CT:150:LEU:HD12 | 3:CT:150:LEU:HA   | 1.79                     | 0.47              |
| 2:BP:140:LEU:HD23 | 2:BP:140:LEU:N    | 2.30                     | 0.47              |
| 2:B6:140:LEU:N    | 2:B6:140:LEU:HD23 | 2.30                     | 0.47              |
| 1:AJ:234:LYS:HD2  | 3:CK:75:GLN:HB3   | 1.96                     | 0.47              |
| 3:CB:130:ALA:O    | 3:CB:131:ALA:HB3  | 2.13                     | 0.47              |
| 1:A8:174:TRP:CZ2  | 2:B8:139:ALA:HB3  | 2.49                     | 0.47              |
| 1:AJ:174:TRP:CZ2  | 2:BK:139:ALA:HB3  | 2.49                     | 0.47              |
| 1:AJ:184:TYR:CE1  | 2:BJ:139:ALA:HB2  | 254.17                   | 0.47              |
| 2:BR:139:ALA:HB2  | 1:DE:184:TYR:CE1  | 265.55                   | 0.47              |
| 1:AI:191:HIS:HD2  | 1:AI:193:GLY:N    | 2.08                     | 0.47              |
| 1:AZ:191:HIS:CD2  | 1:AZ:193:GLY:H    | 2.21                     | 0.47              |
| 1:AH:174:TRP:CZ2  | 2:BH:139:ALA:HB3  | 2.49                     | 0.47              |
| 1:AT:181:LYS:O    | 1:AT:182:ALA:CB   | 2.61                     | 0.47              |
| 2:BY:137:GLU:O    | 2:BY:139:ALA:N    | 2.42                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A2:174:TRP:CZ2  | 2:B3:139:ALA:HB3  | 2.49                     | 0.47              |
| 1:AS:184:TYR:CE1  | 2:BT:139:ALA:HB2  | 2.50                     | 0.47              |
| 2:BT:139:ALA:HB2  | 1:DG:184:TYR:CE1  | 244.70                   | 0.47              |
| 1:A7:174:TRP:CZ2  | 2:B7:139:ALA:HB3  | 2.49                     | 0.47              |
| 1:A7:184:TYR:CE1  | 2:B7:139:ALA:HB2  | 2.50                     | 0.47              |
| 2:BA:157:VAL:CG2  | 3:CA:50:THR:HG21  | 2.43                     | 0.47              |
| 1:AY:191:HIS:HD2  | 1:AY:193:GLY:N    | 2.08                     | 0.47              |
| 1:AJ:242:ASN:HD22 | 1:AK:110:GLY:N    | 2.09                     | 0.47              |
| 1:AK:242:ASN:HD22 | 1:AN:110:GLY:N    | 2.10                     | 0.47              |
| 1:AL:74:THR:HG21  | 3:CM:43:PHE:CE1   | 2.45                     | 0.47              |
| 2:BW:83:LEU:HA    | 2:BW:84:PRO:HA    | 1.60                     | 0.47              |
| 1:DE:163:MET:HE1  | 1:DE:189:GLY:HA3  | 1.97                     | 0.47              |
| 1:AW:104:VAL:HG22 | 1:AW:197:LEU:CD2  | 2.44                     | 0.47              |
| 1:AI:104:VAL:HG22 | 1:AI:197:LEU:CD2  | 2.44                     | 0.47              |
| 1:AK:89:LYS:HE3   | 1:AN:128:VAL:HG21 | 1.96                     | 0.47              |
| 1:AJ:128:VAL:HG21 | 1:AM:89:LYS:HE3   | 1.96                     | 0.47              |
| 1:AQ:165:ARG:HG2  | 2:BP:180:PRO:O    | 2.14                     | 0.47              |
| 1:AP:165:ARG:HG2  | 2:BS:180:PRO:O    | 2.14                     | 0.47              |
| 2:BF:86:ASP:HB3   | 2:BF:141:LYS:HA   | 1.96                     | 0.47              |
| 2:BG:53:ARG:HG2   | 2:BG:221:MET:HE3  | 2.12                     | 0.47              |
| 1:AY:234:LYS:HD2  | 3:CZ:75:GLN:HB3   | 1.96                     | 0.47              |
| 1:AR:234:LYS:HD2  | 3:CS:75:GLN:HB3   | 1.96                     | 0.47              |
| 2:B9:140:LEU:HD23 | 2:B9:140:LEU:N    | 2.30                     | 0.47              |
| 2:BT:140:LEU:N    | 2:BT:140:LEU:HD23 | 2.30                     | 0.47              |
| 2:BF:140:LEU:HD23 | 2:BF:140:LEU:N    | 2.30                     | 0.47              |
| 2:BH:140:LEU:HD23 | 2:BH:140:LEU:N    | 2.30                     | 0.47              |
| 2:BZ:140:LEU:N    | 2:BZ:140:LEU:HD23 | 2.30                     | 0.47              |
| 1:DH:89:LYS:HE3   | 1:DI:128:VAL:HG21 | 1.95                     | 0.47              |
| 1:AT:234:LYS:HD2  | 3:CU:75:GLN:HB3   | 1.96                     | 0.47              |
| 1:AU:184:TYR:CE1  | 2:BV:139:ALA:HB2  | 2.50                     | 0.47              |
| 1:AM:174:TRP:CZ2  | 2:BN:139:ALA:HB3  | 2.49                     | 0.47              |
| 1:AL:174:TRP:CZ2  | 2:BL:139:ALA:HB3  | 108.21                   | 0.47              |
| 2:BU:139:ALA:HB2  | 1:DH:184:TYR:CE1  | 279.54                   | 0.47              |
| 2:BM:157:VAL:CG2  | 3:CM:50:THR:HG21  | 2.42                     | 0.47              |
| 1:AW:207:CYS:O    | 1:AW:208:TYR:CB   | 2.57                     | 0.47              |
| 1:AS:181:LYS:O    | 1:AS:182:ALA:CB   | 2.61                     | 0.47              |
| 1:AB:184:TYR:CE1  | 2:BB:139:ALA:HB2  | 2.50                     | 0.47              |
| 1:DJ:191:HIS:HD2  | 1:DJ:193:GLY:N    | 2.08                     | 0.47              |
| 2:BO:157:VAL:CG2  | 3:CP:50:THR:HG21  | 2.42                     | 0.47              |
| 1:A9:174:TRP:CZ2  | 2:B9:139:ALA:HB3  | 2.49                     | 0.47              |
| 1:A3:110:GLY:N    | 1:A6:242:ASN:HD22 | 2.10                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:DC:242:ASN:HD22 | 1:DD:110:GLY:N    | 2.10                     | 0.47              |
| 3:CJ:42:ASN:ND2   | 3:CJ:44:ILE:H     | 2.12                     | 0.47              |
| 3:CB:42:ASN:ND2   | 3:CB:44:ILE:H     | 2.12                     | 0.47              |
| 1:DH:104:VAL:HG22 | 1:DH:197:LEU:CD2  | 2.44                     | 0.47              |
| 1:AB:89:LYS:HE3   | 1:A8:128:VAL:HG21 | 277.09                   | 0.47              |
| 1:AB:89:LYS:HE3   | 1:AE:128:VAL:HG21 | 1.96                     | 0.47              |
| 1:AK:165:ARG:HG2  | 2:BL:180:PRO:O    | 2.14                     | 0.47              |
| 2:BQ:180:PRO:O    | 1:DD:165:ARG:HG2  | 247.49                   | 0.47              |
| 1:AG:225:PRO:HA   | 1:AG:226:PRO:HD3  | 1.78                     | 0.47              |
| 1:AY:89:LYS:HE3   | 1:AZ:128:VAL:HG21 | 1.96                     | 0.47              |
| 2:B5:86:ASP:HB3   | 2:B5:141:LYS:HA   | 1.96                     | 0.47              |
| 2:BK:86:ASP:HB3   | 2:BK:141:LYS:HA   | 1.96                     | 0.47              |
| 2:BA:140:LEU:HD23 | 2:BA:140:LEU:N    | 2.30                     | 0.47              |
| 2:BJ:140:LEU:N    | 2:BJ:140:LEU:HD23 | 2.30                     | 0.47              |
| 2:B0:140:LEU:N    | 2:B0:140:LEU:HD23 | 2.30                     | 0.47              |
| 2:BL:140:LEU:N    | 2:BL:140:LEU:HD23 | 2.30                     | 0.47              |
| 2:B2:140:LEU:HD23 | 2:B2:140:LEU:N    | 2.30                     | 0.47              |
| 2:BO:140:LEU:N    | 2:BO:140:LEU:HD23 | 2.30                     | 0.47              |
| 2:B5:140:LEU:N    | 2:B5:140:LEU:HD23 | 2.30                     | 0.47              |
| 2:B7:140:LEU:N    | 2:B7:140:LEU:HD23 | 2.30                     | 0.47              |
| 3:CT:75:GLN:HB3   | 1:DF:234:LYS:HD2  | 278.75                   | 0.47              |
| 1:DJ:225:PRO:HA   | 1:DJ:226:PRO:HD3  | 1.78                     | 0.47              |
| 1:AI:174:TRP:CZ2  | 2:BI:139:ALA:HB3  | 2.49                     | 0.47              |
| 1:AF:184:TYR:CE1  | 2:BF:139:ALA:HB2  | 2.50                     | 0.47              |
| 1:AM:184:TYR:CE1  | 2:BN:139:ALA:HB2  | 2.49                     | 0.47              |
| 1:AZ:181:LYS:O    | 1:AZ:182:ALA:CB   | 2.62                     | 0.47              |
| 1:AX:174:TRP:CZ2  | 2:BY:139:ALA:HB3  | 2.49                     | 0.47              |
| 1:AY:174:TRP:CZ2  | 2:BZ:139:ALA:HB3  | 2.49                     | 0.47              |
| 2:BH:157:VAL:CG2  | 3:CI:50:THR:HG21  | 57.94                    | 0.47              |
| 1:A7:181:LYS:O    | 1:A7:182:ALA:CB   | 2.61                     | 0.47              |
| 2:B0:157:VAL:CG2  | 3:C0:50:THR:HG21  | 2.43                     | 0.47              |
| 1:AJ:207:CYS:O    | 1:AJ:208:TYR:CB   | 2.57                     | 0.47              |
| 1:A3:174:TRP:CZ2  | 2:B4:139:ALA:HB3  | 2.49                     | 0.47              |
| 1:A9:191:HIS:HD2  | 1:A9:193:GLY:N    | 2.09                     | 0.47              |
| 1:A9:184:TYR:CE1  | 2:B9:139:ALA:HB2  | 2.50                     | 0.47              |
| 2:B7:157:VAL:CG2  | 3:C8:50:THR:HG21  | 2.42                     | 0.47              |
| 1:AP:191:HIS:HD2  | 1:AP:193:GLY:N    | 2.08                     | 0.47              |
| 1:AF:110:GLY:N    | 1:AH:242:ASN:HD22 | 42.15                    | 0.47              |
| 1:AZ:242:ASN:HD22 | 1:A2:110:GLY:N    | 2.10                     | 0.47              |
| 1:AL:74:THR:HG21  | 3:CM:43:PHE:CE2   | 4.65                     | 0.47              |
| 2:BJ:83:LEU:HA    | 2:BJ:84:PRO:HA    | 1.60                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AO:146:ILE:O    | 1:AO:147:ALA:CB   | 2.62                     | 0.47              |
| 1:A5:146:ILE:O    | 1:A5:147:ALA:CB   | 2.62                     | 0.47              |
| 1:DK:104:VAL:HG22 | 1:DK:197:LEU:CD2  | 2.44                     | 0.47              |
| 1:AJ:104:VAL:HG22 | 1:AJ:197:LEU:CD2  | 2.44                     | 0.47              |
| 1:DF:104:VAL:HG22 | 1:DF:197:LEU:CD2  | 2.44                     | 0.47              |
| 1:AB:104:VAL:HG22 | 1:AB:197:LEU:CD2  | 2.44                     | 0.47              |
| 1:AE:89:LYS:HE3   | 1:AH:128:VAL:HG21 | 180.02                   | 0.47              |
| 1:AA:128:VAL:HG21 | 1:AC:89:LYS:HE3   | 23.97                    | 0.47              |
| 1:AM:165:ARG:HG2  | 2:BN:180:PRO:O    | 2.14                     | 0.47              |
| 1:AW:165:ARG:HG2  | 2:BX:180:PRO:O    | 2.14                     | 0.47              |
| 1:AL:165:ARG:HG2  | 2:BM:180:PRO:O    | 2.14                     | 0.47              |
| 1:AV:234:LYS:HD2  | 3:CW:75:GLN:HB3   | 1.96                     | 0.47              |
| 1:AH:234:LYS:HD2  | 3:CI:75:GLN:HB3   | 74.02                    | 0.47              |
| 1:AC:234:LYS:HD2  | 3:CC:75:GLN:HB3   | 1.96                     | 0.47              |
| 1:AE:234:LYS:HD2  | 3:CE:75:GLN:HB3   | 1.96                     | 0.47              |
| 1:AG:234:LYS:HD2  | 3:CG:75:GLN:HB3   | 1.96                     | 0.47              |
| 1:AU:234:LYS:HD2  | 3:CV:75:GLN:HB3   | 1.96                     | 0.47              |
| 1:A6:234:LYS:HD2  | 3:C7:75:GLN:HB3   | 1.96                     | 0.47              |
| 2:BQ:86:ASP:HB3   | 2:BQ:141:LYS:HA   | 1.96                     | 0.47              |
| 2:B8:86:ASP:HB3   | 2:B8:141:LYS:HA   | 1.96                     | 0.47              |
| 2:BD:140:LEU:HD23 | 2:BD:140:LEU:N    | 2.30                     | 0.47              |
| 2:B4:140:LEU:HD23 | 2:B4:140:LEU:N    | 2.30                     | 0.47              |
| 2:BG:140:LEU:HD23 | 2:BG:140:LEU:N    | 2.30                     | 0.47              |
| 2:BQ:140:LEU:N    | 2:BQ:140:LEU:HD23 | 2.30                     | 0.47              |
| 1:A9:234:LYS:HD2  | 3:DA:75:GLN:HB3   | 1.96                     | 0.47              |
| 1:DI:225:PRO:HA   | 1:DI:226:PRO:HD3  | 1.78                     | 0.47              |
| 1:AU:89:LYS:HE3   | 1:AX:128:VAL:HG21 | 1.96                     | 0.47              |
| 1:AO:165:ARG:HG2  | 2:BO:180:PRO:O    | 2.14                     | 0.47              |
| 2:B3:86:ASP:HB3   | 2:B3:141:LYS:HA   | 1.96                     | 0.47              |
| 1:AX:234:LYS:HD2  | 3:CY:75:GLN:HB3   | 1.96                     | 0.47              |
| 1:AZ:89:LYS:HE3   | 1:A2:128:VAL:HG21 | 1.96                     | 0.47              |
| 1:AA:234:LYS:HD2  | 3:DB:75:GLN:HB3   | 285.36                   | 0.47              |
| 2:BM:140:LEU:N    | 2:BM:140:LEU:HD23 | 2.30                     | 0.47              |
| 2:BV:140:LEU:N    | 2:BV:140:LEU:HD23 | 2.30                     | 0.47              |
| 2:BX:140:LEU:N    | 2:BX:140:LEU:HD23 | 2.30                     | 0.47              |
| 2:BY:140:LEU:HD23 | 2:BY:140:LEU:N    | 2.30                     | 0.47              |
| 2:BI:140:LEU:HD23 | 2:BI:140:LEU:N    | 2.30                     | 0.47              |
| 1:AV:89:LYS:HE3   | 1:AW:128:VAL:HG21 | 1.96                     | 0.47              |
| 3:DB:76:MET:HB2   | 3:DB:84:GLU:HG2   | 1.96                     | 0.47              |
| 3:CD:76:MET:HB2   | 3:CD:84:GLU:HG2   | 1.96                     | 0.47              |
| 1:AL:184:TYR:CE1  | 2:BM:139:ALA:HB2  | 2.50                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AM:184:TYR:CE1  | 2:BM:139:ALA:HB2  | 65.16                    | 0.47              |
| 1:AJ:191:HIS:HD2  | 1:AJ:193:GLY:N    | 2.08                     | 0.47              |
| 1:AW:184:TYR:CE1  | 2:BX:139:ALA:HB2  | 2.50                     | 0.47              |
| 1:AT:184:TYR:CE1  | 2:BU:139:ALA:HB2  | 2.50                     | 0.47              |
| 1:AX:184:TYR:CE1  | 2:BY:139:ALA:HB2  | 2.49                     | 0.47              |
| 2:BQ:139:ALA:HB3  | 1:DD:174:TRP:CZ2  | 277.50                   | 0.47              |
| 2:BW:139:ALA:HB3  | 1:DJ:174:TRP:CZ2  | 282.17                   | 0.47              |
| 1:A8:191:HIS:HD2  | 1:A8:193:GLY:N    | 2.08                     | 0.47              |
| 1:AS:207:CYS:O    | 1:AS:208:TYR:CB   | 2.57                     | 0.47              |
| 2:BK:83:LEU:HA    | 2:BK:84:PRO:HA    | 1.60                     | 0.47              |
| 3:C8:42:ASN:ND2   | 3:C8:44:ILE:H     | 2.11                     | 0.47              |
| 3:CL:110:PHE:HE2  | 3:CL:116:THR:HG22 | 1.80                     | 0.47              |
| 3:CV:110:PHE:HE2  | 3:CV:116:THR:HG22 | 1.80                     | 0.47              |
| 3:CX:110:PHE:HE2  | 3:CX:116:THR:HG22 | 1.80                     | 0.47              |
| 3:C2:110:PHE:HE2  | 3:C2:116:THR:HG22 | 1.80                     | 0.47              |
| 1:AD:104:VAL:HG22 | 1:AD:197:LEU:CD2  | 2.44                     | 0.47              |
| 1:AP:104:VAL:HG22 | 1:AP:197:LEU:CD2  | 2.44                     | 0.47              |
| 1:AV:104:VAL:HG22 | 1:AV:197:LEU:CD2  | 2.44                     | 0.47              |
| 1:AN:128:VAL:HG21 | 1:DD:89:LYS:HE3   | 315.39                   | 0.47              |
| 1:AL:89:LYS:HE3   | 1:AM:128:VAL:HG21 | 1.96                     | 0.47              |
| 1:AF:89:LYS:HE3   | 1:AG:128:VAL:HG21 | 1.96                     | 0.47              |
| 3:CX:75:GLN:HB3   | 1:DJ:234:LYS:HD2  | 282.68                   | 0.47              |
| 2:B4:86:ASP:HB3   | 2:B4:141:LYS:HA   | 1.96                     | 0.47              |
| 2:BZ:86:ASP:HB3   | 2:BZ:141:LYS:HA   | 1.96                     | 0.47              |
| 3:CP:150:LEU:HD12 | 3:CP:150:LEU:HA   | 1.79                     | 0.47              |
| 2:BN:140:LEU:HD23 | 2:BN:140:LEU:N    | 2.30                     | 0.47              |
| 1:A9:165:ARG:HG2  | 2:B9:180:PRO:O    | 2.14                     | 0.47              |
| 1:AN:115:THR:OG1  | 1:AN:133:LEU:HB2  | 2.16                     | 0.47              |
| 1:AD:115:THR:OG1  | 1:AD:133:LEU:HB2  | 2.15                     | 0.47              |
| 1:AE:184:TYR:CE1  | 2:BE:139:ALA:HB2  | 2.49                     | 0.47              |
| 2:BJ:139:ALA:HB3  | 1:DK:174:TRP:CZ2  | 2.49                     | 0.47              |
| 1:AZ:184:TYR:CE1  | 2:B0:139:ALA:HB2  | 2.50                     | 0.47              |
| 1:A2:184:TYR:CE1  | 2:B3:139:ALA:HB2  | 2.49                     | 0.47              |
| 1:AV:184:TYR:CE1  | 2:BW:139:ALA:HB2  | 2.50                     | 0.47              |
| 1:AV:174:TRP:CZ2  | 2:BW:139:ALA:HB3  | 2.49                     | 0.47              |
| 1:AI:207:CYS:O    | 1:AI:208:TYR:CB   | 2.57                     | 0.47              |
| 2:BF:157:VAL:CG2  | 3:CG:50:THR:HG21  | 57.94                    | 0.47              |
| 1:AD:242:ASN:HD22 | 1:AE:110:GLY:N    | 68.89                    | 0.47              |
| 1:AB:87:GLN:HE21  | 1:AB:210:ARG:NH2  | 2.12                     | 0.47              |
| 1:AI:74:THR:HG21  | 3:CI:43:PHE:CE1   | 2.45                     | 0.47              |
| 1:AJ:74:THR:HG21  | 3:CK:43:PHE:CE1   | 2.45                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:DI:87:GLN:HE21  | 1:DI:210:ARG:NH2  | 2.12                     | 0.47              |
| 1:AX:74:THR:HG21  | 3:CY:43:PHE:CE2   | 2.45                     | 0.47              |
| 1:AH:146:ILE:O    | 1:AH:147:ALA:CB   | 2.62                     | 0.47              |
| 3:C1:42:ASN:ND2   | 3:C1:44:ILE:H     | 2.12                     | 0.47              |
| 3:CG:110:PHE:HE2  | 3:CG:116:THR:HG22 | 1.80                     | 0.47              |
| 3:CC:110:PHE:HE2  | 3:CC:116:THR:HG22 | 1.80                     | 0.47              |
| 3:DA:110:PHE:HE2  | 3:DA:116:THR:HG22 | 1.80                     | 0.47              |
| 1:DJ:104:VAL:HG22 | 1:DJ:197:LEU:CD2  | 2.44                     | 0.47              |
| 3:CY:110:PHE:HE2  | 3:CY:116:THR:HG22 | 1.80                     | 0.47              |
| 1:AY:104:VAL:HG22 | 1:AY:197:LEU:CD2  | 2.44                     | 0.47              |
| 1:AO:128:VAL:HG21 | 1:AR:89:LYS:HE3   | 1.96                     | 0.47              |
| 3:CJ:75:GLN:HB3   | 1:DK:234:LYS:HD2  | 1.96                     | 0.47              |
| 3:C4:76:MET:HB2   | 3:C4:84:GLU:HG2   | 1.96                     | 0.47              |
| 3:CY:76:MET:HB2   | 3:CY:84:GLU:HG2   | 1.96                     | 0.47              |
| 2:BC:140:LEU:HD23 | 2:BC:140:LEU:N    | 2.30                     | 0.47              |
| 3:CV:61:TYR:HB3   | 3:CV:205:LEU:HD23 | 1.97                     | 0.47              |
| 3:C8:76:MET:HB2   | 3:C8:84:GLU:HG2   | 1.96                     | 0.47              |
| 1:DG:115:THR:OG1  | 1:DG:133:LEU:HB2  | 2.15                     | 0.47              |
| 1:AU:174:TRP:CZ2  | 2:BV:139:ALA:HB3  | 2.49                     | 0.47              |
| 2:BS:157:VAL:CG2  | 3:CQ:50:THR:HG21  | 2.42                     | 0.47              |
| 2:BU:157:VAL:CG2  | 3:CU:50:THR:HG21  | 2.43                     | 0.47              |
| 1:A3:184:TYR:CE1  | 2:B4:139:ALA:HB2  | 2.50                     | 0.47              |
| 1:AG:207:CYS:O    | 1:AG:208:TYR:CB   | 2.57                     | 0.47              |
| 1:A0:184:TYR:CE1  | 2:B1:139:ALA:HB2  | 2.50                     | 0.47              |
| 1:DF:110:GLY:N    | 1:DI:242:ASN:HD22 | 2.10                     | 0.47              |
| 1:A9:87:GLN:HE21  | 1:A9:210:ARG:NH2  | 2.12                     | 0.47              |
| 3:CP:110:PHE:HE2  | 3:CP:116:THR:HG22 | 1.80                     | 0.47              |
| 1:AA:128:VAL:HG21 | 1:AD:89:LYS:HE3   | 1.96                     | 0.47              |
| 2:B8:140:LEU:N    | 2:B8:140:LEU:HD23 | 2.30                     | 0.47              |
| 3:CB:76:MET:HB2   | 3:CB:84:GLU:HG2   | 1.96                     | 0.47              |
| 1:A0:234:LYS:HD2  | 3:C1:75:GLN:HB3   | 1.96                     | 0.47              |
| 3:C2:76:MET:HB2   | 3:C2:84:GLU:HG2   | 1.96                     | 0.47              |
| 3:CN:61:TYR:HB3   | 3:CN:205:LEU:HD23 | 1.97                     | 0.47              |
| 1:DJ:115:THR:OG1  | 1:DJ:133:LEU:HB2  | 2.16                     | 0.46              |
| 1:DK:115:THR:OG1  | 1:DK:133:LEU:HB2  | 2.15                     | 0.46              |
| 1:AT:115:THR:OG1  | 1:AT:133:LEU:HB2  | 2.15                     | 0.46              |
| 1:A3:115:THR:OG1  | 1:A3:133:LEU:HB2  | 2.15                     | 0.46              |
| 1:A4:115:THR:OG1  | 1:A4:133:LEU:HB2  | 2.15                     | 0.46              |
| 1:DE:115:THR:OG1  | 1:DE:133:LEU:HB2  | 2.16                     | 0.46              |
| 2:BV:139:ALA:HB2  | 1:DI:184:TYR:CE1  | 282.98                   | 0.46              |
| 1:AP:174:TRP:CZ2  | 2:BS:139:ALA:HB3  | 2.49                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B8:137:GLU:O    | 2:B8:139:ALA:N    | 2.41                     | 0.46              |
| 1:A4:184:TYR:CE1  | 2:BX:139:ALA:HB2  | 284.16                   | 0.46              |
| 1:DE:87:GLN:HE21  | 1:DE:210:ARG:NH2  | 2.12                     | 0.46              |
| 2:BL:83:LEU:HA    | 2:BL:84:PRO:HA    | 1.60                     | 0.46              |
| 2:BM:83:LEU:HA    | 2:BM:84:PRO:HA    | 1.60                     | 0.46              |
| 1:AU:146:ILE:O    | 1:AU:147:ALA:CB   | 2.62                     | 0.46              |
| 3:C2:42:ASN:ND2   | 3:C2:44:ILE:H     | 2.12                     | 0.46              |
| 3:C4:42:ASN:ND2   | 3:C4:44:ILE:H     | 2.12                     | 0.46              |
| 3:CW:42:ASN:ND2   | 3:CW:44:ILE:H     | 2.12                     | 0.46              |
| 3:C5:110:PHE:HE2  | 3:C5:116:THR:HG22 | 1.80                     | 0.46              |
| 3:CM:110:PHE:HE2  | 3:CM:116:THR:HG22 | 1.80                     | 0.46              |
| 3:C0:110:PHE:HE2  | 3:C0:116:THR:HG22 | 1.80                     | 0.46              |
| 1:AC:89:LYS:HE3   | 1:AD:128:VAL:HG21 | 1.96                     | 0.46              |
| 1:AN:165:ARG:HG2  | 2:BN:180:PRO:O    | 79.62                    | 0.46              |
| 1:AR:165:ARG:HG2  | 2:BQ:180:PRO:O    | 2.14                     | 0.46              |
| 1:AI:234:LYS:HD2  | 3:CJ:75:GLN:HB3   | 119.18                   | 0.46              |
| 1:A7:234:LYS:HD2  | 3:C8:75:GLN:HB3   | 1.96                     | 0.46              |
| 3:CJ:61:TYR:HB3   | 3:CJ:205:LEU:HD23 | 1.98                     | 0.46              |
| 2:BR:140:LEU:HD23 | 2:BR:140:LEU:N    | 2.30                     | 0.46              |
| 2:BK:140:LEU:HD23 | 2:BK:140:LEU:N    | 2.30                     | 0.46              |
| 3:CL:61:TYR:HB3   | 3:CL:205:LEU:HD23 | 1.97                     | 0.46              |
| 3:CO:36:VAL:HA    | 3:CO:37:PRO:HD3   | 1.64                     | 0.46              |
| 1:DH:128:VAL:HG21 | 1:DJ:89:LYS:HE3   | 1.96                     | 0.46              |
| 1:AF:115:THR:OG1  | 1:AF:133:LEU:HB2  | 2.15                     | 0.46              |
| 1:AP:115:THR:OG1  | 1:AP:133:LEU:HB2  | 2.16                     | 0.46              |
| 1:AV:115:THR:OG1  | 1:AV:133:LEU:HB2  | 2.16                     | 0.46              |
| 1:A7:115:THR:OG1  | 1:A7:133:LEU:HB2  | 2.16                     | 0.46              |
| 1:AC:115:THR:OG1  | 1:AC:133:LEU:HB2  | 2.16                     | 0.46              |
| 1:AB:115:THR:OG1  | 1:AB:133:LEU:HB2  | 2.16                     | 0.46              |
| 1:AI:115:THR:OG1  | 1:AI:133:LEU:HB2  | 2.16                     | 0.46              |
| 1:AJ:184:TYR:CE1  | 2:BK:139:ALA:HB2  | 2.50                     | 0.46              |
| 1:AY:184:TYR:CE1  | 2:BZ:139:ALA:HB2  | 2.50                     | 0.46              |
| 1:AR:184:TYR:CE1  | 2:BQ:139:ALA:HB2  | 2.49                     | 0.46              |
| 2:BB:157:VAL:CG2  | 3:CC:50:THR:HG21  | 91.76                    | 0.46              |
| 2:BC:157:VAL:CG2  | 3:CC:50:THR:HG21  | 2.42                     | 0.46              |
| 2:BV:157:VAL:CG2  | 3:CW:50:THR:HG21  | 91.76                    | 0.46              |
| 1:AB:207:CYS:O    | 1:AB:208:TYR:CB   | 2.57                     | 0.46              |
| 1:A1:184:TYR:CE1  | 2:B2:139:ALA:HB2  | 2.50                     | 0.46              |
| 3:CD:110:PHE:HE2  | 3:CD:116:THR:HG22 | 1.80                     | 0.46              |
| 3:CH:110:PHE:HE2  | 3:CH:116:THR:HG22 | 1.80                     | 0.46              |
| 3:CN:110:PHE:HE2  | 3:CN:116:THR:HG22 | 1.80                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AJ:89:LYS:HE3   | 1:AM:128:VAL:HG21 | 39.95                    | 0.46              |
| 1:AS:234:LYS:HD2  | 3:CT:75:GLN:HB3   | 1.97                     | 0.46              |
| 3:C9:61:TYR:HB3   | 3:C9:205:LEU:HD23 | 1.98                     | 0.46              |
| 2:BS:140:LEU:HD23 | 2:BS:140:LEU:N    | 2.30                     | 0.46              |
| 2:BB:140:LEU:HD23 | 2:BB:140:LEU:N    | 2.30                     | 0.46              |
| 2:BU:140:LEU:HD23 | 2:BU:140:LEU:N    | 2.30                     | 0.46              |
| 3:DA:61:TYR:HB3   | 3:DA:205:LEU:HD23 | 1.97                     | 0.46              |
| 3:CC:61:TYR:HB3   | 3:CC:205:LEU:HD23 | 1.98                     | 0.46              |
| 3:DA:76:MET:HB2   | 3:DA:84:GLU:HG2   | 1.96                     | 0.46              |
| 1:A1:234:LYS:HD2  | 3:C2:75:GLN:HB3   | 1.96                     | 0.46              |
| 3:CE:61:TYR:HB3   | 3:CE:205:LEU:HD23 | 1.98                     | 0.46              |
| 1:AO:115:THR:OG1  | 1:AO:133:LEU:HB2  | 2.15                     | 0.46              |
| 1:AL:115:THR:OG1  | 1:AL:133:LEU:HB2  | 2.16                     | 0.46              |
| 1:A9:115:THR:OG1  | 1:A9:133:LEU:HB2  | 2.16                     | 0.46              |
| 1:AJ:115:THR:OG1  | 1:AJ:133:LEU:HB2  | 2.15                     | 0.46              |
| 1:AH:115:THR:OG1  | 1:AH:133:LEU:HB2  | 2.15                     | 0.46              |
| 1:AK:184:TYR:CE1  | 2:BK:139:ALA:HB2  | 65.16                    | 0.46              |
| 2:BH:157:VAL:HG23 | 3:CI:50:THR:CG2   | 58.34                    | 0.46              |
| 2:BL:157:VAL:CG2  | 3:CM:50:THR:HG21  | 91.76                    | 0.46              |
| 1:AR:87:GLN:HE21  | 1:AR:210:ARG:NH2  | 2.12                     | 0.46              |
| 1:AG:74:THR:HG21  | 3:CG:43:PHE:CE1   | 2.45                     | 0.46              |
| 1:AF:87:GLN:HE21  | 1:AF:210:ARG:NH2  | 2.12                     | 0.46              |
| 1:A4:242:ASN:HD22 | 1:A7:110:GLY:N    | 2.10                     | 0.46              |
| 1:DF:87:GLN:HE21  | 1:DF:210:ARG:NH2  | 2.12                     | 0.46              |
| 2:BB:83:LEU:HA    | 2:BB:84:PRO:HA    | 1.60                     | 0.46              |
| 2:BT:83:LEU:HA    | 2:BT:84:PRO:HA    | 1.60                     | 0.46              |
| 3:CI:110:PHE:HE2  | 3:CI:116:THR:HG22 | 1.80                     | 0.46              |
| 3:CU:110:PHE:HE2  | 3:CU:116:THR:HG22 | 1.80                     | 0.46              |
| 3:C8:110:PHE:HE2  | 3:C8:116:THR:HG22 | 1.80                     | 0.46              |
| 1:AE:234:LYS:HD2  | 3:CF:75:GLN:HB3   | 70.16                    | 0.46              |
| 1:A4:89:LYS:HE3   | 1:A7:128:VAL:HG21 | 1.96                     | 0.46              |
| 3:C7:61:TYR:HB3   | 3:C7:205:LEU:HD23 | 1.97                     | 0.46              |
| 2:BR:224:GLY:HA2  | 2:BR:225:PRO:HD2  | 1.81                     | 0.46              |
| 3:CS:61:TYR:HB3   | 3:CS:205:LEU:HD23 | 1.98                     | 0.46              |
| 2:B8:224:GLY:HA2  | 2:B8:225:PRO:HD2  | 1.81                     | 0.46              |
| 2:B1:140:LEU:N    | 2:B1:140:LEU:HD23 | 2.30                     | 0.46              |
| 2:BB:224:GLY:HA2  | 2:BB:225:PRO:HD2  | 1.81                     | 0.46              |
| 1:AA:115:THR:OG1  | 1:AA:133:LEU:HB2  | 2.15                     | 0.46              |
| 1:DH:115:THR:OG1  | 1:DH:133:LEU:HB2  | 2.16                     | 0.46              |
| 1:AX:115:THR:OG1  | 1:AX:133:LEU:HB2  | 2.16                     | 0.46              |
| 1:AQ:184:TYR:CE1  | 2:BP:139:ALA:HB2  | 2.50                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AP:184:TYR:CE1  | 2:BS:139:ALA:HB2  | 2.50                     | 0.46              |
| 1:AO:164:TRP:CE2  | 1:AO:187:LEU:HD13 | 2.51                     | 0.46              |
| 1:AC:242:ASN:HD22 | 1:AD:110:GLY:N    | 2.10                     | 0.46              |
| 1:AG:87:GLN:HE21  | 1:AG:210:ARG:NH2  | 2.12                     | 0.46              |
| 1:AU:74:THR:HG21  | 3:CV:43:PHE:CE2   | 2.45                     | 0.46              |
| 1:AT:74:THR:HG21  | 3:CU:43:PHE:CE2   | 2.45                     | 0.46              |
| 2:BC:83:LEU:HA    | 2:BC:84:PRO:HA    | 1.60                     | 0.46              |
| 2:BX:83:LEU:HA    | 2:BX:84:PRO:HA    | 1.60                     | 0.46              |
| 1:DH:35:ASP:OD1   | 1:DH:212:ARG:HD3  | 2.16                     | 0.46              |
| 1:A7:146:ILE:O    | 1:A7:147:ALA:CB   | 2.62                     | 0.46              |
| 3:CE:110:PHE:HE2  | 3:CE:116:THR:HG22 | 1.80                     | 0.46              |
| 1:AQ:104:VAL:HG22 | 1:AQ:197:LEU:CD2  | 2.44                     | 0.46              |
| 1:AP:234:LYS:HD2  | 3:CQ:75:GLN:HB3   | 1.96                     | 0.46              |
| 1:AD:234:LYS:HD2  | 3:CE:75:GLN:HB3   | 119.19                   | 0.46              |
| 1:AD:234:LYS:HD2  | 3:CD:75:GLN:HB3   | 1.96                     | 0.46              |
| 1:DI:164:TRP:CE2  | 1:DI:187:LEU:HD13 | 2.51                     | 0.46              |
| 3:CR:36:VAL:HA    | 3:CR:37:PRO:HD3   | 1.64                     | 0.46              |
| 1:DC:89:LYS:HE3   | 1:DD:128:VAL:HG21 | 1.96                     | 0.46              |
| 3:CG:61:TYR:HB3   | 3:CG:205:LEU:HD23 | 1.97                     | 0.46              |
| 2:BE:140:LEU:N    | 2:BE:140:LEU:HD23 | 2.30                     | 0.46              |
| 2:BW:140:LEU:N    | 2:BW:140:LEU:HD23 | 2.30                     | 0.46              |
| 1:A3:234:LYS:HD2  | 3:C4:75:GLN:HB3   | 1.96                     | 0.46              |
| 1:AU:115:THR:OG1  | 1:AU:133:LEU:HB2  | 2.15                     | 0.46              |
| 2:BS:139:ALA:HB2  | 1:DF:184:TYR:CE1  | 263.54                   | 0.46              |
| 1:A4:191:HIS:CD2  | 1:A4:193:GLY:H    | 2.21                     | 0.46              |
| 1:A5:184:TYR:CE1  | 2:B5:139:ALA:HB2  | 2.49                     | 0.46              |
| 1:AU:207:CYS:O    | 1:AU:208:TYR:CB   | 2.57                     | 0.46              |
| 1:AC:110:GLY:N    | 1:A9:242:ASN:HD22 | 274.68                   | 0.46              |
| 2:BO:83:LEU:HA    | 2:BO:84:PRO:HA    | 1.60                     | 0.46              |
| 1:AC:35:ASP:OD1   | 1:AC:212:ARG:HD3  | 2.16                     | 0.46              |
| 1:A1:35:ASP:OD1   | 1:A1:212:ARG:HD3  | 2.16                     | 0.46              |
| 1:AK:35:ASP:OD1   | 1:AK:212:ARG:HD3  | 2.16                     | 0.46              |
| 1:AO:35:ASP:OD1   | 1:AO:212:ARG:HD3  | 2.16                     | 0.46              |
| 3:DB:42:ASN:ND2   | 3:DB:44:ILE:H     | 2.12                     | 0.46              |
| 3:C3:42:ASN:ND2   | 3:C3:44:ILE:H     | 2.11                     | 0.46              |
| 3:CO:110:PHE:HE2  | 3:CO:116:THR:HG22 | 1.80                     | 0.46              |
| 3:CA:110:PHE:HE2  | 3:CA:116:THR:HG22 | 1.80                     | 0.46              |
| 1:AI:234:LYS:HD2  | 3:CI:75:GLN:HB3   | 1.96                     | 0.46              |
| 3:CS:75:GLN:HB3   | 1:DE:234:LYS:HD2  | 304.13                   | 0.46              |
| 3:CU:75:GLN:HB3   | 1:DG:234:LYS:HD2  | 312.93                   | 0.46              |
| 1:DG:164:TRP:CE2  | 1:DG:187:LEU:HD13 | 2.51                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:CF:61:TYR:HB3  | 3:CF:205:LEU:HD23 | 1.98                     | 0.46              |
| 1:AZ:225:PRO:HA  | 1:AZ:226:PRO:HD3  | 1.78                     | 0.46              |
| 3:CP:61:TYR:HB3  | 3:CP:205:LEU:HD23 | 1.98                     | 0.46              |
| 3:CH:61:TYR:HB3  | 3:CH:205:LEU:HD23 | 1.98                     | 0.46              |
| 3:CZ:61:TYR:HB3  | 3:CZ:205:LEU:HD23 | 1.98                     | 0.46              |
| 1:AR:164:TRP:CE2 | 1:AR:187:LEU:HD13 | 2.51                     | 0.46              |
| 1:AK:115:THR:OG1 | 1:AK:133:LEU:HB2  | 2.16                     | 0.46              |
| 1:AY:115:THR:OG1 | 1:AY:133:LEU:HB2  | 2.15                     | 0.46              |
| 1:A5:115:THR:OG1 | 1:A5:133:LEU:HB2  | 2.16                     | 0.46              |
| 1:AM:115:THR:OG1 | 1:AM:133:LEU:HB2  | 2.16                     | 0.46              |
| 1:A8:115:THR:OG1 | 1:A8:133:LEU:HB2  | 2.15                     | 0.46              |
| 1:AQ:115:THR:OG1 | 1:AQ:133:LEU:HB2  | 2.16                     | 0.46              |
| 1:AZ:115:THR:OG1 | 1:AZ:133:LEU:HB2  | 2.15                     | 0.46              |
| 1:DD:115:THR:OG1 | 1:DD:133:LEU:HB2  | 2.16                     | 0.46              |
| 1:AN:184:TYR:CE1 | 2:BN:139:ALA:HB2  | 105.31                   | 0.46              |
| 2:BE:157:VAL:CG2 | 3:CE:50:THR:HG21  | 2.42                     | 0.46              |
| 2:BJ:157:VAL:CG2 | 3:CK:50:THR:HG21  | 221.71                   | 0.46              |
| 2:BA:157:VAL:CG2 | 3:DB:50:THR:HG21  | 271.63                   | 0.46              |
| 1:AX:191:HIS:HD2 | 1:AX:193:GLY:N    | 2.08                     | 0.46              |
| 1:AK:164:TRP:CE2 | 1:AK:187:LEU:HD13 | 2.51                     | 0.46              |
| 1:AN:164:TRP:CE2 | 1:AN:187:LEU:HD13 | 2.51                     | 0.46              |
| 1:AZ:164:TRP:CE2 | 1:AZ:187:LEU:HD13 | 2.51                     | 0.46              |
| 1:AI:74:THR:HG21 | 3:CJ:43:PHE:CE2   | 72.82                    | 0.46              |
| 1:A0:87:GLN:HE21 | 1:A0:210:ARG:NH2  | 2.12                     | 0.46              |
| 2:BD:83:LEU:HA   | 2:BD:84:PRO:HA    | 1.60                     | 0.46              |
| 1:DE:35:ASP:OD1  | 1:DE:212:ARG:HD3  | 2.16                     | 0.46              |
| 1:DJ:35:ASP:OD1  | 1:DJ:212:ARG:HD3  | 2.16                     | 0.46              |
| 1:AP:35:ASP:OD1  | 1:AP:212:ARG:HD3  | 2.16                     | 0.46              |
| 1:AM:35:ASP:OD1  | 1:AM:212:ARG:HD3  | 2.16                     | 0.46              |
| 1:AH:35:ASP:OD1  | 1:AH:212:ARG:HD3  | 2.16                     | 0.46              |
| 1:AU:35:ASP:OD1  | 1:AU:212:ARG:HD3  | 2.16                     | 0.46              |
| 1:AX:35:ASP:OD1  | 1:AX:212:ARG:HD3  | 2.16                     | 0.46              |
| 1:AC:146:ILE:O   | 1:AC:147:ALA:CB   | 2.62                     | 0.46              |
| 1:A2:163:MET:HE3 | 1:A2:189:GLY:HA3  | 1.98                     | 0.46              |
| 3:CK:110:PHE:HE2 | 3:CK:116:THR:HG22 | 1.80                     | 0.46              |
| 3:C7:110:PHE:HE2 | 3:C7:116:THR:HG22 | 1.80                     | 0.46              |
| 1:AB:234:LYS:HD2 | 3:CB:75:GLN:HB3   | 1.96                     | 0.46              |
| 3:CS:36:VAL:HA   | 3:CS:37:PRO:HD3   | 1.64                     | 0.46              |
| 3:C6:61:TYR:HB3  | 3:C6:205:LEU:HD23 | 1.98                     | 0.46              |
| 1:A5:164:TRP:CE2 | 1:A5:187:LEU:HD13 | 2.51                     | 0.46              |
| 1:AG:164:TRP:CE2 | 1:AG:187:LEU:HD13 | 2.51                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AI:164:TRP:CE2  | 1:AI:187:LEU:HD13 | 2.51                     | 0.46              |
| 3:CP:36:VAL:HA    | 3:CP:37:PRO:HD3   | 1.64                     | 0.46              |
| 2:BW:139:ALA:HB2  | 1:DJ:184:TYR:CE1  | 281.38                   | 0.46              |
| 2:BD:157:VAL:CG2  | 3:CD:50:THR:HG21  | 2.42                     | 0.46              |
| 1:DG:181:LYS:O    | 1:DG:182:ALA:CB   | 2.62                     | 0.46              |
| 1:AD:191:HIS:HD2  | 1:AD:193:GLY:N    | 2.08                     | 0.46              |
| 2:BA:157:VAL:HG23 | 3:CA:50:THR:CG2   | 2.40                     | 0.46              |
| 1:AC:164:TRP:CE2  | 1:AC:187:LEU:HD13 | 2.51                     | 0.46              |
| 1:AL:164:TRP:CE2  | 1:AL:187:LEU:HD13 | 2.51                     | 0.46              |
| 1:AP:164:TRP:CE2  | 1:AP:187:LEU:HD13 | 2.51                     | 0.46              |
| 1:AV:164:TRP:CE2  | 1:AV:187:LEU:HD13 | 2.51                     | 0.46              |
| 1:AB:164:TRP:CE2  | 1:AB:187:LEU:HD13 | 2.51                     | 0.46              |
| 1:AN:110:GLY:N    | 1:DD:242:ASN:HD22 | 295.48                   | 0.46              |
| 1:AD:74:THR:HG21  | 3:CD:43:PHE:CE1   | 2.45                     | 0.46              |
| 1:DJ:87:GLN:HE21  | 1:DJ:210:ARG:NH2  | 2.12                     | 0.46              |
| 1:AM:74:THR:HG21  | 3:CN:43:PHE:CE1   | 2.45                     | 0.46              |
| 2:B7:83:LEU:HA    | 2:B7:84:PRO:HA    | 1.60                     | 0.46              |
| 1:DC:35:ASP:OD1   | 1:DC:212:ARG:HD3  | 2.16                     | 0.46              |
| 1:AD:35:ASP:OD1   | 1:AD:212:ARG:HD3  | 2.16                     | 0.46              |
| 1:AN:35:ASP:OD1   | 1:AN:212:ARG:HD3  | 2.16                     | 0.46              |
| 1:AB:35:ASP:OD1   | 1:AB:212:ARG:HD3  | 2.16                     | 0.46              |
| 1:DK:35:ASP:OD1   | 1:DK:212:ARG:HD3  | 2.16                     | 0.46              |
| 1:A4:146:ILE:O    | 1:A4:147:ALA:CB   | 2.62                     | 0.46              |
| 3:CJ:110:PHE:HE2  | 3:CJ:116:THR:HG22 | 1.80                     | 0.46              |
| 3:CT:110:PHE:HE2  | 3:CT:116:THR:HG22 | 1.80                     | 0.46              |
| 1:A3:104:VAL:HG22 | 1:A3:197:LEU:CD2  | 2.44                     | 0.46              |
| 1:AH:89:LYS:HE3   | 1:AI:128:VAL:HG21 | 1.96                     | 0.46              |
| 1:AK:128:VAL:HG23 | 1:AM:91:THR:HG22  | 27.99                    | 0.46              |
| 1:A5:128:VAL:HG23 | 1:A7:91:THR:HG22  | 1.98                     | 0.46              |
| 1:AM:165:ARG:HG2  | 2:BM:180:PRO:O    | 48.68                    | 0.46              |
| 1:AA:234:LYS:HD2  | 3:CA:75:GLN:HB3   | 1.96                     | 0.46              |
| 1:A2:164:TRP:CE2  | 1:A2:187:LEU:HD13 | 2.51                     | 0.46              |
| 3:CQ:61:TYR:HB3   | 3:CQ:205:LEU:HD23 | 1.98                     | 0.46              |
| 2:B3:140:LEU:N    | 2:B3:140:LEU:HD23 | 2.30                     | 0.46              |
| 1:AQ:164:TRP:CE2  | 1:AQ:187:LEU:HD13 | 2.51                     | 0.46              |
| 3:CV:36:VAL:HA    | 3:CV:37:PRO:HD3   | 1.64                     | 0.46              |
| 1:AS:164:TRP:CE2  | 1:AS:187:LEU:HD13 | 2.51                     | 0.46              |
| 3:C3:61:TYR:HB3   | 3:C3:205:LEU:HD23 | 1.98                     | 0.46              |
| 1:A2:115:THR:OG1  | 1:A2:133:LEU:HB2  | 2.16                     | 0.46              |
| 1:AE:115:THR:OG1  | 1:AE:133:LEU:HB2  | 2.16                     | 0.46              |
| 1:AD:174:TRP:CE2  | 1:AD:179:LYS:HB3  | 2.51                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:AJ:174:TRP:CE2 | 1:AJ:179:LYS:HB3  | 2.51                     | 0.46              |
| 1:AO:174:TRP:CE2 | 1:AO:179:LYS:HB3  | 2.51                     | 0.46              |
| 1:AK:184:TYR:CE1 | 2:BL:139:ALA:HB2  | 2.50                     | 0.46              |
| 1:DF:174:TRP:CE2 | 1:DF:179:LYS:HB3  | 2.51                     | 0.46              |
| 1:AH:174:TRP:CE2 | 1:AH:179:LYS:HB3  | 2.51                     | 0.46              |
| 1:AR:174:TRP:CE2 | 1:AR:179:LYS:HB3  | 2.51                     | 0.46              |
| 1:AB:174:TRP:CE2 | 1:AB:179:LYS:HB3  | 2.51                     | 0.46              |
| 1:AG:174:TRP:CE2 | 1:AG:179:LYS:HB3  | 2.51                     | 0.46              |
| 1:A6:191:HIS:HD2 | 1:A6:193:GLY:N    | 2.08                     | 0.46              |
| 1:AI:87:GLN:HE21 | 1:AI:210:ARG:NH2  | 2.12                     | 0.46              |
| 1:A7:74:THR:HG21 | 3:C8:43:PHE:CE2   | 2.45                     | 0.46              |
| 1:AQ:87:GLN:HE21 | 1:AQ:210:ARG:NH2  | 2.12                     | 0.46              |
| 3:CR:43:PHE:CE2  | 1:DD:74:THR:HG21  | 244.29                   | 0.46              |
| 1:AS:74:THR:HG21 | 3:CT:43:PHE:CE2   | 2.45                     | 0.46              |
| 2:B9:83:LEU:HA   | 2:B9:84:PRO:HA    | 1.60                     | 0.46              |
| 1:AQ:35:ASP:OD1  | 1:AQ:212:ARG:HD3  | 2.16                     | 0.46              |
| 1:A7:35:ASP:OD1  | 1:A7:212:ARG:HD3  | 2.16                     | 0.46              |
| 1:AG:35:ASP:OD1  | 1:AG:212:ARG:HD3  | 2.16                     | 0.46              |
| 1:AV:35:ASP:OD1  | 1:AV:212:ARG:HD3  | 2.16                     | 0.46              |
| 1:AJ:35:ASP:OD1  | 1:AJ:212:ARG:HD3  | 2.16                     | 0.46              |
| 1:A4:35:ASP:OD1  | 1:A4:212:ARG:HD3  | 2.16                     | 0.46              |
| 3:CS:110:PHE:HE2 | 3:CS:116:THR:HG22 | 1.80                     | 0.46              |
| 3:CD:36:VAL:HA   | 3:CD:37:PRO:HD3   | 1.64                     | 0.46              |
| 1:AW:234:LYS:HD2 | 3:CX:75:GLN:HB3   | 1.96                     | 0.46              |
| 3:CW:61:TYR:HB3  | 3:CW:205:LEU:HD23 | 1.98                     | 0.46              |
| 1:A4:234:LYS:HD2 | 3:C5:75:GLN:HB3   | 1.96                     | 0.46              |
| 1:A3:164:TRP:CE2 | 1:A3:187:LEU:HD13 | 2.51                     | 0.46              |
| 1:AE:164:TRP:CE2 | 1:AE:187:LEU:HD13 | 2.51                     | 0.46              |
| 1:AF:164:TRP:CE2 | 1:AF:187:LEU:HD13 | 2.51                     | 0.46              |
| 3:CU:61:TYR:HB3  | 3:CU:205:LEU:HD23 | 1.98                     | 0.46              |
| 1:AF:225:PRO:HA  | 1:AF:226:PRO:HD3  | 1.78                     | 0.46              |
| 1:AO:225:PRO:HA  | 1:AO:226:PRO:HD3  | 1.78                     | 0.46              |
| 1:AS:115:THR:OG1 | 1:AS:133:LEU:HB2  | 2.16                     | 0.46              |
| 1:DC:115:THR:OG1 | 1:DC:133:LEU:HB2  | 2.16                     | 0.46              |
| 1:AQ:174:TRP:CE2 | 1:AQ:179:LYS:HB3  | 2.51                     | 0.46              |
| 1:A6:174:TRP:CE2 | 1:A6:179:LYS:HB3  | 2.51                     | 0.46              |
| 1:AI:174:TRP:CE2 | 1:AI:179:LYS:HB3  | 2.51                     | 0.46              |
| 1:AW:174:TRP:CE2 | 1:AW:179:LYS:HB3  | 2.51                     | 0.46              |
| 1:A2:174:TRP:CE2 | 1:A2:179:LYS:HB3  | 2.51                     | 0.46              |
| 1:AK:191:HIS:HD2 | 1:AK:193:GLY:N    | 2.08                     | 0.46              |
| 2:BK:157:VAL:CG2 | 3:CL:50:THR:HG21  | 57.94                    | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BR:157:VAL:CG2  | 3:CO:50:THR:HG21  | 2.42                     | 0.46              |
| 1:AA:207:CYS:O    | 1:AA:208:TYR:CB   | 2.57                     | 0.46              |
| 1:A0:174:TRP:CE2  | 1:A0:179:LYS:HB3  | 2.51                     | 0.46              |
| 1:AV:191:HIS:HD2  | 1:AV:193:GLY:N    | 2.08                     | 0.46              |
| 1:AA:164:TRP:CE2  | 1:AA:187:LEU:HD13 | 2.51                     | 0.46              |
| 1:AB:191:HIS:HD2  | 1:AB:193:GLY:N    | 2.08                     | 0.46              |
| 1:AT:191:HIS:HD2  | 1:AT:193:GLY:N    | 2.08                     | 0.46              |
| 1:DD:164:TRP:CE2  | 1:DD:187:LEU:HD13 | 2.51                     | 0.46              |
| 1:A7:87:GLN:HE21  | 1:A7:210:ARG:NH2  | 2.12                     | 0.46              |
| 1:A0:74:THR:HG21  | 3:CP:43:PHE:CE2   | 4.65                     | 0.46              |
| 1:A0:74:THR:HG21  | 3:C1:43:PHE:CE2   | 2.45                     | 0.46              |
| 1:AY:35:ASP:OD1   | 1:AY:212:ARG:HD3  | 2.16                     | 0.46              |
| 1:AL:35:ASP:OD1   | 1:AL:212:ARG:HD3  | 2.16                     | 0.46              |
| 1:A3:163:MET:HE1  | 1:A3:189:GLY:HA3  | 1.96                     | 0.46              |
| 3:CZ:110:PHE:HE2  | 3:CZ:116:THR:HG22 | 1.80                     | 0.46              |
| 1:AH:234:LYS:HD2  | 3:CH:75:GLN:HB3   | 1.96                     | 0.46              |
| 1:A9:164:TRP:CE2  | 1:A9:187:LEU:HD13 | 2.51                     | 0.46              |
| 3:C4:61:TYR:HB3   | 3:C4:205:LEU:HD23 | 1.98                     | 0.46              |
| 1:A1:164:TRP:CE2  | 1:A1:187:LEU:HD13 | 2.51                     | 0.46              |
| 1:DH:164:TRP:CE2  | 1:DH:187:LEU:HD13 | 2.51                     | 0.46              |
| 3:CK:36:VAL:HA    | 3:CK:37:PRO:HD3   | 1.64                     | 0.46              |
| 3:CS:150:LEU:HD12 | 3:CS:150:LEU:HA   | 1.79                     | 0.46              |
| 3:C9:150:LEU:HD12 | 3:C9:150:LEU:HA   | 1.79                     | 0.46              |
| 3:CL:150:LEU:HD12 | 3:CL:150:LEU:HA   | 1.79                     | 0.46              |
| 3:CW:36:VAL:HA    | 3:CW:37:PRO:HD3   | 1.64                     | 0.46              |
| 3:C1:61:TYR:HB3   | 3:C1:205:LEU:HD23 | 1.98                     | 0.46              |
| 2:B9:86:ASP:HB3   | 2:B9:141:LYS:HA   | 1.96                     | 0.46              |
| 3:CM:61:TYR:HB3   | 3:CM:205:LEU:HD23 | 1.98                     | 0.46              |
| 2:B2:224:GLY:HA2  | 2:B2:225:PRO:HD2  | 1.81                     | 0.46              |
| 1:AW:115:THR:OG1  | 1:AW:133:LEU:HB2  | 2.16                     | 0.46              |
| 1:AG:115:THR:OG1  | 1:AG:133:LEU:HB2  | 2.15                     | 0.46              |
| 1:A1:115:THR:OG1  | 1:A1:133:LEU:HB2  | 2.16                     | 0.46              |
| 1:AU:174:TRP:CE2  | 1:AU:179:LYS:HB3  | 2.51                     | 0.46              |
| 1:A8:174:TRP:CE2  | 1:A8:179:LYS:HB3  | 2.51                     | 0.46              |
| 1:AA:191:HIS:HD2  | 1:AA:193:GLY:N    | 2.08                     | 0.46              |
| 1:AO:191:HIS:HD2  | 1:AO:193:GLY:N    | 2.08                     | 0.46              |
| 2:B6:157:VAL:CG2  | 3:C7:50:THR:HG21  | 2.42                     | 0.46              |
| 1:AL:110:GLY:N    | 1:AN:242:ASN:HD22 | 2.10                     | 0.46              |
| 2:BJ:85:SER:HB2   | 2:BJ:190:ASN:ND2  | 2.31                     | 0.46              |
| 2:BP:85:SER:HB2   | 2:BP:190:ASN:ND2  | 2.31                     | 0.46              |
| 2:BN:85:SER:HB2   | 2:BN:190:ASN:ND2  | 2.31                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B8:85:SER:HB2   | 2:B8:190:ASN:ND2  | 2.31                     | 0.46              |
| 1:AE:35:ASP:OD1   | 1:AE:212:ARG:HD3  | 2.16                     | 0.46              |
| 1:DD:35:ASP:OD1   | 1:DD:212:ARG:HD3  | 2.16                     | 0.46              |
| 1:AA:35:ASP:OD1   | 1:AA:212:ARG:HD3  | 2.16                     | 0.46              |
| 1:DG:35:ASP:OD1   | 1:DG:212:ARG:HD3  | 2.16                     | 0.46              |
| 3:CW:110:PHE:HE2  | 3:CW:116:THR:HG22 | 1.80                     | 0.46              |
| 3:DB:110:PHE:HE2  | 3:DB:116:THR:HG22 | 1.80                     | 0.46              |
| 1:AC:128:VAL:HG23 | 1:A9:91:THR:HG22  | 290.40                   | 0.46              |
| 1:AJ:91:THR:HG22  | 1:AM:128:VAL:HG23 | 42.09                    | 0.46              |
| 1:AY:91:THR:HG22  | 1:AZ:128:VAL:HG23 | 1.98                     | 0.46              |
| 1:AU:91:THR:HG22  | 1:AX:128:VAL:HG23 | 1.98                     | 0.46              |
| 1:DE:164:TRP:CE2  | 1:DE:187:LEU:HD13 | 2.51                     | 0.46              |
| 1:AR:115:THR:OG1  | 1:AR:133:LEU:HB2  | 2.16                     | 0.45              |
| 1:DC:174:TRP:CE2  | 1:DC:179:LYS:HB3  | 2.51                     | 0.45              |
| 1:AF:174:TRP:CE2  | 1:AF:179:LYS:HB3  | 2.51                     | 0.45              |
| 1:AM:174:TRP:CE2  | 1:AM:179:LYS:HB3  | 2.51                     | 0.45              |
| 1:AX:174:TRP:CE2  | 1:AX:179:LYS:HB3  | 2.51                     | 0.45              |
| 2:BQ:157:VAL:CG2  | 3:CS:50:THR:HG21  | 2.42                     | 0.45              |
| 2:B8:157:VAL:CG2  | 3:C9:50:THR:HG21  | 2.43                     | 0.45              |
| 1:A7:174:TRP:CE2  | 1:A7:179:LYS:HB3  | 2.51                     | 0.45              |
| 1:AJ:164:TRP:CE2  | 1:AJ:187:LEU:HD13 | 2.51                     | 0.45              |
| 1:AI:242:ASN:HD22 | 1:AJ:110:GLY:N    | 171.39                   | 0.45              |
| 1:AH:74:THR:HG21  | 3:CH:43:PHE:CE1   | 2.45                     | 0.45              |
| 1:AH:74:THR:HG21  | 3:CI:43:PHE:CE2   | 46.55                    | 0.45              |
| 2:B7:85:SER:HB2   | 2:B7:190:ASN:ND2  | 2.31                     | 0.45              |
| 2:BI:85:SER:HB2   | 2:BI:190:ASN:ND2  | 2.31                     | 0.45              |
| 2:BV:85:SER:HB2   | 2:BV:190:ASN:ND2  | 2.31                     | 0.45              |
| 1:AZ:35:ASP:OD1   | 1:AZ:212:ARG:HD3  | 2.16                     | 0.45              |
| 1:A6:35:ASP:OD1   | 1:A6:212:ARG:HD3  | 2.16                     | 0.45              |
| 3:CF:110:PHE:HE2  | 3:CF:116:THR:HG22 | 1.80                     | 0.45              |
| 3:CR:110:PHE:HE2  | 3:CR:116:THR:HG22 | 1.80                     | 0.45              |
| 1:AH:91:THR:HG22  | 1:AI:128:VAL:HG23 | 1.98                     | 0.45              |
| 1:AL:91:THR:HG22  | 1:AM:128:VAL:HG23 | 1.98                     | 0.45              |
| 1:AY:128:VAL:HG23 | 1:A1:91:THR:HG22  | 1.98                     | 0.45              |
| 1:DF:91:THR:HG22  | 1:DG:128:VAL:HG23 | 1.98                     | 0.45              |
| 1:A3:91:THR:HG22  | 1:A4:128:VAL:HG23 | 1.98                     | 0.45              |
| 1:DG:91:THR:HG22  | 1:DJ:128:VAL:HG23 | 1.98                     | 0.45              |
| 1:AT:91:THR:HG22  | 1:AU:128:VAL:HG23 | 1.98                     | 0.45              |
| 3:CH:36:VAL:HA    | 3:CH:37:PRO:HD3   | 1.64                     | 0.45              |
| 1:DH:128:VAL:HG23 | 1:DJ:91:THR:HG22  | 1.98                     | 0.45              |
| 3:CQ:36:VAL:HA    | 3:CQ:37:PRO:HD3   | 1.64                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AT:164:TRP:CE2  | 1:AT:187:LEU:HD13 | 2.51                     | 0.45              |
| 3:CX:61:TYR:HB3   | 3:CX:205:LEU:HD23 | 1.98                     | 0.45              |
| 2:BO:224:GLY:HA2  | 2:BO:225:PRO:HD2  | 1.81                     | 0.45              |
| 3:CB:61:TYR:HB3   | 3:CB:205:LEU:HD23 | 1.97                     | 0.45              |
| 3:CK:61:TYR:HB3   | 3:CK:205:LEU:HD23 | 1.98                     | 0.45              |
| 3:CQ:9:PRO:C      | 3:CQ:11:SER:H     | 2.20                     | 0.45              |
| 1:AM:164:TRP:CE2  | 1:AM:187:LEU:HD13 | 2.51                     | 0.45              |
| 3:CD:61:TYR:HB3   | 3:CD:205:LEU:HD23 | 1.98                     | 0.45              |
| 3:CX:9:PRO:C      | 3:CX:11:SER:H     | 2.20                     | 0.45              |
| 1:DF:115:THR:OG1  | 1:DF:133:LEU:HB2  | 2.15                     | 0.45              |
| 1:DI:174:TRP:CE2  | 1:DI:179:LYS:HB3  | 2.51                     | 0.45              |
| 1:AE:174:TRP:CE2  | 1:AE:179:LYS:HB3  | 2.51                     | 0.45              |
| 1:AN:174:TRP:CE2  | 1:AN:179:LYS:HB3  | 2.51                     | 0.45              |
| 1:AP:174:TRP:CE2  | 1:AP:179:LYS:HB3  | 2.51                     | 0.45              |
| 1:A4:174:TRP:CE2  | 1:A4:179:LYS:HB3  | 2.51                     | 0.45              |
| 1:DD:174:TRP:CE2  | 1:DD:179:LYS:HB3  | 2.51                     | 0.45              |
| 1:AL:207:CYS:O    | 1:AL:208:TYR:CB   | 2.57                     | 0.45              |
| 1:A0:110:GLY:N    | 1:A2:242:ASN:HD22 | 2.10                     | 0.45              |
| 1:AE:242:ASN:HD22 | 1:AH:110:GLY:N    | 171.39                   | 0.45              |
| 1:AJ:74:THR:HG21  | 3:CK:43:PHE:CE2   | 4.65                     | 0.45              |
| 3:CQ:43:PHE:CE2   | 1:DC:74:THR:HG21  | 218.99                   | 0.45              |
| 2:BW:85:SER:HB2   | 2:BW:190:ASN:ND2  | 2.31                     | 0.45              |
| 1:A2:35:ASP:OD1   | 1:A2:212:ARG:HD3  | 2.16                     | 0.45              |
| 3:CQ:110:PHE:HE2  | 3:CQ:116:THR:HG22 | 1.80                     | 0.45              |
| 3:C4:110:PHE:HE2  | 3:C4:116:THR:HG22 | 1.80                     | 0.45              |
| 1:A0:91:THR:HG22  | 1:A1:128:VAL:HG23 | 1.98                     | 0.45              |
| 1:AC:234:LYS:HD2  | 3:CD:75:GLN:HB3   | 74.02                    | 0.45              |
| 1:AY:225:PRO:HA   | 1:AY:226:PRO:HD3  | 1.78                     | 0.45              |
| 3:CL:9:PRO:C      | 3:CL:11:SER:H     | 2.20                     | 0.45              |
| 3:C8:61:TYR:HB3   | 3:C8:205:LEU:HD23 | 1.98                     | 0.45              |
| 1:AE:209:LEU:HD22 | 1:AE:209:LEU:HA   | 1.74                     | 0.45              |
| 1:AO:209:LEU:HA   | 1:AO:209:LEU:HD22 | 1.74                     | 0.45              |
| 3:CE:150:LEU:HA   | 3:CE:150:LEU:HD12 | 1.79                     | 0.45              |
| 1:AH:164:TRP:CE2  | 1:AH:187:LEU:HD13 | 2.51                     | 0.45              |
| 1:A7:164:TRP:CE2  | 1:A7:187:LEU:HD13 | 2.51                     | 0.45              |
| 1:DI:115:THR:OG1  | 1:DI:133:LEU:HB2  | 2.16                     | 0.45              |
| 1:A0:115:THR:OG1  | 1:A0:133:LEU:HB2  | 2.16                     | 0.45              |
| 1:DC:164:TRP:CE2  | 1:DC:187:LEU:HD13 | 2.51                     | 0.45              |
| 1:AX:164:TRP:CE2  | 1:AX:187:LEU:HD13 | 2.51                     | 0.45              |
| 1:AU:242:ASN:HD22 | 1:AX:110:GLY:N    | 2.10                     | 0.45              |
| 2:BA:85:SER:HB2   | 2:BA:190:ASN:ND2  | 2.31                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BM:85:SER:HB2   | 2:BM:190:ASN:ND2  | 2.31                     | 0.45              |
| 2:BU:85:SER:HB2   | 2:BU:190:ASN:ND2  | 2.31                     | 0.45              |
| 2:BG:83:LEU:HA    | 2:BG:84:PRO:HA    | 1.60                     | 0.45              |
| 1:AI:35:ASP:OD1   | 1:AI:212:ARG:HD3  | 2.16                     | 0.45              |
| 1:A5:35:ASP:OD1   | 1:A5:212:ARG:HD3  | 2.16                     | 0.45              |
| 1:AW:35:ASP:OD1   | 1:AW:212:ARG:HD3  | 2.16                     | 0.45              |
| 1:AK:91:THR:HG22  | 1:AL:128:VAL:HG23 | 27.99                    | 0.45              |
| 1:AO:128:VAL:HG23 | 1:AR:91:THR:HG22  | 1.98                     | 0.45              |
| 1:AP:91:THR:HG22  | 1:AS:128:VAL:HG23 | 1.98                     | 0.45              |
| 2:BF:53:ARG:HG2   | 2:BF:221:MET:HE3  | 2.03                     | 0.45              |
| 3:CR:9:PRO:C      | 3:CR:11:SER:H     | 2.20                     | 0.45              |
| 3:CA:9:PRO:C      | 3:CA:11:SER:H     | 2.20                     | 0.45              |
| 1:DK:164:TRP:CE2  | 1:DK:187:LEU:HD13 | 2.51                     | 0.45              |
| 3:CY:150:LEU:HA   | 3:CY:150:LEU:HD12 | 1.79                     | 0.45              |
| 3:DB:61:TYR:HB3   | 3:DB:205:LEU:HD23 | 1.97                     | 0.45              |
| 2:BE:118:PHE:HE2  | 2:BF:118:PHE:CD1  | 1.98                     | 0.45              |
| 3:CO:9:PRO:C      | 3:CO:11:SER:H     | 2.20                     | 0.45              |
| 1:A0:164:TRP:CE2  | 1:A0:187:LEU:HD13 | 2.51                     | 0.45              |
| 1:A6:115:THR:OG1  | 1:A6:133:LEU:HB2  | 2.15                     | 0.45              |
| 1:AL:174:TRP:CE2  | 1:AL:179:LYS:HB3  | 2.51                     | 0.45              |
| 1:DE:174:TRP:CE2  | 1:DE:179:LYS:HB3  | 2.51                     | 0.45              |
| 1:DK:181:LYS:O    | 1:DK:182:ALA:CB   | 2.62                     | 0.45              |
| 1:DH:174:TRP:CE2  | 1:DH:179:LYS:HB3  | 2.51                     | 0.45              |
| 1:AS:174:TRP:CE2  | 1:AS:179:LYS:HB3  | 2.51                     | 0.45              |
| 1:DG:174:TRP:CE2  | 1:DG:179:LYS:HB3  | 2.51                     | 0.45              |
| 1:AI:110:GLY:N    | 1:AL:242:ASN:HD22 | 145.71                   | 0.45              |
| 1:AR:74:THR:HG21  | 3:CS:43:PHE:CE2   | 2.45                     | 0.45              |
| 3:CT:43:PHE:CE2   | 1:DF:74:THR:HG21  | 259.67                   | 0.45              |
| 2:BU:83:LEU:HA    | 2:BU:84:PRO:HA    | 1.60                     | 0.45              |
| 2:BV:83:LEU:HA    | 2:BV:84:PRO:HA    | 1.60                     | 0.45              |
| 1:AS:35:ASP:OD1   | 1:AS:212:ARG:HD3  | 2.16                     | 0.45              |
| 1:A9:35:ASP:OD1   | 1:A9:212:ARG:HD3  | 2.16                     | 0.45              |
| 1:DI:35:ASP:OD1   | 1:DI:212:ARG:HD3  | 2.16                     | 0.45              |
| 1:A8:35:ASP:OD1   | 1:A8:212:ARG:HD3  | 2.16                     | 0.45              |
| 1:AL:128:VAL:HG23 | 1:AN:91:THR:HG22  | 1.98                     | 0.45              |
| 1:AA:91:THR:HG22  | 1:AB:128:VAL:HG23 | 1.98                     | 0.45              |
| 1:DC:128:VAL:HG23 | 1:DE:91:THR:HG22  | 1.98                     | 0.45              |
| 3:CC:36:VAL:HA    | 3:CC:37:PRO:HD3   | 1.64                     | 0.45              |
| 3:CY:61:TYR:HB3   | 3:CY:205:LEU:HD23 | 1.98                     | 0.45              |
| 3:CT:61:TYR:HB3   | 3:CT:205:LEU:HD23 | 1.98                     | 0.45              |
| 3:C0:61:TYR:HB3   | 3:C0:205:LEU:HD23 | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C0:9:PRO:C      | 3:C0:11:SER:H     | 2.20                     | 0.45              |
| 3:CU:9:PRO:C      | 3:CU:11:SER:H     | 2.20                     | 0.45              |
| 3:CQ:150:LEU:HA   | 3:CQ:150:LEU:HD12 | 1.79                     | 0.45              |
| 1:AC:209:LEU:HA   | 1:AC:209:LEU:HD22 | 1.74                     | 0.45              |
| 3:DB:9:PRO:C      | 3:DB:11:SER:H     | 2.20                     | 0.45              |
| 2:BN:53:ARG:HG2   | 2:BN:221:MET:HE2  | 1.99                     | 0.45              |
| 3:CV:9:PRO:C      | 3:CV:11:SER:H     | 2.20                     | 0.45              |
| 3:CF:9:PRO:C      | 3:CF:11:SER:H     | 2.20                     | 0.45              |
| 1:DJ:174:TRP:CE2  | 1:DJ:179:LYS:HB3  | 2.51                     | 0.45              |
| 2:BZ:157:VAL:CG2  | 3:CZ:50:THR:HG21  | 2.42                     | 0.45              |
| 1:A9:174:TRP:CE2  | 1:A9:179:LYS:HB3  | 2.51                     | 0.45              |
| 1:AW:164:TRP:CE2  | 1:AW:187:LEU:HD13 | 2.51                     | 0.45              |
| 2:B1:157:VAL:CG2  | 3:C1:50:THR:HG21  | 2.42                     | 0.45              |
| 1:AY:164:TRP:CE2  | 1:AY:187:LEU:HD13 | 2.51                     | 0.45              |
| 1:AA:87:GLN:HE21  | 1:AA:210:ARG:NH2  | 2.12                     | 0.45              |
| 1:A5:87:GLN:HE21  | 1:A5:210:ARG:NH2  | 2.12                     | 0.45              |
| 1:A3:87:GLN:HE21  | 1:A3:210:ARG:NH2  | 2.12                     | 0.45              |
| 1:A4:74:THR:HG21  | 3:C5:43:PHE:CE2   | 2.45                     | 0.45              |
| 1:AZ:74:THR:HG21  | 3:C0:43:PHE:CE2   | 2.45                     | 0.45              |
| 2:B0:85:SER:HB2   | 2:B0:190:ASN:ND2  | 2.32                     | 0.45              |
| 2:BE:85:SER:HB2   | 2:BE:190:ASN:ND2  | 2.31                     | 0.45              |
| 1:A9:74:THR:HG21  | 3:DA:43:PHE:CE1   | 2.45                     | 0.45              |
| 2:BT:85:SER:HB2   | 2:BT:190:ASN:ND2  | 2.32                     | 0.45              |
| 2:BD:85:SER:HB2   | 2:BD:190:ASN:ND2  | 2.31                     | 0.45              |
| 1:AF:35:ASP:OD1   | 1:AF:212:ARG:HD3  | 2.16                     | 0.45              |
| 1:AN:146:ILE:O    | 1:AN:147:ALA:CB   | 2.62                     | 0.45              |
| 3:CB:110:PHE:HE2  | 3:CB:116:THR:HG22 | 1.80                     | 0.45              |
| 1:AV:128:VAL:HG23 | 1:AX:91:THR:HG22  | 1.98                     | 0.45              |
| 3:CJ:36:VAL:HA    | 3:CJ:37:PRO:HD3   | 1.64                     | 0.45              |
| 1:AL:225:PRO:HA   | 1:AL:226:PRO:HD3  | 1.78                     | 0.45              |
| 3:CC:9:PRO:C      | 3:CC:11:SER:H     | 2.20                     | 0.45              |
| 3:CS:9:PRO:C      | 3:CS:11:SER:H     | 2.20                     | 0.45              |
| 1:A6:164:TRP:CE2  | 1:A6:187:LEU:HD13 | 2.51                     | 0.45              |
| 1:AR:209:LEU:HD22 | 1:AR:209:LEU:HA   | 1.74                     | 0.45              |
| 3:CC:150:LEU:HD12 | 3:CC:150:LEU:HA   | 1.79                     | 0.45              |
| 2:BM:53:ARG:HG2   | 2:BM:221:MET:HE3  | 1.99                     | 0.45              |
| 2:BD:224:GLY:HA2  | 2:BD:225:PRO:HD2  | 1.81                     | 0.45              |
| 1:DK:174:TRP:CE2  | 1:DK:179:LYS:HB3  | 2.51                     | 0.45              |
| 1:AT:174:TRP:CE2  | 1:AT:179:LYS:HB3  | 2.51                     | 0.45              |
| 2:BJ:157:VAL:CG2  | 3:CJ:50:THR:HG21  | 2.42                     | 0.45              |
| 1:A5:174:TRP:CE2  | 1:A5:179:LYS:HB3  | 2.51                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A3:174:TRP:CE2  | 1:A3:179:LYS:HB3  | 2.51                     | 0.45              |
| 1:AQ:191:HIS:HD2  | 1:AQ:193:GLY:N    | 2.08                     | 0.45              |
| 1:A5:110:GLY:N    | 1:A7:242:ASN:HD22 | 2.10                     | 0.45              |
| 1:AT:35:ASP:OD1   | 1:AT:212:ARG:HD3  | 2.16                     | 0.45              |
| 1:AJ:146:ILE:O    | 1:AJ:147:ALA:CB   | 2.62                     | 0.45              |
| 3:C1:110:PHE:HE2  | 3:C1:116:THR:HG22 | 1.80                     | 0.45              |
| 3:C9:110:PHE:HE2  | 3:C9:116:THR:HG22 | 1.80                     | 0.45              |
| 3:C6:110:PHE:HE2  | 3:C6:116:THR:HG22 | 1.80                     | 0.45              |
| 1:AO:91:THR:HG22  | 1:AP:128:VAL:HG23 | 1.98                     | 0.45              |
| 1:AC:128:VAL:HG23 | 1:AE:91:THR:HG22  | 1.98                     | 0.45              |
| 1:AN:128:VAL:HG23 | 1:DD:91:THR:HG22  | 319.52                   | 0.45              |
| 1:AD:91:THR:HG22  | 1:AE:128:VAL:HG23 | 43.31                    | 0.45              |
| 1:A5:91:THR:HG22  | 1:A6:128:VAL:HG23 | 1.98                     | 0.45              |
| 1:A4:91:THR:HG22  | 1:A7:128:VAL:HG23 | 1.98                     | 0.45              |
| 3:CP:9:PRO:C      | 3:CP:11:SER:H     | 2.20                     | 0.45              |
| 3:CY:9:PRO:C      | 3:CY:11:SER:H     | 2.20                     | 0.45              |
| 3:C6:9:PRO:C      | 3:C6:11:SER:H     | 2.20                     | 0.45              |
| 3:C8:36:VAL:HA    | 3:C8:37:PRO:HD3   | 1.64                     | 0.45              |
| 3:DB:36:VAL:HA    | 3:DB:37:PRO:HD3   | 1.64                     | 0.45              |
| 3:CB:9:PRO:C      | 3:CB:11:SER:H     | 2.20                     | 0.45              |
| 3:CW:9:PRO:C      | 3:CW:11:SER:H     | 2.20                     | 0.45              |
| 1:AU:164:TRP:CE2  | 1:AU:187:LEU:HD13 | 2.51                     | 0.45              |
| 1:AA:174:TRP:CE2  | 1:AA:179:LYS:HB3  | 2.51                     | 0.45              |
| 1:A4:207:CYS:O    | 1:A4:208:TYR:CB   | 2.57                     | 0.45              |
| 2:BS:157:VAL:CG2  | 3:CT:50:THR:HG21  | 57.94                    | 0.45              |
| 1:AD:164:TRP:CE2  | 1:AD:187:LEU:HD13 | 2.51                     | 0.45              |
| 1:AR:207:CYS:O    | 1:AR:208:TYR:CB   | 2.57                     | 0.45              |
| 1:A2:74:THR:HG21  | 3:C3:43:PHE:CE2   | 2.45                     | 0.45              |
| 1:DG:87:GLN:HE21  | 1:DG:210:ARG:NH2  | 2.12                     | 0.45              |
| 2:BE:83:LEU:HA    | 2:BE:84:PRO:HA    | 1.60                     | 0.45              |
| 3:C3:110:PHE:HE2  | 3:C3:116:THR:HG22 | 1.80                     | 0.45              |
| 1:AE:91:THR:HG22  | 1:AH:128:VAL:HG23 | 180.34                   | 0.45              |
| 1:AN:91:THR:HG22  | 1:AO:128:VAL:HG23 | 276.32                   | 0.45              |
| 1:AB:91:THR:HG22  | 1:A8:128:VAL:HG23 | 280.33                   | 0.45              |
| 1:AC:91:THR:HG22  | 1:AD:128:VAL:HG23 | 1.98                     | 0.45              |
| 3:C1:9:PRO:C      | 3:C1:11:SER:H     | 2.20                     | 0.45              |
| 3:CI:61:TYR:HB3   | 3:CI:205:LEU:HD23 | 1.98                     | 0.45              |
| 3:CR:61:TYR:HB3   | 3:CR:205:LEU:HD23 | 1.98                     | 0.45              |
| 2:BL:118:PHE:HE2  | 2:B0:118:PHE:CD1  | 266.82                   | 0.45              |
| 3:CT:9:PRO:C      | 3:CT:11:SER:H     | 2.20                     | 0.45              |
| 1:DK:72:LEU:HD23  | 1:DK:72:LEU:HA    | 1.82                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C8:150:LEU:HA   | 3:C8:150:LEU:HD12 | 1.79                     | 0.45              |
| 1:DH:72:LEU:HD23  | 1:DH:72:LEU:HA    | 1.82                     | 0.45              |
| 3:CD:9:PRO:C      | 3:CD:11:SER:H     | 2.20                     | 0.45              |
| 1:AN:225:PRO:HA   | 1:AN:226:PRO:HD3  | 1.78                     | 0.45              |
| 1:DF:164:TRP:CE2  | 1:DF:187:LEU:HD13 | 2.51                     | 0.45              |
| 1:AC:174:TRP:CE2  | 1:AC:179:LYS:HB3  | 2.51                     | 0.45              |
| 1:AZ:174:TRP:CE2  | 1:AZ:179:LYS:HB3  | 2.51                     | 0.45              |
| 1:AV:174:TRP:CE2  | 1:AV:179:LYS:HB3  | 2.51                     | 0.45              |
| 2:BT:157:VAL:CG2  | 3:CU:50:THR:HG21  | 243.74                   | 0.45              |
| 2:BX:157:VAL:CG2  | 3:CX:50:THR:HG21  | 2.42                     | 0.45              |
| 1:AO:242:ASN:HD22 | 1:DE:110:GLY:N    | 280.17                   | 0.45              |
| 1:AQ:74:THR:HG21  | 3:CR:43:PHE:CE1   | 2.45                     | 0.45              |
| 2:BB:85:SER:HB2   | 2:BB:190:ASN:ND2  | 2.31                     | 0.45              |
| 2:B1:85:SER:HB2   | 2:B1:190:ASN:ND2  | 2.31                     | 0.45              |
| 3:CR:44:ILE:HD12  | 3:CR:44:ILE:HA    | 1.88                     | 0.45              |
| 1:AH:128:VAL:HG23 | 1:DK:91:THR:HG22  | 1.98                     | 0.45              |
| 1:AF:128:VAL:HG23 | 1:AI:91:THR:HG22  | 1.98                     | 0.45              |
| 3:CO:61:TYR:HB3   | 3:CO:205:LEU:HD23 | 1.98                     | 0.45              |
| 3:CH:9:PRO:C      | 3:CH:11:SER:H     | 2.20                     | 0.45              |
| 1:DI:209:LEU:HD22 | 1:DI:209:LEU:HA   | 1.74                     | 0.45              |
| 1:AZ:209:LEU:HD22 | 1:AZ:209:LEU:HA   | 1.74                     | 0.45              |
| 2:BL:53:ARG:HG2   | 2:BL:221:MET:HE2  | 2.11                     | 0.45              |
| 1:AD:67:ALA:O     | 1:AD:70:ARG:O     | 2.35                     | 0.45              |
| 1:DD:67:ALA:O     | 1:DD:70:ARG:O     | 2.35                     | 0.45              |
| 1:AX:67:ALA:O     | 1:AX:70:ARG:O     | 2.35                     | 0.45              |
| 1:AK:174:TRP:CE2  | 1:AK:179:LYS:HB3  | 2.51                     | 0.45              |
| 1:AY:174:TRP:CE2  | 1:AY:179:LYS:HB3  | 2.51                     | 0.45              |
| 1:A0:207:CYS:O    | 1:A0:208:TYR:CB   | 2.57                     | 0.45              |
| 1:DK:191:HIS:HD2  | 1:DK:193:GLY:N    | 2.09                     | 0.45              |
| 1:AO:87:GLN:HE21  | 1:AO:210:ARG:NH2  | 2.12                     | 0.45              |
| 1:A2:87:GLN:HE21  | 1:A2:210:ARG:NH2  | 2.12                     | 0.45              |
| 1:AA:74:THR:HG21  | 3:DB:43:PHE:CE1   | 270.81                   | 0.45              |
| 2:BR:85:SER:HB2   | 2:BR:190:ASN:ND2  | 2.31                     | 0.45              |
| 1:AV:242:ASN:HD22 | 1:AW:110:GLY:N    | 2.09                     | 0.45              |
| 2:BL:85:SER:HB2   | 2:BL:190:ASN:ND2  | 2.32                     | 0.45              |
| 2:BO:85:SER:HB2   | 2:BO:190:ASN:ND2  | 2.31                     | 0.45              |
| 1:A8:74:THR:HG21  | 3:C9:43:PHE:CE2   | 2.45                     | 0.45              |
| 2:B6:85:SER:HB2   | 2:B6:190:ASN:ND2  | 2.31                     | 0.45              |
| 1:A3:35:ASP:OD1   | 1:A3:212:ARG:HD3  | 2.16                     | 0.45              |
| 1:A0:35:ASP:OD1   | 1:A0:212:ARG:HD3  | 2.16                     | 0.45              |
| 1:AB:146:ILE:O    | 1:AB:147:ALA:CB   | 2.62                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AF:128:VAL:HG23 | 1:AH:91:THR:HG22  | 27.99                    | 0.45              |
| 1:AJ:128:VAL:HG23 | 1:AM:91:THR:HG22  | 1.98                     | 0.45              |
| 1:AT:128:VAL:HG23 | 1:AW:91:THR:HG22  | 1.98                     | 0.45              |
| 3:C5:9:PRO:C      | 3:C5:11:SER:H     | 2.20                     | 0.45              |
| 3:C5:61:TYR:HB3   | 3:C5:205:LEU:HD23 | 1.97                     | 0.45              |
| 1:AC:225:PRO:HA   | 1:AC:226:PRO:HD3  | 1.78                     | 0.45              |
| 2:BK:53:ARG:HG2   | 2:BK:221:MET:HE3  | 1.99                     | 0.45              |
| 1:A4:164:TRP:CE2  | 1:A4:187:LEU:HD13 | 2.51                     | 0.45              |
| 3:CO:150:LEU:HA   | 3:CO:150:LEU:HD12 | 1.79                     | 0.45              |
| 1:DH:209:LEU:HD22 | 1:DH:209:LEU:HA   | 1.74                     | 0.45              |
| 1:AO:67:ALA:O     | 1:AO:70:ARG:O     | 2.35                     | 0.45              |
| 1:AJ:67:ALA:O     | 1:AJ:70:ARG:O     | 2.35                     | 0.45              |
| 2:BL:137:GLU:O    | 2:BL:139:ALA:N    | 2.41                     | 0.45              |
| 1:DD:207:CYS:O    | 1:DD:208:TYR:CB   | 2.57                     | 0.45              |
| 1:A3:242:ASN:HD22 | 1:A4:110:GLY:N    | 2.10                     | 0.45              |
| 1:AA:110:GLY:N    | 1:AD:242:ASN:HD22 | 2.10                     | 0.45              |
| 1:DC:110:GLY:N    | 1:DE:242:ASN:HD22 | 2.10                     | 0.45              |
| 1:AE:74:THR:HG21  | 3:CF:43:PHE:CE2   | 86.71                    | 0.45              |
| 3:CS:43:PHE:CE2   | 1:DE:74:THR:HG21  | 277.46                   | 0.45              |
| 2:BG:85:SER:HB2   | 2:BG:190:ASN:ND2  | 2.32                     | 0.45              |
| 2:BH:85:SER:HB2   | 2:BH:190:ASN:ND2  | 2.31                     | 0.45              |
| 3:CU:44:ILE:HA    | 3:CU:44:ILE:HD12  | 1.87                     | 0.45              |
| 1:AB:91:THR:HG22  | 1:AE:128:VAL:HG23 | 1.98                     | 0.45              |
| 1:DC:91:THR:HG22  | 1:DD:128:VAL:HG23 | 1.98                     | 0.45              |
| 3:C8:9:PRO:C      | 3:C8:11:SER:H     | 2.20                     | 0.45              |
| 1:A5:225:PRO:HA   | 1:A5:226:PRO:HD3  | 1.78                     | 0.45              |
| 3:CK:9:PRO:C      | 3:CK:11:SER:H     | 2.20                     | 0.45              |
| 1:DJ:164:TRP:CE2  | 1:DJ:187:LEU:HD13 | 2.51                     | 0.45              |
| 3:C9:36:VAL:HA    | 3:C9:37:PRO:HD3   | 1.64                     | 0.45              |
| 3:CA:61:TYR:HB3   | 3:CA:205:LEU:HD23 | 1.98                     | 0.45              |
| 1:A2:225:PRO:HA   | 1:A2:226:PRO:HD3  | 1.78                     | 0.45              |
| 3:CM:9:PRO:C      | 3:CM:11:SER:H     | 2.20                     | 0.45              |
| 3:C2:61:TYR:HB3   | 3:C2:205:LEU:HD23 | 1.98                     | 0.45              |
| 1:A8:164:TRP:CE2  | 1:A8:187:LEU:HD13 | 2.51                     | 0.45              |
| 2:BN:157:VAL:CG2  | 3:CN:50:THR:HG21  | 2.43                     | 0.44              |
| 1:A4:87:GLN:HE21  | 1:A4:210:ARG:NH2  | 2.12                     | 0.44              |
| 3:CJ:43:PHE:CE1   | 1:DK:74:THR:HG21  | 2.45                     | 0.44              |
| 1:A5:242:ASN:HD22 | 1:A6:110:GLY:N    | 2.10                     | 0.44              |
| 1:AK:74:THR:HG21  | 3:CL:43:PHE:CE1   | 2.45                     | 0.44              |
| 3:CV:43:PHE:CE2   | 1:DH:74:THR:HG21  | 277.44                   | 0.44              |
| 1:AA:74:THR:HG21  | 3:CA:43:PHE:CE1   | 2.45                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BC:85:SER:HB2   | 2:BC:190:ASN:ND2  | 2.31                     | 0.44              |
| 1:AR:35:ASP:OD1   | 1:AR:212:ARG:HD3  | 2.16                     | 0.44              |
| 1:AF:91:THR:HG22  | 1:AG:128:VAL:HG23 | 1.98                     | 0.44              |
| 2:BC:53:ARG:HG2   | 2:BC:221:MET:HE3  | 2.03                     | 0.44              |
| 3:CF:150:LEU:HD12 | 3:CF:150:LEU:HA   | 1.79                     | 0.44              |
| 1:A2:209:LEU:HD22 | 1:A2:209:LEU:HA   | 1.74                     | 0.44              |
| 3:C4:9:PRO:C      | 3:C4:11:SER:H     | 2.20                     | 0.44              |
| 1:AC:67:ALA:O     | 1:AC:70:ARG:O     | 2.35                     | 0.44              |
| 1:AG:67:ALA:O     | 1:AG:70:ARG:O     | 2.35                     | 0.44              |
| 1:DG:67:ALA:O     | 1:DG:70:ARG:O     | 2.35                     | 0.44              |
| 1:AA:67:ALA:O     | 1:AA:70:ARG:O     | 2.35                     | 0.44              |
| 1:A1:67:ALA:O     | 1:A1:70:ARG:O     | 2.35                     | 0.44              |
| 1:A4:67:ALA:O     | 1:A4:70:ARG:O     | 2.35                     | 0.44              |
| 1:A4:191:HIS:HD2  | 1:A4:193:GLY:N    | 2.08                     | 0.44              |
| 1:A1:174:TRP:CE2  | 1:A1:179:LYS:HB3  | 2.51                     | 0.44              |
| 1:AV:87:GLN:HE21  | 1:AV:210:ARG:NH2  | 2.12                     | 0.44              |
| 1:AF:74:THR:HG21  | 3:CG:43:PHE:CE2   | 46.55                    | 0.44              |
| 3:CW:43:PHE:CE2   | 1:DI:74:THR:HG21  | 218.68                   | 0.44              |
| 2:BQ:85:SER:HB2   | 2:BQ:190:ASN:ND2  | 2.32                     | 0.44              |
| 1:AI:91:THR:HG22  | 1:AJ:128:VAL:HG23 | 180.33                   | 0.44              |
| 1:AJ:91:THR:HG22  | 1:AK:128:VAL:HG23 | 1.98                     | 0.44              |
| 1:AA:128:VAL:HG23 | 1:AC:91:THR:HG22  | 27.99                    | 0.44              |
| 1:A3:128:VAL:HG23 | 1:A6:91:THR:HG22  | 1.98                     | 0.44              |
| 2:BZ:53:ARG:HG2   | 2:BZ:221:MET:CE   | 2.48                     | 0.44              |
| 3:CZ:9:PRO:C      | 3:CZ:11:SER:H     | 2.20                     | 0.44              |
| 1:AR:225:PRO:HA   | 1:AR:226:PRO:HD3  | 1.78                     | 0.44              |
| 2:BD:124:LEU:HD23 | 2:BD:198:ILE:HA   | 2.00                     | 0.44              |
| 3:CD:150:LEU:HD12 | 3:CD:150:LEU:HA   | 1.79                     | 0.44              |
| 1:AT:209:LEU:HD22 | 1:AT:209:LEU:HA   | 1.74                     | 0.44              |
| 1:DH:225:PRO:HA   | 1:DH:226:PRO:HD3  | 1.78                     | 0.44              |
| 2:BX:53:ARG:HG2   | 2:BX:221:MET:HE3  | 2.00                     | 0.44              |
| 3:CN:9:PRO:C      | 3:CN:11:SER:H     | 2.20                     | 0.44              |
| 2:BK:156:SER:HB2  | 3:CL:51:TYR:O     | 63.55                    | 0.44              |
| 3:CY:36:VAL:HA    | 3:CY:37:PRO:HD3   | 1.64                     | 0.44              |
| 1:DC:67:ALA:O     | 1:DC:70:ARG:O     | 2.35                     | 0.44              |
| 1:AH:67:ALA:O     | 1:AH:70:ARG:O     | 2.35                     | 0.44              |
| 1:AI:67:ALA:O     | 1:AI:70:ARG:O     | 2.35                     | 0.44              |
| 2:BH:157:VAL:CG2  | 3:CH:50:THR:HG21  | 2.43                     | 0.44              |
| 2:B5:157:VAL:CG2  | 3:C6:50:THR:HG21  | 2.43                     | 0.44              |
| 1:DF:242:ASN:HD22 | 1:DG:110:GLY:N    | 2.10                     | 0.44              |
| 1:A1:87:GLN:HE21  | 1:A1:210:ARG:NH2  | 2.12                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B9:85:SER:HB2   | 2:B9:190:ASN:ND2  | 2.31                     | 0.44              |
| 2:BZ:85:SER:HB2   | 2:BZ:190:ASN:ND2  | 2.31                     | 0.44              |
| 1:AA:128:VAL:HG23 | 1:AD:91:THR:HG22  | 1.98                     | 0.44              |
| 1:A0:128:VAL:HG23 | 1:A2:91:THR:HG22  | 1.98                     | 0.44              |
| 1:AZ:91:THR:HG22  | 1:A2:128:VAL:HG23 | 1.98                     | 0.44              |
| 1:AO:219:TYR:CD2  | 3:CP:36:VAL:HG22  | 2.53                     | 0.44              |
| 2:BM:53:ARG:HG2   | 2:BM:221:MET:CE   | 2.48                     | 0.44              |
| 2:BH:156:SER:HB2  | 3:CH:51:TYR:O     | 2.18                     | 0.44              |
| 2:BV:156:SER:HB2  | 3:CW:51:TYR:O     | 100.83                   | 0.44              |
| 1:AX:219:TYR:CD2  | 3:CY:36:VAL:HG22  | 2.53                     | 0.44              |
| 2:B1:156:SER:HB2  | 3:C1:51:TYR:O     | 2.18                     | 0.44              |
| 2:BZ:156:SER:HB2  | 3:CZ:51:TYR:O     | 2.18                     | 0.44              |
| 2:B6:156:SER:HB2  | 3:C7:51:TYR:O     | 2.18                     | 0.44              |
| 1:AI:225:PRO:HA   | 1:AI:226:PRO:HD3  | 1.78                     | 0.44              |
| 2:BB:53:ARG:HG2   | 2:BB:221:MET:CE   | 2.48                     | 0.44              |
| 2:BC:124:LEU:HD23 | 2:BC:198:ILE:HA   | 2.00                     | 0.44              |
| 2:B2:124:LEU:HD23 | 2:B2:198:ILE:HA   | 2.00                     | 0.44              |
| 2:BJ:124:LEU:HD23 | 2:BJ:198:ILE:HA   | 2.00                     | 0.44              |
| 3:C4:150:LEU:HA   | 3:C4:150:LEU:HD12 | 1.79                     | 0.44              |
| 2:B4:124:LEU:HD23 | 2:B4:198:ILE:HA   | 2.00                     | 0.44              |
| 2:BP:53:ARG:HG2   | 2:BP:221:MET:CE   | 2.48                     | 0.44              |
| 1:AT:67:ALA:O     | 1:AT:70:ARG:O     | 2.35                     | 0.44              |
| 1:AN:67:ALA:O     | 1:AN:70:ARG:O     | 2.35                     | 0.44              |
| 1:A0:67:ALA:O     | 1:A0:70:ARG:O     | 2.35                     | 0.44              |
| 2:BW:157:VAL:CG2  | 3:CX:50:THR:HG21  | 57.94                    | 0.44              |
| 1:AF:191:HIS:HD2  | 1:AF:193:GLY:N    | 2.08                     | 0.44              |
| 1:DF:207:CYS:O    | 1:DF:208:TYR:CB   | 2.57                     | 0.44              |
| 1:AU:87:GLN:HE21  | 1:AU:210:ARG:NH2  | 2.11                     | 0.44              |
| 1:AO:91:THR:HG22  | 1:DE:128:VAL:HG23 | 313.95                   | 0.44              |
| 1:AD:128:VAL:HG23 | 1:AG:91:THR:HG22  | 171.92                   | 0.44              |
| 1:AG:91:THR:HG22  | 1:DK:128:VAL:HG23 | 1.98                     | 0.44              |
| 1:AQ:91:THR:HG22  | 1:AR:128:VAL:HG23 | 1.98                     | 0.44              |
| 1:A8:91:THR:HG22  | 1:A9:128:VAL:HG23 | 1.98                     | 0.44              |
| 3:CE:36:VAL:HA    | 3:CE:37:PRO:HD3   | 1.64                     | 0.44              |
| 1:AF:219:TYR:CD2  | 3:CG:36:VAL:HG22  | 46.04                    | 0.44              |
| 1:AR:219:TYR:CD2  | 3:CS:36:VAL:HG22  | 2.53                     | 0.44              |
| 2:BF:53:ARG:HG2   | 2:BF:221:MET:CE   | 2.48                     | 0.44              |
| 2:BW:156:SER:HB2  | 3:CX:51:TYR:O     | 63.55                    | 0.44              |
| 2:BX:156:SER:HB2  | 3:C5:51:TYR:O     | 243.62                   | 0.44              |
| 2:BC:156:SER:HB2  | 3:CD:51:TYR:O     | 63.55                    | 0.44              |
| 2:B6:53:ARG:HG2   | 2:B6:221:MET:CE   | 2.48                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BN:124:LEU:HD23 | 2:BN:198:ILE:HA   | 2.00                     | 0.44              |
| 2:BI:124:LEU:HD23 | 2:BI:198:ILE:HA   | 2.00                     | 0.44              |
| 3:CG:9:PRO:C      | 3:CG:11:SER:H     | 2.20                     | 0.44              |
| 2:BS:124:LEU:HD23 | 2:BS:198:ILE:HA   | 2.00                     | 0.44              |
| 2:B8:53:ARG:HG2   | 2:B8:221:MET:CE   | 2.48                     | 0.44              |
| 2:BJ:53:ARG:HG2   | 2:BJ:221:MET:HE2  | 2.10                     | 0.44              |
| 2:BK:124:LEU:HD23 | 2:BK:198:ILE:HA   | 2.00                     | 0.44              |
| 3:C7:9:PRO:C      | 3:C7:11:SER:H     | 2.20                     | 0.44              |
| 3:CI:9:PRO:C      | 3:CI:11:SER:H     | 2.20                     | 0.44              |
| 2:B0:53:ARG:HG2   | 2:B0:221:MET:CE   | 2.48                     | 0.44              |
| 2:B7:156:SER:HB2  | 3:C8:51:TYR:O     | 2.18                     | 0.44              |
| 2:B8:156:SER:HB2  | 3:C9:51:TYR:O     | 2.18                     | 0.44              |
| 1:AK:209:LEU:HD22 | 1:AK:209:LEU:HA   | 1.74                     | 0.44              |
| 1:AU:209:LEU:HD22 | 1:AU:209:LEU:HA   | 1.74                     | 0.44              |
| 2:B9:53:ARG:HG2   | 2:B9:221:MET:CE   | 2.48                     | 0.44              |
| 2:BX:124:LEU:HD23 | 2:BX:198:ILE:HA   | 2.00                     | 0.44              |
| 2:BP:124:LEU:HD23 | 2:BP:198:ILE:HA   | 2.00                     | 0.44              |
| 2:BH:124:LEU:HD23 | 2:BH:198:ILE:HA   | 2.00                     | 0.44              |
| 2:BQ:124:LEU:HD23 | 2:BQ:198:ILE:HA   | 2.00                     | 0.44              |
| 2:BZ:124:LEU:HD23 | 2:BZ:198:ILE:HA   | 2.00                     | 0.44              |
| 1:DK:67:ALA:O     | 1:DK:70:ARG:O     | 2.35                     | 0.44              |
| 1:AM:67:ALA:O     | 1:AM:70:ARG:O     | 2.35                     | 0.44              |
| 1:AS:191:HIS:HD2  | 1:AS:193:GLY:N    | 2.08                     | 0.44              |
| 1:AJ:110:GLY:N    | 1:AM:242:ASN:HD22 | 2.10                     | 0.44              |
| 2:BI:83:LEU:HA    | 2:BI:84:PRO:HA    | 1.60                     | 0.44              |
| 2:BO:84:PRO:CD    | 2:BO:85:SER:H     | 2.31                     | 0.44              |
| 2:BX:85:SER:HB2   | 2:BX:190:ASN:ND2  | 2.31                     | 0.44              |
| 1:AI:128:VAL:HG23 | 1:AL:91:THR:HG22  | 169.67                   | 0.44              |
| 1:DF:128:VAL:HG23 | 1:DI:91:THR:HG22  | 1.98                     | 0.44              |
| 1:AQ:128:VAL:HG23 | 1:AS:91:THR:HG22  | 1.98                     | 0.44              |
| 1:AS:219:TYR:CD2  | 3:CT:36:VAL:HG22  | 2.53                     | 0.44              |
| 3:CG:36:VAL:HA    | 3:CG:37:PRO:HD3   | 1.64                     | 0.44              |
| 1:AQ:219:TYR:CD2  | 3:CR:36:VAL:HG22  | 2.53                     | 0.44              |
| 1:AV:219:TYR:CD2  | 3:CW:36:VAL:HG22  | 2.53                     | 0.44              |
| 3:CQ:36:VAL:HG22  | 1:DC:219:TYR:CD2  | 218.66                   | 0.44              |
| 1:AA:219:TYR:CD2  | 3:DB:36:VAL:HG22  | 266.57                   | 0.44              |
| 2:BL:53:ARG:HG2   | 2:BL:221:MET:CE   | 2.48                     | 0.44              |
| 2:BG:156:SER:HB2  | 3:CG:51:TYR:O     | 2.18                     | 0.44              |
| 2:BM:156:SER:HB2  | 3:CN:51:TYR:O     | 63.55                    | 0.44              |
| 2:BS:156:SER:HB2  | 3:CQ:51:TYR:O     | 2.18                     | 0.44              |
| 1:AL:219:TYR:CD2  | 3:CM:36:VAL:HG22  | 2.53                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:CZ:36:VAL:HA    | 3:CZ:37:PRO:HD3   | 1.64                     | 0.44              |
| 2:BR:124:LEU:HD23 | 2:BR:198:ILE:HA   | 2.00                     | 0.44              |
| 2:BG:124:LEU:HD23 | 2:BG:198:ILE:HA   | 2.00                     | 0.44              |
| 2:B3:156:SER:HB2  | 3:C3:51:TYR:O     | 2.18                     | 0.44              |
| 2:B5:224:GLY:HA2  | 2:B5:225:PRO:HD2  | 1.81                     | 0.44              |
| 2:BU:124:LEU:HD23 | 2:BU:198:ILE:HA   | 2.00                     | 0.44              |
| 2:BU:53:ARG:HG2   | 2:BU:221:MET:CE   | 2.48                     | 0.44              |
| 2:BM:124:LEU:HD23 | 2:BM:198:ILE:HA   | 2.00                     | 0.44              |
| 3:CV:150:LEU:HA   | 3:CV:150:LEU:HD12 | 1.79                     | 0.44              |
| 1:AD:209:LEU:HA   | 1:AD:209:LEU:HD22 | 1.74                     | 0.44              |
| 2:BA:156:SER:HB2  | 3:DB:51:TYR:O     | 274.78                   | 0.44              |
| 2:BE:53:ARG:HG2   | 2:BE:221:MET:CE   | 2.48                     | 0.44              |
| 2:B4:53:ARG:HG2   | 2:B4:221:MET:CE   | 2.48                     | 0.44              |
| 3:C3:9:PRO:C      | 3:C3:11:SER:H     | 2.20                     | 0.44              |
| 2:BE:124:LEU:HD23 | 2:BE:198:ILE:HA   | 2.00                     | 0.44              |
| 1:AF:67:ALA:O     | 1:AF:70:ARG:O     | 2.35                     | 0.44              |
| 1:AL:67:ALA:O     | 1:AL:70:ARG:O     | 2.35                     | 0.44              |
| 1:AK:67:ALA:O     | 1:AK:70:ARG:O     | 2.35                     | 0.44              |
| 1:DJ:67:ALA:O     | 1:DJ:70:ARG:O     | 2.35                     | 0.44              |
| 1:AY:67:ALA:O     | 1:AY:70:ARG:O     | 2.35                     | 0.44              |
| 2:BE:157:VAL:CG2  | 3:CF:50:THR:HG21  | 67.02                    | 0.44              |
| 2:BP:157:VAL:CG2  | 3:CQ:50:THR:HG21  | 90.55                    | 0.44              |
| 1:A5:191:HIS:HD2  | 1:A5:193:GLY:N    | 2.08                     | 0.44              |
| 1:AK:74:THR:HG21  | 3:CL:43:PHE:CE2   | 4.65                     | 0.44              |
| 2:BR:84:PRO:CD    | 2:BR:85:SER:H     | 2.31                     | 0.44              |
| 2:BK:85:SER:HB2   | 2:BK:190:ASN:ND2  | 2.31                     | 0.44              |
| 2:B3:83:LEU:HA    | 2:B3:84:PRO:HA    | 1.60                     | 0.44              |
| 1:AF:231:PRO:HG2  | 3:CF:83:ALA:CB    | 2.48                     | 0.44              |
| 2:B2:83:LEU:HA    | 2:B2:84:PRO:HA    | 1.60                     | 0.44              |
| 2:B2:84:PRO:CD    | 2:B2:85:SER:H     | 2.31                     | 0.44              |
| 1:A1:146:ILE:O    | 1:A1:147:ALA:CB   | 2.62                     | 0.44              |
| 3:CV:44:ILE:HD12  | 3:CV:44:ILE:HA    | 1.87                     | 0.44              |
| 3:C0:44:ILE:HD12  | 3:C0:44:ILE:HA    | 1.88                     | 0.44              |
| 1:AD:219:TYR:CD2  | 3:CD:36:VAL:HG22  | 2.53                     | 0.44              |
| 1:AF:219:TYR:CD2  | 3:CF:36:VAL:HG22  | 2.53                     | 0.44              |
| 1:AG:219:TYR:CD2  | 3:CH:36:VAL:HG22  | 76.03                    | 0.44              |
| 2:BN:53:ARG:HG2   | 2:BN:221:MET:CE   | 2.48                     | 0.44              |
| 2:BT:156:SER:HB2  | 3:CT:51:TYR:O     | 2.18                     | 0.44              |
| 2:BJ:53:ARG:HG2   | 2:BJ:221:MET:CE   | 2.48                     | 0.44              |
| 1:AY:219:TYR:CD2  | 3:CZ:36:VAL:HG22  | 2.53                     | 0.44              |
| 2:BQ:53:ARG:HG2   | 2:BQ:221:MET:CE   | 2.48                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BW:124:LEU:HD23 | 2:BW:198:ILE:HA   | 2.00                     | 0.44              |
| 3:DA:9:PRO:C      | 3:DA:11:SER:H     | 2.20                     | 0.44              |
| 2:B1:124:LEU:HD23 | 2:B1:198:ILE:HA   | 2.00                     | 0.44              |
| 1:AI:26:VAL:HG11  | 3:CK:28:LYS:HD3   | 146.79                   | 0.44              |
| 3:CJ:9:PRO:C      | 3:CJ:11:SER:H     | 2.20                     | 0.44              |
| 1:AK:219:TYR:CD2  | 3:CL:36:VAL:HG22  | 2.53                     | 0.44              |
| 1:AM:72:LEU:HD23  | 1:AM:72:LEU:HA    | 1.83                     | 0.44              |
| 1:A0:209:LEU:HD22 | 1:A0:209:LEU:HA   | 1.74                     | 0.44              |
| 1:AB:209:LEU:HA   | 1:AB:209:LEU:HD22 | 1.74                     | 0.44              |
| 2:B0:124:LEU:HD23 | 2:B0:198:ILE:HA   | 2.00                     | 0.44              |
| 3:C2:9:PRO:C      | 3:C2:11:SER:H     | 2.20                     | 0.44              |
| 1:A3:219:TYR:CD2  | 3:C4:36:VAL:HG22  | 2.53                     | 0.44              |
| 2:B1:224:GLY:HA2  | 2:B1:225:PRO:HD2  | 1.81                     | 0.44              |
| 2:BU:224:GLY:HA2  | 2:BU:225:PRO:HD2  | 1.81                     | 0.44              |
| 2:B9:156:SER:HB2  | 3:DA:51:TYR:O     | 2.18                     | 0.44              |
| 2:B5:53:ARG:HG2   | 2:B5:221:MET:CE   | 2.48                     | 0.44              |
| 2:BV:53:ARG:HG2   | 2:BV:221:MET:CE   | 2.48                     | 0.44              |
| 1:AB:67:ALA:O     | 1:AB:70:ARG:O     | 2.35                     | 0.44              |
| 1:DE:67:ALA:O     | 1:DE:70:ARG:O     | 2.35                     | 0.44              |
| 1:A8:67:ALA:O     | 1:A8:70:ARG:O     | 2.35                     | 0.44              |
| 1:A9:67:ALA:O     | 1:A9:70:ARG:O     | 2.35                     | 0.44              |
| 1:A0:191:HIS:HD2  | 1:A0:193:GLY:N    | 2.08                     | 0.44              |
| 1:AL:191:HIS:HD2  | 1:AL:193:GLY:N    | 2.08                     | 0.44              |
| 2:BG:157:VAL:CG2  | 3:CG:50:THR:HG21  | 2.43                     | 0.44              |
| 2:BK:157:VAL:CG2  | 3:CK:50:THR:HG21  | 2.43                     | 0.44              |
| 1:AG:74:THR:HG21  | 3:CH:43:PHE:CE2   | 73.69                    | 0.44              |
| 2:BY:85:SER:HB2   | 2:BY:190:ASN:ND2  | 2.31                     | 0.44              |
| 1:AP:87:GLN:HE21  | 1:AP:210:ARG:NH2  | 2.12                     | 0.44              |
| 2:BH:84:PRO:CD    | 2:BH:85:SER:H     | 2.31                     | 0.44              |
| 1:A3:74:THR:HG21  | 3:C4:43:PHE:CE2   | 2.45                     | 0.44              |
| 2:B9:84:PRO:CD    | 2:B9:85:SER:H     | 2.31                     | 0.44              |
| 2:B4:84:PRO:CD    | 2:B4:85:SER:H     | 2.31                     | 0.44              |
| 1:A3:231:PRO:HG2  | 3:C4:83:ALA:CB    | 2.48                     | 0.44              |
| 2:BZ:84:PRO:CD    | 2:BZ:85:SER:H     | 2.31                     | 0.44              |
| 2:BZ:83:LEU:HA    | 2:BZ:84:PRO:HA    | 1.60                     | 0.44              |
| 1:DF:35:ASP:OD1   | 1:DF:212:ARG:HD3  | 2.16                     | 0.44              |
| 1:A2:163:MET:HE1  | 1:A2:189:GLY:HA3  | 2.00                     | 0.44              |
| 3:CX:36:VAL:HG22  | 1:DJ:219:TYR:CD2  | 242.83                   | 0.44              |
| 3:CX:76:MET:HG3   | 3:CX:76:MET:O     | 2.18                     | 0.44              |
| 3:CP:76:MET:O     | 3:CP:76:MET:HG3   | 2.18                     | 0.44              |
| 3:CZ:76:MET:O     | 3:CZ:76:MET:HG3   | 2.18                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AI:219:TYR:CD2  | 3:CI:36:VAL:HG22  | 2.53                     | 0.44              |
| 3:CI:36:VAL:HA    | 3:CI:37:PRO:HD3   | 1.64                     | 0.44              |
| 3:CV:36:VAL:HG22  | 1:DH:219:TYR:CD2  | 266.94                   | 0.44              |
| 2:BC:53:ARG:HG2   | 2:BC:221:MET:CE   | 2.48                     | 0.44              |
| 2:BD:156:SER:HB2  | 3:CE:51:TYR:O     | 99.59                    | 0.44              |
| 2:BL:156:SER:HB2  | 3:CM:51:TYR:O     | 100.83                   | 0.44              |
| 2:BP:156:SER:HB2  | 3:CR:51:TYR:O     | 2.18                     | 0.44              |
| 2:BQ:156:SER:HB2  | 3:CS:51:TYR:O     | 2.18                     | 0.44              |
| 2:BT:156:SER:HB2  | 3:CU:51:TYR:O     | 243.61                   | 0.44              |
| 1:AB:26:VAL:HG11  | 3:C9:28:LYS:HD3   | 210.45                   | 0.44              |
| 2:BT:124:LEU:HD23 | 2:BT:198:ILE:HA   | 2.00                     | 0.44              |
| 2:BH:53:ARG:HG2   | 2:BH:221:MET:CE   | 2.48                     | 0.44              |
| 2:BO:124:LEU:HD23 | 2:BO:198:ILE:HA   | 2.00                     | 0.44              |
| 2:B5:124:LEU:HD23 | 2:B5:198:ILE:HA   | 2.00                     | 0.44              |
| 2:BR:53:ARG:HG2   | 2:BR:221:MET:CE   | 2.48                     | 0.44              |
| 2:BA:124:LEU:HD23 | 2:BA:198:ILE:HA   | 2.00                     | 0.44              |
| 2:B5:156:SER:HB2  | 3:C6:51:TYR:O     | 2.18                     | 0.44              |
| 1:AZ:219:TYR:CD2  | 3:C0:36:VAL:HG22  | 2.53                     | 0.44              |
| 3:CW:28:LYS:HD3   | 1:DH:26:VAL:HG11  | 243.50                   | 0.44              |
| 2:BL:124:LEU:HD23 | 2:BL:198:ILE:HA   | 2.00                     | 0.44              |
| 1:AC:26:VAL:HG11  | 3:CD:28:LYS:HD3   | 2.00                     | 0.44              |
| 1:AL:209:LEU:HA   | 1:AL:209:LEU:HD22 | 1.74                     | 0.44              |
| 2:BW:53:ARG:HG2   | 2:BW:221:MET:CE   | 2.48                     | 0.44              |
| 2:B3:124:LEU:HD23 | 2:B3:198:ILE:HA   | 2.00                     | 0.44              |
| 1:A3:26:VAL:HG11  | 3:C5:28:LYS:HD3   | 2.00                     | 0.44              |
| 1:AE:67:ALA:O     | 1:AE:70:ARG:O     | 2.35                     | 0.44              |
| 1:AS:67:ALA:O     | 1:AS:70:ARG:O     | 2.35                     | 0.44              |
| 2:BV:157:VAL:CG2  | 3:CV:50:THR:HG21  | 2.43                     | 0.44              |
| 1:AC:74:THR:HG21  | 3:CC:43:PHE:CE1   | 2.45                     | 0.44              |
| 1:AD:74:THR:HG21  | 3:CE:43:PHE:CE2   | 72.82                    | 0.44              |
| 2:BY:83:LEU:HA    | 2:BY:84:PRO:HA    | 1.60                     | 0.44              |
| 2:BA:84:PRO:CD    | 2:BA:85:SER:H     | 2.31                     | 0.44              |
| 2:BF:84:PRO:CD    | 2:BF:85:SER:H     | 2.31                     | 0.44              |
| 2:BK:84:PRO:CD    | 2:BK:85:SER:H     | 2.31                     | 0.44              |
| 2:BM:84:PRO:CD    | 2:BM:85:SER:H     | 2.31                     | 0.44              |
| 2:B5:84:PRO:CD    | 2:B5:85:SER:H     | 2.31                     | 0.44              |
| 1:AI:231:PRO:HG2  | 3:CJ:83:ALA:CB    | 103.74                   | 0.44              |
| 1:AK:231:PRO:HG2  | 3:CL:83:ALA:CB    | 2.48                     | 0.44              |
| 3:CL:76:MET:HG3   | 3:CL:76:MET:O     | 2.18                     | 0.44              |
| 3:CE:76:MET:HG3   | 3:CE:76:MET:O     | 2.18                     | 0.44              |
| 1:AC:219:TYR:CD2  | 3:CD:36:VAL:HG22  | 46.03                    | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:DH:91:THR:HG22 | 1:DI:128:VAL:HG23 | 1.98                     | 0.44              |
| 3:DA:76:MET:O    | 3:DA:76:MET:HG3   | 2.18                     | 0.44              |
| 1:AU:219:TYR:CD2 | 3:CV:36:VAL:HG22  | 2.53                     | 0.44              |
| 1:AJ:219:TYR:CD2 | 3:CK:36:VAL:HG22  | 2.53                     | 0.44              |
| 1:AP:219:TYR:CD2 | 3:CQ:36:VAL:HG22  | 2.53                     | 0.44              |
| 2:BK:53:ARG:HG2  | 2:BK:221:MET:CE   | 2.48                     | 0.44              |
| 2:BX:53:ARG:HG2  | 2:BX:221:MET:CE   | 2.48                     | 0.44              |
| 2:BF:156:SER:HB2 | 3:CG:51:TYR:O     | 63.55                    | 0.44              |
| 2:BJ:156:SER:HB2 | 3:CK:51:TYR:O     | 228.49                   | 0.44              |
| 2:BN:156:SER:HB2 | 3:CN:51:TYR:O     | 2.18                     | 0.44              |
| 2:BV:156:SER:HB2 | 3:CV:51:TYR:O     | 2.18                     | 0.44              |
| 1:AP:26:VAL:HG11 | 3:CT:28:LYS:HD3   | 2.00                     | 0.44              |
| 2:BT:53:ARG:HG2  | 2:BT:221:MET:CE   | 2.48                     | 0.44              |
| 1:AA:209:LEU:HA  | 1:AA:209:LEU:HD22 | 1.74                     | 0.44              |
| 1:AM:219:TYR:CD2 | 3:CN:36:VAL:HG22  | 2.53                     | 0.44              |
| 3:CV:28:LYS:HD3  | 1:DJ:26:VAL:HG11  | 257.87                   | 0.44              |
| 1:AQ:67:ALA:O    | 1:AQ:70:ARG:O     | 2.35                     | 0.44              |
| 1:A7:67:ALA:O    | 1:A7:70:ARG:O     | 2.35                     | 0.44              |
| 2:BY:84:PRO:CD   | 2:BY:85:SER:H     | 2.31                     | 0.44              |
| 2:BT:84:PRO:CD   | 2:BT:85:SER:H     | 2.31                     | 0.44              |
| 2:BG:84:PRO:CD   | 2:BG:85:SER:H     | 2.31                     | 0.44              |
| 2:BD:84:PRO:CD   | 2:BD:85:SER:H     | 2.31                     | 0.44              |
| 1:AN:231:PRO:HG2 | 3:CO:83:ALA:CB    | 2.48                     | 0.44              |
| 1:AM:212:ARG:NH2 | 3:CN:18:VAL:O     | 2.46                     | 0.44              |
| 1:A0:212:ARG:NH2 | 3:C1:18:VAL:O     | 2.46                     | 0.44              |
| 3:CK:44:ILE:HA   | 3:CK:44:ILE:HD12  | 1.88                     | 0.44              |
| 3:CQ:74:PHE:HE2  | 3:CQ:183:LEU:HD13 | 1.83                     | 0.44              |
| 3:CP:74:PHE:HE2  | 3:CP:183:LEU:HD13 | 1.84                     | 0.44              |
| 3:CE:74:PHE:HE2  | 3:CE:183:LEU:HD13 | 1.83                     | 0.44              |
| 3:CR:74:PHE:HE2  | 3:CR:183:LEU:HD13 | 1.83                     | 0.44              |
| 3:C0:76:MET:O    | 3:C0:76:MET:HG3   | 2.18                     | 0.44              |
| 3:CG:76:MET:HG3  | 3:CG:76:MET:O     | 2.18                     | 0.44              |
| 3:CQ:76:MET:HG3  | 3:CQ:76:MET:O     | 2.18                     | 0.44              |
| 3:CT:36:VAL:HG22 | 1:DF:219:TYR:CD2  | 245.96                   | 0.44              |
| 1:AH:219:TYR:CD2 | 3:CH:36:VAL:HG22  | 2.53                     | 0.44              |
| 1:AH:219:TYR:CD2 | 3:CI:36:VAL:HG22  | 46.04                    | 0.44              |
| 1:AI:219:TYR:CD2 | 3:CJ:36:VAL:HG22  | 77.01                    | 0.44              |
| 1:AN:219:TYR:CD2 | 3:CO:36:VAL:HG22  | 2.53                     | 0.44              |
| 2:BI:156:SER:HB2 | 3:CI:51:TYR:O     | 2.18                     | 0.44              |
| 2:BU:156:SER:HB2 | 3:CV:51:TYR:O     | 63.55                    | 0.44              |
| 2:BA:156:SER:HB2 | 3:CA:51:TYR:O     | 2.18                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AD:26:VAL:HG11  | 3:CA:28:LYS:HD3   | 2.00                     | 0.44              |
| 1:A5:26:VAL:HG11  | 3:C7:28:LYS:HD3   | 2.00                     | 0.44              |
| 2:B7:124:LEU:HD23 | 2:B7:198:ILE:HA   | 2.00                     | 0.44              |
| 1:AY:26:VAL:HG11  | 3:C0:28:LYS:HD3   | 2.00                     | 0.44              |
| 2:B9:124:LEU:HD23 | 2:B9:198:ILE:HA   | 2.00                     | 0.44              |
| 3:CU:36:VAL:HG22  | 1:DG:219:TYR:CD2  | 247.18                   | 0.44              |
| 2:BV:124:LEU:HD23 | 2:BV:198:ILE:HA   | 2.00                     | 0.44              |
| 3:CX:150:LEU:HD12 | 3:CX:150:LEU:HA   | 1.79                     | 0.44              |
| 2:BD:53:ARG:HG2   | 2:BD:221:MET:CE   | 2.48                     | 0.44              |
| 1:AK:26:VAL:HG11  | 3:CO:28:LYS:HD3   | 2.00                     | 0.44              |
| 2:BO:53:ARG:HG2   | 2:BO:221:MET:CE   | 2.48                     | 0.44              |
| 3:CE:9:PRO:C      | 3:CE:11:SER:H     | 2.20                     | 0.44              |
| 2:BB:124:LEU:HD23 | 2:BB:198:ILE:HA   | 2.00                     | 0.44              |
| 1:AQ:26:VAL:HG11  | 3:CS:28:LYS:HD3   | 2.00                     | 0.44              |
| 3:CQ:28:LYS:HD3   | 1:DE:26:VAL:HG11  | 243.51                   | 0.44              |
| 1:AR:67:ALA:O     | 1:AR:70:ARG:O     | 2.35                     | 0.43              |
| 1:A3:67:ALA:O     | 1:A3:70:ARG:O     | 2.35                     | 0.43              |
| 2:BN:157:VAL:CG2  | 3:CO:50:THR:HG21  | 90.55                    | 0.43              |
| 1:AG:242:ASN:HD22 | 1:DK:110:GLY:N    | 2.10                     | 0.43              |
| 1:AD:87:GLN:HE21  | 1:AD:210:ARG:NH2  | 2.12                     | 0.43              |
| 1:AW:87:GLN:HE21  | 1:AW:210:ARG:NH2  | 2.12                     | 0.43              |
| 1:AB:74:THR:HG21  | 3:CC:43:PHE:CE2   | 73.69                    | 0.43              |
| 2:B0:84:PRO:CD    | 2:B0:85:SER:H     | 2.31                     | 0.43              |
| 2:BS:84:PRO:CD    | 2:BS:85:SER:H     | 2.31                     | 0.43              |
| 2:BI:84:PRO:CD    | 2:BI:85:SER:H     | 2.31                     | 0.43              |
| 2:BP:84:PRO:CD    | 2:BP:85:SER:H     | 2.31                     | 0.43              |
| 2:B2:85:SER:HB2   | 2:B2:190:ASN:ND2  | 2.31                     | 0.43              |
| 1:AP:146:ILE:O    | 1:AP:147:ALA:CB   | 2.62                     | 0.43              |
| 3:DB:74:PHE:HE2   | 3:DB:183:LEU:HD13 | 1.83                     | 0.43              |
| 3:CI:74:PHE:HE2   | 3:CI:183:LEU:HD13 | 1.84                     | 0.43              |
| 3:CC:76:MET:O     | 3:CC:76:MET:HG3   | 2.18                     | 0.43              |
| 3:C6:76:MET:O     | 3:C6:76:MET:HG3   | 2.18                     | 0.43              |
| 3:CH:76:MET:O     | 3:CH:76:MET:HG3   | 2.18                     | 0.43              |
| 1:AC:219:TYR:CD2  | 3:CC:36:VAL:HG22  | 2.53                     | 0.43              |
| 1:AE:219:TYR:CD2  | 3:CF:36:VAL:HG22  | 83.06                    | 0.43              |
| 3:CW:36:VAL:HG22  | 1:DI:219:TYR:CD2  | 218.64                   | 0.43              |
| 1:A7:219:TYR:CD2  | 3:C8:36:VAL:HG22  | 2.53                     | 0.43              |
| 2:BG:156:SER:HB2  | 3:CH:51:TYR:O     | 100.83                   | 0.43              |
| 2:BX:156:SER:HB2  | 3:CX:51:TYR:O     | 2.18                     | 0.43              |
| 2:BB:156:SER:HB2  | 3:CC:51:TYR:O     | 100.83                   | 0.43              |
| 2:BL:156:SER:HB2  | 3:CL:51:TYR:O     | 2.18                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:AD:26:VAL:HG11 | 3:CF:28:LYS:HD3   | 158.06                   | 0.43              |
| 3:CN:36:VAL:HA   | 3:CN:37:PRO:HD3   | 1.64                     | 0.43              |
| 2:BX:224:GLY:HA2 | 2:BX:225:PRO:HD2  | 1.81                     | 0.43              |
| 1:AH:26:VAL:HG11 | 3:CG:28:LYS:HD3   | 50.98                    | 0.43              |
| 1:AM:209:LEU:HA  | 1:AM:209:LEU:HD22 | 1.74                     | 0.43              |
| 2:BK:224:GLY:HA2 | 2:BK:225:PRO:HD2  | 1.81                     | 0.43              |
| 3:CX:28:LYS:HD3  | 1:DG:26:VAL:HG11  | 234.05                   | 0.43              |
| 1:AS:26:VAL:HG11 | 3:CR:28:LYS:HD3   | 2.00                     | 0.43              |
| 3:CR:28:LYS:HD3  | 1:DC:26:VAL:HG11  | 213.80                   | 0.43              |
| 2:B0:156:SER:HB2 | 3:C0:51:TYR:O     | 2.18                     | 0.43              |
| 1:DH:67:ALA:O    | 1:DH:70:ARG:O     | 2.35                     | 0.43              |
| 1:DF:67:ALA:O    | 1:DF:70:ARG:O     | 2.35                     | 0.43              |
| 1:AW:74:THR:HG21 | 3:CX:43:PHE:CE2   | 2.45                     | 0.43              |
| 2:BB:84:PRO:CD   | 2:BB:85:SER:H     | 2.31                     | 0.43              |
| 2:BU:84:PRO:CD   | 2:BU:85:SER:H     | 2.31                     | 0.43              |
| 1:DC:87:GLN:HE21 | 1:DC:210:ARG:NH2  | 2.12                     | 0.43              |
| 2:B1:84:PRO:CD   | 2:B1:85:SER:H     | 2.31                     | 0.43              |
| 2:BV:84:PRO:CD   | 2:BV:85:SER:H     | 2.31                     | 0.43              |
| 2:BH:83:LEU:HA   | 2:BH:84:PRO:HA    | 1.60                     | 0.43              |
| 1:AY:231:PRO:HG2 | 3:CZ:83:ALA:CB    | 2.48                     | 0.43              |
| 1:AD:231:PRO:HG2 | 3:CE:83:ALA:CB    | 103.74                   | 0.43              |
| 1:AF:231:PRO:HG2 | 3:CG:83:ALA:CB    | 63.69                    | 0.43              |
| 1:AA:146:ILE:O   | 1:AA:147:ALA:CB   | 2.62                     | 0.43              |
| 3:CB:74:PHE:HE2  | 3:CB:183:LEU:HD13 | 1.83                     | 0.43              |
| 3:CG:74:PHE:HE2  | 3:CG:183:LEU:HD13 | 1.83                     | 0.43              |
| 3:CC:74:PHE:HE2  | 3:CC:183:LEU:HD13 | 1.83                     | 0.43              |
| 3:C5:74:PHE:HE2  | 3:C5:183:LEU:HD13 | 1.84                     | 0.43              |
| 3:C6:74:PHE:HE2  | 3:C6:183:LEU:HD13 | 1.83                     | 0.43              |
| 2:B0:166:ARG:HB3 | 3:C0:112:GLY:O    | 2.19                     | 0.43              |
| 3:CW:76:MET:HG3  | 3:CW:76:MET:O     | 2.18                     | 0.43              |
| 1:AG:165:ARG:HA  | 3:CG:32:PRO:HG2   | 2.01                     | 0.43              |
| 1:AG:165:ARG:HA  | 3:CH:32:PRO:HG2   | 70.33                    | 0.43              |
| 3:CS:76:MET:HG3  | 3:CS:76:MET:O     | 2.18                     | 0.43              |
| 1:A5:165:ARG:HA  | 3:C6:32:PRO:HG2   | 2.01                     | 0.43              |
| 3:CB:76:MET:O    | 3:CB:76:MET:HG3   | 2.18                     | 0.43              |
| 1:A8:219:TYR:CD2 | 3:C9:36:VAL:HG22  | 2.53                     | 0.43              |
| 2:BE:156:SER:HB2 | 3:CE:51:TYR:O     | 2.18                     | 0.43              |
| 3:CL:36:VAL:HA   | 3:CL:37:PRO:HD3   | 1.64                     | 0.43              |
| 3:CO:28:LYS:HD3  | 1:DD:26:VAL:HG11  | 263.57                   | 0.43              |
| 2:BO:156:SER:HB2 | 3:CP:51:TYR:O     | 2.18                     | 0.43              |
| 2:BF:224:GLY:HA2 | 2:BF:225:PRO:HD2  | 1.81                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BI:53:ARG:HG2   | 2:BI:221:MET:CE   | 2.48                     | 0.43              |
| 2:B7:224:GLY:HA2  | 2:B7:225:PRO:HD2  | 1.81                     | 0.43              |
| 1:A2:219:TYR:CD2  | 3:C3:36:VAL:HG22  | 2.53                     | 0.43              |
| 3:C9:9:PRO:C      | 3:C9:11:SER:H     | 2.20                     | 0.43              |
| 3:CH:150:LEU:HA   | 3:CH:150:LEU:HD12 | 1.79                     | 0.43              |
| 1:A9:209:LEU:HD22 | 1:A9:209:LEU:HA   | 1.74                     | 0.43              |
| 2:BI:157:VAL:CG2  | 3:CI:50:THR:HG21  | 2.42                     | 0.43              |
| 2:BW:84:PRO:CD    | 2:BW:85:SER:H     | 2.31                     | 0.43              |
| 2:BL:84:PRO:CD    | 2:BL:85:SER:H     | 2.31                     | 0.43              |
| 2:BE:84:PRO:CD    | 2:BE:85:SER:H     | 2.31                     | 0.43              |
| 2:BA:83:LEU:HA    | 2:BA:84:PRO:HA    | 1.60                     | 0.43              |
| 2:BC:84:PRO:CD    | 2:BC:85:SER:H     | 2.31                     | 0.43              |
| 2:BQ:83:LEU:HA    | 2:BQ:84:PRO:HA    | 1.60                     | 0.43              |
| 2:BN:83:LEU:HA    | 2:BN:84:PRO:HA    | 1.60                     | 0.43              |
| 2:BX:84:PRO:CD    | 2:BX:85:SER:H     | 2.31                     | 0.43              |
| 3:CN:74:PHE:HE2   | 3:CN:183:LEU:HD13 | 1.84                     | 0.43              |
| 3:CM:74:PHE:HE2   | 3:CM:183:LEU:HD13 | 1.84                     | 0.43              |
| 3:C2:74:PHE:HE2   | 3:C2:183:LEU:HD13 | 1.84                     | 0.43              |
| 3:CW:74:PHE:HE2   | 3:CW:183:LEU:HD13 | 1.83                     | 0.43              |
| 3:CF:74:PHE:HE2   | 3:CF:183:LEU:HD13 | 1.83                     | 0.43              |
| 3:CJ:74:PHE:HE2   | 3:CJ:183:LEU:HD13 | 1.84                     | 0.43              |
| 2:BX:166:ARG:HB3  | 3:C5:112:GLY:O    | 246.15                   | 0.43              |
| 3:CA:76:MET:HG3   | 3:CA:76:MET:O     | 2.18                     | 0.43              |
| 3:CT:32:PRO:HG2   | 1:DF:165:ARG:HA   | 250.15                   | 0.43              |
| 1:A0:165:ARG:HA   | 3:C1:32:PRO:HG2   | 2.00                     | 0.43              |
| 1:AD:219:TYR:CD2  | 3:CE:36:VAL:HG22  | 77.01                    | 0.43              |
| 2:BG:53:ARG:HG2   | 2:BG:221:MET:CE   | 2.48                     | 0.43              |
| 1:AV:91:THR:HG22  | 1:AW:128:VAL:HG23 | 1.98                     | 0.43              |
| 3:CR:36:VAL:HG22  | 1:DD:219:TYR:CD2  | 222.71                   | 0.43              |
| 2:BD:156:SER:HB2  | 3:CD:51:TYR:O     | 2.18                     | 0.43              |
| 2:BK:156:SER:HB2  | 3:CK:51:TYR:O     | 2.18                     | 0.43              |
| 2:BQ:156:SER:HB2  | 3:CR:51:TYR:O     | 60.32                    | 0.43              |
| 2:BB:156:SER:HB2  | 3:CB:51:TYR:O     | 2.18                     | 0.43              |
| 2:BE:156:SER:HB2  | 3:CF:51:TYR:O     | 58.50                    | 0.43              |
| 2:BN:156:SER:HB2  | 3:CO:51:TYR:O     | 99.59                    | 0.43              |
| 2:BR:156:SER:HB2  | 3:CO:51:TYR:O     | 2.18                     | 0.43              |
| 1:AC:26:VAL:HG11  | 3:DB:28:LYS:HD3   | 257.78                   | 0.43              |
| 1:A5:219:TYR:CD2  | 3:C6:36:VAL:HG22  | 2.53                     | 0.43              |
| 2:B3:224:GLY:HA2  | 2:B3:225:PRO:HD2  | 1.81                     | 0.43              |
| 1:A6:219:TYR:CD2  | 3:C7:36:VAL:HG22  | 2.53                     | 0.43              |
| 2:BA:53:ARG:HG2   | 2:BA:221:MET:CE   | 2.48                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B4:156:SER:HB2  | 3:C4:51:TYR:O     | 2.18                     | 0.43              |
| 2:B1:53:ARG:HG2   | 2:B1:221:MET:CE   | 2.48                     | 0.43              |
| 1:AB:225:PRO:HA   | 1:AB:226:PRO:HD3  | 1.78                     | 0.43              |
| 1:A4:219:TYR:CD2  | 3:C5:36:VAL:HG22  | 2.53                     | 0.43              |
| 2:BM:224:GLY:HA2  | 2:BM:225:PRO:HD2  | 1.81                     | 0.43              |
| 1:AP:67:ALA:O     | 1:AP:70:ARG:O     | 2.35                     | 0.43              |
| 1:AV:67:ALA:O     | 1:AV:70:ARG:O     | 2.35                     | 0.43              |
| 1:AW:67:ALA:O     | 1:AW:70:ARG:O     | 2.35                     | 0.43              |
| 1:AT:242:ASN:HD22 | 1:AU:110:GLY:N    | 2.10                     | 0.43              |
| 1:A5:74:THR:HG21  | 3:C6:43:PHE:CE2   | 2.45                     | 0.43              |
| 2:BJ:84:PRO:CD    | 2:BJ:85:SER:H     | 2.31                     | 0.43              |
| 2:BN:84:PRO:CD    | 2:BN:85:SER:H     | 2.31                     | 0.43              |
| 1:A0:146:ILE:O    | 1:A0:147:ALA:CB   | 2.62                     | 0.43              |
| 3:C1:44:ILE:HD12  | 3:C1:44:ILE:HA    | 1.88                     | 0.43              |
| 3:CF:44:ILE:HA    | 3:CF:44:ILE:HD12  | 1.88                     | 0.43              |
| 3:CU:74:PHE:HE2   | 3:CU:183:LEU:HD13 | 1.83                     | 0.43              |
| 3:C1:74:PHE:HE2   | 3:C1:183:LEU:HD13 | 1.83                     | 0.43              |
| 2:BE:166:ARG:HB3  | 3:CF:112:GLY:O    | 23.81                    | 0.43              |
| 2:BX:166:ARG:HB3  | 3:CX:112:GLY:O    | 2.19                     | 0.43              |
| 2:BN:166:ARG:HB3  | 3:CN:112:GLY:O    | 2.19                     | 0.43              |
| 2:BU:166:ARG:HB3  | 3:CU:112:GLY:O    | 2.19                     | 0.43              |
| 2:BA:166:ARG:HB3  | 3:DB:112:GLY:O    | 287.97                   | 0.43              |
| 2:B7:166:ARG:HB3  | 3:C8:112:GLY:O    | 2.19                     | 0.43              |
| 1:AK:91:THR:HG22  | 1:AN:128:VAL:HG23 | 1.98                     | 0.43              |
| 3:CU:76:MET:O     | 3:CU:76:MET:HG3   | 2.18                     | 0.43              |
| 1:AJ:165:ARG:HA   | 3:CK:32:PRO:HG2   | 2.00                     | 0.43              |
| 1:AK:165:ARG:HA   | 3:CL:32:PRO:HG2   | 2.01                     | 0.43              |
| 3:CS:36:VAL:HG22  | 1:DE:219:TYR:CD2  | 266.96                   | 0.43              |
| 2:BH:156:SER:HB2  | 3:CI:51:TYR:O     | 63.55                    | 0.43              |
| 2:BI:156:SER:HB2  | 3:CJ:51:TYR:O     | 99.59                    | 0.43              |
| 2:BU:156:SER:HB2  | 3:CU:51:TYR:O     | 2.18                     | 0.43              |
| 1:AI:26:VAL:HG11  | 3:CF:28:LYS:HD3   | 2.00                     | 0.43              |
| 1:AL:26:VAL:HG11  | 3:CN:28:LYS:HD3   | 2.00                     | 0.43              |
| 1:AE:26:VAL:HG11  | 3:CC:28:LYS:HD3   | 2.00                     | 0.43              |
| 3:CH:28:LYS:HD3   | 1:DK:26:VAL:HG11  | 2.00                     | 0.43              |
| 1:AW:26:VAL:HG11  | 3:CU:28:LYS:HD3   | 2.00                     | 0.43              |
| 1:A9:219:TYR:CD2  | 3:DA:36:VAL:HG22  | 2.53                     | 0.43              |
| 1:A0:219:TYR:CD2  | 3:C1:36:VAL:HG22  | 2.53                     | 0.43              |
| 1:A7:209:LEU:HA   | 1:A7:209:LEU:HD22 | 1.74                     | 0.43              |
| 1:AU:72:LEU:HD23  | 1:AU:72:LEU:HA    | 1.83                     | 0.43              |
| 1:A6:26:VAL:HG11  | 3:C4:28:LYS:HD3   | 2.00                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A5:67:ALA:O    | 1:A5:70:ARG:O     | 2.35                     | 0.43              |
| 1:AX:207:CYS:O   | 1:AX:208:TYR:CB   | 2.58                     | 0.43              |
| 1:AC:87:GLN:HE21 | 1:AC:210:ARG:NH2  | 2.12                     | 0.43              |
| 1:AH:87:GLN:HE21 | 1:AH:210:ARG:NH2  | 2.12                     | 0.43              |
| 3:CX:74:PHE:HE2  | 3:CX:183:LEU:HD13 | 1.84                     | 0.43              |
| 3:C8:74:PHE:HE2  | 3:C8:183:LEU:HD13 | 1.83                     | 0.43              |
| 3:CL:74:PHE:HE2  | 3:CL:183:LEU:HD13 | 1.83                     | 0.43              |
| 2:BK:166:ARG:HB3 | 3:CK:112:GLY:O    | 2.19                     | 0.43              |
| 2:BS:166:ARG:HB3 | 3:CT:112:GLY:O    | 85.79                    | 0.43              |
| 2:BV:166:ARG:HB3 | 3:CV:112:GLY:O    | 2.19                     | 0.43              |
| 2:BC:166:ARG:HB3 | 3:CC:112:GLY:O    | 2.19                     | 0.43              |
| 2:BH:166:ARG:HB3 | 3:CH:112:GLY:O    | 2.19                     | 0.43              |
| 2:BH:166:ARG:HB3 | 3:CI:112:GLY:O    | 85.79                    | 0.43              |
| 2:BT:166:ARG:HB3 | 3:CT:112:GLY:O    | 2.19                     | 0.43              |
| 2:BT:166:ARG:HB3 | 3:CU:112:GLY:O    | 246.13                   | 0.43              |
| 2:BZ:166:ARG:HB3 | 3:CZ:112:GLY:O    | 2.19                     | 0.43              |
| 2:BO:166:ARG:HB3 | 3:CP:112:GLY:O    | 2.19                     | 0.43              |
| 3:CM:76:MET:O    | 3:CM:76:MET:HG3   | 2.18                     | 0.43              |
| 3:CV:76:MET:O    | 3:CV:76:MET:HG3   | 2.18                     | 0.43              |
| 3:CJ:76:MET:HG3  | 3:CJ:76:MET:O     | 2.18                     | 0.43              |
| 1:AR:165:ARG:HA  | 3:CS:32:PRO:HG2   | 2.00                     | 0.43              |
| 1:A4:165:ARG:HA  | 3:C5:32:PRO:HG2   | 2.01                     | 0.43              |
| 1:AN:165:ARG:HA  | 3:CO:32:PRO:HG2   | 2.01                     | 0.43              |
| 1:AA:165:ARG:HA  | 3:DB:32:PRO:HG2   | 272.44                   | 0.43              |
| 2:BY:86:ASP:CB   | 2:BY:141:LYS:HA   | 2.49                     | 0.43              |
| 1:AB:219:TYR:CD2 | 3:CB:36:VAL:HG22  | 2.53                     | 0.43              |
| 1:AO:165:ARG:HA  | 3:CP:32:PRO:HG2   | 2.01                     | 0.43              |
| 2:BS:156:SER:HB2 | 3:CT:51:TYR:O     | 63.55                    | 0.43              |
| 2:BC:156:SER:HB2 | 3:CC:51:TYR:O     | 2.18                     | 0.43              |
| 1:AX:26:VAL:HG11 | 3:CW:28:LYS:HD3   | 2.00                     | 0.43              |
| 3:CT:28:LYS:HD3  | 1:DI:26:VAL:HG11  | 244.36                   | 0.43              |
| 2:BN:224:GLY:HA2 | 2:BN:225:PRO:HD2  | 1.81                     | 0.43              |
| 2:B4:166:ARG:HB3 | 3:C4:112:GLY:O    | 2.19                     | 0.43              |
| 2:BY:156:SER:HB2 | 3:CY:51:TYR:O     | 2.18                     | 0.43              |
| 1:DG:225:PRO:HA  | 1:DG:226:PRO:HD3  | 1.77                     | 0.43              |
| 1:AQ:240:PRO:HG2 | 1:AR:114:LYS:HB2  | 2.01                     | 0.43              |
| 1:A1:219:TYR:CD2 | 3:C2:36:VAL:HG22  | 2.53                     | 0.43              |
| 3:CR:150:LEU:HA  | 3:CR:150:LEU:HD12 | 1.79                     | 0.43              |
| 1:AT:72:LEU:HD23 | 1:AT:72:LEU:HA    | 1.82                     | 0.43              |
| 1:AA:240:PRO:HG2 | 1:AB:114:LYS:HB2  | 2.01                     | 0.43              |
| 2:B3:166:ARG:HB3 | 3:C3:112:GLY:O    | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A2:67:ALA:O     | 1:A2:70:ARG:O     | 2.35                     | 0.43              |
| 1:AZ:67:ALA:O     | 1:AZ:70:ARG:O     | 2.35                     | 0.43              |
| 3:CG:175:THR:HG23 | 3:CG:176:VAL:N    | 2.34                     | 0.43              |
| 3:CP:175:THR:HG23 | 3:CP:176:VAL:N    | 2.34                     | 0.43              |
| 1:A8:242:ASN:HD22 | 1:A9:110:GLY:N    | 2.10                     | 0.43              |
| 1:AM:87:GLN:HE21  | 1:AM:210:ARG:NH2  | 2.12                     | 0.43              |
| 2:BF:85:SER:HB2   | 2:BF:190:ASN:ND2  | 2.31                     | 0.43              |
| 2:B6:83:LEU:HA    | 2:B6:84:PRO:HA    | 1.60                     | 0.43              |
| 2:B6:84:PRO:CD    | 2:B6:85:SER:H     | 2.31                     | 0.43              |
| 2:BR:152:TYR:CB   | 2:BR:197:LEU:HD11 | 2.49                     | 0.43              |
| 1:AH:163:MET:HE3  | 1:AH:189:GLY:HA3  | 2.07                     | 0.43              |
| 3:C2:44:ILE:HA    | 3:C2:44:ILE:HD12  | 1.88                     | 0.43              |
| 3:CV:74:PHE:HE2   | 3:CV:183:LEU:HD13 | 1.84                     | 0.43              |
| 2:BD:166:ARG:HB3  | 3:CE:112:GLY:O    | 136.25                   | 0.43              |
| 2:BL:166:ARG:HB3  | 3:CL:112:GLY:O    | 2.19                     | 0.43              |
| 2:BQ:166:ARG:HB3  | 3:CR:112:GLY:O    | 83.24                    | 0.43              |
| 2:BD:166:ARG:HB3  | 3:CD:112:GLY:O    | 2.19                     | 0.43              |
| 2:BR:86:ASP:CB    | 2:BR:141:LYS:HA   | 2.49                     | 0.43              |
| 2:BC:86:ASP:CB    | 2:BC:141:LYS:HA   | 2.49                     | 0.43              |
| 1:AV:165:ARG:HA   | 3:CW:32:PRO:HG2   | 2.01                     | 0.43              |
| 3:CO:76:MET:O     | 3:CO:76:MET:HG3   | 2.18                     | 0.43              |
| 3:CR:76:MET:O     | 3:CR:76:MET:HG3   | 2.18                     | 0.43              |
| 1:A2:165:ARG:HA   | 3:C3:32:PRO:HG2   | 2.01                     | 0.43              |
| 3:CI:76:MET:HG3   | 3:CI:76:MET:O     | 2.18                     | 0.43              |
| 1:AG:219:TYR:CD2  | 3:CG:36:VAL:HG22  | 2.53                     | 0.43              |
| 1:AZ:165:ARG:HA   | 3:C0:32:PRO:HG2   | 2.00                     | 0.43              |
| 1:AV:26:VAL:HG11  | 3:CX:28:LYS:HD3   | 2.00                     | 0.43              |
| 1:AZ:26:VAL:HG11  | 3:C3:28:LYS:HD3   | 2.00                     | 0.43              |
| 2:B1:166:ARG:HB3  | 3:C1:112:GLY:O    | 2.19                     | 0.43              |
| 2:BY:53:ARG:HG2   | 2:BY:221:MET:CE   | 2.48                     | 0.43              |
| 2:BU:118:PHE:CD1  | 2:B6:118:PHE:HE2  | 251.94                   | 0.43              |
| 3:CW:150:LEU:HD12 | 3:CW:150:LEU:HA   | 1.79                     | 0.43              |
| 2:B2:156:SER:HB2  | 3:C2:51:TYR:O     | 2.18                     | 0.43              |
| 2:BS:53:ARG:HG2   | 2:BS:221:MET:CE   | 2.48                     | 0.43              |
| 1:AF:114:LYS:HB2  | 1:AH:240:PRO:HG2  | 46.58                    | 0.43              |
| 1:AL:240:PRO:HG2  | 1:AM:114:LYS:HB2  | 2.01                     | 0.43              |
| 2:B8:166:ARG:HB3  | 3:C9:112:GLY:O    | 2.19                     | 0.43              |
| 1:A1:26:VAL:HG11  | 3:CZ:28:LYS:HD3   | 2.00                     | 0.43              |
| 1:DI:67:ALA:O     | 1:DI:70:ARG:O     | 2.35                     | 0.43              |
| 1:AU:67:ALA:O     | 1:AU:70:ARG:O     | 2.35                     | 0.43              |
| 1:A6:67:ALA:O     | 1:A6:70:ARG:O     | 2.35                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AC:191:HIS:HD2  | 1:AC:193:GLY:N    | 2.08                     | 0.43              |
| 3:CV:175:THR:HG23 | 3:CV:176:VAL:N    | 2.34                     | 0.43              |
| 3:C4:175:THR:HG23 | 3:C4:176:VAL:N    | 2.34                     | 0.43              |
| 3:C1:175:THR:HG23 | 3:C1:176:VAL:N    | 2.34                     | 0.43              |
| 3:CA:175:THR:HG23 | 3:CA:176:VAL:N    | 2.34                     | 0.43              |
| 2:BQ:84:PRO:CD    | 2:BQ:85:SER:H     | 2.31                     | 0.43              |
| 1:AJ:231:PRO:HG2  | 3:CK:83:ALA:CB    | 2.48                     | 0.43              |
| 2:BY:152:TYR:CB   | 2:BY:197:LEU:HD11 | 2.49                     | 0.43              |
| 2:BJ:152:TYR:CB   | 2:BJ:197:LEU:HD11 | 2.49                     | 0.43              |
| 1:AK:146:ILE:O    | 1:AK:147:ALA:CB   | 2.62                     | 0.43              |
| 3:CH:74:PHE:HE2   | 3:CH:183:LEU:HD13 | 1.83                     | 0.43              |
| 3:CK:74:PHE:HE2   | 3:CK:183:LEU:HD13 | 1.84                     | 0.43              |
| 2:BI:166:ARG:HB3  | 3:CI:112:GLY:O    | 2.19                     | 0.43              |
| 2:BJ:166:ARG:HB3  | 3:CJ:112:GLY:O    | 2.19                     | 0.43              |
| 2:BW:166:ARG:HB3  | 3:CX:112:GLY:O    | 85.79                    | 0.43              |
| 2:BM:166:ARG:HB3  | 3:CM:112:GLY:O    | 2.19                     | 0.43              |
| 2:BM:166:ARG:HB3  | 3:CN:112:GLY:O    | 85.79                    | 0.43              |
| 3:CZ:74:PHE:HE2   | 3:CZ:183:LEU:HD13 | 1.83                     | 0.43              |
| 2:B6:166:ARG:HB3  | 3:C7:112:GLY:O    | 2.19                     | 0.43              |
| 2:BD:86:ASP:CB    | 2:BD:141:LYS:HA   | 2.49                     | 0.43              |
| 2:BX:86:ASP:CB    | 2:BX:141:LYS:HA   | 2.49                     | 0.43              |
| 1:AF:165:ARG:HA   | 3:CF:32:PRO:HG2   | 2.00                     | 0.43              |
| 1:AI:165:ARG:HA   | 3:CJ:32:PRO:HG2   | 71.30                    | 0.43              |
| 3:CV:32:PRO:HG2   | 1:DH:165:ARG:HA   | 269.17                   | 0.43              |
| 1:AW:165:ARG:HA   | 3:CX:32:PRO:HG2   | 2.01                     | 0.43              |
| 2:BA:86:ASP:CB    | 2:BA:141:LYS:HA   | 2.49                     | 0.43              |
| 3:C5:76:MET:O     | 3:C5:76:MET:HG3   | 2.18                     | 0.43              |
| 3:CJ:36:VAL:HG22  | 1:DK:219:TYR:CD2  | 2.53                     | 0.43              |
| 3:C4:76:MET:O     | 3:C4:76:MET:HG3   | 2.18                     | 0.43              |
| 3:CA:36:VAL:HA    | 3:CA:37:PRO:HD3   | 1.64                     | 0.43              |
| 1:AG:26:VAL:HG11  | 3:CJ:28:LYS:HD3   | 2.00                     | 0.43              |
| 1:AN:26:VAL:HG11  | 3:CM:28:LYS:HD3   | 2.00                     | 0.43              |
| 1:AO:26:VAL:HG11  | 3:CQ:28:LYS:HD3   | 2.00                     | 0.43              |
| 1:AF:114:LYS:HB2  | 1:AI:240:PRO:HG2  | 2.01                     | 0.43              |
| 1:AK:114:LYS:HB2  | 1:AM:240:PRO:HG2  | 46.58                    | 0.43              |
| 1:A2:26:VAL:HG11  | 3:C1:28:LYS:HD3   | 2.00                     | 0.43              |
| 2:B2:53:ARG:HG2   | 2:B2:221:MET:CE   | 2.48                     | 0.43              |
| 2:B6:224:GLY:HA2  | 2:B6:225:PRO:HD2  | 1.81                     | 0.43              |
| 1:AN:72:LEU:HD23  | 1:AN:72:LEU:HA    | 1.83                     | 0.43              |
| 2:B3:53:ARG:HG2   | 2:B3:221:MET:CE   | 2.48                     | 0.43              |
| 2:BF:124:LEU:HD23 | 2:BF:198:ILE:HA   | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:DG:240:PRO:HG2  | 1:DJ:114:LYS:HB2  | 2.01                     | 0.43              |
| 1:AV:225:PRO:HA   | 1:AV:226:PRO:HD3  | 1.78                     | 0.43              |
| 1:A1:191:HIS:HD2  | 1:A1:193:GLY:N    | 2.08                     | 0.43              |
| 3:DA:175:THR:HG23 | 3:DA:176:VAL:N    | 2.34                     | 0.43              |
| 1:AL:187:LEU:HA   | 1:AL:188:PRO:HD2  | 1.95                     | 0.43              |
| 3:CW:175:THR:HG23 | 3:CW:176:VAL:N    | 2.34                     | 0.43              |
| 2:B4:157:VAL:CG2  | 3:C4:50:THR:HG21  | 2.42                     | 0.43              |
| 1:AV:187:LEU:HA   | 1:AV:188:PRO:HD2  | 1.95                     | 0.43              |
| 3:C7:175:THR:HG23 | 3:C7:176:VAL:N    | 2.34                     | 0.43              |
| 1:AN:74:THR:HG21  | 3:CO:43:PHE:CE2   | 4.65                     | 0.43              |
| 2:B7:84:PRO:CD    | 2:B7:85:SER:H     | 2.31                     | 0.43              |
| 2:BS:85:SER:HB2   | 2:BS:190:ASN:ND2  | 2.32                     | 0.43              |
| 1:AA:231:PRO:HG2  | 3:DB:83:ALA:CB    | 288.88                   | 0.43              |
| 1:AB:231:PRO:HG2  | 3:CB:83:ALA:CB    | 2.48                     | 0.43              |
| 1:AQ:212:ARG:NH2  | 3:CR:18:VAL:O     | 2.46                     | 0.43              |
| 2:BT:152:TYR:CB   | 2:BT:197:LEU:HD11 | 2.49                     | 0.43              |
| 2:BA:152:TYR:CB   | 2:BA:197:LEU:HD11 | 2.49                     | 0.43              |
| 2:BL:152:TYR:CB   | 2:BL:197:LEU:HD11 | 2.49                     | 0.43              |
| 3:CY:74:PHE:HE2   | 3:CY:183:LEU:HD13 | 1.83                     | 0.43              |
| 2:BA:166:ARG:HB3  | 3:CA:112:GLY:O    | 2.19                     | 0.43              |
| 1:AW:219:TYR:CD2  | 3:CX:36:VAL:HG22  | 2.53                     | 0.43              |
| 2:B0:86:ASP:CB    | 2:B0:141:LYS:HA   | 2.49                     | 0.43              |
| 2:BB:86:ASP:CB    | 2:BB:141:LYS:HA   | 2.49                     | 0.43              |
| 3:CW:32:PRO:HG2   | 1:DI:165:ARG:HA   | 234.36                   | 0.43              |
| 2:B7:86:ASP:CB    | 2:B7:141:LYS:HA   | 2.49                     | 0.43              |
| 1:A7:165:ARG:HA   | 3:C8:32:PRO:HG2   | 2.00                     | 0.43              |
| 2:B5:86:ASP:CB    | 2:B5:141:LYS:HA   | 2.49                     | 0.43              |
| 2:BQ:86:ASP:CB    | 2:BQ:141:LYS:HA   | 2.49                     | 0.43              |
| 1:AT:26:VAL:HG11  | 3:CV:28:LYS:HD3   | 2.00                     | 0.43              |
| 1:AT:219:TYR:CD2  | 3:CU:36:VAL:HG22  | 2.53                     | 0.43              |
| 1:AA:26:VAL:HG11  | 3:CB:28:LYS:HD3   | 2.00                     | 0.43              |
| 1:AF:26:VAL:HG11  | 3:CG:28:LYS:HD3   | 2.00                     | 0.43              |
| 1:A8:26:VAL:HG11  | 3:DA:28:LYS:HD3   | 2.00                     | 0.43              |
| 3:CS:40:PHE:CD2   | 1:DE:221:PRO:HD3  | 270.49                   | 0.43              |
| 2:BZ:224:GLY:HA2  | 2:BZ:225:PRO:HD2  | 1.81                     | 0.43              |
| 1:AI:209:LEU:HD22 | 1:AI:209:LEU:HA   | 1.74                     | 0.43              |
| 1:AN:114:LYS:HB2  | 1:DD:240:PRO:HG2  | 318.98                   | 0.43              |
| 3:CW:40:PHE:CD2   | 1:DI:221:PRO:HD3  | 213.25                   | 0.43              |
| 1:AD:240:PRO:HG2  | 1:AE:114:LYS:HB2  | 76.63                    | 0.43              |
| 1:A4:221:PRO:HD3  | 3:C5:40:PHE:CD2   | 2.54                     | 0.43              |
| 1:AE:191:HIS:HD2  | 1:AE:193:GLY:N    | 2.08                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:CH:175:THR:HG23 | 3:CH:176:VAL:N    | 2.34                     | 0.43              |
| 3:CI:175:THR:HG23 | 3:CI:176:VAL:N    | 2.34                     | 0.43              |
| 3:CJ:175:THR:HG23 | 3:CJ:176:VAL:N    | 2.34                     | 0.43              |
| 3:CL:175:THR:HG23 | 3:CL:176:VAL:N    | 2.34                     | 0.43              |
| 3:CO:175:THR:HG23 | 3:CO:176:VAL:N    | 2.34                     | 0.43              |
| 3:C9:175:THR:HG23 | 3:C9:176:VAL:N    | 2.34                     | 0.43              |
| 3:DB:175:THR:HG23 | 3:DB:176:VAL:N    | 2.34                     | 0.43              |
| 3:CX:83:ALA:CB    | 1:DJ:231:PRO:HG2  | 284.00                   | 0.43              |
| 2:BO:152:TYR:CB   | 2:BO:197:LEU:HD11 | 2.49                     | 0.43              |
| 2:BD:152:TYR:CB   | 2:BD:197:LEU:HD11 | 2.49                     | 0.43              |
| 2:BF:152:TYR:CB   | 2:BF:197:LEU:HD11 | 2.49                     | 0.43              |
| 2:B2:152:TYR:CB   | 2:B2:197:LEU:HD11 | 2.49                     | 0.43              |
| 2:BQ:152:TYR:CB   | 2:BQ:197:LEU:HD11 | 2.49                     | 0.43              |
| 2:BK:152:TYR:CB   | 2:BK:197:LEU:HD11 | 2.49                     | 0.43              |
| 2:B7:152:TYR:CB   | 2:B7:197:LEU:HD11 | 2.49                     | 0.43              |
| 2:BX:152:TYR:CB   | 2:BX:197:LEU:HD11 | 2.49                     | 0.43              |
| 2:B1:152:TYR:CB   | 2:B1:197:LEU:HD11 | 2.49                     | 0.43              |
| 3:C3:74:PHE:HE2   | 3:C3:183:LEU:HD13 | 1.83                     | 0.43              |
| 2:BB:166:ARG:HB3  | 3:CB:112:GLY:O    | 2.19                     | 0.43              |
| 2:BG:166:ARG:HB3  | 3:CG:112:GLY:O    | 2.19                     | 0.43              |
| 2:B2:166:ARG:HB3  | 3:C2:112:GLY:O    | 2.19                     | 0.43              |
| 2:BY:166:ARG:HB3  | 3:CY:112:GLY:O    | 2.19                     | 0.43              |
| 1:AB:165:ARG:HA   | 3:CB:32:PRO:HG2   | 2.01                     | 0.43              |
| 1:AC:165:ARG:HA   | 3:CC:32:PRO:HG2   | 2.01                     | 0.43              |
| 2:BH:86:ASP:CB    | 2:BH:141:LYS:HA   | 2.49                     | 0.43              |
| 2:BJ:86:ASP:CB    | 2:BJ:141:LYS:HA   | 2.49                     | 0.43              |
| 1:AX:165:ARG:HA   | 3:CY:32:PRO:HG2   | 2.00                     | 0.43              |
| 2:BW:86:ASP:CB    | 2:BW:141:LYS:HA   | 2.49                     | 0.43              |
| 1:AE:219:TYR:CD2  | 3:CE:36:VAL:HG22  | 2.53                     | 0.43              |
| 2:BF:156:SER:HB2  | 3:CF:51:TYR:O     | 2.18                     | 0.43              |
| 2:BJ:156:SER:HB2  | 3:CJ:51:TYR:O     | 2.18                     | 0.43              |
| 1:AL:26:VAL:HG11  | 3:CJ:28:LYS:HD3   | 169.78                   | 0.43              |
| 1:A9:26:VAL:HG11  | 3:CD:28:LYS:HD3   | 255.14                   | 0.43              |
| 3:CU:28:LYS:HD3   | 1:DF:26:VAL:HG11  | 221.86                   | 0.43              |
| 1:AN:240:PRO:HG2  | 1:AO:114:LYS:HB2  | 264.01                   | 0.43              |
| 1:AP:221:PRO:HD3  | 3:CQ:40:PHE:CD1   | 2.54                     | 0.43              |
| 2:B7:53:ARG:HG2   | 2:B7:221:MET:CE   | 2.48                     | 0.43              |
| 1:A6:225:PRO:HA   | 1:A6:226:PRO:HD3  | 1.78                     | 0.43              |
| 1:AD:221:PRO:HD3  | 3:CE:40:PHE:CD2   | 76.67                    | 0.43              |
| 1:A4:26:VAL:HG11  | 3:C8:28:LYS:HD3   | 2.00                     | 0.43              |
| 3:CT:40:PHE:CD2   | 1:DF:221:PRO:HD3  | 251.05                   | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A0:26:VAL:HG11  | 3:C2:28:LYS:HD3   | 2.00                     | 0.43              |
| 2:BI:224:GLY:HA2  | 2:BI:225:PRO:HD2  | 1.81                     | 0.43              |
| 1:AV:114:LYS:HB2  | 1:AX:240:PRO:HG2  | 2.01                     | 0.43              |
| 1:AZ:240:PRO:HG2  | 1:A2:114:LYS:HB2  | 2.01                     | 0.43              |
| 2:BJ:224:GLY:HA2  | 2:BJ:225:PRO:HD2  | 1.81                     | 0.43              |
| 1:AY:114:LYS:HB2  | 1:A1:240:PRO:HG2  | 2.01                     | 0.43              |
| 2:B6:124:LEU:HD23 | 2:B6:198:ILE:HA   | 2.00                     | 0.43              |
| 1:A4:225:PRO:HA   | 1:A4:226:PRO:HD3  | 1.78                     | 0.43              |
| 1:DF:114:LYS:HB2  | 1:DI:240:PRO:HG2  | 2.01                     | 0.43              |
| 3:CB:175:THR:HG23 | 3:CB:176:VAL:N    | 2.34                     | 0.43              |
| 3:CC:175:THR:HG23 | 3:CC:176:VAL:N    | 2.34                     | 0.43              |
| 3:CK:175:THR:HG23 | 3:CK:176:VAL:N    | 2.34                     | 0.43              |
| 3:CU:175:THR:HG23 | 3:CU:176:VAL:N    | 2.34                     | 0.43              |
| 3:CT:175:THR:HG23 | 3:CT:176:VAL:N    | 2.34                     | 0.43              |
| 3:CQ:175:THR:HG23 | 3:CQ:176:VAL:N    | 2.34                     | 0.43              |
| 1:A6:87:GLN:HE21  | 1:A6:210:ARG:NH2  | 2.12                     | 0.43              |
| 1:AF:74:THR:HG21  | 3:CF:43:PHE:CE1   | 2.45                     | 0.43              |
| 1:A1:74:THR:HG21  | 3:C2:43:PHE:CE2   | 2.45                     | 0.43              |
| 2:B8:84:PRO:CD    | 2:B8:85:SER:H     | 2.31                     | 0.43              |
| 1:AH:231:PRO:HG2  | 3:CH:83:ALA:CB    | 2.48                     | 0.43              |
| 1:A9:212:ARG:NH2  | 3:DA:18:VAL:O     | 2.46                     | 0.43              |
| 2:BH:152:TYR:CB   | 2:BH:197:LEU:HD11 | 2.49                     | 0.43              |
| 2:BU:152:TYR:CB   | 2:BU:197:LEU:HD11 | 2.49                     | 0.43              |
| 2:BG:152:TYR:CB   | 2:BG:197:LEU:HD11 | 2.49                     | 0.43              |
| 2:BR:152:TYR:HB3  | 2:BR:197:LEU:HD11 | 2.01                     | 0.43              |
| 2:BV:152:TYR:CB   | 2:BV:197:LEU:HD11 | 2.49                     | 0.43              |
| 2:BE:152:TYR:HB3  | 2:BE:197:LEU:HD11 | 2.01                     | 0.43              |
| 3:CO:74:PHE:HE2   | 3:CO:183:LEU:HD13 | 1.84                     | 0.43              |
| 2:BR:166:ARG:HB3  | 3:CS:112:GLY:O    | 197.41                   | 0.43              |
| 2:BS:166:ARG:HB3  | 3:CQ:112:GLY:O    | 2.19                     | 0.43              |
| 2:BE:86:ASP:CB    | 2:BE:141:LYS:HA   | 2.49                     | 0.43              |
| 2:BL:86:ASP:CB    | 2:BL:141:LYS:HA   | 2.49                     | 0.43              |
| 1:AM:165:ARG:HA   | 3:CN:32:PRO:HG2   | 2.00                     | 0.43              |
| 1:AQ:165:ARG:HA   | 3:CR:32:PRO:HG2   | 2.01                     | 0.43              |
| 1:AS:165:ARG:HA   | 3:CT:32:PRO:HG2   | 2.00                     | 0.43              |
| 3:CU:32:PRO:HG2   | 1:DG:165:ARG:HA   | 239.15                   | 0.43              |
| 2:BS:86:ASP:CB    | 2:BS:141:LYS:HA   | 2.49                     | 0.43              |
| 3:CK:76:MET:HG3   | 3:CK:76:MET:O     | 2.18                     | 0.43              |
| 2:BV:86:ASP:CB    | 2:BV:141:LYS:HA   | 2.49                     | 0.43              |
| 2:B1:86:ASP:CB    | 2:B1:141:LYS:HA   | 2.49                     | 0.43              |
| 2:B6:86:ASP:CB    | 2:B6:141:LYS:HA   | 2.49                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BI:86:ASP:CB    | 2:BI:141:LYS:HA   | 2.49                     | 0.43              |
| 2:B3:86:ASP:CB    | 2:B3:141:LYS:HA   | 2.49                     | 0.43              |
| 1:AH:187:LEU:HD23 | 1:AH:187:LEU:HA   | 1.90                     | 0.43              |
| 1:AA:219:TYR:CD2  | 3:CA:36:VAL:HG22  | 2.53                     | 0.43              |
| 2:BM:156:SER:HB2  | 3:CM:51:TYR:O     | 2.18                     | 0.43              |
| 2:BW:156:SER:HB2  | 3:CW:51:TYR:O     | 2.18                     | 0.43              |
| 2:BP:156:SER:HB2  | 3:CQ:51:TYR:O     | 99.59                    | 0.43              |
| 1:AJ:26:VAL:HG11  | 3:CL:28:LYS:HD3   | 2.00                     | 0.43              |
| 1:AE:221:PRO:HD3  | 3:CE:40:PHE:CD1   | 2.54                     | 0.43              |
| 1:AC:221:PRO:HD3  | 3:CD:40:PHE:CD2   | 49.74                    | 0.43              |
| 1:AF:221:PRO:HD3  | 3:CF:40:PHE:CD1   | 2.54                     | 0.43              |
| 1:A3:240:PRO:HG2  | 1:A4:114:LYS:HB2  | 2.01                     | 0.43              |
| 1:A7:221:PRO:HD3  | 3:C8:40:PHE:CD2   | 2.54                     | 0.43              |
| 1:AC:114:LYS:HB2  | 1:AE:240:PRO:HG2  | 2.01                     | 0.43              |
| 1:A0:221:PRO:HD3  | 3:C1:40:PHE:CD2   | 2.54                     | 0.43              |
| 1:AK:221:PRO:HD3  | 3:CL:40:PHE:CD1   | 2.54                     | 0.43              |
| 1:AK:221:PRO:HD3  | 3:CL:40:PHE:CD2   | 4.39                     | 0.43              |
| 3:CU:40:PHE:CD2   | 1:DG:221:PRO:HD3  | 258.60                   | 0.43              |
| 1:AP:209:LEU:HD22 | 1:AP:209:LEU:HA   | 1.74                     | 0.43              |
| 2:BY:124:LEU:HD23 | 2:BY:198:ILE:HA   | 2.00                     | 0.43              |
| 1:AO:221:PRO:HD3  | 3:CP:40:PHE:CD1   | 2.54                     | 0.43              |
| 2:BT:157:VAL:CG2  | 3:CT:50:THR:HG21  | 2.43                     | 0.42              |
| 3:CD:175:THR:HG23 | 3:CD:176:VAL:N    | 2.34                     | 0.42              |
| 3:CS:175:THR:HG23 | 3:CS:176:VAL:N    | 2.34                     | 0.42              |
| 1:AZ:187:LEU:HA   | 1:AZ:188:PRO:HD2  | 1.95                     | 0.42              |
| 3:CZ:175:THR:HG23 | 3:CZ:176:VAL:N    | 2.34                     | 0.42              |
| 3:CY:175:THR:HG23 | 3:CY:176:VAL:N    | 2.34                     | 0.42              |
| 1:AK:87:GLN:HE21  | 1:AK:210:ARG:NH2  | 2.12                     | 0.42              |
| 2:B5:85:SER:HB2   | 2:B5:190:ASN:ND2  | 2.31                     | 0.42              |
| 2:B3:84:PRO:CD    | 2:B3:85:SER:H     | 2.31                     | 0.42              |
| 2:BW:152:TYR:HB3  | 2:BW:197:LEU:HD11 | 2.02                     | 0.42              |
| 2:BK:152:TYR:HB3  | 2:BK:197:LEU:HD11 | 2.02                     | 0.42              |
| 2:BE:152:TYR:CB   | 2:BE:197:LEU:HD11 | 2.49                     | 0.42              |
| 3:CA:44:ILE:HD12  | 3:CA:44:ILE:HA    | 1.88                     | 0.42              |
| 3:CO:44:ILE:HD12  | 3:CO:44:ILE:HA    | 1.88                     | 0.42              |
| 3:CT:74:PHE:HE2   | 3:CT:183:LEU:HD13 | 1.84                     | 0.42              |
| 3:CD:74:PHE:HE2   | 3:CD:183:LEU:HD13 | 1.84                     | 0.42              |
| 2:BB:166:ARG:HB3  | 3:CC:112:GLY:O    | 137.22                   | 0.42              |
| 2:BF:166:ARG:HB3  | 3:CG:112:GLY:O    | 85.79                    | 0.42              |
| 2:BJ:166:ARG:HB3  | 3:CK:112:GLY:O    | 255.37                   | 0.42              |
| 2:BE:166:ARG:HB3  | 3:CE:112:GLY:O    | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BF:166:ARG:HB3  | 3:CF:112:GLY:O    | 2.19                     | 0.42              |
| 2:BK:166:ARG:HB3  | 3:CL:112:GLY:O    | 85.79                    | 0.42              |
| 2:BQ:166:ARG:HB3  | 3:CS:112:GLY:O    | 2.19                     | 0.42              |
| 2:BU:86:ASP:CB    | 2:BU:141:LYS:HA   | 2.49                     | 0.42              |
| 1:AF:165:ARG:HA   | 3:CG:32:PRO:HG2   | 42.51                    | 0.42              |
| 2:BM:86:ASP:CB    | 2:BM:141:LYS:HA   | 2.49                     | 0.42              |
| 2:BN:86:ASP:CB    | 2:BN:141:LYS:HA   | 2.49                     | 0.42              |
| 2:BR:156:SER:HB2  | 3:CS:51:TYR:O     | 205.62                   | 0.42              |
| 1:AI:114:LYS:HB2  | 1:AL:240:PRO:HG2  | 154.40                   | 0.42              |
| 1:AB:240:PRO:HG2  | 1:A8:114:LYS:HB2  | 237.63                   | 0.42              |
| 1:AB:221:PRO:HD3  | 3:CB:40:PHE:CD1   | 2.54                     | 0.42              |
| 1:AC:221:PRO:HD3  | 3:CC:40:PHE:CD1   | 2.54                     | 0.42              |
| 1:A5:221:PRO:HD3  | 3:C6:40:PHE:CD2   | 2.54                     | 0.42              |
| 1:A8:209:LEU:HD22 | 1:A8:209:LEU:HA   | 1.74                     | 0.42              |
| 1:DC:114:LYS:HB2  | 1:DE:240:PRO:HG2  | 2.01                     | 0.42              |
| 1:DF:191:HIS:HD2  | 1:DF:193:GLY:N    | 2.08                     | 0.42              |
| 1:AJ:187:LEU:HA   | 1:AJ:187:LEU:HD23 | 1.91                     | 0.42              |
| 3:CN:175:THR:HG23 | 3:CN:176:VAL:N    | 2.34                     | 0.42              |
| 3:CR:175:THR:HG23 | 3:CR:176:VAL:N    | 2.34                     | 0.42              |
| 1:AL:242:ASN:HD22 | 1:AM:110:GLY:N    | 2.09                     | 0.42              |
| 1:AO:231:PRO:HG2  | 3:CP:83:ALA:CB    | 2.48                     | 0.42              |
| 1:AP:231:PRO:HG2  | 3:CQ:83:ALA:CB    | 2.48                     | 0.42              |
| 2:BO:152:TYR:HB3  | 2:BO:197:LEU:HD11 | 2.02                     | 0.42              |
| 2:BN:152:TYR:CB   | 2:BN:197:LEU:HD11 | 2.49                     | 0.42              |
| 2:BN:152:TYR:HB3  | 2:BN:197:LEU:HD11 | 2.01                     | 0.42              |
| 2:BM:152:TYR:CB   | 2:BM:197:LEU:HD11 | 2.49                     | 0.42              |
| 2:B6:152:TYR:CB   | 2:B6:197:LEU:HD11 | 2.49                     | 0.42              |
| 2:BB:152:TYR:HB3  | 2:BB:197:LEU:HD11 | 2.02                     | 0.42              |
| 1:AF:146:ILE:O    | 1:AF:147:ALA:CB   | 2.62                     | 0.42              |
| 2:BY:152:TYR:HB3  | 2:BY:197:LEU:HD11 | 2.01                     | 0.42              |
| 2:BP:166:ARG:HB3  | 3:CR:112:GLY:O    | 2.19                     | 0.42              |
| 2:BG:166:ARG:HB3  | 3:CH:112:GLY:O    | 137.22                   | 0.42              |
| 2:BI:166:ARG:HB3  | 3:CJ:112:GLY:O    | 136.25                   | 0.42              |
| 2:BL:166:ARG:HB3  | 3:CM:112:GLY:O    | 137.22                   | 0.42              |
| 2:BZ:70:PRO:HG2   | 2:BZ:73:GLN:HB2   | 2.02                     | 0.42              |
| 3:C0:84:GLU:H     | 3:C0:84:GLU:CD    | 2.23                     | 0.42              |
| 3:CG:84:GLU:CD    | 3:CG:84:GLU:H     | 2.23                     | 0.42              |
| 1:AE:165:ARG:HA   | 3:CF:32:PRO:HG2   | 102.15                   | 0.42              |
| 1:AB:165:ARG:HA   | 3:CC:32:PRO:HG2   | 70.33                    | 0.42              |
| 1:AL:165:ARG:HA   | 3:CM:32:PRO:HG2   | 2.01                     | 0.42              |
| 2:B2:86:ASP:CB    | 2:B2:141:LYS:HA   | 2.49                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:CF:76:MET:HG3   | 3:CF:76:MET:O     | 2.18                     | 0.42              |
| 1:A8:165:ARG:HA   | 3:C9:32:PRO:HG2   | 2.01                     | 0.42              |
| 2:BK:86:ASP:CB    | 2:BK:141:LYS:HA   | 2.49                     | 0.42              |
| 3:CD:76:MET:O     | 3:CD:76:MET:HG3   | 2.18                     | 0.42              |
| 2:BZ:86:ASP:CB    | 2:BZ:141:LYS:HA   | 2.49                     | 0.42              |
| 3:CY:76:MET:HG3   | 3:CY:76:MET:O     | 2.18                     | 0.42              |
| 1:AK:26:VAL:HG11  | 3:CM:28:LYS:HD3   | 31.20                    | 0.42              |
| 1:AN:26:VAL:HG11  | 3:CP:28:LYS:HD3   | 221.84                   | 0.42              |
| 1:AO:26:VAL:HG11  | 3:CS:28:LYS:HD3   | 51.32                    | 0.42              |
| 3:CJ:40:PHE:CD1   | 1:DK:221:PRO:HD3  | 2.54                     | 0.42              |
| 1:AO:221:PRO:HD3  | 3:CP:40:PHE:CD2   | 4.39                     | 0.42              |
| 2:BE:224:GLY:HA2  | 2:BE:225:PRO:HD2  | 1.81                     | 0.42              |
| 1:AQ:221:PRO:HD3  | 3:CR:40:PHE:CD1   | 2.54                     | 0.42              |
| 1:AP:240:PRO:HG2  | 1:AS:114:LYS:HB2  | 2.01                     | 0.42              |
| 3:CG:150:LEU:HA   | 3:CG:150:LEU:HD12 | 1.79                     | 0.42              |
| 3:CV:40:PHE:CD2   | 1:DH:221:PRO:HD3  | 270.47                   | 0.42              |
| 3:C2:150:LEU:HD12 | 3:C2:150:LEU:HA   | 1.79                     | 0.42              |
| 1:A0:240:PRO:HG2  | 1:A1:114:LYS:HB2  | 2.01                     | 0.42              |
| 1:AT:240:PRO:HG2  | 1:AU:114:LYS:HB2  | 2.01                     | 0.42              |
| 1:A2:221:PRO:HD3  | 3:C3:40:PHE:CD2   | 2.54                     | 0.42              |
| 2:BM:115:ASN:HB3  | 2:BM:210:PRO:HG2  | 2.02                     | 0.42              |
| 1:AU:240:PRO:HG2  | 1:AX:114:LYS:HB2  | 2.01                     | 0.42              |
| 1:A3:221:PRO:HD3  | 3:C4:40:PHE:CD2   | 2.54                     | 0.42              |
| 1:AD:207:CYS:O    | 1:AD:208:TYR:CB   | 2.57                     | 0.42              |
| 3:CM:175:THR:HG23 | 3:CM:176:VAL:N    | 2.34                     | 0.42              |
| 3:CX:175:THR:HG23 | 3:CX:176:VAL:N    | 2.34                     | 0.42              |
| 3:C8:175:THR:HG23 | 3:C8:176:VAL:N    | 2.34                     | 0.42              |
| 1:AQ:110:GLY:N    | 1:AS:242:ASN:HD22 | 2.10                     | 0.42              |
| 1:AY:110:GLY:N    | 1:A1:242:ASN:HD22 | 2.10                     | 0.42              |
| 2:B4:85:SER:HB2   | 2:B4:190:ASN:ND2  | 2.31                     | 0.42              |
| 1:AD:212:ARG:NH2  | 3:CD:18:VAL:O     | 2.46                     | 0.42              |
| 1:AE:212:ARG:NH2  | 3:CE:18:VAL:O     | 2.46                     | 0.42              |
| 1:AK:212:ARG:NH2  | 3:CL:18:VAL:O     | 2.46                     | 0.42              |
| 1:AJ:212:ARG:NH2  | 3:CK:18:VAL:O     | 2.46                     | 0.42              |
| 2:BW:152:TYR:CB   | 2:BW:197:LEU:HD11 | 2.49                     | 0.42              |
| 2:BC:152:TYR:CB   | 2:BC:197:LEU:HD11 | 2.49                     | 0.42              |
| 2:BZ:152:TYR:HB3  | 2:BZ:197:LEU:HD11 | 2.02                     | 0.42              |
| 3:C8:44:ILE:HA    | 3:C8:44:ILE:HD12  | 1.88                     | 0.42              |
| 3:C9:74:PHE:HE2   | 3:C9:183:LEU:HD13 | 1.83                     | 0.42              |
| 2:BV:166:ARG:HB3  | 3:CW:112:GLY:O    | 137.22                   | 0.42              |
| 2:BR:166:ARG:HB3  | 3:CO:112:GLY:O    | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:CS:74:PHE:HE2   | 3:CS:183:LEU:HD13 | 1.83                     | 0.42              |
| 2:BX:70:PRO:HG2   | 2:BX:73:GLN:HB2   | 2.02                     | 0.42              |
| 2:BK:70:PRO:HG2   | 2:BK:73:GLN:HB2   | 2.02                     | 0.42              |
| 2:BN:70:PRO:HG2   | 2:BN:73:GLN:HB2   | 2.01                     | 0.42              |
| 2:BG:86:ASP:CB    | 2:BG:141:LYS:HA   | 2.49                     | 0.42              |
| 2:BT:86:ASP:CB    | 2:BT:141:LYS:HA   | 2.49                     | 0.42              |
| 1:AC:165:ARG:HA   | 3:CD:32:PRO:HG2   | 42.51                    | 0.42              |
| 3:CS:32:PRO:HG2   | 1:DE:165:ARG:HA   | 269.18                   | 0.42              |
| 1:AT:165:ARG:HA   | 3:CU:32:PRO:HG2   | 2.01                     | 0.42              |
| 2:BF:86:ASP:CB    | 2:BF:141:LYS:HA   | 2.49                     | 0.42              |
| 3:C2:76:MET:HG3   | 3:C2:76:MET:O     | 2.18                     | 0.42              |
| 1:A2:187:LEU:HD23 | 1:A2:187:LEU:HA   | 1.91                     | 0.42              |
| 1:AJ:26:VAL:HG11  | 3:CN:28:LYS:HD3   | 51.32                    | 0.42              |
| 1:AI:240:PRO:HG2  | 1:AJ:114:LYS:HB2  | 178.44                   | 0.42              |
| 1:AF:221:PRO:HD3  | 3:CG:40:PHE:CD2   | 49.74                    | 0.42              |
| 2:BG:115:ASN:HB3  | 2:BG:210:PRO:HG2  | 2.02                     | 0.42              |
| 1:AO:240:PRO:HG2  | 1:DE:114:LYS:HB2  | 302.92                   | 0.42              |
| 1:AZ:221:PRO:HD3  | 3:C0:40:PHE:CD2   | 2.54                     | 0.42              |
| 2:BL:228:ASN:CG   | 3:CL:140:ALA:HB2  | 82.01                    | 0.42              |
| 1:A9:221:PRO:HD3  | 3:DA:40:PHE:CD1   | 2.54                     | 0.42              |
| 2:BS:115:ASN:HB3  | 2:BS:210:PRO:HG2  | 2.02                     | 0.42              |
| 1:AY:209:LEU:HA   | 1:AY:209:LEU:HD22 | 1.74                     | 0.42              |
| 1:A6:209:LEU:HD22 | 1:A6:209:LEU:HA   | 1.74                     | 0.42              |
| 3:CU:150:LEU:HA   | 3:CU:150:LEU:HD12 | 1.79                     | 0.42              |
| 1:AM:221:PRO:HD3  | 3:CN:40:PHE:CD2   | 4.39                     | 0.42              |
| 2:BT:115:ASN:HB3  | 2:BT:210:PRO:HG2  | 2.02                     | 0.42              |
| 1:AU:191:HIS:HD2  | 1:AU:193:GLY:N    | 2.08                     | 0.42              |
| 1:AK:187:LEU:HD23 | 1:AK:187:LEU:HA   | 1.91                     | 0.42              |
| 3:C0:175:THR:HG23 | 3:C0:176:VAL:N    | 2.34                     | 0.42              |
| 2:BS:83:LEU:HA    | 2:BS:84:PRO:HA    | 1.60                     | 0.42              |
| 2:BC:152:TYR:HB3  | 2:BC:197:LEU:HD11 | 2.02                     | 0.42              |
| 2:BI:152:TYR:HB3  | 2:BI:197:LEU:HD11 | 2.02                     | 0.42              |
| 2:BI:152:TYR:CB   | 2:BI:197:LEU:HD11 | 2.49                     | 0.42              |
| 2:B9:152:TYR:HB3  | 2:B9:197:LEU:HD11 | 2.02                     | 0.42              |
| 2:BT:152:TYR:HB3  | 2:BT:197:LEU:HD11 | 2.02                     | 0.42              |
| 2:BZ:152:TYR:CB   | 2:BZ:197:LEU:HD11 | 2.49                     | 0.42              |
| 3:CH:44:ILE:HD12  | 3:CH:44:ILE:HA    | 1.88                     | 0.42              |
| 3:CB:148:VAL:CG1  | 3:CB:149:GLY:N    | 2.83                     | 0.42              |
| 3:CH:148:VAL:CG1  | 3:CH:149:GLY:N    | 2.83                     | 0.42              |
| 2:BH:70:PRO:HG2   | 2:BH:73:GLN:HB2   | 2.02                     | 0.42              |
| 2:BY:70:PRO:HG2   | 2:BY:73:GLN:HB2   | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B2:70:PRO:HG2   | 2:B2:73:GLN:HB2   | 2.01                     | 0.42              |
| 2:BP:86:ASP:CB    | 2:BP:141:LYS:HA   | 2.49                     | 0.42              |
| 1:AI:165:ARG:HA   | 3:CI:32:PRO:HG2   | 2.01                     | 0.42              |
| 3:C1:84:GLU:CD    | 3:C1:84:GLU:H     | 2.23                     | 0.42              |
| 1:A3:165:ARG:HA   | 3:C4:32:PRO:HG2   | 2.01                     | 0.42              |
| 1:AE:26:VAL:HG11  | 3:CI:28:LYS:HD3   | 139.51                   | 0.42              |
| 1:AH:240:PRO:HG2  | 1:AI:114:LYS:HB2  | 2.01                     | 0.42              |
| 1:AC:240:PRO:HG2  | 1:AD:114:LYS:HB2  | 2.01                     | 0.42              |
| 1:AO:240:PRO:HG2  | 1:AP:114:LYS:HB2  | 2.01                     | 0.42              |
| 2:BL:228:ASN:CG   | 3:CK:140:ALA:HB2  | 2.40                     | 0.42              |
| 1:AM:221:PRO:HD3  | 3:CN:40:PHE:CD1   | 2.54                     | 0.42              |
| 2:BC:228:ASN:CG   | 3:DA:140:ALA:HB2  | 280.73                   | 0.42              |
| 2:BV:228:ASN:CG   | 3:CU:140:ALA:HB2  | 2.40                     | 0.42              |
| 1:AU:26:VAL:HG11  | 3:CY:28:LYS:HD3   | 2.00                     | 0.42              |
| 2:BP:115:ASN:HB3  | 2:BP:210:PRO:HG2  | 2.02                     | 0.42              |
| 2:BG:224:GLY:HA2  | 2:BG:225:PRO:HD2  | 1.81                     | 0.42              |
| 2:BP:224:GLY:HA2  | 2:BP:225:PRO:HD2  | 1.81                     | 0.42              |
| 1:AN:209:LEU:HD22 | 1:AN:209:LEU:HA   | 1.75                     | 0.42              |
| 2:BA:228:ASN:CG   | 3:CD:140:ALA:HB2  | 2.40                     | 0.42              |
| 2:BL:115:ASN:HB3  | 2:BL:210:PRO:HG2  | 2.02                     | 0.42              |
| 2:B2:115:ASN:HB3  | 2:B2:210:PRO:HG2  | 2.02                     | 0.42              |
| 3:CX:40:PHE:CD2   | 1:DJ:221:PRO:HD3  | 251.20                   | 0.42              |
| 1:A7:26:VAL:HG11  | 3:C6:28:LYS:HD3   | 2.00                     | 0.42              |
| 2:BE:115:ASN:HB3  | 2:BE:210:PRO:HG2  | 2.02                     | 0.42              |
| 1:AD:174:TRP:CH2  | 2:BD:139:ALA:HB3  | 2.55                     | 0.42              |
| 1:AE:174:TRP:CH2  | 2:BE:139:ALA:HB3  | 2.55                     | 0.42              |
| 1:AA:187:LEU:HA   | 1:AA:187:LEU:HD23 | 1.91                     | 0.42              |
| 3:CF:175:THR:HG23 | 3:CF:176:VAL:N    | 2.34                     | 0.42              |
| 3:C2:175:THR:HG23 | 3:C2:176:VAL:N    | 2.34                     | 0.42              |
| 1:DK:87:GLN:HE21  | 1:DK:210:ARG:NH2  | 2.12                     | 0.42              |
| 1:AP:74:THR:HG21  | 3:CQ:43:PHE:CE1   | 2.45                     | 0.42              |
| 1:AG:212:ARG:NH2  | 3:CH:18:VAL:O     | 37.15                    | 0.42              |
| 2:B4:152:TYR:HB3  | 2:B4:197:LEU:HD11 | 2.01                     | 0.42              |
| 2:B5:152:TYR:HB3  | 2:B5:197:LEU:HD11 | 2.01                     | 0.42              |
| 2:BF:152:TYR:HB3  | 2:BF:197:LEU:HD11 | 2.02                     | 0.42              |
| 2:BH:152:TYR:HB3  | 2:BH:197:LEU:HD11 | 2.02                     | 0.42              |
| 2:BA:152:TYR:HB3  | 2:BA:197:LEU:HD11 | 2.02                     | 0.42              |
| 2:BS:152:TYR:CB   | 2:BS:197:LEU:HD11 | 2.49                     | 0.42              |
| 2:BB:152:TYR:CB   | 2:BB:197:LEU:HD11 | 2.49                     | 0.42              |
| 2:BP:152:TYR:CB   | 2:BP:197:LEU:HD11 | 2.49                     | 0.42              |
| 3:CG:148:VAL:CG1  | 3:CG:149:GLY:N    | 2.83                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BC:166:ARG:HB3  | 3:CD:112:GLY:O    | 85.79                    | 0.42              |
| 3:CD:148:VAL:CG1  | 3:CD:149:GLY:N    | 2.83                     | 0.42              |
| 3:CE:148:VAL:CG1  | 3:CE:149:GLY:N    | 2.83                     | 0.42              |
| 2:BU:166:ARG:HB3  | 3:CV:112:GLY:O    | 85.79                    | 0.42              |
| 3:C0:148:VAL:CG1  | 3:C0:149:GLY:N    | 2.83                     | 0.42              |
| 3:C9:148:VAL:CG1  | 3:C9:149:GLY:N    | 2.83                     | 0.42              |
| 2:B0:70:PRO:HG2   | 2:B0:73:GLN:HB2   | 2.01                     | 0.42              |
| 1:AE:165:ARG:HA   | 3:CE:32:PRO:HG2   | 2.00                     | 0.42              |
| 3:CJ:32:PRO:HG2   | 1:DK:165:ARG:HA   | 2.01                     | 0.42              |
| 3:CN:84:GLU:H     | 3:CN:84:GLU:CD    | 2.23                     | 0.42              |
| 1:AB:219:TYR:CD2  | 3:CC:36:VAL:HG22  | 76.03                    | 0.42              |
| 1:AM:26:VAL:HG11  | 3:CL:28:LYS:HD3   | 31.20                    | 0.42              |
| 1:AR:26:VAL:HG11  | 3:CP:28:LYS:HD3   | 2.00                     | 0.42              |
| 1:AA:26:VAL:HG11  | 3:CC:28:LYS:HD3   | 50.98                    | 0.42              |
| 1:AB:240:PRO:HG2  | 1:AE:114:LYS:HB2  | 2.01                     | 0.42              |
| 1:AI:221:PRO:HD3  | 3:CJ:40:PHE:CD2   | 76.67                    | 0.42              |
| 1:AH:114:LYS:HB2  | 1:DK:240:PRO:HG2  | 2.01                     | 0.42              |
| 2:BP:228:ASN:CG   | 3:CT:140:ALA:HB2  | 2.40                     | 0.42              |
| 2:BS:228:ASN:CG   | 3:CW:140:ALA:HB2  | 296.65                   | 0.42              |
| 2:BM:228:ASN:CG   | 3:CO:140:ALA:HB2  | 2.40                     | 0.42              |
| 1:AW:220:CYS:HA   | 1:AW:221:PRO:HD2  | 1.95                     | 0.42              |
| 2:B3:228:ASN:CG   | 3:C0:140:ALA:HB2  | 2.40                     | 0.42              |
| 2:BC:115:ASN:HB3  | 2:BC:210:PRO:HG2  | 2.02                     | 0.42              |
| 1:AF:240:PRO:HG2  | 1:AG:114:LYS:HB2  | 2.01                     | 0.42              |
| 2:BR:115:ASN:HB3  | 2:BR:210:PRO:HG2  | 2.02                     | 0.42              |
| 2:BJ:115:ASN:HB3  | 2:BJ:210:PRO:HG2  | 2.02                     | 0.42              |
| 1:AS:225:PRO:HA   | 1:AS:226:PRO:HD3  | 1.78                     | 0.42              |
| 1:AK:225:PRO:HA   | 1:AK:226:PRO:HD3  | 1.78                     | 0.42              |
| 3:C5:150:LEU:HA   | 3:C5:150:LEU:HD12 | 1.79                     | 0.42              |
| 3:C1:150:LEU:HA   | 3:C1:150:LEU:HD12 | 1.79                     | 0.42              |
| 2:BU:115:ASN:HB3  | 2:BU:210:PRO:HG2  | 2.02                     | 0.42              |
| 1:AA:221:PRO:HD3  | 3:DB:40:PHE:CD1   | 266.48                   | 0.42              |
| 1:AN:221:PRO:HD3  | 3:CO:40:PHE:CD2   | 4.39                     | 0.42              |
| 1:AI:174:TRP:CH2  | 2:BI:139:ALA:HB3  | 2.55                     | 0.42              |
| 1:AO:174:TRP:CH2  | 2:BO:139:ALA:HB3  | 2.55                     | 0.42              |
| 1:AH:174:TRP:CH2  | 2:BH:139:ALA:HB3  | 2.55                     | 0.42              |
| 1:AZ:174:TRP:CH2  | 2:B0:139:ALA:HB3  | 2.55                     | 0.42              |
| 1:AY:174:TRP:CH2  | 2:BZ:139:ALA:HB3  | 2.55                     | 0.42              |
| 3:CE:175:THR:HG23 | 3:CE:176:VAL:N    | 2.34                     | 0.42              |
| 3:C5:175:THR:HG23 | 3:C5:176:VAL:N    | 2.34                     | 0.42              |
| 2:BF:83:LEU:HA    | 2:BF:84:PRO:HA    | 1.60                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:BD:152:TYR:HB3 | 2:BD:197:LEU:HD11 | 2.01                     | 0.42              |
| 1:AW:212:ARG:NH2 | 3:CX:18:VAL:O     | 2.46                     | 0.42              |
| 2:BS:152:TYR:HB3 | 2:BS:197:LEU:HD11 | 2.02                     | 0.42              |
| 2:BU:152:TYR:HB3 | 2:BU:197:LEU:HD11 | 2.02                     | 0.42              |
| 2:BQ:152:TYR:HB3 | 2:BQ:197:LEU:HD11 | 2.02                     | 0.42              |
| 2:BP:152:TYR:HB3 | 2:BP:197:LEU:HD11 | 2.02                     | 0.42              |
| 2:B3:152:TYR:CB  | 2:B3:197:LEU:HD11 | 2.49                     | 0.42              |
| 3:C5:44:ILE:HD12 | 3:C5:44:ILE:HA    | 1.87                     | 0.42              |
| 1:A3:163:MET:HE3 | 1:A3:189:GLY:HA3  | 2.02                     | 0.42              |
| 3:C7:74:PHE:HE2  | 3:C7:183:LEU:HD13 | 1.84                     | 0.42              |
| 3:CM:110:PHE:CD2 | 3:CM:148:VAL:HG11 | 2.55                     | 0.42              |
| 3:CT:148:VAL:CG1 | 3:CT:149:GLY:N    | 2.83                     | 0.42              |
| 3:C0:74:PHE:HE2  | 3:C0:183:LEU:HD13 | 1.84                     | 0.42              |
| 3:DA:74:PHE:HE2  | 3:DA:183:LEU:HD13 | 1.84                     | 0.42              |
| 3:CR:110:PHE:CD2 | 3:CR:148:VAL:HG11 | 2.55                     | 0.42              |
| 2:BI:70:PRO:HG2  | 2:BI:73:GLN:HB2   | 2.02                     | 0.42              |
| 3:CZ:110:PHE:CD2 | 3:CZ:148:VAL:HG11 | 2.55                     | 0.42              |
| 2:BO:70:PRO:HG2  | 2:BO:73:GLN:HB2   | 2.02                     | 0.42              |
| 3:C9:110:PHE:CD2 | 3:C9:148:VAL:HG11 | 2.55                     | 0.42              |
| 3:DA:148:VAL:CG1 | 3:DA:149:GLY:N    | 2.83                     | 0.42              |
| 2:BU:70:PRO:HG2  | 2:BU:73:GLN:HB2   | 2.02                     | 0.42              |
| 3:CA:110:PHE:CD2 | 3:CA:148:VAL:HG11 | 2.55                     | 0.42              |
| 3:CA:148:VAL:CG1 | 3:CA:149:GLY:N    | 2.83                     | 0.42              |
| 2:BV:70:PRO:HG2  | 2:BV:73:GLN:HB2   | 2.02                     | 0.42              |
| 2:B5:166:ARG:HB3 | 3:C6:112:GLY:O    | 2.19                     | 0.42              |
| 3:CN:110:PHE:CD2 | 3:CN:148:VAL:HG11 | 2.55                     | 0.42              |
| 2:BB:70:PRO:HG2  | 2:BB:73:GLN:HB2   | 2.01                     | 0.42              |
| 3:C7:110:PHE:CD2 | 3:C7:148:VAL:HG11 | 2.55                     | 0.42              |
| 2:BW:70:PRO:HG2  | 2:BW:73:GLN:HB2   | 2.02                     | 0.42              |
| 3:CC:84:GLU:CD   | 3:CC:84:GLU:H     | 2.23                     | 0.42              |
| 2:BO:86:ASP:CB   | 2:BO:141:LYS:HA   | 2.49                     | 0.42              |
| 1:AH:165:ARG:HA  | 3:CI:32:PRO:HG2   | 42.50                    | 0.42              |
| 1:AA:165:ARG:HA  | 3:CA:32:PRO:HG2   | 2.00                     | 0.42              |
| 1:A1:165:ARG:HA  | 3:C2:32:PRO:HG2   | 2.01                     | 0.42              |
| 2:B8:86:ASP:CB   | 2:B8:141:LYS:HA   | 2.49                     | 0.42              |
| 3:DB:76:MET:O    | 3:DB:76:MET:HG3   | 2.18                     | 0.42              |
| 2:B8:53:ARG:HG2  | 2:B8:221:MET:HE2  | 2.02                     | 0.42              |
| 3:CM:36:VAL:HA   | 3:CM:37:PRO:HD3   | 1.64                     | 0.42              |
| 1:AB:26:VAL:HG11 | 3:CE:28:LYS:HD3   | 2.00                     | 0.42              |
| 1:AM:26:VAL:HG11 | 3:CK:28:LYS:HD3   | 2.00                     | 0.42              |
| 1:AO:114:LYS:HB2 | 1:AR:240:PRO:HG2  | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:CQ:40:PHE:CD2   | 1:DC:221:PRO:HD3  | 212.56                   | 0.42              |
| 1:AB:221:PRO:HD3  | 3:CC:40:PHE:CD2   | 78.07                    | 0.42              |
| 1:AC:114:LYS:HB2  | 1:A9:240:PRO:HG2  | 290.78                   | 0.42              |
| 2:BI:228:ASN:CG   | 3:CM:140:ALA:HB2  | 120.05                   | 0.42              |
| 2:BM:228:ASN:CG   | 3:CK:140:ALA:HB2  | 133.74                   | 0.42              |
| 2:BC:228:ASN:CG   | 3:CE:140:ALA:HB2  | 2.40                     | 0.42              |
| 2:BW:228:ASN:CG   | 3:CY:140:ALA:HB2  | 2.40                     | 0.42              |
| 2:BV:228:ASN:CG   | 3:CV:140:ALA:HB2  | 82.01                    | 0.42              |
| 1:DH:240:PRO:HG2  | 1:DI:114:LYS:HB2  | 2.01                     | 0.42              |
| 2:B2:228:ASN:CG   | 3:C1:140:ALA:HB2  | 2.40                     | 0.42              |
| 1:A1:221:PRO:HD3  | 3:C2:40:PHE:CD2   | 2.54                     | 0.42              |
| 2:BZ:115:ASN:HB3  | 2:BZ:210:PRO:HG2  | 2.02                     | 0.42              |
| 1:DF:240:PRO:HG2  | 1:DG:114:LYS:HB2  | 2.01                     | 0.42              |
| 1:A3:114:LYS:HB2  | 1:A6:240:PRO:HG2  | 2.01                     | 0.42              |
| 2:B0:115:ASN:HB3  | 2:B0:210:PRO:HG2  | 2.02                     | 0.42              |
| 3:CN:150:LEU:HD12 | 3:CN:150:LEU:HA   | 1.79                     | 0.42              |
| 1:A9:72:LEU:HD23  | 1:A9:72:LEU:HA    | 1.82                     | 0.42              |
| 2:BB:228:ASN:CG   | 3:CA:140:ALA:HB2  | 2.40                     | 0.42              |
| 2:BF:228:ASN:CG   | 3:CI:140:ALA:HB2  | 2.40                     | 0.42              |
| 2:BH:228:ASN:CG   | 3:CF:140:ALA:HB2  | 133.74                   | 0.42              |
| 2:BW:115:ASN:HB3  | 2:BW:210:PRO:HG2  | 2.02                     | 0.42              |
| 2:B9:166:ARG:HB3  | 3:DA:112:GLY:O    | 2.19                     | 0.42              |
| 1:AL:174:TRP:CH2  | 2:BM:139:ALA:HB3  | 2.55                     | 0.42              |
| 2:BS:139:ALA:HB3  | 1:DF:174:TRP:CH2  | 266.27                   | 0.42              |
| 1:AX:174:TRP:CH2  | 2:BY:139:ALA:HB3  | 2.55                     | 0.42              |
| 1:A9:174:TRP:CH2  | 2:B9:139:ALA:HB3  | 2.55                     | 0.42              |
| 3:C6:175:THR:HG23 | 3:C6:176:VAL:N    | 2.34                     | 0.42              |
| 1:AO:242:ASN:HD22 | 1:AP:110:GLY:N    | 2.10                     | 0.42              |
| 1:AB:242:ASN:HD22 | 1:AE:110:GLY:N    | 2.10                     | 0.42              |
| 1:DI:92:THR:CG2   | 1:DI:93:THR:H     | 2.26                     | 0.42              |
| 3:CR:18:VAL:O     | 1:DD:212:ARG:NH2  | 249.67                   | 0.42              |
| 1:AU:231:PRO:HG2  | 3:CV:83:ALA:CB    | 2.48                     | 0.42              |
| 1:AF:212:ARG:NH2  | 3:CG:18:VAL:O     | 24.16                    | 0.42              |
| 2:B4:152:TYR:CB   | 2:B4:197:LEU:HD11 | 2.49                     | 0.42              |
| 2:B4:149:ALA:O    | 2:B4:153:GLN:HG3  | 2.20                     | 0.42              |
| 2:B9:149:ALA:O    | 2:B9:153:GLN:HG3  | 2.20                     | 0.42              |
| 2:BH:149:ALA:O    | 2:BH:153:GLN:HG3  | 2.20                     | 0.42              |
| 2:B2:149:ALA:O    | 2:B2:153:GLN:HG3  | 2.20                     | 0.42              |
| 2:BG:152:TYR:HB3  | 2:BG:197:LEU:HD11 | 2.02                     | 0.42              |
| 1:AL:146:ILE:O    | 1:AL:147:ALA:CB   | 2.62                     | 0.42              |
| 1:AD:146:ILE:O    | 1:AD:147:ALA:CB   | 2.62                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:CM:44:ILE:HD12  | 3:CM:44:ILE:HA    | 1.88                     | 0.42              |
| 3:CG:110:PHE:CD2  | 3:CG:148:VAL:HG11 | 2.55                     | 0.42              |
| 2:BW:166:ARG:HB3  | 3:CW:112:GLY:O    | 2.19                     | 0.42              |
| 3:CE:110:PHE:CD2  | 3:CE:148:VAL:HG11 | 2.55                     | 0.42              |
| 3:CI:110:PHE:CD2  | 3:CI:148:VAL:HG11 | 2.55                     | 0.42              |
| 2:BL:70:PRO:HG2   | 2:BL:73:GLN:HB2   | 2.02                     | 0.42              |
| 3:CP:148:VAL:CG1  | 3:CP:149:GLY:N    | 2.83                     | 0.42              |
| 2:BC:70:PRO:HG2   | 2:BC:73:GLN:HB2   | 2.02                     | 0.42              |
| 2:BT:70:PRO:HG2   | 2:BT:73:GLN:HB2   | 2.01                     | 0.42              |
| 2:B1:70:PRO:HG2   | 2:B1:73:GLN:HB2   | 2.01                     | 0.42              |
| 2:B9:70:PRO:HG2   | 2:B9:73:GLN:HB2   | 2.02                     | 0.42              |
| 3:CT:76:MET:HG3   | 3:CT:76:MET:O     | 2.18                     | 0.42              |
| 1:AU:165:ARG:HA   | 3:CV:32:PRO:HG2   | 2.01                     | 0.42              |
| 3:CQ:32:PRO:HG2   | 1:DC:165:ARG:HA   | 234.37                   | 0.42              |
| 3:CK:84:GLU:H     | 3:CK:84:GLU:CD    | 2.23                     | 0.42              |
| 3:C3:76:MET:O     | 3:C3:76:MET:HG3   | 2.18                     | 0.42              |
| 1:AG:26:VAL:HG11  | 3:CE:28:LYS:HD3   | 133.19                   | 0.42              |
| 1:AH:26:VAL:HG11  | 3:CI:28:LYS:HD3   | 2.00                     | 0.42              |
| 1:AJ:240:PRO:HG2  | 1:AM:114:LYS:HB2  | 77.43                    | 0.42              |
| 1:AJ:114:LYS:HB2  | 1:AM:240:PRO:HG2  | 2.01                     | 0.42              |
| 1:AD:114:LYS:HB2  | 1:AG:240:PRO:HG2  | 193.59                   | 0.42              |
| 1:AE:221:PRO:HD3  | 3:CF:40:PHE:CD2   | 78.33                    | 0.42              |
| 1:AE:240:PRO:HG2  | 1:AH:114:LYS:HB2  | 178.45                   | 0.42              |
| 1:AT:221:PRO:HD3  | 3:CU:40:PHE:CD2   | 2.54                     | 0.42              |
| 1:AU:221:PRO:HD3  | 3:CV:40:PHE:CD2   | 2.54                     | 0.42              |
| 2:BO:228:ASN:CG   | 3:CO:140:ALA:HB2  | 242.31                   | 0.42              |
| 2:BR:228:ASN:CG   | 3:CP:140:ALA:HB2  | 252.10                   | 0.42              |
| 2:BX:228:ASN:CG   | 3:C4:140:ALA:HB2  | 288.36                   | 0.42              |
| 2:BN:228:ASN:CG   | 3:CM:140:ALA:HB2  | 2.40                     | 0.42              |
| 1:AA:221:PRO:HD3  | 3:CA:40:PHE:CD1   | 2.54                     | 0.42              |
| 2:BX:115:ASN:HB3  | 2:BX:210:PRO:HG2  | 2.02                     | 0.42              |
| 1:AY:221:PRO:HD3  | 3:CZ:40:PHE:CD2   | 2.54                     | 0.42              |
| 2:B4:228:ASN:CG   | 3:C7:140:ALA:HB2  | 2.40                     | 0.42              |
| 2:B8:124:LEU:HD23 | 2:B8:198:ILE:HA   | 2.00                     | 0.42              |
| 1:DC:240:PRO:HG2  | 1:DD:114:LYS:HB2  | 2.01                     | 0.42              |
| 2:B6:228:ASN:CG   | 3:C6:140:ALA:HB2  | 2.40                     | 0.42              |
| 2:B8:115:ASN:HB3  | 2:B8:210:PRO:HG2  | 2.02                     | 0.42              |
| 3:CK:150:LEU:HA   | 3:CK:150:LEU:HD12 | 1.79                     | 0.42              |
| 1:A5:114:LYS:HB2  | 1:A7:240:PRO:HG2  | 2.01                     | 0.42              |
| 1:AV:240:PRO:HG2  | 1:AW:114:LYS:HB2  | 2.01                     | 0.42              |
| 2:BO:115:ASN:HB3  | 2:BO:210:PRO:HG2  | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BV:139:ALA:HB3  | 1:DI:174:TRP:CH2  | 283.21                   | 0.42              |
| 1:AJ:174:TRP:CH2  | 2:BJ:139:ALA:HB3  | 257.78                   | 0.42              |
| 1:AM:174:TRP:CH2  | 2:BM:139:ALA:HB3  | 65.71                    | 0.42              |
| 2:BJ:139:ALA:HB3  | 1:DK:174:TRP:CH2  | 2.55                     | 0.42              |
| 2:BQ:139:ALA:HB3  | 1:DD:174:TRP:CH2  | 276.17                   | 0.42              |
| 2:BW:139:ALA:HB3  | 1:DJ:174:TRP:CH2  | 281.63                   | 0.42              |
| 2:BQ:157:VAL:CG2  | 3:CR:50:THR:HG21  | 54.76                    | 0.42              |
| 1:A7:174:TRP:CH2  | 2:B7:139:ALA:HB3  | 2.55                     | 0.42              |
| 1:AB:174:TRP:CH2  | 2:BB:139:ALA:HB3  | 2.55                     | 0.42              |
| 1:A3:174:TRP:CH2  | 2:B4:139:ALA:HB3  | 2.55                     | 0.42              |
| 1:A1:174:TRP:CH2  | 2:B2:139:ALA:HB3  | 2.55                     | 0.42              |
| 3:C3:175:THR:HG23 | 3:C3:176:VAL:N    | 2.34                     | 0.42              |
| 1:AB:242:ASN:HD22 | 1:A8:110:GLY:N    | 222.32                   | 0.42              |
| 2:B3:85:SER:HB2   | 2:B3:190:ASN:ND2  | 2.31                     | 0.42              |
| 1:AM:231:PRO:HG2  | 3:CN:83:ALA:CB    | 2.48                     | 0.42              |
| 1:AD:231:PRO:HG2  | 3:CD:83:ALA:CB    | 2.48                     | 0.42              |
| 1:AE:231:PRO:HG2  | 3:CF:83:ALA:CB    | 78.51                    | 0.42              |
| 1:AT:212:ARG:NH2  | 3:CU:18:VAL:O     | 2.46                     | 0.42              |
| 1:A8:212:ARG:NH2  | 3:C9:18:VAL:O     | 2.46                     | 0.42              |
| 2:BM:149:ALA:O    | 2:BM:153:GLN:HG3  | 2.20                     | 0.42              |
| 2:BR:149:ALA:O    | 2:BR:153:GLN:HG3  | 2.20                     | 0.42              |
| 2:BV:152:TYR:HB3  | 2:BV:197:LEU:HD11 | 2.02                     | 0.42              |
| 3:CH:110:PHE:CD2  | 3:CH:148:VAL:HG11 | 2.55                     | 0.42              |
| 3:CJ:110:PHE:CD2  | 3:CJ:148:VAL:HG11 | 2.55                     | 0.42              |
| 3:CT:110:PHE:CD2  | 3:CT:148:VAL:HG11 | 2.55                     | 0.42              |
| 3:CO:110:PHE:CD2  | 3:CO:148:VAL:HG11 | 2.55                     | 0.42              |
| 2:BJ:70:PRO:HG2   | 2:BJ:73:GLN:HB2   | 2.02                     | 0.42              |
| 3:CC:110:PHE:CD2  | 3:CC:148:VAL:HG11 | 2.55                     | 0.42              |
| 2:BE:70:PRO:HG2   | 2:BE:73:GLN:HB2   | 2.02                     | 0.42              |
| 2:B6:70:PRO:HG2   | 2:B6:73:GLN:HB2   | 2.02                     | 0.42              |
| 3:C7:148:VAL:CG1  | 3:C7:149:GLY:N    | 2.83                     | 0.42              |
| 3:CY:110:PHE:CD2  | 3:CY:148:VAL:HG11 | 2.55                     | 0.42              |
| 3:CM:84:GLU:CD    | 3:CM:84:GLU:H     | 2.23                     | 0.42              |
| 1:AD:165:ARG:HA   | 3:CE:32:PRO:HG2   | 71.30                    | 0.42              |
| 3:CH:84:GLU:H     | 3:CH:84:GLU:CD    | 2.23                     | 0.42              |
| 3:CF:84:GLU:H     | 3:CF:84:GLU:CD    | 2.23                     | 0.42              |
| 3:C9:76:MET:O     | 3:C9:76:MET:HG3   | 2.18                     | 0.42              |
| 2:B4:86:ASP:CB    | 2:B4:141:LYS:HA   | 2.49                     | 0.42              |
| 3:C8:84:GLU:H     | 3:C8:84:GLU:CD    | 2.23                     | 0.42              |
| 3:C2:84:GLU:CD    | 3:C2:84:GLU:H     | 2.23                     | 0.42              |
| 1:AF:26:VAL:HG11  | 3:CH:28:LYS:HD3   | 50.98                    | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BI:53:ARG:HG2   | 2:BI:221:MET:HE3  | 2.01                     | 0.42              |
| 1:AR:221:PRO:HD3  | 3:CS:40:PHE:CD2   | 2.54                     | 0.42              |
| 1:AD:221:PRO:HD3  | 3:CD:40:PHE:CD1   | 2.54                     | 0.42              |
| 2:BT:228:ASN:CG   | 3:CQ:140:ALA:HB2  | 2.40                     | 0.42              |
| 2:BE:228:ASN:CG   | 3:CB:140:ALA:HB2  | 2.40                     | 0.42              |
| 2:BG:228:ASN:CG   | 3:CF:140:ALA:HB2  | 2.40                     | 0.42              |
| 2:BH:228:ASN:CG   | 3:CJ:140:ALA:HB2  | 2.40                     | 0.42              |
| 2:BU:228:ASN:CG   | 3:CX:140:ALA:HB2  | 2.40                     | 0.42              |
| 1:AJ:221:PRO:HD3  | 3:CK:40:PHE:CD1   | 2.54                     | 0.42              |
| 1:AL:221:PRO:HD3  | 3:CM:40:PHE:CD1   | 2.54                     | 0.42              |
| 1:AY:72:LEU:HD23  | 1:AY:72:LEU:HA    | 1.82                     | 0.42              |
| 1:AH:209:LEU:HD22 | 1:AH:209:LEU:HA   | 1.74                     | 0.42              |
| 2:BD:115:ASN:HB3  | 2:BD:210:PRO:HG2  | 2.02                     | 0.42              |
| 2:BV:224:GLY:HA2  | 2:BV:225:PRO:HD2  | 1.81                     | 0.42              |
| 1:AL:174:TRP:CH2  | 2:BL:139:ALA:HB3  | 108.73                   | 0.42              |
| 1:A2:174:TRP:CH2  | 2:B3:139:ALA:HB3  | 2.55                     | 0.42              |
| 2:BP:157:VAL:CG2  | 3:CR:50:THR:HG21  | 2.42                     | 0.42              |
| 1:AQ:207:CYS:O    | 1:AQ:208:TYR:CB   | 2.57                     | 0.42              |
| 1:AB:187:LEU:HA   | 1:AB:188:PRO:HD2  | 1.95                     | 0.42              |
| 1:AL:87:GLN:HE21  | 1:AL:210:ARG:NH2  | 2.11                     | 0.42              |
| 1:A4:231:PRO:HG2  | 3:C5:83:ALA:CB    | 2.48                     | 0.42              |
| 1:AR:231:PRO:HG2  | 3:CS:83:ALA:CB    | 2.48                     | 0.42              |
| 1:AF:212:ARG:NH2  | 3:CF:18:VAL:O     | 2.46                     | 0.42              |
| 2:BT:149:ALA:O    | 2:BT:153:GLN:HG3  | 2.20                     | 0.42              |
| 2:BU:149:ALA:O    | 2:BU:153:GLN:HG3  | 2.20                     | 0.42              |
| 2:BE:149:ALA:O    | 2:BE:153:GLN:HG3  | 2.20                     | 0.42              |
| 3:CT:44:ILE:HD12  | 3:CT:44:ILE:HA    | 1.88                     | 0.42              |
| 3:CA:74:PHE:HE2   | 3:CA:183:LEU:HD13 | 1.83                     | 0.42              |
| 2:BN:166:ARG:HB3  | 3:CO:112:GLY:O    | 136.25                   | 0.42              |
| 3:CI:148:VAL:CG1  | 3:CI:149:GLY:N    | 2.83                     | 0.42              |
| 3:CU:148:VAL:CG1  | 3:CU:149:GLY:N    | 2.83                     | 0.42              |
| 3:CV:148:VAL:CG1  | 3:CV:149:GLY:N    | 2.83                     | 0.42              |
| 2:BP:70:PRO:HG2   | 2:BP:73:GLN:HB2   | 2.02                     | 0.42              |
| 3:CK:110:PHE:CD2  | 3:CK:148:VAL:HG11 | 2.55                     | 0.42              |
| 3:CX:84:GLU:H     | 3:CX:84:GLU:CD    | 2.23                     | 0.42              |
| 3:CR:32:PRO:HG2   | 1:DD:165:ARG:HA   | 217.66                   | 0.42              |
| 1:AY:165:ARG:HA   | 3:CZ:32:PRO:HG2   | 2.00                     | 0.42              |
| 3:C1:76:MET:O     | 3:C1:76:MET:HG3   | 2.18                     | 0.42              |
| 3:CD:84:GLU:H     | 3:CD:84:GLU:CD    | 2.23                     | 0.42              |
| 3:CY:84:GLU:H     | 3:CY:84:GLU:CD    | 2.23                     | 0.42              |
| 1:AI:187:LEU:HD23 | 1:AI:187:LEU:HA   | 1.91                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BR:53:ARG:HG2   | 2:BR:221:MET:HE2  | 2.14                     | 0.42              |
| 1:AA:114:LYS:HB2  | 1:AC:240:PRO:HG2  | 46.58                    | 0.42              |
| 1:AG:221:PRO:HD3  | 3:CH:40:PHE:CD2   | 78.07                    | 0.42              |
| 3:CR:40:PHE:CD2   | 1:DD:221:PRO:HD3  | 233.60                   | 0.42              |
| 2:BI:228:ASN:CG   | 3:CH:140:ALA:HB2  | 2.40                     | 0.42              |
| 2:BX:228:ASN:CG   | 3:CW:140:ALA:HB2  | 2.40                     | 0.42              |
| 2:BD:228:ASN:CG   | 3:CC:140:ALA:HB2  | 2.40                     | 0.42              |
| 1:AN:221:PRO:HD3  | 3:CO:40:PHE:CD1   | 2.54                     | 0.42              |
| 2:BB:228:ASN:CG   | 3:DB:140:ALA:HB2  | 261.90                   | 0.42              |
| 2:B5:115:ASN:HB3  | 2:B5:210:PRO:HG2  | 2.02                     | 0.42              |
| 1:A4:240:PRO:HG2  | 1:A7:114:LYS:HB2  | 2.01                     | 0.42              |
| 2:B6:115:ASN:HB3  | 2:B6:210:PRO:HG2  | 2.02                     | 0.42              |
| 2:B0:228:ASN:CG   | 3:CZ:140:ALA:HB2  | 2.40                     | 0.42              |
| 2:BH:115:ASN:HB3  | 2:BH:210:PRO:HG2  | 2.02                     | 0.42              |
| 2:B1:228:ASN:CG   | 3:C3:140:ALA:HB2  | 2.40                     | 0.42              |
| 1:A0:114:LYS:HB2  | 1:A2:240:PRO:HG2  | 2.01                     | 0.42              |
| 1:AJ:225:PRO:HA   | 1:AJ:226:PRO:HD3  | 1.78                     | 0.42              |
| 2:BA:115:ASN:HB3  | 2:BA:210:PRO:HG2  | 2.02                     | 0.42              |
| 2:BK:115:ASN:HB3  | 2:BK:210:PRO:HG2  | 2.02                     | 0.42              |
| 1:AF:209:LEU:HA   | 1:AF:209:LEU:HD22 | 1.74                     | 0.42              |
| 3:CA:150:LEU:HD12 | 3:CA:150:LEU:HA   | 1.79                     | 0.42              |
| 1:AE:225:PRO:HA   | 1:AE:226:PRO:HD3  | 1.78                     | 0.42              |
| 1:AU:174:TRP:CH2  | 2:BV:139:ALA:HB3  | 2.55                     | 0.42              |
| 1:AS:174:TRP:CH2  | 2:BT:139:ALA:HB3  | 2.55                     | 0.42              |
| 2:B3:157:VAL:CG2  | 3:C3:50:THR:HG21  | 2.42                     | 0.42              |
| 1:DC:187:LEU:HA   | 1:DC:188:PRO:HD2  | 1.95                     | 0.42              |
| 1:AB:74:THR:HG21  | 3:CB:43:PHE:CE1   | 2.45                     | 0.42              |
| 2:B5:83:LEU:HA    | 2:B5:84:PRO:HA    | 1.60                     | 0.42              |
| 1:AN:212:ARG:NH2  | 3:CO:18:VAL:O     | 2.46                     | 0.42              |
| 2:BW:149:ALA:O    | 2:BW:153:GLN:HG3  | 2.20                     | 0.42              |
| 2:B9:152:TYR:CB   | 2:B9:197:LEU:HD11 | 2.49                     | 0.42              |
| 2:BS:149:ALA:O    | 2:BS:153:GLN:HG3  | 2.20                     | 0.42              |
| 2:B8:152:TYR:CB   | 2:B8:197:LEU:HD11 | 2.49                     | 0.42              |
| 3:CQ:110:PHE:CD2  | 3:CQ:148:VAL:HG11 | 2.55                     | 0.42              |
| 3:CQ:148:VAL:CG1  | 3:CQ:149:GLY:N    | 2.83                     | 0.42              |
| 2:BP:166:ARG:HB3  | 3:CQ:112:GLY:O    | 136.25                   | 0.42              |
| 3:CJ:148:VAL:CG1  | 3:CJ:149:GLY:N    | 2.83                     | 0.42              |
| 3:CU:110:PHE:CD2  | 3:CU:148:VAL:HG11 | 2.55                     | 0.42              |
| 3:CW:148:VAL:CG1  | 3:CW:149:GLY:N    | 2.83                     | 0.42              |
| 3:C0:110:PHE:CD2  | 3:C0:148:VAL:HG11 | 2.55                     | 0.42              |
| 3:C2:110:PHE:CD2  | 3:C2:148:VAL:HG11 | 2.55                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C1:110:PHE:CD2 | 3:C1:148:VAL:HG11 | 2.55                     | 0.42              |
| 2:BM:70:PRO:HG2  | 2:BM:73:GLN:HB2   | 2.02                     | 0.42              |
| 3:CK:148:VAL:CG1 | 3:CK:149:GLY:N    | 2.83                     | 0.42              |
| 3:C3:110:PHE:CD2 | 3:C3:148:VAL:HG11 | 2.55                     | 0.42              |
| 1:AH:165:ARG:HA  | 3:CH:32:PRO:HG2   | 2.01                     | 0.42              |
| 1:AP:165:ARG:HA  | 3:CQ:32:PRO:HG2   | 2.01                     | 0.42              |
| 3:CE:84:GLU:CD   | 3:CE:84:GLU:H     | 2.23                     | 0.42              |
| 3:CI:84:GLU:CD   | 3:CI:84:GLU:H     | 2.23                     | 0.42              |
| 2:B9:86:ASP:CB   | 2:B9:141:LYS:HA   | 2.49                     | 0.42              |
| 3:C4:36:VAL:HA   | 3:C4:37:PRO:HD3   | 1.64                     | 0.42              |
| 1:AH:221:PRO:HD3 | 3:CI:40:PHE:CD2   | 49.74                    | 0.42              |
| 1:AS:221:PRO:HD3 | 3:CT:40:PHE:CD2   | 2.54                     | 0.42              |
| 1:AK:220:CYS:HA  | 1:AK:221:PRO:HD2  | 1.95                     | 0.42              |
| 2:B8:228:ASN:CG  | 3:CC:140:ALA:HB2  | 252.10                   | 0.42              |
| 2:B7:115:ASN:HB3 | 2:B7:210:PRO:HG2  | 2.02                     | 0.42              |
| 2:BQ:224:GLY:HA2 | 2:BQ:225:PRO:HD2  | 1.81                     | 0.42              |
| 2:BB:115:ASN:HB3 | 2:BB:210:PRO:HG2  | 2.02                     | 0.42              |
| 3:CI:150:LEU:HA  | 3:CI:150:LEU:HD12 | 1.79                     | 0.42              |
| 1:DG:209:LEU:HA  | 1:DG:209:LEU:HD22 | 1.74                     | 0.42              |
| 2:BN:115:ASN:HB3 | 2:BN:210:PRO:HG2  | 2.02                     | 0.42              |
| 2:B9:228:ASN:CG  | 3:C9:140:ALA:HB2  | 2.40                     | 0.42              |
| 2:BP:139:ALA:HB3 | 1:DC:174:TRP:CH2  | 243.67                   | 0.41              |
| 1:AK:174:TRP:CH2 | 2:BK:139:ALA:HB3  | 65.71                    | 0.41              |
| 1:AT:174:TRP:CH2 | 2:BU:139:ALA:HB3  | 2.55                     | 0.41              |
| 1:AD:187:LEU:HA  | 1:AD:188:PRO:HD2  | 1.95                     | 0.41              |
| 1:AW:231:PRO:HG2 | 3:CX:83:ALA:CB    | 2.48                     | 0.41              |
| 2:B3:149:ALA:O   | 2:B3:153:GLN:HG3  | 2.20                     | 0.41              |
| 2:B0:152:TYR:CB  | 2:B0:197:LEU:HD11 | 2.49                     | 0.41              |
| 3:CN:44:ILE:HA   | 3:CN:44:ILE:HD12  | 1.87                     | 0.41              |
| 3:CF:110:PHE:CD2 | 3:CF:148:VAL:HG11 | 2.55                     | 0.41              |
| 3:CM:148:VAL:CG1 | 3:CM:149:GLY:N    | 2.83                     | 0.41              |
| 3:CS:110:PHE:CD2 | 3:CS:148:VAL:HG11 | 2.55                     | 0.41              |
| 3:CX:148:VAL:CG1 | 3:CX:149:GLY:N    | 2.83                     | 0.41              |
| 2:BR:70:PRO:HG2  | 2:BR:73:GLN:HB2   | 2.01                     | 0.41              |
| 3:DB:110:PHE:CD2 | 3:DB:148:VAL:HG11 | 2.55                     | 0.41              |
| 2:B8:70:PRO:HG2  | 2:B8:73:GLN:HB2   | 2.02                     | 0.41              |
| 3:CT:84:GLU:CD   | 3:CT:84:GLU:H     | 2.23                     | 0.41              |
| 3:CV:84:GLU:CD   | 3:CV:84:GLU:H     | 2.23                     | 0.41              |
| 1:AD:165:ARG:HA  | 3:CD:32:PRO:HG2   | 2.01                     | 0.41              |
| 1:A6:165:ARG:HA  | 3:C7:32:PRO:HG2   | 2.01                     | 0.41              |
| 3:C6:36:VAL:HA   | 3:C6:37:PRO:HD3   | 1.64                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:AV:221:PRO:HD3 | 3:CW:40:PHE:CD2   | 2.54                     | 0.41              |
| 1:A2:220:CYS:HA  | 1:A2:221:PRO:HD2  | 1.95                     | 0.41              |
| 2:BS:228:ASN:CG  | 3:CP:140:ALA:HB2  | 2.40                     | 0.41              |
| 2:BW:228:ASN:CG  | 3:CU:140:ALA:HB2  | 133.74                   | 0.41              |
| 1:AX:221:PRO:HD3 | 3:CY:40:PHE:CD2   | 2.54                     | 0.41              |
| 1:DH:114:LYS:HB2 | 1:DJ:240:PRO:HG2  | 2.01                     | 0.41              |
| 3:CD:4:ARG:HD3   | 3:CD:4:ARG:HH11   | 1.74                     | 0.41              |
| 1:AP:72:LEU:HA   | 1:AP:72:LEU:HD23  | 1.82                     | 0.41              |
| 3:CP:4:ARG:HH11  | 3:CP:4:ARG:HD3    | 1.75                     | 0.41              |
| 3:C8:4:ARG:HH11  | 3:C8:4:ARG:HD3    | 1.75                     | 0.41              |
| 2:BV:115:ASN:HB3 | 2:BV:210:PRO:HG2  | 2.02                     | 0.41              |
| 1:AQ:174:TRP:CH2 | 2:BP:139:ALA:HB3  | 2.55                     | 0.41              |
| 1:A8:174:TRP:CH2 | 2:B8:139:ALA:HB3  | 2.55                     | 0.41              |
| 1:AJ:174:TRP:CH2 | 2:BK:139:ALA:HB3  | 2.55                     | 0.41              |
| 1:AM:174:TRP:CH2 | 2:BN:139:ALA:HB3  | 2.55                     | 0.41              |
| 1:AN:174:TRP:CH2 | 2:BN:139:ALA:HB3  | 110.22                   | 0.41              |
| 2:BR:139:ALA:HB3 | 1:DE:174:TRP:CH2  | 265.23                   | 0.41              |
| 1:AW:174:TRP:CH2 | 2:BX:139:ALA:HB3  | 2.55                     | 0.41              |
| 1:A4:174:TRP:CH2 | 2:BX:139:ALA:HB3  | 287.27                   | 0.41              |
| 2:BU:139:ALA:HB3 | 1:DH:174:TRP:CH2  | 281.35                   | 0.41              |
| 1:A0:174:TRP:CH2 | 2:B1:139:ALA:HB3  | 2.55                     | 0.41              |
| 1:AE:231:PRO:HG2 | 3:CE:83:ALA:CB    | 2.48                     | 0.41              |
| 2:BN:149:ALA:O   | 2:BN:153:GLN:HG3  | 2.20                     | 0.41              |
| 2:BV:149:ALA:O   | 2:BV:153:GLN:HG3  | 2.20                     | 0.41              |
| 2:BJ:149:ALA:O   | 2:BJ:153:GLN:HG3  | 2.20                     | 0.41              |
| 2:BJ:152:TYR:HB3 | 2:BJ:197:LEU:HD11 | 2.01                     | 0.41              |
| 3:CC:44:ILE:HA   | 3:CC:44:ILE:HD12  | 1.88                     | 0.41              |
| 3:CD:110:PHE:CD2 | 3:CD:148:VAL:HG11 | 2.55                     | 0.41              |
| 3:CL:148:VAL:CG1 | 3:CL:149:GLY:N    | 2.83                     | 0.41              |
| 3:CV:110:PHE:CD2 | 3:CV:148:VAL:HG11 | 2.55                     | 0.41              |
| 3:CW:110:PHE:CD2 | 3:CW:148:VAL:HG11 | 2.55                     | 0.41              |
| 2:BQ:70:PRO:HG2  | 2:BQ:73:GLN:HB2   | 2.02                     | 0.41              |
| 3:C8:110:PHE:CD2 | 3:C8:148:VAL:HG11 | 2.55                     | 0.41              |
| 3:CN:148:VAL:CG1 | 3:CN:149:GLY:N    | 2.83                     | 0.41              |
| 3:CX:32:PRO:HG2  | 1:DJ:165:ARG:HA   | 243.59                   | 0.41              |
| 3:CQ:84:GLU:CD   | 3:CQ:84:GLU:H     | 2.23                     | 0.41              |
| 3:C4:84:GLU:H    | 3:C4:84:GLU:CD    | 2.23                     | 0.41              |
| 1:AG:221:PRO:HD3 | 3:CG:40:PHE:CD1   | 2.54                     | 0.41              |
| 1:AH:221:PRO:HD3 | 3:CH:40:PHE:CD1   | 2.54                     | 0.41              |
| 1:AJ:221:PRO:HD3 | 3:CK:40:PHE:CD2   | 4.39                     | 0.41              |
| 3:CU:91:ALA:O    | 3:CU:94:SER:HB2   | 2.21                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:CM:91:ALA:O    | 3:CM:94:SER:HB2   | 2.21                     | 0.41              |
| 2:BO:129:VAL:HA  | 2:BO:130:PRO:HD3  | 1.98                     | 0.41              |
| 2:BK:228:ASN:CG  | 3:CN:140:ALA:HB2  | 2.40                     | 0.41              |
| 1:A8:240:PRO:HG2 | 1:A9:114:LYS:HB2  | 2.01                     | 0.41              |
| 2:BI:115:ASN:HB3 | 2:BI:210:PRO:HG2  | 2.02                     | 0.41              |
| 2:B7:228:ASN:CG  | 3:C5:140:ALA:HB2  | 2.40                     | 0.41              |
| 1:DK:209:LEU:HA  | 1:DK:209:LEU:HD22 | 1.74                     | 0.41              |
| 3:CB:4:ARG:HD3   | 3:CB:4:ARG:HH11   | 1.75                     | 0.41              |
| 3:CT:91:ALA:O    | 3:CT:94:SER:HB2   | 2.21                     | 0.41              |
| 1:AK:174:TRP:CH2 | 2:BL:139:ALA:HB3  | 2.55                     | 0.41              |
| 1:AA:174:TRP:CH2 | 2:BA:139:ALA:HB3  | 2.55                     | 0.41              |
| 2:BR:157:VAL:CG2 | 3:CS:50:THR:HG21  | 207.45                   | 0.41              |
| 1:AG:174:TRP:CH2 | 2:BG:139:ALA:HB3  | 2.55                     | 0.41              |
| 1:AE:74:THR:HG21 | 3:CE:43:PHE:CE1   | 2.45                     | 0.41              |
| 1:A6:74:THR:HG21 | 3:C7:43:PHE:CE2   | 2.45                     | 0.41              |
| 1:A9:74:THR:CG2  | 1:A9:74:THR:O     | 2.68                     | 0.41              |
| 1:AC:212:ARG:NH2 | 3:CD:18:VAL:O     | 24.16                    | 0.41              |
| 3:CJ:18:VAL:O    | 1:DK:212:ARG:NH2  | 2.46                     | 0.41              |
| 1:AG:212:ARG:NH2 | 3:CG:18:VAL:O     | 2.46                     | 0.41              |
| 2:B5:152:TYR:CB  | 2:B5:197:LEU:HD11 | 2.49                     | 0.41              |
| 2:BA:149:ALA:O   | 2:BA:153:GLN:HG3  | 2.20                     | 0.41              |
| 2:BG:149:ALA:O   | 2:BG:153:GLN:HG3  | 2.20                     | 0.41              |
| 2:B3:152:TYR:HB3 | 2:B3:197:LEU:HD11 | 2.02                     | 0.41              |
| 2:BY:149:ALA:O   | 2:BY:153:GLN:HG3  | 2.20                     | 0.41              |
| 2:BX:149:ALA:O   | 2:BX:153:GLN:HG3  | 2.20                     | 0.41              |
| 2:B0:152:TYR:HB3 | 2:B0:197:LEU:HD11 | 2.02                     | 0.41              |
| 1:A2:146:ILE:O   | 1:A2:147:ALA:CB   | 2.62                     | 0.41              |
| 2:BV:101:HIS:CG  | 2:BV:222:VAL:HG13 | 2.56                     | 0.41              |
| 2:B0:101:HIS:CG  | 2:B0:222:VAL:HG13 | 2.56                     | 0.41              |
| 3:CF:148:VAL:CG1 | 3:CF:149:GLY:N    | 2.83                     | 0.41              |
| 3:CL:110:PHE:CD2 | 3:CL:148:VAL:HG11 | 2.55                     | 0.41              |
| 3:CX:110:PHE:CD2 | 3:CX:148:VAL:HG11 | 2.55                     | 0.41              |
| 3:C1:148:VAL:CG1 | 3:C1:149:GLY:N    | 2.83                     | 0.41              |
| 3:C6:110:PHE:CD2 | 3:C6:148:VAL:HG11 | 2.55                     | 0.41              |
| 2:B4:70:PRO:HG2  | 2:B4:73:GLN:HB2   | 2.02                     | 0.41              |
| 3:C6:84:GLU:CD   | 3:C6:84:GLU:H     | 2.23                     | 0.41              |
| 3:CJ:84:GLU:H    | 3:CJ:84:GLU:CD    | 2.23                     | 0.41              |
| 3:CO:84:GLU:CD   | 3:CO:84:GLU:H     | 2.23                     | 0.41              |
| 3:CS:84:GLU:H    | 3:CS:84:GLU:CD    | 2.23                     | 0.41              |
| 1:A9:165:ARG:HA  | 3:DA:32:PRO:HG2   | 2.01                     | 0.41              |
| 1:AJ:240:PRO:HG2 | 1:AK:114:LYS:HB2  | 2.01                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AL:114:LYS:HB2  | 1:AN:240:PRO:HG2  | 2.01                     | 0.41              |
| 1:AA:114:LYS:HB2  | 1:AD:240:PRO:HG2  | 2.01                     | 0.41              |
| 2:B7:53:ARG:HG2   | 2:B7:221:MET:HE3  | 2.01                     | 0.41              |
| 1:AD:220:CYS:HA   | 1:AD:221:PRO:HD2  | 1.95                     | 0.41              |
| 2:BO:228:ASN:CG   | 3:CS:140:ALA:HB2  | 2.40                     | 0.41              |
| 2:BN:228:ASN:CG   | 3:CR:140:ALA:HB2  | 253.60                   | 0.41              |
| 2:BQ:115:ASN:HB3  | 2:BQ:210:PRO:HG2  | 2.02                     | 0.41              |
| 3:CX:101:ARG:O    | 3:CX:214:PHE:HA   | 2.21                     | 0.41              |
| 3:CP:101:ARG:O    | 3:CP:214:PHE:HA   | 2.21                     | 0.41              |
| 2:BZ:228:ASN:CG   | 3:C2:140:ALA:HB2  | 2.40                     | 0.41              |
| 3:CG:91:ALA:O     | 3:CG:94:SER:HB2   | 2.21                     | 0.41              |
| 3:CP:91:ALA:O     | 3:CP:94:SER:HB2   | 2.21                     | 0.41              |
| 3:CY:91:ALA:O     | 3:CY:94:SER:HB2   | 2.21                     | 0.41              |
| 3:C7:101:ARG:O    | 3:C7:214:PHE:HA   | 2.21                     | 0.41              |
| 1:AW:209:LEU:HA   | 1:AW:209:LEU:HD22 | 1.74                     | 0.41              |
| 3:CM:178:ASN:HD22 | 3:CM:178:ASN:HA   | 1.65                     | 0.41              |
| 3:CL:101:ARG:O    | 3:CL:214:PHE:HA   | 2.21                     | 0.41              |
| 3:DA:101:ARG:O    | 3:DA:214:PHE:HA   | 2.20                     | 0.41              |
| 2:BL:129:VAL:HA   | 2:BL:130:PRO:HD3  | 1.98                     | 0.41              |
| 3:CC:101:ARG:O    | 3:CC:214:PHE:HA   | 2.21                     | 0.41              |
| 1:AF:174:TRP:CH2  | 2:BF:139:ALA:HB3  | 2.55                     | 0.41              |
| 1:AW:191:HIS:HD2  | 1:AW:193:GLY:N    | 2.08                     | 0.41              |
| 1:DD:87:GLN:HE21  | 1:DD:210:ARG:NH2  | 2.12                     | 0.41              |
| 3:CX:43:PHE:CE2   | 1:DJ:74:THR:HG21  | 259.31                   | 0.41              |
| 1:AA:212:ARG:NH2  | 3:CA:18:VAL:O     | 2.46                     | 0.41              |
| 1:AL:231:PRO:HG2  | 3:CM:83:ALA:CB    | 2.48                     | 0.41              |
| 2:BC:149:ALA:O    | 2:BC:153:GLN:HG3  | 2.20                     | 0.41              |
| 2:BL:149:ALA:O    | 2:BL:153:GLN:HG3  | 2.20                     | 0.41              |
| 2:BL:152:TYR:HB3  | 2:BL:197:LEU:HD11 | 2.02                     | 0.41              |
| 2:B6:152:TYR:HB3  | 2:B6:197:LEU:HD11 | 2.01                     | 0.41              |
| 1:AS:146:ILE:O    | 1:AS:147:ALA:CB   | 2.62                     | 0.41              |
| 3:CJ:44:ILE:HA    | 3:CJ:44:ILE:HD12  | 1.88                     | 0.41              |
| 3:CX:44:ILE:HD12  | 3:CX:44:ILE:HA    | 1.88                     | 0.41              |
| 2:BA:101:HIS:CG   | 2:BA:222:VAL:HG13 | 2.56                     | 0.41              |
| 2:B6:101:HIS:CG   | 2:B6:222:VAL:HG13 | 2.56                     | 0.41              |
| 2:BH:101:HIS:CG   | 2:BH:222:VAL:HG13 | 2.56                     | 0.41              |
| 3:C5:148:VAL:CG1  | 3:C5:149:GLY:N    | 2.83                     | 0.41              |
| 3:CS:148:VAL:CG1  | 3:CS:149:GLY:N    | 2.83                     | 0.41              |
| 3:CC:148:VAL:CG1  | 3:CC:149:GLY:N    | 2.83                     | 0.41              |
| 3:C2:148:VAL:CG1  | 3:C2:149:GLY:N    | 2.83                     | 0.41              |
| 2:BG:70:PRO:HG2   | 2:BG:73:GLN:HB2   | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BF:70:PRO:HG2   | 2:BF:73:GLN:HB2   | 2.01                     | 0.41              |
| 2:BA:70:PRO:HG2   | 2:BA:73:GLN:HB2   | 2.02                     | 0.41              |
| 2:BD:70:PRO:HG2   | 2:BD:73:GLN:HB2   | 2.02                     | 0.41              |
| 3:C0:127:PRO:HD3  | 3:C0:180:SER:O    | 2.21                     | 0.41              |
| 3:CN:127:PRO:HD3  | 3:CN:180:SER:O    | 2.21                     | 0.41              |
| 3:C2:127:PRO:HD3  | 3:C2:180:SER:O    | 2.21                     | 0.41              |
| 3:CN:76:MET:HG3   | 3:CN:76:MET:O     | 2.18                     | 0.41              |
| 3:C3:84:GLU:H     | 3:C3:84:GLU:CD    | 2.23                     | 0.41              |
| 3:CZ:84:GLU:H     | 3:CZ:84:GLU:CD    | 2.23                     | 0.41              |
| 3:C1:36:VAL:HA    | 3:C1:37:PRO:HD3   | 1.64                     | 0.41              |
| 3:C2:36:VAL:HA    | 3:C2:37:PRO:HD3   | 1.64                     | 0.41              |
| 1:AR:220:CYS:HA   | 1:AR:221:PRO:HD2  | 1.95                     | 0.41              |
| 1:AK:240:PRO:HG2  | 1:AN:114:LYS:HB2  | 2.01                     | 0.41              |
| 1:AI:221:PRO:HD3  | 3:CI:40:PHE:CD1   | 2.54                     | 0.41              |
| 2:BP:228:ASN:CG   | 3:CS:140:ALA:HB2  | 133.33                   | 0.41              |
| 2:BT:228:ASN:CG   | 3:CT:140:ALA:HB2  | 82.01                    | 0.41              |
| 1:AQ:114:LYS:HB2  | 1:AS:240:PRO:HG2  | 2.01                     | 0.41              |
| 2:BF:115:ASN:HB3  | 2:BF:210:PRO:HG2  | 2.02                     | 0.41              |
| 3:CD:91:ALA:O     | 3:CD:94:SER:HB2   | 2.21                     | 0.41              |
| 3:C4:101:ARG:O    | 3:C4:214:PHE:HA   | 2.21                     | 0.41              |
| 1:A6:221:PRO:HD3  | 3:C7:40:PHE:CD2   | 2.54                     | 0.41              |
| 3:C6:101:ARG:O    | 3:C6:214:PHE:HA   | 2.21                     | 0.41              |
| 1:AY:240:PRO:HG2  | 1:AZ:114:LYS:HB2  | 2.01                     | 0.41              |
| 3:CJ:101:ARG:O    | 3:CJ:214:PHE:HA   | 2.21                     | 0.41              |
| 3:CH:91:ALA:O     | 3:CH:94:SER:HB2   | 2.21                     | 0.41              |
| 1:A8:221:PRO:HD3  | 3:C9:40:PHE:CD2   | 2.54                     | 0.41              |
| 3:CQ:101:ARG:O    | 3:CQ:214:PHE:HA   | 2.21                     | 0.41              |
| 3:CS:101:ARG:O    | 3:CS:214:PHE:HA   | 2.21                     | 0.41              |
| 3:DB:150:LEU:HD12 | 3:DB:150:LEU:HA   | 1.79                     | 0.41              |
| 1:A1:209:LEU:HA   | 1:A1:209:LEU:HD22 | 1.75                     | 0.41              |
| 3:CM:101:ARG:O    | 3:CM:214:PHE:HA   | 2.21                     | 0.41              |
| 3:CJ:91:ALA:O     | 3:CJ:94:SER:HB2   | 2.21                     | 0.41              |
| 1:AP:174:TRP:CH2  | 2:BS:139:ALA:HB3  | 2.55                     | 0.41              |
| 1:AC:174:TRP:CH2  | 2:BC:139:ALA:HB3  | 2.55                     | 0.41              |
| 1:AR:191:HIS:HD2  | 1:AR:193:GLY:N    | 2.08                     | 0.41              |
| 1:DD:187:LEU:HA   | 1:DD:188:PRO:HD2  | 1.95                     | 0.41              |
| 1:AY:74:THR:CG2   | 1:AY:74:THR:O     | 2.68                     | 0.41              |
| 1:A6:74:THR:O     | 1:A6:74:THR:CG2   | 2.69                     | 0.41              |
| 1:AC:231:PRO:HG2  | 3:CD:83:ALA:CB    | 63.69                    | 0.41              |
| 1:AL:212:ARG:NH2  | 3:CM:18:VAL:O     | 2.46                     | 0.41              |
| 2:B2:152:TYR:HB3  | 2:B2:197:LEU:HD11 | 2.01                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BM:152:TYR:HB3  | 2:BM:197:LEU:HD11 | 2.02                     | 0.41              |
| 2:BK:149:ALA:O    | 2:BK:153:GLN:HG3  | 2.20                     | 0.41              |
| 1:AG:146:ILE:O    | 1:AG:147:ALA:CB   | 2.62                     | 0.41              |
| 2:B7:152:TYR:HB3  | 2:B7:197:LEU:HD11 | 2.01                     | 0.41              |
| 2:BX:152:TYR:HB3  | 2:BX:197:LEU:HD11 | 2.02                     | 0.41              |
| 2:B1:149:ALA:O    | 2:B1:153:GLN:HG3  | 2.20                     | 0.41              |
| 2:BJ:101:HIS:CG   | 2:BJ:222:VAL:HG13 | 2.56                     | 0.41              |
| 2:BB:101:HIS:CG   | 2:BB:222:VAL:HG13 | 2.56                     | 0.41              |
| 2:BO:101:HIS:CG   | 2:BO:222:VAL:HG13 | 2.56                     | 0.41              |
| 2:BX:101:HIS:CG   | 2:BX:222:VAL:HG13 | 2.56                     | 0.41              |
| 2:BW:101:HIS:CG   | 2:BW:222:VAL:HG13 | 2.56                     | 0.41              |
| 2:BD:101:HIS:CG   | 2:BD:222:VAL:HG13 | 2.56                     | 0.41              |
| 3:C4:74:PHE:HE2   | 3:C4:183:LEU:HD13 | 1.84                     | 0.41              |
| 2:B5:70:PRO:HG2   | 2:B5:73:GLN:HB2   | 2.01                     | 0.41              |
| 3:CZ:148:VAL:CG1  | 3:CZ:149:GLY:N    | 2.83                     | 0.41              |
| 3:DA:110:PHE:CD2  | 3:DA:148:VAL:HG11 | 2.55                     | 0.41              |
| 3:CP:110:PHE:CD2  | 3:CP:148:VAL:HG11 | 2.55                     | 0.41              |
| 3:CY:148:VAL:CG1  | 3:CY:149:GLY:N    | 2.83                     | 0.41              |
| 3:CH:127:PRO:HD3  | 3:CH:180:SER:O    | 2.21                     | 0.41              |
| 3:CK:127:PRO:HD3  | 3:CK:180:SER:O    | 2.21                     | 0.41              |
| 3:CM:127:PRO:HD3  | 3:CM:180:SER:O    | 2.21                     | 0.41              |
| 3:CD:127:PRO:HD3  | 3:CD:180:SER:O    | 2.21                     | 0.41              |
| 2:BQ:228:ASN:CG   | 3:CR:140:ALA:HB2  | 2.40                     | 0.41              |
| 2:BE:228:ASN:CG   | 3:CE:140:ALA:HB2  | 82.01                    | 0.41              |
| 2:BY:228:ASN:CG   | 3:CV:140:ALA:HB2  | 2.40                     | 0.41              |
| 1:AW:221:PRO:HD3  | 3:CX:40:PHE:CD2   | 2.54                     | 0.41              |
| 2:BG:228:ASN:CG   | 3:CG:140:ALA:HB2  | 82.01                    | 0.41              |
| 2:BJ:228:ASN:CG   | 3:CG:140:ALA:HB2  | 2.40                     | 0.41              |
| 1:AL:221:PRO:HD3  | 3:CM:40:PHE:CD2   | 4.39                     | 0.41              |
| 2:BI:43:PRO:HA    | 2:BI:44:PRO:HD3   | 1.96                     | 0.41              |
| 3:CV:91:ALA:O     | 3:CV:94:SER:HB2   | 2.21                     | 0.41              |
| 3:CO:101:ARG:O    | 3:CO:214:PHE:HA   | 2.21                     | 0.41              |
| 2:B5:228:ASN:CG   | 3:C8:140:ALA:HB2  | 2.40                     | 0.41              |
| 3:C4:91:ALA:O     | 3:C4:94:SER:HB2   | 2.21                     | 0.41              |
| 3:CO:91:ALA:O     | 3:CO:94:SER:HB2   | 2.21                     | 0.41              |
| 3:C5:91:ALA:O     | 3:C5:94:SER:HB2   | 2.21                     | 0.41              |
| 3:CI:101:ARG:O    | 3:CI:214:PHE:HA   | 2.21                     | 0.41              |
| 1:AX:209:LEU:HD22 | 1:AX:209:LEU:HA   | 1.74                     | 0.41              |
| 3:CB:178:ASN:HD22 | 3:CB:178:ASN:HA   | 1.65                     | 0.41              |
| 1:AL:72:LEU:HA    | 1:AL:72:LEU:HD23  | 1.83                     | 0.41              |
| 3:CI:91:ALA:O     | 3:CI:94:SER:HB2   | 2.21                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:CQ:91:ALA:O    | 3:CQ:94:SER:HB2   | 2.21                     | 0.41              |
| 3:C9:101:ARG:O   | 3:C9:214:PHE:HA   | 2.21                     | 0.41              |
| 3:CU:101:ARG:O   | 3:CU:214:PHE:HA   | 2.21                     | 0.41              |
| 3:CD:101:ARG:O   | 3:CD:214:PHE:HA   | 2.21                     | 0.41              |
| 1:A6:174:TRP:CH2 | 2:B6:139:ALA:HB3  | 2.55                     | 0.41              |
| 1:AN:174:TRP:CH2 | 2:BR:139:ALA:HB3  | 2.55                     | 0.41              |
| 1:AV:174:TRP:CH2 | 2:BW:139:ALA:HB3  | 2.55                     | 0.41              |
| 1:A5:174:TRP:CH2 | 2:B5:139:ALA:HB3  | 2.55                     | 0.41              |
| 1:AN:187:LEU:HA  | 1:AN:188:PRO:HD2  | 1.95                     | 0.41              |
| 1:A4:74:THR:O    | 1:A4:74:THR:CG2   | 2.68                     | 0.41              |
| 2:BO:149:ALA:O   | 2:BO:153:GLN:HG3  | 2.20                     | 0.41              |
| 2:B5:149:ALA:O   | 2:B5:153:GLN:HG3  | 2.20                     | 0.41              |
| 2:BI:149:ALA:O   | 2:BI:153:GLN:HG3  | 2.20                     | 0.41              |
| 2:BQ:149:ALA:O   | 2:BQ:153:GLN:HG3  | 2.20                     | 0.41              |
| 2:B6:149:ALA:O   | 2:B6:153:GLN:HG3  | 2.20                     | 0.41              |
| 2:BP:149:ALA:O   | 2:BP:153:GLN:HG3  | 2.20                     | 0.41              |
| 2:B0:149:ALA:O   | 2:B0:153:GLN:HG3  | 2.20                     | 0.41              |
| 1:AK:163:MET:HE3 | 1:AK:189:GLY:HA3  | 2.08                     | 0.41              |
| 2:BU:101:HIS:CG  | 2:BU:222:VAL:HG13 | 2.56                     | 0.41              |
| 2:BN:101:HIS:CG  | 2:BN:222:VAL:HG13 | 2.56                     | 0.41              |
| 2:B8:101:HIS:CG  | 2:B8:222:VAL:HG13 | 2.56                     | 0.41              |
| 3:C5:110:PHE:CD2 | 3:C5:148:VAL:HG11 | 2.55                     | 0.41              |
| 3:C4:148:VAL:CG1 | 3:C4:149:GLY:N    | 2.83                     | 0.41              |
| 3:CC:127:PRO:HD3 | 3:CC:180:SER:O    | 2.21                     | 0.41              |
| 3:CR:127:PRO:HD3 | 3:CR:180:SER:O    | 2.21                     | 0.41              |
| 3:CS:127:PRO:HD3 | 3:CS:180:SER:O    | 2.21                     | 0.41              |
| 3:CA:127:PRO:HD3 | 3:CA:180:SER:O    | 2.21                     | 0.41              |
| 3:C5:127:PRO:HD3 | 3:C5:180:SER:O    | 2.21                     | 0.41              |
| 3:C8:76:MET:O    | 3:C8:76:MET:HG3   | 2.18                     | 0.41              |
| 2:BI:53:ARG:HG2  | 2:BI:221:MET:HE2  | 2.14                     | 0.41              |
| 1:AG:240:PRO:HG2 | 1:DK:114:LYS:HB2  | 2.01                     | 0.41              |
| 1:AH:220:CYS:HA  | 1:AH:221:PRO:HD2  | 1.95                     | 0.41              |
| 3:C1:91:ALA:O    | 3:C1:94:SER:HB2   | 2.21                     | 0.41              |
| 3:CF:101:ARG:O   | 3:CF:214:PHE:HA   | 2.21                     | 0.41              |
| 3:CW:101:ARG:O   | 3:CW:214:PHE:HA   | 2.21                     | 0.41              |
| 3:CE:91:ALA:O    | 3:CE:94:SER:HB2   | 2.21                     | 0.41              |
| 3:C5:101:ARG:O   | 3:C5:214:PHE:HA   | 2.21                     | 0.41              |
| 3:CZ:101:ARG:O   | 3:CZ:214:PHE:HA   | 2.21                     | 0.41              |
| 3:CG:4:ARG:HD3   | 3:CG:4:ARG:HH11   | 1.75                     | 0.41              |
| 3:C7:91:ALA:O    | 3:C7:94:SER:HB2   | 2.21                     | 0.41              |
| 3:C1:101:ARG:O   | 3:C1:214:PHE:HA   | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:CN:101:ARG:O    | 3:CN:214:PHE:HA   | 2.21                     | 0.41              |
| 2:BH:43:PRO:HA    | 2:BH:44:PRO:HD3   | 1.96                     | 0.41              |
| 3:DA:91:ALA:O     | 3:DA:94:SER:HB2   | 2.21                     | 0.41              |
| 1:AZ:191:HIS:HD2  | 1:AZ:193:GLY:N    | 2.08                     | 0.41              |
| 1:AC:187:LEU:HD23 | 1:AC:187:LEU:HA   | 1.90                     | 0.41              |
| 1:AX:187:LEU:HD23 | 1:AX:187:LEU:HA   | 1.91                     | 0.41              |
| 1:AN:87:GLN:HE21  | 1:AN:210:ARG:NH2  | 2.12                     | 0.41              |
| 1:DH:87:GLN:HE21  | 1:DH:210:ARG:NH2  | 2.12                     | 0.41              |
| 2:BB:82:PRO:HA    | 2:BB:193:THR:HA   | 2.03                     | 0.41              |
| 1:DE:146:ILE:O    | 1:DE:147:ALA:CB   | 2.62                     | 0.41              |
| 2:B8:152:TYR:HB3  | 2:B8:197:LEU:HD11 | 2.02                     | 0.41              |
| 2:BF:101:HIS:CG   | 2:BF:222:VAL:HG13 | 2.56                     | 0.41              |
| 2:BK:101:HIS:CG   | 2:BK:222:VAL:HG13 | 2.56                     | 0.41              |
| 3:C4:127:PRO:HD3  | 3:C4:180:SER:O    | 2.21                     | 0.41              |
| 3:CL:127:PRO:HD3  | 3:CL:180:SER:O    | 2.21                     | 0.41              |
| 3:C6:127:PRO:HD3  | 3:C6:180:SER:O    | 2.21                     | 0.41              |
| 3:CW:84:GLU:H     | 3:CW:84:GLU:CD    | 2.23                     | 0.41              |
| 3:C7:76:MET:O     | 3:C7:76:MET:HG3   | 2.18                     | 0.41              |
| 3:CR:84:GLU:CD    | 3:CR:84:GLU:H     | 2.23                     | 0.41              |
| 1:AG:187:LEU:HD23 | 1:AG:187:LEU:HA   | 1.90                     | 0.41              |
| 2:BQ:53:ARG:HG2   | 2:BQ:221:MET:HE3  | 2.03                     | 0.41              |
| 3:C5:36:VAL:HA    | 3:C5:37:PRO:HD3   | 1.64                     | 0.41              |
| 2:BD:228:ASN:CG   | 3:CH:140:ALA:HB2  | 183.81                   | 0.41              |
| 2:BJ:228:ASN:CG   | 3:CJ:140:ALA:HB2  | 82.01                    | 0.41              |
| 3:CC:91:ALA:O     | 3:CC:94:SER:HB2   | 2.21                     | 0.41              |
| 3:CY:101:ARG:O    | 3:CY:214:PHE:HA   | 2.21                     | 0.41              |
| 2:BG:129:VAL:HA   | 2:BG:130:PRO:HD3  | 1.98                     | 0.41              |
| 3:CN:91:ALA:O     | 3:CN:94:SER:HB2   | 2.21                     | 0.41              |
| 3:CX:91:ALA:O     | 3:CX:94:SER:HB2   | 2.21                     | 0.41              |
| 3:CA:101:ARG:O    | 3:CA:214:PHE:HA   | 2.21                     | 0.41              |
| 1:A1:72:LEU:HD23  | 1:A1:72:LEU:HA    | 1.83                     | 0.41              |
| 3:C3:178:ASN:HA   | 3:C3:178:ASN:HD22 | 1.66                     | 0.41              |
| 3:CS:91:ALA:O     | 3:CS:94:SER:HB2   | 2.21                     | 0.41              |
| 2:B3:115:ASN:HB3  | 2:B3:210:PRO:HG2  | 2.02                     | 0.41              |
| 3:CK:91:ALA:O     | 3:CK:94:SER:HB2   | 2.21                     | 0.41              |
| 1:AL:187:LEU:HD23 | 1:AL:187:LEU:HA   | 1.91                     | 0.41              |
| 2:BW:82:PRO:HA    | 2:BW:193:THR:HA   | 2.03                     | 0.41              |
| 2:BF:82:PRO:HA    | 2:BF:193:THR:HA   | 2.03                     | 0.41              |
| 2:BM:82:PRO:HA    | 2:BM:193:THR:HA   | 2.03                     | 0.41              |
| 2:BP:82:PRO:HA    | 2:BP:193:THR:HA   | 2.03                     | 0.41              |
| 2:BX:82:PRO:HA    | 2:BX:193:THR:HA   | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AD:212:ARG:NH2  | 3:CE:18:VAL:O     | 35.99                    | 0.41              |
| 2:BZ:149:ALA:O    | 2:BZ:153:GLN:HG3  | 2.20                     | 0.41              |
| 3:DB:44:ILE:HD12  | 3:DB:44:ILE:HA    | 1.88                     | 0.41              |
| 2:BI:101:HIS:CG   | 2:BI:222:VAL:HG13 | 2.56                     | 0.41              |
| 2:BM:101:HIS:CG   | 2:BM:222:VAL:HG13 | 2.56                     | 0.41              |
| 2:BG:101:HIS:CG   | 2:BG:222:VAL:HG13 | 2.56                     | 0.41              |
| 3:C6:148:VAL:CG1  | 3:C6:149:GLY:N    | 2.83                     | 0.41              |
| 3:C3:148:VAL:CG1  | 3:C3:149:GLY:N    | 2.83                     | 0.41              |
| 3:C4:110:PHE:CD2  | 3:C4:148:VAL:HG11 | 2.55                     | 0.41              |
| 3:CK:127:PRO:HD3  | 3:CK:180:SER:C    | 2.41                     | 0.41              |
| 3:CO:127:PRO:HD3  | 3:CO:180:SER:O    | 2.21                     | 0.41              |
| 3:CQ:127:PRO:HD3  | 3:CQ:180:SER:O    | 2.21                     | 0.41              |
| 3:CT:127:PRO:HD3  | 3:CT:180:SER:O    | 2.21                     | 0.41              |
| 3:CG:127:PRO:HD3  | 3:CG:180:SER:O    | 2.21                     | 0.41              |
| 3:CJ:127:PRO:HD3  | 3:CJ:180:SER:O    | 2.21                     | 0.41              |
| 3:C3:127:PRO:HD3  | 3:C3:180:SER:O    | 2.21                     | 0.41              |
| 3:CV:127:PRO:HD3  | 3:CV:180:SER:C    | 2.41                     | 0.41              |
| 3:CV:127:PRO:HD3  | 3:CV:180:SER:O    | 2.21                     | 0.41              |
| 3:CI:127:PRO:HD3  | 3:CI:180:SER:C    | 2.41                     | 0.41              |
| 3:CI:127:PRO:HD3  | 3:CI:180:SER:O    | 2.21                     | 0.41              |
| 1:A7:224:ILE:HA   | 1:A7:225:PRO:HD2  | 1.95                     | 0.41              |
| 3:C9:84:GLU:CD    | 3:C9:84:GLU:H     | 2.23                     | 0.41              |
| 3:C5:84:GLU:CD    | 3:C5:84:GLU:H     | 2.23                     | 0.41              |
| 3:DA:84:GLU:CD    | 3:DA:84:GLU:H     | 2.23                     | 0.41              |
| 2:BP:53:ARG:HG2   | 2:BP:221:MET:HE3  | 2.01                     | 0.41              |
| 2:B4:53:ARG:HG2   | 2:B4:221:MET:HE2  | 2.03                     | 0.41              |
| 2:B5:53:ARG:HG2   | 2:B5:221:MET:HE3  | 2.01                     | 0.41              |
| 3:C7:36:VAL:HA    | 3:C7:37:PRO:HD3   | 1.64                     | 0.41              |
| 2:B3:53:ARG:HG2   | 2:B3:221:MET:HE2  | 2.03                     | 0.41              |
| 3:C3:101:ARG:O    | 3:C3:214:PHE:HA   | 2.21                     | 0.41              |
| 3:C2:91:ALA:O     | 3:C2:94:SER:HB2   | 2.21                     | 0.41              |
| 2:BY:115:ASN:HB3  | 2:BY:210:PRO:HG2  | 2.02                     | 0.41              |
| 1:A5:240:PRO:HG2  | 1:A6:114:LYS:HB2  | 2.01                     | 0.41              |
| 3:CF:91:ALA:O     | 3:CF:94:SER:HB2   | 2.21                     | 0.41              |
| 1:DC:209:LEU:HD22 | 1:DC:209:LEU:HA   | 1.74                     | 0.41              |
| 3:CK:101:ARG:O    | 3:CK:214:PHE:HA   | 2.21                     | 0.41              |
| 3:CE:101:ARG:O    | 3:CE:214:PHE:HA   | 2.21                     | 0.41              |
| 1:AP:187:LEU:HA   | 1:AP:188:PRO:HD2  | 1.95                     | 0.41              |
| 1:A8:87:GLN:HE21  | 1:A8:210:ARG:NH2  | 2.12                     | 0.41              |
| 1:AE:87:GLN:HE21  | 1:AE:210:ARG:NH2  | 2.12                     | 0.41              |
| 1:AV:74:THR:CG2   | 1:AV:74:THR:O     | 2.69                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B0:83:LEU:HA   | 2:B0:84:PRO:HA    | 1.60                     | 0.41              |
| 2:BJ:82:PRO:HA   | 2:BJ:193:THR:HA   | 2.03                     | 0.41              |
| 2:BU:82:PRO:HA   | 2:BU:193:THR:HA   | 2.03                     | 0.41              |
| 2:BS:82:PRO:HA   | 2:BS:193:THR:HA   | 2.03                     | 0.41              |
| 2:BC:82:PRO:HA   | 2:BC:193:THR:HA   | 2.03                     | 0.41              |
| 2:BO:82:PRO:HA   | 2:BO:193:THR:HA   | 2.03                     | 0.41              |
| 2:B5:82:PRO:HA   | 2:B5:193:THR:HA   | 2.03                     | 0.41              |
| 2:BD:82:PRO:HA   | 2:BD:193:THR:HA   | 2.03                     | 0.41              |
| 1:AS:231:PRO:HG2 | 3:CT:83:ALA:CB    | 2.48                     | 0.41              |
| 1:AG:231:PRO:HG2 | 3:CG:83:ALA:CB    | 2.48                     | 0.41              |
| 1:AI:212:ARG:NH2 | 3:CJ:18:VAL:O     | 35.99                    | 0.41              |
| 2:BF:149:ALA:O   | 2:BF:153:GLN:HG3  | 2.20                     | 0.41              |
| 2:BB:149:ALA:O   | 2:BB:153:GLN:HG3  | 2.20                     | 0.41              |
| 2:B7:149:ALA:O   | 2:B7:153:GLN:HG3  | 2.20                     | 0.41              |
| 3:C9:29:VAL:HG23 | 3:C9:29:VAL:O     | 2.21                     | 0.41              |
| 3:DA:44:ILE:HA   | 3:DA:44:ILE:HD12  | 1.87                     | 0.41              |
| 2:BQ:101:HIS:CG  | 2:BQ:222:VAL:HG13 | 2.56                     | 0.41              |
| 2:B7:101:HIS:CG  | 2:B7:222:VAL:HG13 | 2.56                     | 0.41              |
| 2:BB:166:ARG:NH2 | 3:CB:116:THR:O    | 2.54                     | 0.41              |
| 3:CR:148:VAL:CG1 | 3:CR:149:GLY:N    | 2.83                     | 0.41              |
| 3:CO:148:VAL:CG1 | 3:CO:149:GLY:N    | 2.83                     | 0.41              |
| 2:BS:70:PRO:HG2  | 2:BS:73:GLN:HB2   | 2.02                     | 0.41              |
| 2:BV:68:GLU:O    | 2:BV:70:PRO:HD3   | 2.21                     | 0.41              |
| 3:CW:127:PRO:HD3 | 3:CW:180:SER:C    | 2.41                     | 0.41              |
| 3:CW:127:PRO:HD3 | 3:CW:180:SER:O    | 2.21                     | 0.41              |
| 3:CP:127:PRO:HD3 | 3:CP:180:SER:C    | 2.42                     | 0.41              |
| 3:CT:127:PRO:HD3 | 3:CT:180:SER:C    | 2.42                     | 0.41              |
| 3:CD:127:PRO:HD3 | 3:CD:180:SER:C    | 2.41                     | 0.41              |
| 3:C1:127:PRO:HD3 | 3:C1:180:SER:C    | 2.41                     | 0.41              |
| 3:CX:127:PRO:HD3 | 3:CX:180:SER:C    | 2.42                     | 0.41              |
| 3:DB:127:PRO:HD3 | 3:DB:180:SER:C    | 2.41                     | 0.41              |
| 3:CY:127:PRO:HD3 | 3:CY:180:SER:O    | 2.21                     | 0.41              |
| 3:C5:127:PRO:HD3 | 3:C5:180:SER:C    | 2.42                     | 0.41              |
| 3:C8:127:PRO:HD3 | 3:C8:180:SER:C    | 2.42                     | 0.41              |
| 3:C2:127:PRO:HD3 | 3:C2:180:SER:C    | 2.41                     | 0.41              |
| 3:CU:84:GLU:CD   | 3:CU:84:GLU:H     | 2.23                     | 0.41              |
| 3:DB:84:GLU:CD   | 3:DB:84:GLU:H     | 2.23                     | 0.41              |
| 2:BR:53:ARG:HG2  | 2:BR:221:MET:HE3  | 2.01                     | 0.41              |
| 1:AK:240:PRO:HG2 | 1:AL:114:LYS:HB2  | 46.58                    | 0.41              |
| 2:BQ:228:ASN:CG  | 3:CQ:140:ALA:HB2  | 133.74                   | 0.41              |
| 1:AJ:220:CYS:HA  | 1:AJ:221:PRO:HD2  | 1.95                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B4:129:VAL:HA  | 2:B4:130:PRO:HD3  | 1.98                     | 0.41              |
| 3:CW:91:ALA:O    | 3:CW:94:SER:HB2   | 2.21                     | 0.41              |
| 3:CR:101:ARG:O   | 3:CR:214:PHE:HA   | 2.21                     | 0.41              |
| 3:CU:4:ARG:HH11  | 3:CU:4:ARG:HD3    | 1.75                     | 0.41              |
| 1:AO:72:LEU:HA   | 1:AO:72:LEU:HD23  | 1.83                     | 0.41              |
| 1:A7:72:LEU:HA   | 1:A7:72:LEU:HD23  | 1.82                     | 0.41              |
| 1:DG:72:LEU:HD23 | 1:DG:72:LEU:HA    | 1.83                     | 0.41              |
| 2:BB:129:VAL:HA  | 2:BB:130:PRO:HD3  | 1.98                     | 0.41              |
| 3:CR:91:ALA:O    | 3:CR:94:SER:HB2   | 2.21                     | 0.41              |
| 3:CT:101:ARG:O   | 3:CT:214:PHE:HA   | 2.21                     | 0.41              |
| 3:C0:91:ALA:O    | 3:C0:94:SER:HB2   | 2.21                     | 0.41              |
| 2:BA:43:PRO:HA   | 2:BA:44:PRO:HD3   | 1.96                     | 0.41              |
| 1:AH:72:LEU:HA   | 1:AH:72:LEU:HD23  | 1.82                     | 0.41              |
| 2:BT:224:GLY:HA2 | 2:BT:225:PRO:HD2  | 1.81                     | 0.41              |
| 3:CA:91:ALA:O    | 3:CA:94:SER:HB2   | 2.21                     | 0.41              |
| 2:B1:115:ASN:HB3 | 2:B1:210:PRO:HG2  | 2.02                     | 0.41              |
| 3:CV:101:ARG:O   | 3:CV:214:PHE:HA   | 2.21                     | 0.41              |
| 1:DC:207:CYS:O   | 1:DC:208:TYR:CB   | 2.57                     | 0.41              |
| 1:AA:187:LEU:HA  | 1:AA:188:PRO:HD2  | 1.95                     | 0.41              |
| 1:AX:187:LEU:HA  | 1:AX:188:PRO:HD2  | 1.95                     | 0.41              |
| 1:AB:74:THR:O    | 1:AB:74:THR:CG2   | 2.68                     | 0.41              |
| 2:BL:82:PRO:HA   | 2:BL:193:THR:HA   | 2.03                     | 0.41              |
| 2:BN:82:PRO:HA   | 2:BN:193:THR:HA   | 2.03                     | 0.41              |
| 1:AT:87:GLN:HE21 | 1:AT:210:ARG:NH2  | 2.12                     | 0.41              |
| 2:B4:83:LEU:HA   | 2:B4:84:PRO:HA    | 1.60                     | 0.41              |
| 2:B1:152:TYR:HB3 | 2:B1:197:LEU:HD11 | 2.01                     | 0.41              |
| 3:CC:29:VAL:O    | 3:CC:29:VAL:HG23  | 2.22                     | 0.41              |
| 3:C5:29:VAL:O    | 3:C5:29:VAL:HG23  | 2.21                     | 0.41              |
| 3:C8:29:VAL:HG23 | 3:C8:29:VAL:O     | 2.21                     | 0.41              |
| 3:DA:29:VAL:O    | 3:DA:29:VAL:HG23  | 2.21                     | 0.41              |
| 3:C6:29:VAL:HG23 | 3:C6:29:VAL:O     | 2.21                     | 0.41              |
| 2:BY:101:HIS:CG  | 2:BY:222:VAL:HG13 | 2.56                     | 0.41              |
| 2:B5:101:HIS:CG  | 2:B5:222:VAL:HG13 | 2.56                     | 0.41              |
| 2:B9:101:HIS:CG  | 2:B9:222:VAL:HG13 | 2.56                     | 0.41              |
| 2:BT:166:ARG:NH2 | 3:CU:116:THR:O    | 240.80                   | 0.41              |
| 2:BX:166:ARG:NH2 | 3:C5:116:THR:O    | 240.82                   | 0.41              |
| 3:CB:110:PHE:CD2 | 3:CB:148:VAL:HG11 | 2.55                     | 0.41              |
| 2:BE:166:ARG:NH2 | 3:CF:116:THR:O    | 23.73                    | 0.41              |
| 2:BU:166:ARG:NH2 | 3:CV:116:THR:O    | 88.50                    | 0.41              |
| 2:B7:70:PRO:HG2  | 2:B7:73:GLN:HB2   | 2.02                     | 0.41              |
| 2:B0:166:ARG:NH2 | 3:C0:116:THR:O    | 2.54                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B2:166:ARG:NH2  | 3:C2:116:THR:O    | 2.54                     | 0.41              |
| 2:BQ:68:GLU:O     | 2:BQ:70:PRO:HD3   | 2.21                     | 0.41              |
| 2:BF:68:GLU:O     | 2:BF:70:PRO:HD3   | 2.22                     | 0.41              |
| 2:B7:166:ARG:NH2  | 3:C8:116:THR:O    | 2.54                     | 0.41              |
| 2:B3:70:PRO:HG2   | 2:B3:73:GLN:HB2   | 2.02                     | 0.41              |
| 2:BN:68:GLU:O     | 2:BN:70:PRO:HD3   | 2.21                     | 0.41              |
| 3:CS:127:PRO:HD3  | 3:CS:180:SER:C    | 2.41                     | 0.41              |
| 3:CF:127:PRO:HD3  | 3:CF:180:SER:O    | 2.21                     | 0.41              |
| 3:CX:127:PRO:HD3  | 3:CX:180:SER:O    | 2.21                     | 0.41              |
| 3:C0:127:PRO:HD3  | 3:C0:180:SER:C    | 2.41                     | 0.41              |
| 2:B4:68:GLU:O     | 2:B4:70:PRO:HD3   | 2.21                     | 0.41              |
| 2:BG:53:ARG:HG2   | 2:BG:221:MET:HE2  | 2.03                     | 0.41              |
| 3:CB:84:GLU:H     | 3:CB:84:GLU:CD    | 2.23                     | 0.41              |
| 2:BU:53:ARG:HG2   | 2:BU:221:MET:HE3  | 2.03                     | 0.41              |
| 2:BR:228:ASN:CG   | 3:CL:140:ALA:HB2  | 2.40                     | 0.41              |
| 2:BE:129:VAL:HA   | 2:BE:130:PRO:HD3  | 1.98                     | 0.41              |
| 3:DB:91:ALA:O     | 3:DB:94:SER:HB2   | 2.21                     | 0.41              |
| 1:AT:114:LYS:HB2  | 1:AW:240:PRO:HG2  | 2.01                     | 0.41              |
| 3:C6:91:ALA:O     | 3:C6:94:SER:HB2   | 2.21                     | 0.41              |
| 1:AG:72:LEU:HA    | 1:AG:72:LEU:HD23  | 1.82                     | 0.41              |
| 3:C8:178:ASN:HA   | 3:C8:178:ASN:HD22 | 1.65                     | 0.41              |
| 3:C3:150:LEU:HD12 | 3:C3:150:LEU:HA   | 1.79                     | 0.41              |
| 2:BO:43:PRO:HA    | 2:BO:44:PRO:HD3   | 1.96                     | 0.41              |
| 3:CB:101:ARG:O    | 3:CB:214:PHE:HA   | 2.21                     | 0.41              |
| 2:B3:43:PRO:HA    | 2:B3:44:PRO:HD3   | 1.96                     | 0.41              |
| 1:AR:174:TRP:CH2  | 2:BQ:139:ALA:HB3  | 2.55                     | 0.40              |
| 2:BK:154:GLN:O    | 2:BK:157:VAL:HB   | 2.22                     | 0.40              |
| 2:BS:154:GLN:O    | 2:BS:157:VAL:HB   | 2.22                     | 0.40              |
| 1:AW:187:LEU:HA   | 1:AW:188:PRO:HD2  | 1.95                     | 0.40              |
| 1:AD:74:THR:CG2   | 1:AD:74:THR:O     | 2.68                     | 0.40              |
| 1:A3:74:THR:CG2   | 1:A3:74:THR:O     | 2.69                     | 0.40              |
| 2:BD:149:ALA:O    | 2:BD:153:GLN:HG3  | 2.20                     | 0.40              |
| 2:B8:149:ALA:O    | 2:B8:153:GLN:HG3  | 2.20                     | 0.40              |
| 3:CD:29:VAL:HG23  | 3:CD:29:VAL:O     | 2.21                     | 0.40              |
| 3:CI:29:VAL:O     | 3:CI:29:VAL:HG23  | 2.21                     | 0.40              |
| 3:CV:29:VAL:HG23  | 3:CV:29:VAL:O     | 2.21                     | 0.40              |
| 3:C3:29:VAL:O     | 3:C3:29:VAL:HG23  | 2.21                     | 0.40              |
| 3:CO:29:VAL:HG23  | 3:CO:29:VAL:O     | 2.21                     | 0.40              |
| 2:BC:101:HIS:CG   | 2:BC:222:VAL:HG13 | 2.56                     | 0.40              |
| 2:BP:101:HIS:CG   | 2:BP:222:VAL:HG13 | 2.56                     | 0.40              |
| 2:BT:101:HIS:CG   | 2:BT:222:VAL:HG13 | 2.56                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B3:101:HIS:CG   | 2:B3:222:VAL:HG13 | 2.56                     | 0.40              |
| 2:BI:166:ARG:NH2  | 3:CI:116:THR:O    | 2.54                     | 0.40              |
| 2:BM:166:ARG:NH2  | 3:CM:116:THR:O    | 2.55                     | 0.40              |
| 2:BT:166:ARG:NH2  | 3:CT:116:THR:O    | 2.54                     | 0.40              |
| 2:BH:68:GLU:O     | 2:BH:70:PRO:HD3   | 2.21                     | 0.40              |
| 2:BZ:166:ARG:NH2  | 3:CZ:116:THR:O    | 2.55                     | 0.40              |
| 2:BO:68:GLU:O     | 2:BO:70:PRO:HD3   | 2.21                     | 0.40              |
| 2:BZ:68:GLU:O     | 2:BZ:70:PRO:HD3   | 2.21                     | 0.40              |
| 3:C8:148:VAL:CG1  | 3:C8:149:GLY:N    | 2.83                     | 0.40              |
| 2:BO:166:ARG:NH2  | 3:CP:116:THR:O    | 2.54                     | 0.40              |
| 2:BX:68:GLU:O     | 2:BX:70:PRO:HD3   | 2.21                     | 0.40              |
| 2:B6:166:ARG:NH2  | 3:C7:116:THR:O    | 2.54                     | 0.40              |
| 3:CE:127:PRO:HD3  | 3:CE:180:SER:C    | 2.42                     | 0.40              |
| 2:B0:68:GLU:O     | 2:B0:70:PRO:HD3   | 2.22                     | 0.40              |
| 3:CC:127:PRO:HD3  | 3:CC:180:SER:C    | 2.41                     | 0.40              |
| 3:CP:127:PRO:HD3  | 3:CP:180:SER:O    | 2.21                     | 0.40              |
| 3:CQ:127:PRO:HD3  | 3:CQ:180:SER:C    | 2.42                     | 0.40              |
| 3:CR:127:PRO:HD3  | 3:CR:180:SER:C    | 2.41                     | 0.40              |
| 3:C1:127:PRO:HD3  | 3:C1:180:SER:O    | 2.21                     | 0.40              |
| 3:C7:127:PRO:HD3  | 3:C7:180:SER:O    | 2.21                     | 0.40              |
| 3:CU:127:PRO:HD3  | 3:CU:180:SER:O    | 2.21                     | 0.40              |
| 1:DK:220:CYS:HA   | 1:DK:221:PRO:HD2  | 1.95                     | 0.40              |
| 1:AL:220:CYS:HA   | 1:AL:221:PRO:HD2  | 1.95                     | 0.40              |
| 2:B4:115:ASN:HB3  | 2:B4:210:PRO:HG2  | 2.02                     | 0.40              |
| 2:B4:224:GLY:HA2  | 2:B4:225:PRO:HD2  | 1.81                     | 0.40              |
| 3:CG:101:ARG:O    | 3:CG:214:PHE:HA   | 2.21                     | 0.40              |
| 2:B9:115:ASN:HB3  | 2:B9:210:PRO:HG2  | 2.02                     | 0.40              |
| 1:DD:209:LEU:HD22 | 1:DD:209:LEU:HA   | 1.74                     | 0.40              |
| 3:C8:91:ALA:O     | 3:C8:94:SER:HB2   | 2.21                     | 0.40              |
| 3:C2:101:ARG:O    | 3:C2:214:PHE:HA   | 2.21                     | 0.40              |
| 1:AX:224:ILE:HA   | 1:AX:225:PRO:HD2  | 1.95                     | 0.40              |
| 2:BM:154:GLN:O    | 2:BM:157:VAL:HB   | 2.22                     | 0.40              |
| 1:DG:191:HIS:HD2  | 1:DG:193:GLY:N    | 2.08                     | 0.40              |
| 1:AJ:187:LEU:HA   | 1:AJ:188:PRO:HD2  | 1.95                     | 0.40              |
| 1:AL:241:THR:CG2  | 1:AL:242:ASN:N    | 2.85                     | 0.40              |
| 1:AE:241:THR:CG2  | 1:AE:242:ASN:N    | 2.85                     | 0.40              |
| 1:AD:241:THR:CG2  | 1:AD:242:ASN:N    | 2.85                     | 0.40              |
| 1:AN:241:THR:CG2  | 1:AN:242:ASN:N    | 2.85                     | 0.40              |
| 1:AS:87:GLN:HE21  | 1:AS:210:ARG:NH2  | 2.12                     | 0.40              |
| 1:AM:74:THR:HG21  | 3:CN:43:PHE:CE2   | 4.65                     | 0.40              |
| 2:B0:82:PRO:HA    | 2:B0:193:THR:HA   | 2.03                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:BG:82:PRO:HA    | 2:BG:193:THR:HA   | 2.03                     | 0.40              |
| 1:A0:74:THR:CG2   | 1:A0:74:THR:O     | 2.68                     | 0.40              |
| 1:A3:212:ARG:NH2  | 3:C4:18:VAL:O     | 2.46                     | 0.40              |
| 3:CS:83:ALA:CB    | 1:DE:231:PRO:HG2  | 304.73                   | 0.40              |
| 1:DJ:146:ILE:O    | 1:DJ:147:ALA:CB   | 2.62                     | 0.40              |
| 3:CX:29:VAL:O     | 3:CX:29:VAL:HG23  | 2.21                     | 0.40              |
| 3:CM:29:VAL:HG23  | 3:CM:29:VAL:O     | 2.21                     | 0.40              |
| 2:BL:101:HIS:CG   | 2:BL:222:VAL:HG13 | 2.56                     | 0.40              |
| 2:BR:101:HIS:CG   | 2:BR:222:VAL:HG13 | 2.56                     | 0.40              |
| 3:CP:56:ILE:HD12  | 3:CP:74:PHE:CD1   | 2.57                     | 0.40              |
| 3:C9:56:ILE:HD12  | 3:C9:74:PHE:CD1   | 2.57                     | 0.40              |
| 2:BU:166:ARG:NH2  | 3:CU:116:THR:O    | 2.54                     | 0.40              |
| 2:BC:166:ARG:NH2  | 3:CD:116:THR:O    | 88.50                    | 0.40              |
| 2:BQ:166:ARG:NH2  | 3:CS:116:THR:O    | 2.55                     | 0.40              |
| 2:BS:166:ARG:NH2  | 3:CT:116:THR:O    | 88.50                    | 0.40              |
| 2:BI:68:GLU:O     | 2:BI:70:PRO:HD3   | 2.22                     | 0.40              |
| 2:B8:68:GLU:O     | 2:B8:70:PRO:HD3   | 2.22                     | 0.40              |
| 2:BK:68:GLU:O     | 2:BK:70:PRO:HD3   | 2.21                     | 0.40              |
| 2:B3:68:GLU:O     | 2:B3:70:PRO:HD3   | 2.22                     | 0.40              |
| 2:B2:68:GLU:O     | 2:B2:70:PRO:HD3   | 2.21                     | 0.40              |
| 3:CB:127:PRO:HD3  | 3:CB:180:SER:C    | 2.41                     | 0.40              |
| 3:CE:127:PRO:HD3  | 3:CE:180:SER:O    | 2.21                     | 0.40              |
| 3:CL:127:PRO:HD3  | 3:CL:180:SER:C    | 2.42                     | 0.40              |
| 3:CM:127:PRO:HD3  | 3:CM:180:SER:C    | 2.42                     | 0.40              |
| 3:C3:127:PRO:HD3  | 3:C3:180:SER:C    | 2.42                     | 0.40              |
| 2:B9:68:GLU:O     | 2:B9:70:PRO:HD3   | 2.21                     | 0.40              |
| 3:CN:127:PRO:HD3  | 3:CN:180:SER:C    | 2.41                     | 0.40              |
| 3:CP:84:GLU:H     | 3:CP:84:GLU:CD    | 2.23                     | 0.40              |
| 3:C7:84:GLU:CD    | 3:C7:84:GLU:H     | 2.23                     | 0.40              |
| 3:CL:91:ALA:O     | 3:CL:94:SER:HB2   | 2.21                     | 0.40              |
| 2:BN:43:PRO:HA    | 2:BN:44:PRO:HD3   | 1.96                     | 0.40              |
| 3:CK:178:ASN:HD22 | 3:CK:178:ASN:HA   | 1.65                     | 0.40              |
| 3:CD:178:ASN:HA   | 3:CD:178:ASN:HD22 | 1.65                     | 0.40              |
| 2:BF:154:GLN:O    | 2:BF:157:VAL:HB   | 2.22                     | 0.40              |
| 2:BG:154:GLN:O    | 2:BG:157:VAL:HB   | 2.22                     | 0.40              |
| 2:BT:139:ALA:HB3  | 1:DG:174:TRP:CH2  | 243.65                   | 0.40              |
| 1:AC:187:LEU:HA   | 1:AC:188:PRO:HD2  | 1.95                     | 0.40              |
| 1:AK:187:LEU:HA   | 1:AK:188:PRO:HD2  | 1.95                     | 0.40              |
| 1:AO:187:LEU:HA   | 1:AO:188:PRO:HD2  | 1.95                     | 0.40              |
| 1:AQ:241:THR:CG2  | 1:AQ:242:ASN:N    | 2.85                     | 0.40              |
| 1:AX:241:THR:CG2  | 1:AX:242:ASN:N    | 2.85                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:DI:74:THR:O    | 1:DI:74:THR:CG2   | 2.69                     | 0.40              |
| 1:AR:74:THR:CG2  | 1:AR:74:THR:O     | 2.68                     | 0.40              |
| 1:A1:241:THR:CG2 | 1:A1:242:ASN:N    | 2.85                     | 0.40              |
| 2:BQ:82:PRO:HA   | 2:BQ:193:THR:HA   | 2.03                     | 0.40              |
| 2:B8:83:LEU:HA   | 2:B8:84:PRO:HA    | 1.60                     | 0.40              |
| 1:A8:74:THR:CG2  | 1:A8:74:THR:O     | 2.69                     | 0.40              |
| 3:CW:29:VAL:O    | 3:CW:29:VAL:HG23  | 2.22                     | 0.40              |
| 3:C0:29:VAL:HG23 | 3:C0:29:VAL:O     | 2.21                     | 0.40              |
| 2:BS:101:HIS:CG  | 2:BS:222:VAL:HG13 | 2.56                     | 0.40              |
| 3:CD:56:ILE:HD12 | 3:CD:74:PHE:CD1   | 2.57                     | 0.40              |
| 3:CG:56:ILE:HD12 | 3:CG:74:PHE:CD1   | 2.57                     | 0.40              |
| 3:CC:56:ILE:HD12 | 3:CC:74:PHE:CD1   | 2.57                     | 0.40              |
| 3:C5:56:ILE:HD12 | 3:C5:74:PHE:CD1   | 2.57                     | 0.40              |
| 3:CI:56:ILE:HD12 | 3:CI:74:PHE:CD1   | 2.57                     | 0.40              |
| 2:BE:166:ARG:NH2 | 3:CE:116:THR:O    | 2.54                     | 0.40              |
| 2:BH:166:ARG:NH2 | 3:CI:116:THR:O    | 88.50                    | 0.40              |
| 2:BR:68:GLU:O    | 2:BR:70:PRO:HD3   | 2.22                     | 0.40              |
| 2:BS:68:GLU:O    | 2:BS:70:PRO:HD3   | 2.21                     | 0.40              |
| 2:BA:166:ARG:NH2 | 3:CA:116:THR:O    | 2.55                     | 0.40              |
| 2:BA:166:ARG:NH2 | 3:DB:116:THR:O    | 285.16                   | 0.40              |
| 2:BC:68:GLU:O    | 2:BC:70:PRO:HD3   | 2.22                     | 0.40              |
| 2:BY:166:ARG:NH2 | 3:CY:116:THR:O    | 2.54                     | 0.40              |
| 3:CH:127:PRO:HD3 | 3:CH:180:SER:C    | 2.41                     | 0.40              |
| 3:C9:127:PRO:HD3 | 3:C9:180:SER:C    | 2.41                     | 0.40              |
| 3:C6:127:PRO:HD3 | 3:C6:180:SER:C    | 2.41                     | 0.40              |
| 3:DB:127:PRO:HD3 | 3:DB:180:SER:O    | 2.21                     | 0.40              |
| 3:CU:127:PRO:HD3 | 3:CU:180:SER:C    | 2.42                     | 0.40              |
| 3:CY:127:PRO:HD3 | 3:CY:180:SER:C    | 2.42                     | 0.40              |
| 3:C8:127:PRO:HD3 | 3:C8:180:SER:O    | 2.21                     | 0.40              |
| 3:CL:84:GLU:H    | 3:CL:84:GLU:CD    | 2.23                     | 0.40              |
| 1:A7:220:CYS:HA  | 1:A7:221:PRO:HD2  | 1.95                     | 0.40              |
| 3:CM:15:MET:HB2  | 3:CN:25:LEU:HD21  | 2.03                     | 0.40              |
| 3:C8:101:ARG:O   | 3:C8:214:PHE:HA   | 2.21                     | 0.40              |
| 3:CC:15:MET:HB2  | 3:C9:25:LEU:HD21  | 256.30                   | 0.40              |
| 3:CC:15:MET:HB2  | 3:CD:25:LEU:HD21  | 2.04                     | 0.40              |
| 2:BR:129:VAL:HA  | 2:BR:130:PRO:HD3  | 1.98                     | 0.40              |
| 3:DB:4:ARG:HH11  | 3:DB:4:ARG:HD3    | 1.75                     | 0.40              |
| 3:CM:150:LEU:HA  | 3:CM:150:LEU:HD12 | 1.79                     | 0.40              |
| 2:BS:224:GLY:HA2 | 2:BS:225:PRO:HD2  | 1.81                     | 0.40              |
| 3:CB:91:ALA:O    | 3:CB:94:SER:HB2   | 2.21                     | 0.40              |
| 1:AG:191:HIS:HD2 | 1:AG:193:GLY:N    | 2.08                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:BH:154:GLN:O   | 2:BH:157:VAL:HB   | 2.22                     | 0.40              |
| 2:BQ:154:GLN:O   | 2:BQ:157:VAL:HB   | 2.22                     | 0.40              |
| 2:BA:154:GLN:O   | 2:BA:157:VAL:HB   | 2.22                     | 0.40              |
| 1:A6:241:THR:CG2 | 1:A6:242:ASN:N    | 2.85                     | 0.40              |
| 2:BY:82:PRO:HA   | 2:BY:193:THR:HA   | 2.03                     | 0.40              |
| 2:BK:82:PRO:HA   | 2:BK:193:THR:HA   | 2.03                     | 0.40              |
| 1:AP:241:THR:CG2 | 1:AP:242:ASN:N    | 2.85                     | 0.40              |
| 2:BP:83:LEU:HA   | 2:BP:84:PRO:HA    | 1.60                     | 0.40              |
| 3:CT:83:ALA:CB   | 1:DF:231:PRO:HG2  | 282.39                   | 0.40              |
| 3:CV:83:ALA:CB   | 1:DH:231:PRO:HG2  | 304.71                   | 0.40              |
| 2:BZ:82:PRO:HA   | 2:BZ:193:THR:HA   | 2.03                     | 0.40              |
| 1:AO:212:ARG:NH2 | 3:CP:18:VAL:O     | 2.46                     | 0.40              |
| 1:AH:212:ARG:NH2 | 3:CI:18:VAL:O     | 24.16                    | 0.40              |
| 1:DI:146:ILE:O   | 1:DI:147:ALA:CB   | 2.62                     | 0.40              |
| 3:CH:29:VAL:HG23 | 3:CH:29:VAL:O     | 2.22                     | 0.40              |
| 3:CJ:29:VAL:O    | 3:CJ:29:VAL:HG23  | 2.21                     | 0.40              |
| 3:CQ:29:VAL:HG23 | 3:CQ:29:VAL:O     | 2.21                     | 0.40              |
| 3:CL:29:VAL:HG23 | 3:CL:29:VAL:O     | 2.22                     | 0.40              |
| 3:CU:29:VAL:O    | 3:CU:29:VAL:HG23  | 2.21                     | 0.40              |
| 3:CR:29:VAL:HG23 | 3:CR:29:VAL:O     | 2.22                     | 0.40              |
| 2:B1:101:HIS:CG  | 2:B1:222:VAL:HG13 | 2.56                     | 0.40              |
| 3:CT:56:ILE:HD12 | 3:CT:74:PHE:CD1   | 2.57                     | 0.40              |
| 3:CH:56:ILE:HD12 | 3:CH:74:PHE:CD1   | 2.57                     | 0.40              |
| 3:CF:56:ILE:HD12 | 3:CF:74:PHE:CD1   | 2.57                     | 0.40              |
| 3:CE:56:ILE:HD12 | 3:CE:74:PHE:CD1   | 2.57                     | 0.40              |
| 3:CR:56:ILE:HD12 | 3:CR:74:PHE:CD1   | 2.57                     | 0.40              |
| 2:BK:166:ARG:NH2 | 3:CL:116:THR:O    | 88.50                    | 0.40              |
| 3:CS:56:ILE:HD12 | 3:CS:74:PHE:CD1   | 2.57                     | 0.40              |
| 3:CY:56:ILE:HD12 | 3:CY:74:PHE:CD1   | 2.57                     | 0.40              |
| 2:BA:68:GLU:O    | 2:BA:70:PRO:HD3   | 2.22                     | 0.40              |
| 2:BT:68:GLU:O    | 2:BT:70:PRO:HD3   | 2.22                     | 0.40              |
| 2:BD:68:GLU:O    | 2:BD:70:PRO:HD3   | 2.21                     | 0.40              |
| 3:CA:84:GLU:H    | 3:CA:84:GLU:CD    | 2.23                     | 0.40              |
| 2:BW:53:ARG:HG2  | 2:BW:221:MET:HE3  | 2.08                     | 0.40              |
| 3:CQ:15:MET:HB2  | 3:CR:25:LEU:HD21  | 21.86                    | 0.40              |
| 3:CT:25:LEU:HD21 | 3:CW:15:MET:HB2   | 263.96                   | 0.40              |
| 3:CC:25:LEU:HD21 | 3:CE:15:MET:HB2   | 2.04                     | 0.40              |
| 3:CG:25:LEU:HD21 | 3:CI:15:MET:HB2   | 21.86                    | 0.40              |
| 1:AE:72:LEU:HA   | 1:AE:72:LEU:HD23  | 1.83                     | 0.40              |
| 1:AW:72:LEU:HD23 | 1:AW:72:LEU:HA    | 1.83                     | 0.40              |
| 3:CL:15:MET:HB2  | 3:CO:25:LEU:HD21  | 2.04                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B1:129:VAL:HA  | 2:B1:130:PRO:HD3  | 1.98                     | 0.40              |
| 2:BC:154:GLN:O   | 2:BC:157:VAL:HB   | 2.22                     | 0.40              |
| 2:BE:154:GLN:O   | 2:BE:157:VAL:HB   | 2.22                     | 0.40              |
| 2:BP:154:GLN:O   | 2:BP:157:VAL:HB   | 2.22                     | 0.40              |
| 2:BR:154:GLN:O   | 2:BR:157:VAL:HB   | 2.22                     | 0.40              |
| 2:B0:154:GLN:O   | 2:B0:157:VAL:HB   | 2.22                     | 0.40              |
| 2:BO:154:GLN:O   | 2:BO:157:VAL:HB   | 2.22                     | 0.40              |
| 1:AY:187:LEU:HA  | 1:AY:188:PRO:HD2  | 1.95                     | 0.40              |
| 1:AT:74:THR:CG2  | 1:AT:74:THR:O     | 2.69                     | 0.40              |
| 2:B1:82:PRO:HA   | 2:B1:193:THR:HA   | 2.03                     | 0.40              |
| 2:B1:83:LEU:HA   | 2:B1:84:PRO:HA    | 1.60                     | 0.40              |
| 2:BV:82:PRO:HA   | 2:BV:193:THR:HA   | 2.03                     | 0.40              |
| 1:AH:231:PRO:HG2 | 3:CI:83:ALA:CB    | 63.69                    | 0.40              |
| 3:CR:83:ALA:CB   | 1:DD:231:PRO:HG2  | 281.85                   | 0.40              |
| 1:AB:212:ARG:NH2 | 3:CB:18:VAL:O     | 2.46                     | 0.40              |
| 3:CT:29:VAL:O    | 3:CT:29:VAL:HG23  | 2.21                     | 0.40              |
| 3:CK:29:VAL:HG23 | 3:CK:29:VAL:O     | 2.21                     | 0.40              |
| 3:DB:29:VAL:O    | 3:DB:29:VAL:HG23  | 2.21                     | 0.40              |
| 3:CP:29:VAL:HG23 | 3:CP:29:VAL:O     | 2.21                     | 0.40              |
| 2:B2:101:HIS:CG  | 2:B2:222:VAL:HG13 | 2.56                     | 0.40              |
| 3:CN:56:ILE:HD12 | 3:CN:74:PHE:CD1   | 2.57                     | 0.40              |
| 3:CO:56:ILE:HD12 | 3:CO:74:PHE:CD1   | 2.57                     | 0.40              |
| 3:CX:56:ILE:HD11 | 3:CX:206:VAL:HG13 | 2.04                     | 0.40              |
| 3:C7:56:ILE:HD12 | 3:C7:74:PHE:CD1   | 2.57                     | 0.40              |
| 3:CU:56:ILE:HD12 | 3:CU:74:PHE:CD1   | 2.57                     | 0.40              |
| 3:DB:56:ILE:HD12 | 3:DB:74:PHE:CD1   | 2.57                     | 0.40              |
| 3:C4:56:ILE:HD12 | 3:C4:74:PHE:CD1   | 2.57                     | 0.40              |
| 3:CJ:56:ILE:HD12 | 3:CJ:74:PHE:CD1   | 2.57                     | 0.40              |
| 2:BL:166:ARG:NH2 | 3:CM:116:THR:O    | 142.07                   | 0.40              |
| 2:BG:166:ARG:NH2 | 3:CH:116:THR:O    | 142.07                   | 0.40              |
| 2:BJ:166:ARG:NH2 | 3:CJ:116:THR:O    | 2.54                     | 0.40              |
| 3:C6:56:ILE:HD12 | 3:C6:74:PHE:CD1   | 2.57                     | 0.40              |
| 3:DA:56:ILE:HD12 | 3:DA:74:PHE:CD1   | 2.57                     | 0.40              |
| 2:BM:68:GLU:O    | 2:BM:70:PRO:HD3   | 2.22                     | 0.40              |
| 2:B5:166:ARG:NH2 | 3:C6:116:THR:O    | 2.54                     | 0.40              |
| 3:CB:127:PRO:HD3 | 3:CB:180:SER:O    | 2.21                     | 0.40              |
| 3:DA:127:PRO:HD3 | 3:DA:180:SER:O    | 2.21                     | 0.40              |
| 3:CG:127:PRO:HD3 | 3:CG:180:SER:C    | 2.42                     | 0.40              |
| 2:BW:68:GLU:O    | 2:BW:70:PRO:HD3   | 2.22                     | 0.40              |
| 3:CZ:127:PRO:HD3 | 3:CZ:180:SER:O    | 2.21                     | 0.40              |
| 2:BE:118:PHE:CD1 | 2:BN:118:PHE:HE2  | 218.53                   | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A2:224:ILE:HA  | 1:A2:225:PRO:HD2 | 1.95                     | 0.40              |
| 2:BV:53:ARG:HG2  | 2:BV:221:MET:HE2 | 2.10                     | 0.40              |
| 1:AF:220:CYS:HA  | 1:AF:221:PRO:HD2 | 1.95                     | 0.40              |
| 1:AG:220:CYS:HA  | 1:AG:221:PRO:HD2 | 1.95                     | 0.40              |
| 3:CE:15:MET:HB2  | 3:CF:25:LEU:HD21 | 136.57                   | 0.40              |
| 3:CF:25:LEU:HD21 | 3:CI:15:MET:HB2  | 2.04                     | 0.40              |
| 2:BW:129:VAL:HA  | 2:BW:130:PRO:HD3 | 1.98                     | 0.40              |
| 3:CP:15:MET:HB2  | 3:CQ:25:LEU:HD21 | 2.04                     | 0.40              |
| 3:CQ:25:LEU:HD21 | 3:CS:15:MET:HB2  | 21.86                    | 0.40              |
| 1:A1:225:PRO:HA  | 1:A1:226:PRO:HD3 | 1.78                     | 0.40              |
| 3:CH:101:ARG:O   | 3:CH:214:PHE:HA  | 2.21                     | 0.40              |
| 3:CA:25:LEU:HD21 | 3:CD:15:MET:HB2  | 2.04                     | 0.40              |
| 2:B8:129:VAL:HA  | 2:B8:130:PRO:HD3 | 1.98                     | 0.40              |
| 2:B4:43:PRO:HA   | 2:B4:44:PRO:HD3  | 1.96                     | 0.40              |
| 3:DB:101:ARG:O   | 3:DB:214:PHE:HA  | 2.21                     | 0.40              |
| 3:C9:91:ALA:O    | 3:C9:94:SER:HB2  | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 1   | A0    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | A1    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | A2    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | A3    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | A4    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | A5    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | A6    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 1   | A7    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | A8    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | A9    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | AA    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | AB    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | AC    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | AD    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | AE    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | AF    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | AG    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | AH    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | AI    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | AJ    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | AK    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | AL    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | AM    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | AN    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | AO    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | AP    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | AQ    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | AR    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | AS    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | AT    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | AU    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | AV    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | AW    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | AX    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | AY    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | AZ    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | Aa    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | Ab    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 1   | Ac    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | Ad    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | Ae    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | Af    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | Ag    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | Ah    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | Ai    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | Aj    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | Ak    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | Al    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | Am    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | An    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | Ao    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | DC    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | DD    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | DE    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | DF    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | DG    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | DH    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | DI    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | DJ    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 1   | DK    | 244/246 (99%) | 206 (84%) | 24 (10%) | 14 (6%)  | 2           | 28 |
| 2   | B0    | 198/200 (99%) | 183 (92%) | 7 (4%)   | 8 (4%)   | 4           | 35 |
| 2   | B1    | 198/200 (99%) | 183 (92%) | 7 (4%)   | 8 (4%)   | 4           | 35 |
| 2   | B2    | 198/200 (99%) | 183 (92%) | 7 (4%)   | 8 (4%)   | 4           | 35 |
| 2   | B3    | 198/200 (99%) | 183 (92%) | 7 (4%)   | 8 (4%)   | 4           | 35 |
| 2   | B4    | 198/200 (99%) | 184 (93%) | 6 (3%)   | 8 (4%)   | 4           | 35 |
| 2   | B5    | 198/200 (99%) | 183 (92%) | 7 (4%)   | 8 (4%)   | 4           | 35 |
| 2   | B6    | 198/200 (99%) | 183 (92%) | 7 (4%)   | 8 (4%)   | 4           | 35 |
| 2   | B7    | 198/200 (99%) | 183 (92%) | 7 (4%)   | 8 (4%)   | 4           | 35 |
| 2   | B8    | 198/200 (99%) | 183 (92%) | 7 (4%)   | 8 (4%)   | 4           | 35 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|---------|----------|-------------|----|
| 2   | B9    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | BA    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | BB    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | BC    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | BD    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | BE    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | BF    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | BG    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | BH    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | BI    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | BJ    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | BK    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | BL    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | BM    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | BN    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | BO    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | BP    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | BQ    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | BR    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | BS    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | BT    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | BU    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | BV    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | BW    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | BX    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | BY    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | BZ    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | Ba    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | Bb    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | Bc    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | Bd    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|---------|----------|-------------|----|
| 2   | Be    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | Bf    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | Bg    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | Bh    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | Bi    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | Bj    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | Bk    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | Bl    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | Bm    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | Bn    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | Bo    | 198/200 (99%) | 184 (93%) | 6 (3%)  | 8 (4%)   | 4           | 35 |
| 2   | Bp    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | Bq    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | Br    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | Bs    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | Bt    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | Bu    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | Bv    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | Bw    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 2   | Bx    | 198/200 (99%) | 183 (92%) | 7 (4%)  | 8 (4%)   | 4           | 35 |
| 3   | C0    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | C1    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | C2    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | C3    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | C4    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | C5    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | C6    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | C7    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | C8    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | C9    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | CA    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|---------|----------|-------------|----|
| 3   | CB    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | CC    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | CD    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | CE    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | CF    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | CG    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | CH    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | CI    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | CJ    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | CK    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | CL    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | CM    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | CN    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | CO    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | CP    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | CQ    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | CR    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | CS    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | CT    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | CU    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | CV    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | CW    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | CX    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | CY    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | CZ    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | Cc    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | Cd    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | Ce    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | Cf    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | Cg    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |
| 3   | Ch    | 224/226 (99%) | 204 (91%) | 14 (6%) | 6 (3%)   | 6           | 45 |

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| Mol | Chain | Analysed          | Favoured    | Allowed   | Outliers  | Percentiles |    |
|-----|-------|-------------------|-------------|-----------|-----------|-------------|----|
| 3   | Ci    | 224/226 (99%)     | 204 (91%)   | 14 (6%)   | 6 (3%)    | 6           | 45 |
| 3   | Cj    | 224/226 (99%)     | 204 (91%)   | 14 (6%)   | 6 (3%)    | 6           | 45 |
| 3   | Ck    | 224/226 (99%)     | 204 (91%)   | 14 (6%)   | 6 (3%)    | 6           | 45 |
| 3   | Cl    | 224/226 (99%)     | 204 (91%)   | 14 (6%)   | 6 (3%)    | 6           | 45 |
| 3   | Cm    | 224/226 (99%)     | 204 (91%)   | 14 (6%)   | 6 (3%)    | 6           | 45 |
| 3   | Cn    | 224/226 (99%)     | 204 (91%)   | 14 (6%)   | 6 (3%)    | 6           | 45 |
| 3   | Co    | 224/226 (99%)     | 204 (91%)   | 14 (6%)   | 6 (3%)    | 6           | 45 |
| 3   | Cp    | 224/226 (99%)     | 204 (91%)   | 14 (6%)   | 6 (3%)    | 6           | 45 |
| 3   | Cq    | 224/226 (99%)     | 204 (91%)   | 14 (6%)   | 6 (3%)    | 6           | 45 |
| 3   | Cr    | 224/226 (99%)     | 204 (91%)   | 14 (6%)   | 6 (3%)    | 6           | 45 |
| 3   | Cs    | 224/226 (99%)     | 204 (91%)   | 14 (6%)   | 6 (3%)    | 6           | 45 |
| 3   | Ct    | 224/226 (99%)     | 204 (91%)   | 14 (6%)   | 6 (3%)    | 6           | 45 |
| 3   | Cu    | 224/226 (99%)     | 204 (91%)   | 14 (6%)   | 6 (3%)    | 6           | 45 |
| 3   | Cv    | 224/226 (99%)     | 204 (91%)   | 14 (6%)   | 6 (3%)    | 6           | 45 |
| 3   | Cw    | 224/226 (99%)     | 204 (91%)   | 14 (6%)   | 6 (3%)    | 6           | 45 |
| 3   | Cx    | 224/226 (99%)     | 204 (91%)   | 14 (6%)   | 6 (3%)    | 6           | 45 |
| 3   | DA    | 224/226 (99%)     | 204 (91%)   | 14 (6%)   | 6 (3%)    | 6           | 45 |
| 3   | DB    | 224/226 (99%)     | 204 (91%)   | 14 (6%)   | 6 (3%)    | 6           | 45 |
| All | All   | 39960/40320 (99%) | 35582 (89%) | 2698 (7%) | 1680 (4%) | 6           | 34 |

All (1680) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 2   | THR  |
| 1   | AA    | 5   | GLY  |
| 1   | AA    | 41  | GLU  |
| 1   | AA    | 202 | HIS  |
| 1   | AA    | 244 | ASN  |
| 1   | AB    | 2   | THR  |
| 1   | AB    | 5   | GLY  |
| 1   | AB    | 41  | GLU  |
| 1   | AB    | 202 | HIS  |
| 1   | AB    | 244 | ASN  |
| 1   | AC    | 2   | THR  |
| 1   | AC    | 5   | GLY  |
| 1   | AC    | 41  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AC    | 202 | HIS  |
| 1   | AC    | 244 | ASN  |
| 1   | AD    | 2   | THR  |
| 1   | AD    | 5   | GLY  |
| 1   | AD    | 41  | GLU  |
| 1   | AD    | 202 | HIS  |
| 1   | AD    | 244 | ASN  |
| 1   | AE    | 2   | THR  |
| 1   | AE    | 5   | GLY  |
| 1   | AE    | 41  | GLU  |
| 1   | AE    | 202 | HIS  |
| 1   | AE    | 244 | ASN  |
| 1   | AF    | 2   | THR  |
| 1   | AF    | 5   | GLY  |
| 1   | AF    | 41  | GLU  |
| 1   | AF    | 202 | HIS  |
| 1   | AF    | 244 | ASN  |
| 1   | AG    | 2   | THR  |
| 1   | AG    | 5   | GLY  |
| 1   | AG    | 41  | GLU  |
| 1   | AG    | 202 | HIS  |
| 1   | AG    | 244 | ASN  |
| 1   | AH    | 2   | THR  |
| 1   | AH    | 5   | GLY  |
| 1   | AH    | 41  | GLU  |
| 1   | AH    | 202 | HIS  |
| 1   | AH    | 244 | ASN  |
| 1   | AI    | 2   | THR  |
| 1   | AI    | 5   | GLY  |
| 1   | AI    | 41  | GLU  |
| 1   | AI    | 202 | HIS  |
| 1   | AI    | 244 | ASN  |
| 1   | AJ    | 2   | THR  |
| 1   | AJ    | 5   | GLY  |
| 1   | AJ    | 41  | GLU  |
| 1   | AJ    | 202 | HIS  |
| 1   | AJ    | 244 | ASN  |
| 1   | AK    | 2   | THR  |
| 1   | AK    | 5   | GLY  |
| 1   | AK    | 41  | GLU  |
| 1   | AK    | 202 | HIS  |
| 1   | AK    | 244 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AL    | 2   | THR  |
| 1   | AL    | 5   | GLY  |
| 1   | AL    | 41  | GLU  |
| 1   | AL    | 202 | HIS  |
| 1   | AL    | 244 | ASN  |
| 1   | AM    | 2   | THR  |
| 1   | AM    | 5   | GLY  |
| 1   | AM    | 41  | GLU  |
| 1   | AM    | 202 | HIS  |
| 1   | AM    | 244 | ASN  |
| 1   | AN    | 2   | THR  |
| 1   | AN    | 5   | GLY  |
| 1   | AN    | 41  | GLU  |
| 1   | AN    | 202 | HIS  |
| 1   | AN    | 244 | ASN  |
| 1   | AO    | 2   | THR  |
| 1   | AO    | 5   | GLY  |
| 1   | AO    | 41  | GLU  |
| 1   | AO    | 202 | HIS  |
| 1   | AO    | 244 | ASN  |
| 1   | AP    | 2   | THR  |
| 1   | AP    | 5   | GLY  |
| 1   | AP    | 41  | GLU  |
| 1   | AP    | 202 | HIS  |
| 1   | AP    | 244 | ASN  |
| 1   | AQ    | 2   | THR  |
| 1   | AQ    | 5   | GLY  |
| 1   | AQ    | 41  | GLU  |
| 1   | AQ    | 202 | HIS  |
| 1   | AQ    | 244 | ASN  |
| 1   | AR    | 2   | THR  |
| 1   | AR    | 5   | GLY  |
| 1   | AR    | 41  | GLU  |
| 1   | AR    | 202 | HIS  |
| 1   | AR    | 244 | ASN  |
| 1   | AS    | 2   | THR  |
| 1   | AS    | 5   | GLY  |
| 1   | AS    | 41  | GLU  |
| 1   | AS    | 202 | HIS  |
| 1   | AS    | 244 | ASN  |
| 1   | AT    | 2   | THR  |
| 1   | AT    | 5   | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AT    | 41  | GLU  |
| 1   | AT    | 202 | HIS  |
| 1   | AT    | 244 | ASN  |
| 1   | AU    | 2   | THR  |
| 1   | AU    | 5   | GLY  |
| 1   | AU    | 41  | GLU  |
| 1   | AU    | 202 | HIS  |
| 1   | AU    | 244 | ASN  |
| 1   | AV    | 2   | THR  |
| 1   | AV    | 5   | GLY  |
| 1   | AV    | 41  | GLU  |
| 1   | AV    | 202 | HIS  |
| 1   | AV    | 244 | ASN  |
| 1   | AW    | 2   | THR  |
| 1   | AW    | 5   | GLY  |
| 1   | AW    | 41  | GLU  |
| 1   | AW    | 202 | HIS  |
| 1   | AW    | 244 | ASN  |
| 1   | AX    | 2   | THR  |
| 1   | AX    | 5   | GLY  |
| 1   | AX    | 41  | GLU  |
| 1   | AX    | 202 | HIS  |
| 1   | AX    | 244 | ASN  |
| 1   | AY    | 2   | THR  |
| 1   | AY    | 5   | GLY  |
| 1   | AY    | 41  | GLU  |
| 1   | AY    | 202 | HIS  |
| 1   | AY    | 244 | ASN  |
| 1   | AZ    | 2   | THR  |
| 1   | AZ    | 5   | GLY  |
| 1   | AZ    | 41  | GLU  |
| 1   | AZ    | 202 | HIS  |
| 1   | AZ    | 244 | ASN  |
| 1   | A0    | 2   | THR  |
| 1   | A0    | 5   | GLY  |
| 1   | A0    | 41  | GLU  |
| 1   | A0    | 202 | HIS  |
| 1   | A0    | 244 | ASN  |
| 1   | A1    | 2   | THR  |
| 1   | A1    | 5   | GLY  |
| 1   | A1    | 41  | GLU  |
| 1   | A1    | 202 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A1    | 244 | ASN  |
| 1   | A2    | 2   | THR  |
| 1   | A2    | 5   | GLY  |
| 1   | A2    | 41  | GLU  |
| 1   | A2    | 202 | HIS  |
| 1   | A2    | 244 | ASN  |
| 1   | A3    | 2   | THR  |
| 1   | A3    | 5   | GLY  |
| 1   | A3    | 41  | GLU  |
| 1   | A3    | 202 | HIS  |
| 1   | A3    | 244 | ASN  |
| 1   | A4    | 2   | THR  |
| 1   | A4    | 5   | GLY  |
| 1   | A4    | 41  | GLU  |
| 1   | A4    | 202 | HIS  |
| 1   | A4    | 244 | ASN  |
| 1   | A5    | 2   | THR  |
| 1   | A5    | 5   | GLY  |
| 1   | A5    | 41  | GLU  |
| 1   | A5    | 202 | HIS  |
| 1   | A5    | 244 | ASN  |
| 1   | A6    | 2   | THR  |
| 1   | A6    | 5   | GLY  |
| 1   | A6    | 41  | GLU  |
| 1   | A6    | 202 | HIS  |
| 1   | A6    | 244 | ASN  |
| 1   | A7    | 2   | THR  |
| 1   | A7    | 5   | GLY  |
| 1   | A7    | 41  | GLU  |
| 1   | A7    | 202 | HIS  |
| 1   | A7    | 244 | ASN  |
| 1   | A8    | 2   | THR  |
| 1   | A8    | 5   | GLY  |
| 1   | A8    | 41  | GLU  |
| 1   | A8    | 202 | HIS  |
| 1   | A8    | 244 | ASN  |
| 1   | A9    | 2   | THR  |
| 1   | A9    | 5   | GLY  |
| 1   | A9    | 41  | GLU  |
| 1   | A9    | 202 | HIS  |
| 1   | A9    | 244 | ASN  |
| 1   | Aa    | 2   | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Aa    | 5   | GLY  |
| 1   | Aa    | 41  | GLU  |
| 1   | Aa    | 202 | HIS  |
| 1   | Aa    | 244 | ASN  |
| 1   | Ab    | 2   | THR  |
| 1   | Ab    | 5   | GLY  |
| 1   | Ab    | 41  | GLU  |
| 1   | Ab    | 202 | HIS  |
| 1   | Ab    | 244 | ASN  |
| 1   | Ac    | 2   | THR  |
| 1   | Ac    | 5   | GLY  |
| 1   | Ac    | 41  | GLU  |
| 1   | Ac    | 202 | HIS  |
| 1   | Ac    | 244 | ASN  |
| 1   | Ad    | 2   | THR  |
| 1   | Ad    | 5   | GLY  |
| 1   | Ad    | 41  | GLU  |
| 1   | Ad    | 202 | HIS  |
| 1   | Ad    | 244 | ASN  |
| 1   | Ae    | 2   | THR  |
| 1   | Ae    | 5   | GLY  |
| 1   | Ae    | 41  | GLU  |
| 1   | Ae    | 202 | HIS  |
| 1   | Ae    | 244 | ASN  |
| 1   | Af    | 2   | THR  |
| 1   | Af    | 5   | GLY  |
| 1   | Af    | 41  | GLU  |
| 1   | Af    | 202 | HIS  |
| 1   | Af    | 244 | ASN  |
| 1   | Ag    | 2   | THR  |
| 1   | Ag    | 5   | GLY  |
| 1   | Ag    | 41  | GLU  |
| 1   | Ag    | 202 | HIS  |
| 1   | Ag    | 244 | ASN  |
| 1   | Ah    | 2   | THR  |
| 1   | Ah    | 5   | GLY  |
| 1   | Ah    | 41  | GLU  |
| 1   | Ah    | 202 | HIS  |
| 1   | Ah    | 244 | ASN  |
| 1   | Ai    | 2   | THR  |
| 1   | Ai    | 5   | GLY  |
| 1   | Ai    | 41  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Ai    | 202 | HIS  |
| 1   | Ai    | 244 | ASN  |
| 1   | Aj    | 2   | THR  |
| 1   | Aj    | 5   | GLY  |
| 1   | Aj    | 41  | GLU  |
| 1   | Aj    | 202 | HIS  |
| 1   | Aj    | 244 | ASN  |
| 1   | Ak    | 2   | THR  |
| 1   | Ak    | 5   | GLY  |
| 1   | Ak    | 41  | GLU  |
| 1   | Ak    | 202 | HIS  |
| 1   | Ak    | 244 | ASN  |
| 1   | Al    | 2   | THR  |
| 1   | Al    | 5   | GLY  |
| 1   | Al    | 41  | GLU  |
| 1   | Al    | 202 | HIS  |
| 1   | Al    | 244 | ASN  |
| 1   | Am    | 2   | THR  |
| 1   | Am    | 5   | GLY  |
| 1   | Am    | 41  | GLU  |
| 1   | Am    | 202 | HIS  |
| 1   | Am    | 244 | ASN  |
| 1   | An    | 2   | THR  |
| 1   | An    | 5   | GLY  |
| 1   | An    | 41  | GLU  |
| 1   | An    | 202 | HIS  |
| 1   | An    | 244 | ASN  |
| 1   | Ao    | 2   | THR  |
| 1   | Ao    | 5   | GLY  |
| 1   | Ao    | 41  | GLU  |
| 1   | Ao    | 202 | HIS  |
| 1   | Ao    | 244 | ASN  |
| 2   | BA    | 84  | PRO  |
| 2   | BA    | 85  | SER  |
| 2   | BA    | 134 | HIS  |
| 2   | BA    | 135 | THR  |
| 2   | BB    | 84  | PRO  |
| 2   | BB    | 85  | SER  |
| 2   | BB    | 134 | HIS  |
| 2   | BB    | 135 | THR  |
| 2   | BC    | 84  | PRO  |
| 2   | BC    | 85  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | BC    | 134 | HIS  |
| 2   | BC    | 135 | THR  |
| 2   | BD    | 84  | PRO  |
| 2   | BD    | 85  | SER  |
| 2   | BD    | 134 | HIS  |
| 2   | BD    | 135 | THR  |
| 2   | BE    | 84  | PRO  |
| 2   | BE    | 85  | SER  |
| 2   | BE    | 134 | HIS  |
| 2   | BE    | 135 | THR  |
| 2   | BF    | 84  | PRO  |
| 2   | BF    | 85  | SER  |
| 2   | BF    | 134 | HIS  |
| 2   | BF    | 135 | THR  |
| 2   | BG    | 84  | PRO  |
| 2   | BG    | 85  | SER  |
| 2   | BG    | 134 | HIS  |
| 2   | BG    | 135 | THR  |
| 2   | BH    | 84  | PRO  |
| 2   | BH    | 85  | SER  |
| 2   | BH    | 134 | HIS  |
| 2   | BH    | 135 | THR  |
| 2   | BI    | 84  | PRO  |
| 2   | BI    | 85  | SER  |
| 2   | BI    | 134 | HIS  |
| 2   | BI    | 135 | THR  |
| 2   | BJ    | 84  | PRO  |
| 2   | BJ    | 85  | SER  |
| 2   | BJ    | 134 | HIS  |
| 2   | BJ    | 135 | THR  |
| 2   | BK    | 84  | PRO  |
| 2   | BK    | 85  | SER  |
| 2   | BK    | 134 | HIS  |
| 2   | BK    | 135 | THR  |
| 2   | BL    | 84  | PRO  |
| 2   | BL    | 85  | SER  |
| 2   | BL    | 134 | HIS  |
| 2   | BL    | 135 | THR  |
| 2   | BM    | 84  | PRO  |
| 2   | BM    | 85  | SER  |
| 2   | BM    | 134 | HIS  |
| 2   | BM    | 135 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | BN    | 84  | PRO  |
| 2   | BN    | 85  | SER  |
| 2   | BN    | 134 | HIS  |
| 2   | BN    | 135 | THR  |
| 2   | BR    | 84  | PRO  |
| 2   | BR    | 85  | SER  |
| 2   | BR    | 134 | HIS  |
| 2   | BR    | 135 | THR  |
| 2   | BO    | 84  | PRO  |
| 2   | BO    | 85  | SER  |
| 2   | BO    | 134 | HIS  |
| 2   | BO    | 135 | THR  |
| 2   | BS    | 84  | PRO  |
| 2   | BS    | 85  | SER  |
| 2   | BS    | 134 | HIS  |
| 2   | BS    | 135 | THR  |
| 2   | BP    | 84  | PRO  |
| 2   | BP    | 85  | SER  |
| 2   | BP    | 134 | HIS  |
| 2   | BP    | 135 | THR  |
| 2   | BQ    | 84  | PRO  |
| 2   | BQ    | 85  | SER  |
| 2   | BQ    | 134 | HIS  |
| 2   | BQ    | 135 | THR  |
| 2   | BT    | 84  | PRO  |
| 2   | BT    | 85  | SER  |
| 2   | BT    | 134 | HIS  |
| 2   | BT    | 135 | THR  |
| 2   | BU    | 84  | PRO  |
| 2   | BU    | 85  | SER  |
| 2   | BU    | 134 | HIS  |
| 2   | BU    | 135 | THR  |
| 2   | BV    | 84  | PRO  |
| 2   | BV    | 85  | SER  |
| 2   | BV    | 134 | HIS  |
| 2   | BV    | 135 | THR  |
| 2   | BW    | 84  | PRO  |
| 2   | BW    | 85  | SER  |
| 2   | BW    | 134 | HIS  |
| 2   | BW    | 135 | THR  |
| 2   | BX    | 84  | PRO  |
| 2   | BX    | 85  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | BX    | 134 | HIS  |
| 2   | BX    | 135 | THR  |
| 2   | BY    | 84  | PRO  |
| 2   | BY    | 85  | SER  |
| 2   | BY    | 134 | HIS  |
| 2   | BY    | 135 | THR  |
| 2   | BZ    | 84  | PRO  |
| 2   | BZ    | 85  | SER  |
| 2   | BZ    | 134 | HIS  |
| 2   | BZ    | 135 | THR  |
| 2   | B0    | 84  | PRO  |
| 2   | B0    | 85  | SER  |
| 2   | B0    | 134 | HIS  |
| 2   | B0    | 135 | THR  |
| 2   | B1    | 84  | PRO  |
| 2   | B1    | 85  | SER  |
| 2   | B1    | 134 | HIS  |
| 2   | B1    | 135 | THR  |
| 2   | B2    | 84  | PRO  |
| 2   | B2    | 85  | SER  |
| 2   | B2    | 134 | HIS  |
| 2   | B2    | 135 | THR  |
| 2   | B3    | 84  | PRO  |
| 2   | B3    | 85  | SER  |
| 2   | B3    | 134 | HIS  |
| 2   | B3    | 135 | THR  |
| 2   | B4    | 84  | PRO  |
| 2   | B4    | 85  | SER  |
| 2   | B4    | 134 | HIS  |
| 2   | B4    | 135 | THR  |
| 2   | B5    | 84  | PRO  |
| 2   | B5    | 85  | SER  |
| 2   | B5    | 134 | HIS  |
| 2   | B5    | 135 | THR  |
| 2   | B6    | 84  | PRO  |
| 2   | B6    | 85  | SER  |
| 2   | B6    | 134 | HIS  |
| 2   | B6    | 135 | THR  |
| 2   | B7    | 84  | PRO  |
| 2   | B7    | 85  | SER  |
| 2   | B7    | 134 | HIS  |
| 2   | B7    | 135 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B8    | 84  | PRO  |
| 2   | B8    | 85  | SER  |
| 2   | B8    | 134 | HIS  |
| 2   | B8    | 135 | THR  |
| 2   | B9    | 84  | PRO  |
| 2   | B9    | 85  | SER  |
| 2   | B9    | 134 | HIS  |
| 2   | B9    | 135 | THR  |
| 2   | Ba    | 84  | PRO  |
| 2   | Ba    | 85  | SER  |
| 2   | Ba    | 134 | HIS  |
| 2   | Ba    | 135 | THR  |
| 2   | Bb    | 84  | PRO  |
| 2   | Bb    | 85  | SER  |
| 2   | Bb    | 134 | HIS  |
| 2   | Bb    | 135 | THR  |
| 2   | Bc    | 84  | PRO  |
| 2   | Bc    | 85  | SER  |
| 2   | Bc    | 134 | HIS  |
| 2   | Bc    | 135 | THR  |
| 2   | Bd    | 84  | PRO  |
| 2   | Bd    | 85  | SER  |
| 2   | Bd    | 134 | HIS  |
| 2   | Bd    | 135 | THR  |
| 2   | Be    | 84  | PRO  |
| 2   | Be    | 85  | SER  |
| 2   | Be    | 134 | HIS  |
| 2   | Be    | 135 | THR  |
| 2   | Bf    | 84  | PRO  |
| 2   | Bf    | 85  | SER  |
| 2   | Bf    | 134 | HIS  |
| 2   | Bf    | 135 | THR  |
| 2   | Bg    | 84  | PRO  |
| 2   | Bg    | 85  | SER  |
| 2   | Bg    | 134 | HIS  |
| 2   | Bg    | 135 | THR  |
| 2   | Bh    | 84  | PRO  |
| 2   | Bh    | 85  | SER  |
| 2   | Bh    | 134 | HIS  |
| 2   | Bh    | 135 | THR  |
| 2   | Bi    | 84  | PRO  |
| 2   | Bi    | 85  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Bi    | 134 | HIS  |
| 2   | Bi    | 135 | THR  |
| 2   | Bj    | 84  | PRO  |
| 2   | Bj    | 85  | SER  |
| 2   | Bj    | 134 | HIS  |
| 2   | Bj    | 135 | THR  |
| 2   | Bk    | 84  | PRO  |
| 2   | Bk    | 85  | SER  |
| 2   | Bk    | 134 | HIS  |
| 2   | Bk    | 135 | THR  |
| 2   | Bl    | 84  | PRO  |
| 2   | Bl    | 85  | SER  |
| 2   | Bl    | 134 | HIS  |
| 2   | Bl    | 135 | THR  |
| 2   | Bm    | 84  | PRO  |
| 2   | Bm    | 85  | SER  |
| 2   | Bm    | 134 | HIS  |
| 2   | Bm    | 135 | THR  |
| 2   | Bn    | 84  | PRO  |
| 2   | Bn    | 85  | SER  |
| 2   | Bn    | 134 | HIS  |
| 2   | Bn    | 135 | THR  |
| 2   | Bo    | 84  | PRO  |
| 2   | Bo    | 85  | SER  |
| 2   | Bo    | 134 | HIS  |
| 2   | Bo    | 135 | THR  |
| 2   | Bp    | 84  | PRO  |
| 2   | Bp    | 85  | SER  |
| 2   | Bp    | 134 | HIS  |
| 2   | Bp    | 135 | THR  |
| 2   | Bq    | 84  | PRO  |
| 2   | Bq    | 85  | SER  |
| 2   | Bq    | 134 | HIS  |
| 2   | Bq    | 135 | THR  |
| 2   | Br    | 84  | PRO  |
| 2   | Br    | 85  | SER  |
| 2   | Br    | 134 | HIS  |
| 2   | Br    | 135 | THR  |
| 2   | Bs    | 84  | PRO  |
| 2   | Bs    | 85  | SER  |
| 2   | Bs    | 134 | HIS  |
| 2   | Bs    | 135 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Bt    | 84  | PRO  |
| 2   | Bt    | 85  | SER  |
| 2   | Bt    | 134 | HIS  |
| 2   | Bt    | 135 | THR  |
| 2   | Bu    | 84  | PRO  |
| 2   | Bu    | 85  | SER  |
| 2   | Bu    | 134 | HIS  |
| 2   | Bu    | 135 | THR  |
| 2   | Bv    | 84  | PRO  |
| 2   | Bv    | 85  | SER  |
| 2   | Bv    | 134 | HIS  |
| 2   | Bv    | 135 | THR  |
| 2   | Bw    | 84  | PRO  |
| 2   | Bw    | 85  | SER  |
| 2   | Bw    | 134 | HIS  |
| 2   | Bw    | 135 | THR  |
| 2   | Bx    | 84  | PRO  |
| 2   | Bx    | 85  | SER  |
| 2   | Bx    | 134 | HIS  |
| 2   | Bx    | 135 | THR  |
| 3   | CA    | 11  | SER  |
| 3   | CA    | 36  | VAL  |
| 3   | CB    | 11  | SER  |
| 3   | CB    | 36  | VAL  |
| 3   | CC    | 11  | SER  |
| 3   | CC    | 36  | VAL  |
| 3   | CD    | 11  | SER  |
| 3   | CD    | 36  | VAL  |
| 3   | CE    | 11  | SER  |
| 3   | CE    | 36  | VAL  |
| 3   | CF    | 11  | SER  |
| 3   | CF    | 36  | VAL  |
| 3   | CG    | 11  | SER  |
| 3   | CG    | 36  | VAL  |
| 3   | CH    | 11  | SER  |
| 3   | CH    | 36  | VAL  |
| 3   | CI    | 11  | SER  |
| 3   | CI    | 36  | VAL  |
| 3   | CJ    | 11  | SER  |
| 3   | CJ    | 36  | VAL  |
| 3   | CK    | 11  | SER  |
| 3   | CK    | 36  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CL    | 11  | SER  |
| 3   | CL    | 36  | VAL  |
| 3   | CM    | 11  | SER  |
| 3   | CM    | 36  | VAL  |
| 3   | CN    | 11  | SER  |
| 3   | CN    | 36  | VAL  |
| 3   | CO    | 11  | SER  |
| 3   | CO    | 36  | VAL  |
| 3   | CP    | 11  | SER  |
| 3   | CP    | 36  | VAL  |
| 3   | CQ    | 11  | SER  |
| 3   | CQ    | 36  | VAL  |
| 3   | CR    | 11  | SER  |
| 3   | CR    | 36  | VAL  |
| 3   | CS    | 11  | SER  |
| 3   | CS    | 36  | VAL  |
| 3   | CT    | 11  | SER  |
| 3   | CT    | 36  | VAL  |
| 3   | CU    | 11  | SER  |
| 3   | CU    | 36  | VAL  |
| 3   | CV    | 11  | SER  |
| 3   | CV    | 36  | VAL  |
| 3   | CW    | 11  | SER  |
| 3   | CW    | 36  | VAL  |
| 3   | CX    | 11  | SER  |
| 3   | CX    | 36  | VAL  |
| 3   | CY    | 11  | SER  |
| 3   | CY    | 36  | VAL  |
| 3   | CZ    | 11  | SER  |
| 3   | CZ    | 36  | VAL  |
| 3   | C0    | 11  | SER  |
| 3   | C0    | 36  | VAL  |
| 3   | C1    | 11  | SER  |
| 3   | C1    | 36  | VAL  |
| 3   | C2    | 11  | SER  |
| 3   | C2    | 36  | VAL  |
| 3   | C3    | 11  | SER  |
| 3   | C3    | 36  | VAL  |
| 3   | C4    | 11  | SER  |
| 3   | C4    | 36  | VAL  |
| 3   | C5    | 11  | SER  |
| 3   | C5    | 36  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C6    | 11  | SER  |
| 3   | C6    | 36  | VAL  |
| 3   | C7    | 11  | SER  |
| 3   | C7    | 36  | VAL  |
| 3   | C8    | 11  | SER  |
| 3   | C8    | 36  | VAL  |
| 3   | C9    | 11  | SER  |
| 3   | C9    | 36  | VAL  |
| 3   | Cc    | 11  | SER  |
| 3   | Cc    | 36  | VAL  |
| 3   | Cd    | 11  | SER  |
| 3   | Cd    | 36  | VAL  |
| 3   | Ce    | 11  | SER  |
| 3   | Ce    | 36  | VAL  |
| 3   | Cf    | 11  | SER  |
| 3   | Cf    | 36  | VAL  |
| 3   | Cg    | 11  | SER  |
| 3   | Cg    | 36  | VAL  |
| 3   | Ch    | 11  | SER  |
| 3   | Ch    | 36  | VAL  |
| 3   | Ci    | 11  | SER  |
| 3   | Ci    | 36  | VAL  |
| 3   | Cj    | 11  | SER  |
| 3   | Cj    | 36  | VAL  |
| 3   | Ck    | 11  | SER  |
| 3   | Ck    | 36  | VAL  |
| 3   | Cl    | 11  | SER  |
| 3   | Cl    | 36  | VAL  |
| 3   | Cm    | 11  | SER  |
| 3   | Cm    | 36  | VAL  |
| 3   | Cn    | 11  | SER  |
| 3   | Cn    | 36  | VAL  |
| 3   | Co    | 11  | SER  |
| 3   | Co    | 36  | VAL  |
| 3   | Cp    | 11  | SER  |
| 3   | Cp    | 36  | VAL  |
| 3   | Cq    | 11  | SER  |
| 3   | Cq    | 36  | VAL  |
| 3   | Cr    | 11  | SER  |
| 3   | Cr    | 36  | VAL  |
| 3   | Cs    | 11  | SER  |
| 3   | Cs    | 36  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Ct    | 11  | SER  |
| 3   | Ct    | 36  | VAL  |
| 3   | Cu    | 11  | SER  |
| 3   | Cu    | 36  | VAL  |
| 3   | Cv    | 11  | SER  |
| 3   | Cv    | 36  | VAL  |
| 3   | Cw    | 11  | SER  |
| 3   | Cw    | 36  | VAL  |
| 3   | Cx    | 11  | SER  |
| 3   | Cx    | 36  | VAL  |
| 3   | DA    | 11  | SER  |
| 3   | DA    | 36  | VAL  |
| 3   | DB    | 11  | SER  |
| 3   | DB    | 36  | VAL  |
| 1   | DC    | 2   | THR  |
| 1   | DC    | 5   | GLY  |
| 1   | DC    | 41  | GLU  |
| 1   | DC    | 202 | HIS  |
| 1   | DC    | 244 | ASN  |
| 1   | DD    | 2   | THR  |
| 1   | DD    | 5   | GLY  |
| 1   | DD    | 41  | GLU  |
| 1   | DD    | 202 | HIS  |
| 1   | DD    | 244 | ASN  |
| 1   | DE    | 2   | THR  |
| 1   | DE    | 5   | GLY  |
| 1   | DE    | 41  | GLU  |
| 1   | DE    | 202 | HIS  |
| 1   | DE    | 244 | ASN  |
| 1   | DF    | 2   | THR  |
| 1   | DF    | 5   | GLY  |
| 1   | DF    | 41  | GLU  |
| 1   | DF    | 202 | HIS  |
| 1   | DF    | 244 | ASN  |
| 1   | DG    | 2   | THR  |
| 1   | DG    | 5   | GLY  |
| 1   | DG    | 41  | GLU  |
| 1   | DG    | 202 | HIS  |
| 1   | DG    | 244 | ASN  |
| 1   | DH    | 2   | THR  |
| 1   | DH    | 5   | GLY  |
| 1   | DH    | 41  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | DH    | 202 | HIS  |
| 1   | DH    | 244 | ASN  |
| 1   | DI    | 2   | THR  |
| 1   | DI    | 5   | GLY  |
| 1   | DI    | 41  | GLU  |
| 1   | DI    | 202 | HIS  |
| 1   | DI    | 244 | ASN  |
| 1   | DJ    | 2   | THR  |
| 1   | DJ    | 5   | GLY  |
| 1   | DJ    | 41  | GLU  |
| 1   | DJ    | 202 | HIS  |
| 1   | DJ    | 244 | ASN  |
| 1   | DK    | 2   | THR  |
| 1   | DK    | 5   | GLY  |
| 1   | DK    | 41  | GLU  |
| 1   | DK    | 202 | HIS  |
| 1   | DK    | 244 | ASN  |
| 1   | AA    | 22  | VAL  |
| 1   | AA    | 71  | LEU  |
| 1   | AA    | 147 | ALA  |
| 1   | AA    | 182 | ALA  |
| 1   | AA    | 184 | TYR  |
| 1   | AB    | 22  | VAL  |
| 1   | AB    | 71  | LEU  |
| 1   | AB    | 147 | ALA  |
| 1   | AB    | 182 | ALA  |
| 1   | AB    | 184 | TYR  |
| 1   | AC    | 22  | VAL  |
| 1   | AC    | 71  | LEU  |
| 1   | AC    | 147 | ALA  |
| 1   | AC    | 182 | ALA  |
| 1   | AC    | 184 | TYR  |
| 1   | AD    | 22  | VAL  |
| 1   | AD    | 71  | LEU  |
| 1   | AD    | 147 | ALA  |
| 1   | AD    | 182 | ALA  |
| 1   | AD    | 184 | TYR  |
| 1   | AE    | 22  | VAL  |
| 1   | AE    | 71  | LEU  |
| 1   | AE    | 147 | ALA  |
| 1   | AE    | 182 | ALA  |
| 1   | AE    | 184 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AF    | 22  | VAL  |
| 1   | AF    | 71  | LEU  |
| 1   | AF    | 147 | ALA  |
| 1   | AF    | 182 | ALA  |
| 1   | AF    | 184 | TYR  |
| 1   | AG    | 22  | VAL  |
| 1   | AG    | 71  | LEU  |
| 1   | AG    | 147 | ALA  |
| 1   | AG    | 182 | ALA  |
| 1   | AG    | 184 | TYR  |
| 1   | AH    | 22  | VAL  |
| 1   | AH    | 71  | LEU  |
| 1   | AH    | 147 | ALA  |
| 1   | AH    | 182 | ALA  |
| 1   | AH    | 184 | TYR  |
| 1   | AI    | 22  | VAL  |
| 1   | AI    | 71  | LEU  |
| 1   | AI    | 147 | ALA  |
| 1   | AI    | 182 | ALA  |
| 1   | AI    | 184 | TYR  |
| 1   | AJ    | 22  | VAL  |
| 1   | AJ    | 71  | LEU  |
| 1   | AJ    | 147 | ALA  |
| 1   | AJ    | 182 | ALA  |
| 1   | AJ    | 184 | TYR  |
| 1   | AK    | 22  | VAL  |
| 1   | AK    | 71  | LEU  |
| 1   | AK    | 147 | ALA  |
| 1   | AK    | 182 | ALA  |
| 1   | AK    | 184 | TYR  |
| 1   | AL    | 22  | VAL  |
| 1   | AL    | 71  | LEU  |
| 1   | AL    | 147 | ALA  |
| 1   | AL    | 182 | ALA  |
| 1   | AL    | 184 | TYR  |
| 1   | AM    | 22  | VAL  |
| 1   | AM    | 71  | LEU  |
| 1   | AM    | 147 | ALA  |
| 1   | AM    | 182 | ALA  |
| 1   | AM    | 184 | TYR  |
| 1   | AN    | 22  | VAL  |
| 1   | AN    | 71  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AN    | 147 | ALA  |
| 1   | AN    | 182 | ALA  |
| 1   | AN    | 184 | TYR  |
| 1   | AO    | 22  | VAL  |
| 1   | AO    | 71  | LEU  |
| 1   | AO    | 147 | ALA  |
| 1   | AO    | 182 | ALA  |
| 1   | AO    | 184 | TYR  |
| 1   | AP    | 22  | VAL  |
| 1   | AP    | 71  | LEU  |
| 1   | AP    | 147 | ALA  |
| 1   | AP    | 182 | ALA  |
| 1   | AP    | 184 | TYR  |
| 1   | AQ    | 22  | VAL  |
| 1   | AQ    | 71  | LEU  |
| 1   | AQ    | 147 | ALA  |
| 1   | AQ    | 182 | ALA  |
| 1   | AQ    | 184 | TYR  |
| 1   | AR    | 22  | VAL  |
| 1   | AR    | 71  | LEU  |
| 1   | AR    | 147 | ALA  |
| 1   | AR    | 182 | ALA  |
| 1   | AR    | 184 | TYR  |
| 1   | AS    | 22  | VAL  |
| 1   | AS    | 71  | LEU  |
| 1   | AS    | 147 | ALA  |
| 1   | AS    | 182 | ALA  |
| 1   | AS    | 184 | TYR  |
| 1   | AT    | 22  | VAL  |
| 1   | AT    | 71  | LEU  |
| 1   | AT    | 147 | ALA  |
| 1   | AT    | 182 | ALA  |
| 1   | AT    | 184 | TYR  |
| 1   | AU    | 22  | VAL  |
| 1   | AU    | 71  | LEU  |
| 1   | AU    | 147 | ALA  |
| 1   | AU    | 182 | ALA  |
| 1   | AU    | 184 | TYR  |
| 1   | AV    | 22  | VAL  |
| 1   | AV    | 71  | LEU  |
| 1   | AV    | 147 | ALA  |
| 1   | AV    | 182 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AV    | 184 | TYR  |
| 1   | AW    | 22  | VAL  |
| 1   | AW    | 71  | LEU  |
| 1   | AW    | 147 | ALA  |
| 1   | AW    | 182 | ALA  |
| 1   | AW    | 184 | TYR  |
| 1   | AX    | 22  | VAL  |
| 1   | AX    | 71  | LEU  |
| 1   | AX    | 147 | ALA  |
| 1   | AX    | 182 | ALA  |
| 1   | AX    | 184 | TYR  |
| 1   | AY    | 22  | VAL  |
| 1   | AY    | 71  | LEU  |
| 1   | AY    | 147 | ALA  |
| 1   | AY    | 182 | ALA  |
| 1   | AY    | 184 | TYR  |
| 1   | AZ    | 22  | VAL  |
| 1   | AZ    | 71  | LEU  |
| 1   | AZ    | 147 | ALA  |
| 1   | AZ    | 182 | ALA  |
| 1   | AZ    | 184 | TYR  |
| 1   | A0    | 22  | VAL  |
| 1   | A0    | 71  | LEU  |
| 1   | A0    | 147 | ALA  |
| 1   | A0    | 182 | ALA  |
| 1   | A0    | 184 | TYR  |
| 1   | A1    | 22  | VAL  |
| 1   | A1    | 71  | LEU  |
| 1   | A1    | 147 | ALA  |
| 1   | A1    | 182 | ALA  |
| 1   | A1    | 184 | TYR  |
| 1   | A2    | 22  | VAL  |
| 1   | A2    | 71  | LEU  |
| 1   | A2    | 147 | ALA  |
| 1   | A2    | 182 | ALA  |
| 1   | A2    | 184 | TYR  |
| 1   | A3    | 22  | VAL  |
| 1   | A3    | 71  | LEU  |
| 1   | A3    | 147 | ALA  |
| 1   | A3    | 182 | ALA  |
| 1   | A3    | 184 | TYR  |
| 1   | A4    | 22  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A4    | 71  | LEU  |
| 1   | A4    | 147 | ALA  |
| 1   | A4    | 182 | ALA  |
| 1   | A4    | 184 | TYR  |
| 1   | A5    | 22  | VAL  |
| 1   | A5    | 71  | LEU  |
| 1   | A5    | 147 | ALA  |
| 1   | A5    | 182 | ALA  |
| 1   | A5    | 184 | TYR  |
| 1   | A6    | 22  | VAL  |
| 1   | A6    | 71  | LEU  |
| 1   | A6    | 147 | ALA  |
| 1   | A6    | 182 | ALA  |
| 1   | A6    | 184 | TYR  |
| 1   | A7    | 22  | VAL  |
| 1   | A7    | 71  | LEU  |
| 1   | A7    | 147 | ALA  |
| 1   | A7    | 182 | ALA  |
| 1   | A7    | 184 | TYR  |
| 1   | A8    | 22  | VAL  |
| 1   | A8    | 71  | LEU  |
| 1   | A8    | 147 | ALA  |
| 1   | A8    | 182 | ALA  |
| 1   | A8    | 184 | TYR  |
| 1   | A9    | 22  | VAL  |
| 1   | A9    | 71  | LEU  |
| 1   | A9    | 147 | ALA  |
| 1   | A9    | 182 | ALA  |
| 1   | A9    | 184 | TYR  |
| 1   | Aa    | 22  | VAL  |
| 1   | Aa    | 71  | LEU  |
| 1   | Aa    | 147 | ALA  |
| 1   | Aa    | 182 | ALA  |
| 1   | Aa    | 184 | TYR  |
| 1   | Ab    | 22  | VAL  |
| 1   | Ab    | 71  | LEU  |
| 1   | Ab    | 147 | ALA  |
| 1   | Ab    | 182 | ALA  |
| 1   | Ab    | 184 | TYR  |
| 1   | Ac    | 22  | VAL  |
| 1   | Ac    | 71  | LEU  |
| 1   | Ac    | 147 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Ac    | 182 | ALA  |
| 1   | Ac    | 184 | TYR  |
| 1   | Ad    | 22  | VAL  |
| 1   | Ad    | 71  | LEU  |
| 1   | Ad    | 147 | ALA  |
| 1   | Ad    | 182 | ALA  |
| 1   | Ad    | 184 | TYR  |
| 1   | Ae    | 22  | VAL  |
| 1   | Ae    | 71  | LEU  |
| 1   | Ae    | 147 | ALA  |
| 1   | Ae    | 182 | ALA  |
| 1   | Ae    | 184 | TYR  |
| 1   | Af    | 22  | VAL  |
| 1   | Af    | 71  | LEU  |
| 1   | Af    | 147 | ALA  |
| 1   | Af    | 182 | ALA  |
| 1   | Af    | 184 | TYR  |
| 1   | Ag    | 22  | VAL  |
| 1   | Ag    | 71  | LEU  |
| 1   | Ag    | 147 | ALA  |
| 1   | Ag    | 182 | ALA  |
| 1   | Ag    | 184 | TYR  |
| 1   | Ah    | 22  | VAL  |
| 1   | Ah    | 71  | LEU  |
| 1   | Ah    | 147 | ALA  |
| 1   | Ah    | 182 | ALA  |
| 1   | Ah    | 184 | TYR  |
| 1   | Ai    | 22  | VAL  |
| 1   | Ai    | 71  | LEU  |
| 1   | Ai    | 147 | ALA  |
| 1   | Ai    | 182 | ALA  |
| 1   | Ai    | 184 | TYR  |
| 1   | Aj    | 22  | VAL  |
| 1   | Aj    | 71  | LEU  |
| 1   | Aj    | 147 | ALA  |
| 1   | Aj    | 182 | ALA  |
| 1   | Aj    | 184 | TYR  |
| 1   | Ak    | 22  | VAL  |
| 1   | Ak    | 71  | LEU  |
| 1   | Ak    | 147 | ALA  |
| 1   | Ak    | 182 | ALA  |
| 1   | Ak    | 184 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Al    | 22  | VAL  |
| 1   | Al    | 71  | LEU  |
| 1   | Al    | 147 | ALA  |
| 1   | Al    | 182 | ALA  |
| 1   | Al    | 184 | TYR  |
| 1   | Am    | 22  | VAL  |
| 1   | Am    | 71  | LEU  |
| 1   | Am    | 147 | ALA  |
| 1   | Am    | 182 | ALA  |
| 1   | Am    | 184 | TYR  |
| 1   | An    | 22  | VAL  |
| 1   | An    | 71  | LEU  |
| 1   | An    | 147 | ALA  |
| 1   | An    | 182 | ALA  |
| 1   | An    | 184 | TYR  |
| 1   | Ao    | 22  | VAL  |
| 1   | Ao    | 71  | LEU  |
| 1   | Ao    | 147 | ALA  |
| 1   | Ao    | 182 | ALA  |
| 1   | Ao    | 184 | TYR  |
| 2   | BA    | 92  | GLY  |
| 2   | BA    | 224 | GLY  |
| 2   | BB    | 92  | GLY  |
| 2   | BB    | 224 | GLY  |
| 2   | BC    | 92  | GLY  |
| 2   | BC    | 224 | GLY  |
| 2   | BD    | 92  | GLY  |
| 2   | BD    | 224 | GLY  |
| 2   | BE    | 92  | GLY  |
| 2   | BE    | 224 | GLY  |
| 2   | BF    | 92  | GLY  |
| 2   | BF    | 224 | GLY  |
| 2   | BG    | 92  | GLY  |
| 2   | BG    | 224 | GLY  |
| 2   | BH    | 92  | GLY  |
| 2   | BH    | 224 | GLY  |
| 2   | BI    | 92  | GLY  |
| 2   | BI    | 224 | GLY  |
| 2   | BJ    | 92  | GLY  |
| 2   | BJ    | 224 | GLY  |
| 2   | BK    | 92  | GLY  |
| 2   | BK    | 224 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | BL    | 92  | GLY  |
| 2   | BL    | 224 | GLY  |
| 2   | BM    | 92  | GLY  |
| 2   | BM    | 224 | GLY  |
| 2   | BN    | 92  | GLY  |
| 2   | BN    | 224 | GLY  |
| 2   | BR    | 92  | GLY  |
| 2   | BR    | 224 | GLY  |
| 2   | BO    | 92  | GLY  |
| 2   | BO    | 224 | GLY  |
| 2   | BS    | 92  | GLY  |
| 2   | BS    | 224 | GLY  |
| 2   | BP    | 92  | GLY  |
| 2   | BP    | 224 | GLY  |
| 2   | BQ    | 92  | GLY  |
| 2   | BQ    | 224 | GLY  |
| 2   | BT    | 92  | GLY  |
| 2   | BT    | 224 | GLY  |
| 2   | BU    | 92  | GLY  |
| 2   | BU    | 224 | GLY  |
| 2   | BV    | 92  | GLY  |
| 2   | BV    | 224 | GLY  |
| 2   | BW    | 92  | GLY  |
| 2   | BW    | 224 | GLY  |
| 2   | BX    | 92  | GLY  |
| 2   | BX    | 224 | GLY  |
| 2   | BY    | 92  | GLY  |
| 2   | BY    | 224 | GLY  |
| 2   | BZ    | 92  | GLY  |
| 2   | BZ    | 224 | GLY  |
| 2   | B0    | 92  | GLY  |
| 2   | B0    | 224 | GLY  |
| 2   | B1    | 92  | GLY  |
| 2   | B1    | 224 | GLY  |
| 2   | B2    | 92  | GLY  |
| 2   | B2    | 224 | GLY  |
| 2   | B3    | 92  | GLY  |
| 2   | B3    | 224 | GLY  |
| 2   | B4    | 92  | GLY  |
| 2   | B4    | 224 | GLY  |
| 2   | B5    | 92  | GLY  |
| 2   | B5    | 224 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B6    | 92  | GLY  |
| 2   | B6    | 224 | GLY  |
| 2   | B7    | 92  | GLY  |
| 2   | B7    | 224 | GLY  |
| 2   | B8    | 92  | GLY  |
| 2   | B8    | 224 | GLY  |
| 2   | B9    | 92  | GLY  |
| 2   | B9    | 224 | GLY  |
| 2   | Ba    | 92  | GLY  |
| 2   | Ba    | 224 | GLY  |
| 2   | Bb    | 92  | GLY  |
| 2   | Bb    | 224 | GLY  |
| 2   | Bc    | 92  | GLY  |
| 2   | Bc    | 224 | GLY  |
| 2   | Bd    | 92  | GLY  |
| 2   | Bd    | 224 | GLY  |
| 2   | Be    | 92  | GLY  |
| 2   | Be    | 224 | GLY  |
| 2   | Bf    | 92  | GLY  |
| 2   | Bf    | 224 | GLY  |
| 2   | Bg    | 92  | GLY  |
| 2   | Bg    | 224 | GLY  |
| 2   | Bh    | 92  | GLY  |
| 2   | Bh    | 224 | GLY  |
| 2   | Bi    | 92  | GLY  |
| 2   | Bi    | 224 | GLY  |
| 2   | Bj    | 92  | GLY  |
| 2   | Bj    | 224 | GLY  |
| 2   | Bk    | 92  | GLY  |
| 2   | Bk    | 224 | GLY  |
| 2   | Bl    | 92  | GLY  |
| 2   | Bl    | 224 | GLY  |
| 2   | Bm    | 92  | GLY  |
| 2   | Bm    | 224 | GLY  |
| 2   | Bn    | 92  | GLY  |
| 2   | Bn    | 224 | GLY  |
| 2   | Bo    | 92  | GLY  |
| 2   | Bo    | 224 | GLY  |
| 2   | Bp    | 92  | GLY  |
| 2   | Bp    | 224 | GLY  |
| 2   | Bq    | 92  | GLY  |
| 2   | Bq    | 224 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Br    | 92  | GLY  |
| 2   | Br    | 224 | GLY  |
| 2   | Bs    | 92  | GLY  |
| 2   | Bs    | 224 | GLY  |
| 2   | Bt    | 92  | GLY  |
| 2   | Bt    | 224 | GLY  |
| 2   | Bu    | 92  | GLY  |
| 2   | Bu    | 224 | GLY  |
| 2   | Bv    | 92  | GLY  |
| 2   | Bv    | 224 | GLY  |
| 2   | Bw    | 92  | GLY  |
| 2   | Bw    | 224 | GLY  |
| 2   | Bx    | 92  | GLY  |
| 2   | Bx    | 224 | GLY  |
| 3   | CA    | 15  | MET  |
| 3   | CA    | 35  | GLN  |
| 3   | CA    | 70  | ASP  |
| 3   | CB    | 15  | MET  |
| 3   | CB    | 35  | GLN  |
| 3   | CB    | 70  | ASP  |
| 3   | CC    | 15  | MET  |
| 3   | CC    | 35  | GLN  |
| 3   | CC    | 70  | ASP  |
| 3   | CD    | 15  | MET  |
| 3   | CD    | 35  | GLN  |
| 3   | CD    | 70  | ASP  |
| 3   | CE    | 15  | MET  |
| 3   | CE    | 35  | GLN  |
| 3   | CE    | 70  | ASP  |
| 3   | CF    | 15  | MET  |
| 3   | CF    | 35  | GLN  |
| 3   | CF    | 70  | ASP  |
| 3   | CG    | 15  | MET  |
| 3   | CG    | 35  | GLN  |
| 3   | CG    | 70  | ASP  |
| 3   | CH    | 15  | MET  |
| 3   | CH    | 35  | GLN  |
| 3   | CH    | 70  | ASP  |
| 3   | CI    | 15  | MET  |
| 3   | CI    | 35  | GLN  |
| 3   | CI    | 70  | ASP  |
| 3   | CJ    | 15  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CJ    | 35  | GLN  |
| 3   | CJ    | 70  | ASP  |
| 3   | CK    | 15  | MET  |
| 3   | CK    | 35  | GLN  |
| 3   | CK    | 70  | ASP  |
| 3   | CL    | 15  | MET  |
| 3   | CL    | 35  | GLN  |
| 3   | CL    | 70  | ASP  |
| 3   | CM    | 15  | MET  |
| 3   | CM    | 35  | GLN  |
| 3   | CM    | 70  | ASP  |
| 3   | CN    | 15  | MET  |
| 3   | CN    | 35  | GLN  |
| 3   | CN    | 70  | ASP  |
| 3   | CO    | 15  | MET  |
| 3   | CO    | 35  | GLN  |
| 3   | CO    | 70  | ASP  |
| 3   | CP    | 15  | MET  |
| 3   | CP    | 35  | GLN  |
| 3   | CP    | 70  | ASP  |
| 3   | CQ    | 15  | MET  |
| 3   | CQ    | 35  | GLN  |
| 3   | CQ    | 70  | ASP  |
| 3   | CR    | 15  | MET  |
| 3   | CR    | 35  | GLN  |
| 3   | CR    | 70  | ASP  |
| 3   | CS    | 15  | MET  |
| 3   | CS    | 35  | GLN  |
| 3   | CS    | 70  | ASP  |
| 3   | CT    | 15  | MET  |
| 3   | CT    | 35  | GLN  |
| 3   | CT    | 70  | ASP  |
| 3   | CU    | 15  | MET  |
| 3   | CU    | 35  | GLN  |
| 3   | CU    | 70  | ASP  |
| 3   | CV    | 15  | MET  |
| 3   | CV    | 35  | GLN  |
| 3   | CV    | 70  | ASP  |
| 3   | CW    | 15  | MET  |
| 3   | CW    | 35  | GLN  |
| 3   | CW    | 70  | ASP  |
| 3   | CX    | 15  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CX    | 35  | GLN  |
| 3   | CX    | 70  | ASP  |
| 3   | CY    | 15  | MET  |
| 3   | CY    | 35  | GLN  |
| 3   | CY    | 70  | ASP  |
| 3   | CZ    | 15  | MET  |
| 3   | CZ    | 35  | GLN  |
| 3   | CZ    | 70  | ASP  |
| 3   | C0    | 15  | MET  |
| 3   | C0    | 35  | GLN  |
| 3   | C0    | 70  | ASP  |
| 3   | C1    | 15  | MET  |
| 3   | C1    | 35  | GLN  |
| 3   | C1    | 70  | ASP  |
| 3   | C2    | 15  | MET  |
| 3   | C2    | 35  | GLN  |
| 3   | C2    | 70  | ASP  |
| 3   | C3    | 15  | MET  |
| 3   | C3    | 35  | GLN  |
| 3   | C3    | 70  | ASP  |
| 3   | C4    | 15  | MET  |
| 3   | C4    | 35  | GLN  |
| 3   | C4    | 70  | ASP  |
| 3   | C5    | 15  | MET  |
| 3   | C5    | 35  | GLN  |
| 3   | C5    | 70  | ASP  |
| 3   | C6    | 15  | MET  |
| 3   | C6    | 35  | GLN  |
| 3   | C6    | 70  | ASP  |
| 3   | C7    | 15  | MET  |
| 3   | C7    | 35  | GLN  |
| 3   | C7    | 70  | ASP  |
| 3   | C8    | 15  | MET  |
| 3   | C8    | 35  | GLN  |
| 3   | C8    | 70  | ASP  |
| 3   | C9    | 15  | MET  |
| 3   | C9    | 35  | GLN  |
| 3   | C9    | 70  | ASP  |
| 3   | Cc    | 15  | MET  |
| 3   | Cc    | 35  | GLN  |
| 3   | Cc    | 70  | ASP  |
| 3   | Cd    | 15  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Cd    | 35  | GLN  |
| 3   | Cd    | 70  | ASP  |
| 3   | Ce    | 15  | MET  |
| 3   | Ce    | 35  | GLN  |
| 3   | Ce    | 70  | ASP  |
| 3   | Cf    | 15  | MET  |
| 3   | Cf    | 35  | GLN  |
| 3   | Cf    | 70  | ASP  |
| 3   | Cg    | 15  | MET  |
| 3   | Cg    | 35  | GLN  |
| 3   | Cg    | 70  | ASP  |
| 3   | Ch    | 15  | MET  |
| 3   | Ch    | 35  | GLN  |
| 3   | Ch    | 70  | ASP  |
| 3   | Ci    | 15  | MET  |
| 3   | Ci    | 35  | GLN  |
| 3   | Ci    | 70  | ASP  |
| 3   | Cj    | 15  | MET  |
| 3   | Cj    | 35  | GLN  |
| 3   | Cj    | 70  | ASP  |
| 3   | Ck    | 15  | MET  |
| 3   | Ck    | 35  | GLN  |
| 3   | Ck    | 70  | ASP  |
| 3   | Cl    | 15  | MET  |
| 3   | Cl    | 35  | GLN  |
| 3   | Cl    | 70  | ASP  |
| 3   | Cm    | 15  | MET  |
| 3   | Cm    | 35  | GLN  |
| 3   | Cm    | 70  | ASP  |
| 3   | Cn    | 15  | MET  |
| 3   | Cn    | 35  | GLN  |
| 3   | Cn    | 70  | ASP  |
| 3   | Co    | 15  | MET  |
| 3   | Co    | 35  | GLN  |
| 3   | Co    | 70  | ASP  |
| 3   | Cp    | 15  | MET  |
| 3   | Cp    | 35  | GLN  |
| 3   | Cp    | 70  | ASP  |
| 3   | Cq    | 15  | MET  |
| 3   | Cq    | 35  | GLN  |
| 3   | Cq    | 70  | ASP  |
| 3   | Cr    | 15  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Cr    | 35  | GLN  |
| 3   | Cr    | 70  | ASP  |
| 3   | Cs    | 15  | MET  |
| 3   | Cs    | 35  | GLN  |
| 3   | Cs    | 70  | ASP  |
| 3   | Ct    | 15  | MET  |
| 3   | Ct    | 35  | GLN  |
| 3   | Ct    | 70  | ASP  |
| 3   | Cu    | 15  | MET  |
| 3   | Cu    | 35  | GLN  |
| 3   | Cu    | 70  | ASP  |
| 3   | Cv    | 15  | MET  |
| 3   | Cv    | 35  | GLN  |
| 3   | Cv    | 70  | ASP  |
| 3   | Cw    | 15  | MET  |
| 3   | Cw    | 35  | GLN  |
| 3   | Cw    | 70  | ASP  |
| 3   | Cx    | 15  | MET  |
| 3   | Cx    | 35  | GLN  |
| 3   | Cx    | 70  | ASP  |
| 3   | DA    | 15  | MET  |
| 3   | DA    | 35  | GLN  |
| 3   | DA    | 70  | ASP  |
| 3   | DB    | 15  | MET  |
| 3   | DB    | 35  | GLN  |
| 3   | DB    | 70  | ASP  |
| 1   | DC    | 22  | VAL  |
| 1   | DC    | 71  | LEU  |
| 1   | DC    | 147 | ALA  |
| 1   | DC    | 182 | ALA  |
| 1   | DC    | 184 | TYR  |
| 1   | DD    | 22  | VAL  |
| 1   | DD    | 71  | LEU  |
| 1   | DD    | 147 | ALA  |
| 1   | DD    | 182 | ALA  |
| 1   | DD    | 184 | TYR  |
| 1   | DE    | 22  | VAL  |
| 1   | DE    | 71  | LEU  |
| 1   | DE    | 147 | ALA  |
| 1   | DE    | 182 | ALA  |
| 1   | DE    | 184 | TYR  |
| 1   | DF    | 22  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | DF    | 71  | LEU  |
| 1   | DF    | 147 | ALA  |
| 1   | DF    | 182 | ALA  |
| 1   | DF    | 184 | TYR  |
| 1   | DG    | 22  | VAL  |
| 1   | DG    | 71  | LEU  |
| 1   | DG    | 147 | ALA  |
| 1   | DG    | 182 | ALA  |
| 1   | DG    | 184 | TYR  |
| 1   | DH    | 22  | VAL  |
| 1   | DH    | 71  | LEU  |
| 1   | DH    | 147 | ALA  |
| 1   | DH    | 182 | ALA  |
| 1   | DH    | 184 | TYR  |
| 1   | DI    | 22  | VAL  |
| 1   | DI    | 71  | LEU  |
| 1   | DI    | 147 | ALA  |
| 1   | DI    | 182 | ALA  |
| 1   | DI    | 184 | TYR  |
| 1   | DJ    | 22  | VAL  |
| 1   | DJ    | 71  | LEU  |
| 1   | DJ    | 147 | ALA  |
| 1   | DJ    | 182 | ALA  |
| 1   | DJ    | 184 | TYR  |
| 1   | DK    | 22  | VAL  |
| 1   | DK    | 71  | LEU  |
| 1   | DK    | 147 | ALA  |
| 1   | DK    | 182 | ALA  |
| 1   | DK    | 184 | TYR  |
| 1   | AA    | 3   | ASN  |
| 1   | AB    | 3   | ASN  |
| 1   | AC    | 3   | ASN  |
| 1   | AD    | 3   | ASN  |
| 1   | AE    | 3   | ASN  |
| 1   | AF    | 3   | ASN  |
| 1   | AG    | 3   | ASN  |
| 1   | AH    | 3   | ASN  |
| 1   | AI    | 3   | ASN  |
| 1   | AJ    | 3   | ASN  |
| 1   | AK    | 3   | ASN  |
| 1   | AL    | 3   | ASN  |
| 1   | AM    | 3   | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AN    | 3   | ASN  |
| 1   | AO    | 3   | ASN  |
| 1   | AP    | 3   | ASN  |
| 1   | AQ    | 3   | ASN  |
| 1   | AR    | 3   | ASN  |
| 1   | AS    | 3   | ASN  |
| 1   | AT    | 3   | ASN  |
| 1   | AU    | 3   | ASN  |
| 1   | AV    | 3   | ASN  |
| 1   | AW    | 3   | ASN  |
| 1   | AX    | 3   | ASN  |
| 1   | AY    | 3   | ASN  |
| 1   | AZ    | 3   | ASN  |
| 1   | A0    | 3   | ASN  |
| 1   | A1    | 3   | ASN  |
| 1   | A2    | 3   | ASN  |
| 1   | A3    | 3   | ASN  |
| 1   | A4    | 3   | ASN  |
| 1   | A5    | 3   | ASN  |
| 1   | A6    | 3   | ASN  |
| 1   | A7    | 3   | ASN  |
| 1   | A8    | 3   | ASN  |
| 1   | A9    | 3   | ASN  |
| 1   | Aa    | 3   | ASN  |
| 1   | Ab    | 3   | ASN  |
| 1   | Ac    | 3   | ASN  |
| 1   | Ad    | 3   | ASN  |
| 1   | Ae    | 3   | ASN  |
| 1   | Af    | 3   | ASN  |
| 1   | Ag    | 3   | ASN  |
| 1   | Ah    | 3   | ASN  |
| 1   | Ai    | 3   | ASN  |
| 1   | Aj    | 3   | ASN  |
| 1   | Ak    | 3   | ASN  |
| 1   | Al    | 3   | ASN  |
| 1   | Am    | 3   | ASN  |
| 1   | An    | 3   | ASN  |
| 1   | Ao    | 3   | ASN  |
| 1   | DC    | 3   | ASN  |
| 1   | DD    | 3   | ASN  |
| 1   | DE    | 3   | ASN  |
| 1   | DF    | 3   | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | DG    | 3   | ASN  |
| 1   | DH    | 3   | ASN  |
| 1   | DI    | 3   | ASN  |
| 1   | DJ    | 3   | ASN  |
| 1   | DK    | 3   | ASN  |
| 1   | AA    | 187 | LEU  |
| 1   | AA    | 208 | TYR  |
| 1   | AB    | 187 | LEU  |
| 1   | AB    | 208 | TYR  |
| 1   | AC    | 187 | LEU  |
| 1   | AC    | 208 | TYR  |
| 1   | AD    | 187 | LEU  |
| 1   | AD    | 208 | TYR  |
| 1   | AE    | 187 | LEU  |
| 1   | AE    | 208 | TYR  |
| 1   | AF    | 187 | LEU  |
| 1   | AF    | 208 | TYR  |
| 1   | AG    | 187 | LEU  |
| 1   | AG    | 208 | TYR  |
| 1   | AH    | 187 | LEU  |
| 1   | AH    | 208 | TYR  |
| 1   | AI    | 187 | LEU  |
| 1   | AI    | 208 | TYR  |
| 1   | AJ    | 187 | LEU  |
| 1   | AJ    | 208 | TYR  |
| 1   | AK    | 187 | LEU  |
| 1   | AK    | 208 | TYR  |
| 1   | AL    | 187 | LEU  |
| 1   | AL    | 208 | TYR  |
| 1   | AM    | 187 | LEU  |
| 1   | AM    | 208 | TYR  |
| 1   | AN    | 187 | LEU  |
| 1   | AN    | 208 | TYR  |
| 1   | AO    | 187 | LEU  |
| 1   | AO    | 208 | TYR  |
| 1   | AP    | 187 | LEU  |
| 1   | AP    | 208 | TYR  |
| 1   | AQ    | 187 | LEU  |
| 1   | AQ    | 208 | TYR  |
| 1   | AR    | 187 | LEU  |
| 1   | AR    | 208 | TYR  |
| 1   | AS    | 187 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AS    | 208 | TYR  |
| 1   | AT    | 187 | LEU  |
| 1   | AT    | 208 | TYR  |
| 1   | AU    | 187 | LEU  |
| 1   | AU    | 208 | TYR  |
| 1   | AV    | 187 | LEU  |
| 1   | AV    | 208 | TYR  |
| 1   | AW    | 187 | LEU  |
| 1   | AW    | 208 | TYR  |
| 1   | AX    | 187 | LEU  |
| 1   | AX    | 208 | TYR  |
| 1   | AY    | 187 | LEU  |
| 1   | AY    | 208 | TYR  |
| 1   | AZ    | 187 | LEU  |
| 1   | AZ    | 208 | TYR  |
| 1   | A0    | 187 | LEU  |
| 1   | A0    | 208 | TYR  |
| 1   | A1    | 187 | LEU  |
| 1   | A1    | 208 | TYR  |
| 1   | A2    | 187 | LEU  |
| 1   | A2    | 208 | TYR  |
| 1   | A3    | 187 | LEU  |
| 1   | A3    | 208 | TYR  |
| 1   | A4    | 187 | LEU  |
| 1   | A4    | 208 | TYR  |
| 1   | A5    | 187 | LEU  |
| 1   | A5    | 208 | TYR  |
| 1   | A6    | 187 | LEU  |
| 1   | A6    | 208 | TYR  |
| 1   | A7    | 187 | LEU  |
| 1   | A7    | 208 | TYR  |
| 1   | A8    | 187 | LEU  |
| 1   | A8    | 208 | TYR  |
| 1   | A9    | 187 | LEU  |
| 1   | A9    | 208 | TYR  |
| 1   | Aa    | 187 | LEU  |
| 1   | Aa    | 208 | TYR  |
| 1   | Ab    | 187 | LEU  |
| 1   | Ab    | 208 | TYR  |
| 1   | Ac    | 187 | LEU  |
| 1   | Ac    | 208 | TYR  |
| 1   | Ad    | 187 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Ad    | 208 | TYR  |
| 1   | Ae    | 187 | LEU  |
| 1   | Ae    | 208 | TYR  |
| 1   | Af    | 187 | LEU  |
| 1   | Af    | 208 | TYR  |
| 1   | Ag    | 187 | LEU  |
| 1   | Ag    | 208 | TYR  |
| 1   | Ah    | 187 | LEU  |
| 1   | Ah    | 208 | TYR  |
| 1   | Ai    | 187 | LEU  |
| 1   | Ai    | 208 | TYR  |
| 1   | Aj    | 187 | LEU  |
| 1   | Aj    | 208 | TYR  |
| 1   | Ak    | 187 | LEU  |
| 1   | Ak    | 208 | TYR  |
| 1   | Al    | 187 | LEU  |
| 1   | Al    | 208 | TYR  |
| 1   | Am    | 187 | LEU  |
| 1   | Am    | 208 | TYR  |
| 1   | An    | 187 | LEU  |
| 1   | An    | 208 | TYR  |
| 1   | Ao    | 187 | LEU  |
| 1   | Ao    | 208 | TYR  |
| 2   | BA    | 149 | ALA  |
| 2   | BB    | 149 | ALA  |
| 2   | BC    | 149 | ALA  |
| 2   | BD    | 149 | ALA  |
| 2   | BE    | 149 | ALA  |
| 2   | BF    | 149 | ALA  |
| 2   | BG    | 149 | ALA  |
| 2   | BH    | 149 | ALA  |
| 2   | BI    | 149 | ALA  |
| 2   | BJ    | 149 | ALA  |
| 2   | BK    | 149 | ALA  |
| 2   | BL    | 149 | ALA  |
| 2   | BM    | 149 | ALA  |
| 2   | BN    | 149 | ALA  |
| 2   | BR    | 149 | ALA  |
| 2   | BO    | 149 | ALA  |
| 2   | BS    | 149 | ALA  |
| 2   | BP    | 149 | ALA  |
| 2   | BQ    | 149 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | BT    | 149 | ALA  |
| 2   | BU    | 149 | ALA  |
| 2   | BV    | 149 | ALA  |
| 2   | BW    | 149 | ALA  |
| 2   | BX    | 149 | ALA  |
| 2   | BY    | 149 | ALA  |
| 2   | BZ    | 149 | ALA  |
| 2   | B0    | 149 | ALA  |
| 2   | B1    | 149 | ALA  |
| 2   | B2    | 149 | ALA  |
| 2   | B3    | 149 | ALA  |
| 2   | B4    | 149 | ALA  |
| 2   | B5    | 149 | ALA  |
| 2   | B6    | 149 | ALA  |
| 2   | B7    | 149 | ALA  |
| 2   | B8    | 149 | ALA  |
| 2   | B9    | 149 | ALA  |
| 2   | Ba    | 149 | ALA  |
| 2   | Bb    | 149 | ALA  |
| 2   | Bc    | 149 | ALA  |
| 2   | Bd    | 149 | ALA  |
| 2   | Be    | 149 | ALA  |
| 2   | Bf    | 149 | ALA  |
| 2   | Bg    | 149 | ALA  |
| 2   | Bh    | 149 | ALA  |
| 2   | Bi    | 149 | ALA  |
| 2   | Bj    | 149 | ALA  |
| 2   | Bk    | 149 | ALA  |
| 2   | Bl    | 149 | ALA  |
| 2   | Bm    | 149 | ALA  |
| 2   | Bn    | 149 | ALA  |
| 2   | Bo    | 149 | ALA  |
| 2   | Bp    | 149 | ALA  |
| 2   | Bq    | 149 | ALA  |
| 2   | Br    | 149 | ALA  |
| 2   | Bs    | 149 | ALA  |
| 2   | Bt    | 149 | ALA  |
| 2   | Bu    | 149 | ALA  |
| 2   | Bv    | 149 | ALA  |
| 2   | Bw    | 149 | ALA  |
| 2   | Bx    | 149 | ALA  |
| 3   | CA    | 131 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CB    | 131 | ALA  |
| 3   | CC    | 131 | ALA  |
| 3   | CD    | 131 | ALA  |
| 3   | CE    | 131 | ALA  |
| 3   | CF    | 131 | ALA  |
| 3   | CG    | 131 | ALA  |
| 3   | CH    | 131 | ALA  |
| 3   | CI    | 131 | ALA  |
| 3   | CJ    | 131 | ALA  |
| 3   | CK    | 131 | ALA  |
| 3   | CL    | 131 | ALA  |
| 3   | CM    | 131 | ALA  |
| 3   | CN    | 131 | ALA  |
| 3   | CO    | 131 | ALA  |
| 3   | CP    | 131 | ALA  |
| 3   | CQ    | 131 | ALA  |
| 3   | CR    | 131 | ALA  |
| 3   | CS    | 131 | ALA  |
| 3   | CT    | 131 | ALA  |
| 3   | CU    | 131 | ALA  |
| 3   | CV    | 131 | ALA  |
| 3   | CW    | 131 | ALA  |
| 3   | CX    | 131 | ALA  |
| 3   | CY    | 131 | ALA  |
| 3   | CZ    | 131 | ALA  |
| 3   | C0    | 131 | ALA  |
| 3   | C1    | 131 | ALA  |
| 3   | C2    | 131 | ALA  |
| 3   | C3    | 131 | ALA  |
| 3   | C4    | 131 | ALA  |
| 3   | C5    | 131 | ALA  |
| 3   | C6    | 131 | ALA  |
| 3   | C7    | 131 | ALA  |
| 3   | C8    | 131 | ALA  |
| 3   | C9    | 131 | ALA  |
| 3   | Cc    | 131 | ALA  |
| 3   | Cd    | 131 | ALA  |
| 3   | Ce    | 131 | ALA  |
| 3   | Cf    | 131 | ALA  |
| 3   | Cg    | 131 | ALA  |
| 3   | Ch    | 131 | ALA  |
| 3   | Ci    | 131 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Cj    | 131 | ALA  |
| 3   | Ck    | 131 | ALA  |
| 3   | Cl    | 131 | ALA  |
| 3   | Cm    | 131 | ALA  |
| 3   | Cn    | 131 | ALA  |
| 3   | Co    | 131 | ALA  |
| 3   | Cp    | 131 | ALA  |
| 3   | Cq    | 131 | ALA  |
| 3   | Cr    | 131 | ALA  |
| 3   | Cs    | 131 | ALA  |
| 3   | Ct    | 131 | ALA  |
| 3   | Cu    | 131 | ALA  |
| 3   | Cv    | 131 | ALA  |
| 3   | Cw    | 131 | ALA  |
| 3   | Cx    | 131 | ALA  |
| 3   | DA    | 131 | ALA  |
| 3   | DB    | 131 | ALA  |
| 1   | DC    | 187 | LEU  |
| 1   | DC    | 208 | TYR  |
| 1   | DD    | 187 | LEU  |
| 1   | DD    | 208 | TYR  |
| 1   | DE    | 187 | LEU  |
| 1   | DE    | 208 | TYR  |
| 1   | DF    | 187 | LEU  |
| 1   | DF    | 208 | TYR  |
| 1   | DG    | 187 | LEU  |
| 1   | DG    | 208 | TYR  |
| 1   | DH    | 187 | LEU  |
| 1   | DH    | 208 | TYR  |
| 1   | DI    | 187 | LEU  |
| 1   | DI    | 208 | TYR  |
| 1   | DJ    | 187 | LEU  |
| 1   | DJ    | 208 | TYR  |
| 1   | DK    | 187 | LEU  |
| 1   | DK    | 208 | TYR  |
| 2   | BA    | 60  | ARG  |
| 2   | BB    | 60  | ARG  |
| 2   | BC    | 60  | ARG  |
| 2   | BD    | 60  | ARG  |
| 2   | BE    | 60  | ARG  |
| 2   | BF    | 60  | ARG  |
| 2   | BG    | 60  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | BH    | 60  | ARG  |
| 2   | BI    | 60  | ARG  |
| 2   | BJ    | 60  | ARG  |
| 2   | BK    | 60  | ARG  |
| 2   | BL    | 60  | ARG  |
| 2   | BM    | 60  | ARG  |
| 2   | BN    | 60  | ARG  |
| 2   | BR    | 60  | ARG  |
| 2   | BO    | 60  | ARG  |
| 2   | BS    | 60  | ARG  |
| 2   | BP    | 60  | ARG  |
| 2   | BQ    | 60  | ARG  |
| 2   | BT    | 60  | ARG  |
| 2   | BU    | 60  | ARG  |
| 2   | BV    | 60  | ARG  |
| 2   | BW    | 60  | ARG  |
| 2   | BX    | 60  | ARG  |
| 2   | BY    | 60  | ARG  |
| 2   | BZ    | 60  | ARG  |
| 2   | B0    | 60  | ARG  |
| 2   | B1    | 60  | ARG  |
| 2   | B2    | 60  | ARG  |
| 2   | B3    | 60  | ARG  |
| 2   | B4    | 60  | ARG  |
| 2   | B5    | 60  | ARG  |
| 2   | B6    | 60  | ARG  |
| 2   | B7    | 60  | ARG  |
| 2   | B8    | 60  | ARG  |
| 2   | B9    | 60  | ARG  |
| 2   | Ba    | 60  | ARG  |
| 2   | Bb    | 60  | ARG  |
| 2   | Bc    | 60  | ARG  |
| 2   | Bd    | 60  | ARG  |
| 2   | Be    | 60  | ARG  |
| 2   | Bf    | 60  | ARG  |
| 2   | Bg    | 60  | ARG  |
| 2   | Bh    | 60  | ARG  |
| 2   | Bi    | 60  | ARG  |
| 2   | Bj    | 60  | ARG  |
| 2   | Bk    | 60  | ARG  |
| 2   | Bl    | 60  | ARG  |
| 2   | Bm    | 60  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Bn    | 60  | ARG  |
| 2   | Bo    | 60  | ARG  |
| 2   | Bp    | 60  | ARG  |
| 2   | Bq    | 60  | ARG  |
| 2   | Br    | 60  | ARG  |
| 2   | Bs    | 60  | ARG  |
| 2   | Bt    | 60  | ARG  |
| 2   | Bu    | 60  | ARG  |
| 2   | Bv    | 60  | ARG  |
| 2   | Bw    | 60  | ARG  |
| 2   | Bx    | 60  | ARG  |
| 1   | Ac    | 226 | PRO  |
| 1   | AA    | 226 | PRO  |
| 1   | AB    | 226 | PRO  |
| 1   | AC    | 226 | PRO  |
| 1   | AD    | 226 | PRO  |
| 1   | AE    | 226 | PRO  |
| 1   | AF    | 226 | PRO  |
| 1   | AG    | 226 | PRO  |
| 1   | AH    | 226 | PRO  |
| 1   | AI    | 226 | PRO  |
| 1   | AJ    | 226 | PRO  |
| 1   | AK    | 226 | PRO  |
| 1   | AL    | 226 | PRO  |
| 1   | AM    | 226 | PRO  |
| 1   | AN    | 226 | PRO  |
| 1   | AO    | 226 | PRO  |
| 1   | AP    | 226 | PRO  |
| 1   | AQ    | 226 | PRO  |
| 1   | AR    | 226 | PRO  |
| 1   | AS    | 226 | PRO  |
| 1   | AT    | 226 | PRO  |
| 1   | AU    | 226 | PRO  |
| 1   | AV    | 226 | PRO  |
| 1   | AW    | 226 | PRO  |
| 1   | AX    | 226 | PRO  |
| 1   | AY    | 226 | PRO  |
| 1   | AZ    | 226 | PRO  |
| 1   | A0    | 226 | PRO  |
| 1   | A1    | 226 | PRO  |
| 1   | A2    | 226 | PRO  |
| 1   | A3    | 226 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A4    | 226 | PRO  |
| 1   | A5    | 226 | PRO  |
| 1   | A6    | 226 | PRO  |
| 1   | A7    | 226 | PRO  |
| 1   | A8    | 226 | PRO  |
| 1   | A9    | 226 | PRO  |
| 1   | Aa    | 226 | PRO  |
| 1   | Ab    | 226 | PRO  |
| 1   | Ad    | 226 | PRO  |
| 1   | Ae    | 226 | PRO  |
| 1   | Af    | 226 | PRO  |
| 1   | Ag    | 226 | PRO  |
| 1   | Ah    | 226 | PRO  |
| 1   | Ai    | 226 | PRO  |
| 1   | Aj    | 226 | PRO  |
| 1   | Ak    | 226 | PRO  |
| 1   | Al    | 226 | PRO  |
| 1   | Am    | 226 | PRO  |
| 1   | An    | 226 | PRO  |
| 1   | Ao    | 226 | PRO  |
| 1   | DC    | 226 | PRO  |
| 1   | DD    | 226 | PRO  |
| 1   | DE    | 226 | PRO  |
| 1   | DF    | 226 | PRO  |
| 1   | DG    | 226 | PRO  |
| 1   | DH    | 226 | PRO  |
| 1   | DI    | 226 | PRO  |
| 1   | DJ    | 226 | PRO  |
| 1   | DK    | 226 | PRO  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1   | A0    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | A1    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1   | A2    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | A3    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | A4    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | A5    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | A6    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | A7    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | A8    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | A9    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | AA    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | AB    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | AC    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | AD    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | AE    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | AF    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | AG    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | AH    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | AI    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | AJ    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | AK    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | AL    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | AM    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | AN    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | AO    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | AP    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | AQ    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | AR    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | AS    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | AT    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | AU    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | AV    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | AW    | 208/208 (100%) | 183 (88%) | 25 (12%) | 6           | 31 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1   | AX    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | AY    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | AZ    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | Aa    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | Ab    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | Ac    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | Ad    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | Ae    | 208/208 (100%) | 183 (88%) | 25 (12%) | 6           | 31 |
| 1   | Af    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | Ag    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | Ah    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | Ai    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | Aj    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | Ak    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | Al    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | Am    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | An    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | Ao    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | DC    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | DD    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | DE    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | DF    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | DG    | 208/208 (100%) | 183 (88%) | 25 (12%) | 6           | 31 |
| 1   | DH    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | DI    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | DJ    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 1   | DK    | 208/208 (100%) | 184 (88%) | 24 (12%) | 7           | 32 |
| 2   | B0    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | B1    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | B2    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | B3    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2   | B4    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | B5    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | B6    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | B7    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | B8    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | B9    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | BA    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | BB    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | BC    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | BD    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | BE    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | BF    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | BG    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | BH    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | BI    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | BJ    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | BK    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | BL    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | BM    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | BN    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | BO    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | BP    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | BQ    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | BR    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | BS    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | BT    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | BU    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | BV    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | BW    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | BX    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | BY    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2   | BZ    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | Ba    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | Bb    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | Bc    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | Bd    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | Be    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | Bf    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | Bg    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | Bh    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | Bi    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | Bj    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | Bk    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | Bl    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | Bm    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | Bn    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | Bo    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | Bp    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | Bq    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | Br    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | Bs    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | Bt    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | Bu    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | Bv    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | Bw    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 2   | Bx    | 176/176 (100%) | 150 (85%) | 26 (15%) | 4           | 24 |
| 3   | C0    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9  |
| 3   | C1    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9  |
| 3   | C2    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9  |
| 3   | C3    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9  |
| 3   | C4    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9  |
| 3   | C5    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9  |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |   |
|-----|-------|----------------|-----------|----------|-------------|---|
| 3   | C6    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9 |
| 3   | C7    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9 |
| 3   | C8    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9 |
| 3   | C9    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9 |
| 3   | CA    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9 |
| 3   | CB    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9 |
| 3   | CC    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9 |
| 3   | CD    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9 |
| 3   | CE    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9 |
| 3   | CF    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9 |
| 3   | CG    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9 |
| 3   | CH    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9 |
| 3   | CI    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9 |
| 3   | CJ    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9 |
| 3   | CK    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9 |
| 3   | CL    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9 |
| 3   | CM    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9 |
| 3   | CN    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9 |
| 3   | CO    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9 |
| 3   | CP    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9 |
| 3   | CQ    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9 |
| 3   | CR    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9 |
| 3   | CS    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9 |
| 3   | CT    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9 |
| 3   | CU    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9 |
| 3   | CV    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9 |
| 3   | CW    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9 |
| 3   | CX    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9 |
| 3   | CY    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9 |
| 3   | CZ    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9 |
| 3   | Cc    | 190/190 (100%) | 150 (79%) | 40 (21%) | 1           | 9 |

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| Mol | Chain | Analysed           | Rotameric   | Outliers   | Percentiles |    |
|-----|-------|--------------------|-------------|------------|-------------|----|
| 3   | Cd    | 190/190 (100%)     | 150 (79%)   | 40 (21%)   | 1           | 9  |
| 3   | Ce    | 190/190 (100%)     | 150 (79%)   | 40 (21%)   | 1           | 9  |
| 3   | Cf    | 190/190 (100%)     | 150 (79%)   | 40 (21%)   | 1           | 9  |
| 3   | Cg    | 190/190 (100%)     | 150 (79%)   | 40 (21%)   | 1           | 9  |
| 3   | Ch    | 190/190 (100%)     | 150 (79%)   | 40 (21%)   | 1           | 9  |
| 3   | Ci    | 190/190 (100%)     | 150 (79%)   | 40 (21%)   | 1           | 9  |
| 3   | Cj    | 190/190 (100%)     | 150 (79%)   | 40 (21%)   | 1           | 9  |
| 3   | Ck    | 190/190 (100%)     | 150 (79%)   | 40 (21%)   | 1           | 9  |
| 3   | Cl    | 190/190 (100%)     | 150 (79%)   | 40 (21%)   | 1           | 9  |
| 3   | Cm    | 190/190 (100%)     | 150 (79%)   | 40 (21%)   | 1           | 9  |
| 3   | Cn    | 190/190 (100%)     | 150 (79%)   | 40 (21%)   | 1           | 9  |
| 3   | Co    | 190/190 (100%)     | 150 (79%)   | 40 (21%)   | 1           | 9  |
| 3   | Cp    | 190/190 (100%)     | 150 (79%)   | 40 (21%)   | 1           | 9  |
| 3   | Cq    | 190/190 (100%)     | 150 (79%)   | 40 (21%)   | 1           | 9  |
| 3   | Cr    | 190/190 (100%)     | 150 (79%)   | 40 (21%)   | 1           | 9  |
| 3   | Cs    | 190/190 (100%)     | 150 (79%)   | 40 (21%)   | 1           | 9  |
| 3   | Ct    | 190/190 (100%)     | 150 (79%)   | 40 (21%)   | 1           | 9  |
| 3   | Cu    | 190/190 (100%)     | 150 (79%)   | 40 (21%)   | 1           | 9  |
| 3   | Cv    | 190/190 (100%)     | 150 (79%)   | 40 (21%)   | 1           | 9  |
| 3   | Cw    | 190/190 (100%)     | 150 (79%)   | 40 (21%)   | 1           | 9  |
| 3   | Cx    | 190/190 (100%)     | 150 (79%)   | 40 (21%)   | 1           | 9  |
| 3   | DA    | 190/190 (100%)     | 150 (79%)   | 40 (21%)   | 1           | 9  |
| 3   | DB    | 190/190 (100%)     | 150 (79%)   | 40 (21%)   | 1           | 9  |
| All | All   | 34440/34440 (100%) | 29037 (84%) | 5403 (16%) | 7           | 21 |

All (5403) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 4   | VAL  |
| 1   | AA    | 28  | THR  |
| 1   | AA    | 36  | ARG  |
| 1   | AA    | 39  | ASP  |
| 1   | AA    | 40  | VAL  |
| 1   | AA    | 42  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 45  | LEU  |
| 1   | AA    | 49  | THR  |
| 1   | AA    | 62  | SER  |
| 1   | AA    | 71  | LEU  |
| 1   | AA    | 113 | THR  |
| 1   | AA    | 120 | GLN  |
| 1   | AA    | 150 | ARG  |
| 1   | AA    | 158 | VAL  |
| 1   | AA    | 163 | MET  |
| 1   | AA    | 166 | VAL  |
| 1   | AA    | 187 | LEU  |
| 1   | AA    | 196 | LEU  |
| 1   | AA    | 198 | THR  |
| 1   | AA    | 203 | ASP  |
| 1   | AA    | 209 | LEU  |
| 1   | AA    | 226 | PRO  |
| 1   | AA    | 237 | HIS  |
| 1   | AA    | 246 | GLN  |
| 1   | AB    | 4   | VAL  |
| 1   | AB    | 28  | THR  |
| 1   | AB    | 36  | ARG  |
| 1   | AB    | 39  | ASP  |
| 1   | AB    | 40  | VAL  |
| 1   | AB    | 42  | THR  |
| 1   | AB    | 45  | LEU  |
| 1   | AB    | 49  | THR  |
| 1   | AB    | 62  | SER  |
| 1   | AB    | 71  | LEU  |
| 1   | AB    | 113 | THR  |
| 1   | AB    | 120 | GLN  |
| 1   | AB    | 150 | ARG  |
| 1   | AB    | 158 | VAL  |
| 1   | AB    | 163 | MET  |
| 1   | AB    | 166 | VAL  |
| 1   | AB    | 187 | LEU  |
| 1   | AB    | 196 | LEU  |
| 1   | AB    | 198 | THR  |
| 1   | AB    | 203 | ASP  |
| 1   | AB    | 209 | LEU  |
| 1   | AB    | 226 | PRO  |
| 1   | AB    | 237 | HIS  |
| 1   | AB    | 246 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AC    | 4   | VAL  |
| 1   | AC    | 28  | THR  |
| 1   | AC    | 36  | ARG  |
| 1   | AC    | 39  | ASP  |
| 1   | AC    | 40  | VAL  |
| 1   | AC    | 42  | THR  |
| 1   | AC    | 45  | LEU  |
| 1   | AC    | 49  | THR  |
| 1   | AC    | 62  | SER  |
| 1   | AC    | 71  | LEU  |
| 1   | AC    | 113 | THR  |
| 1   | AC    | 120 | GLN  |
| 1   | AC    | 150 | ARG  |
| 1   | AC    | 158 | VAL  |
| 1   | AC    | 163 | MET  |
| 1   | AC    | 166 | VAL  |
| 1   | AC    | 187 | LEU  |
| 1   | AC    | 196 | LEU  |
| 1   | AC    | 198 | THR  |
| 1   | AC    | 203 | ASP  |
| 1   | AC    | 209 | LEU  |
| 1   | AC    | 226 | PRO  |
| 1   | AC    | 237 | HIS  |
| 1   | AC    | 246 | GLN  |
| 1   | AD    | 4   | VAL  |
| 1   | AD    | 28  | THR  |
| 1   | AD    | 36  | ARG  |
| 1   | AD    | 39  | ASP  |
| 1   | AD    | 40  | VAL  |
| 1   | AD    | 42  | THR  |
| 1   | AD    | 45  | LEU  |
| 1   | AD    | 49  | THR  |
| 1   | AD    | 62  | SER  |
| 1   | AD    | 71  | LEU  |
| 1   | AD    | 113 | THR  |
| 1   | AD    | 120 | GLN  |
| 1   | AD    | 150 | ARG  |
| 1   | AD    | 158 | VAL  |
| 1   | AD    | 163 | MET  |
| 1   | AD    | 166 | VAL  |
| 1   | AD    | 187 | LEU  |
| 1   | AD    | 196 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AD    | 198 | THR  |
| 1   | AD    | 203 | ASP  |
| 1   | AD    | 209 | LEU  |
| 1   | AD    | 226 | PRO  |
| 1   | AD    | 237 | HIS  |
| 1   | AD    | 246 | GLN  |
| 1   | AE    | 4   | VAL  |
| 1   | AE    | 28  | THR  |
| 1   | AE    | 36  | ARG  |
| 1   | AE    | 39  | ASP  |
| 1   | AE    | 40  | VAL  |
| 1   | AE    | 42  | THR  |
| 1   | AE    | 45  | LEU  |
| 1   | AE    | 49  | THR  |
| 1   | AE    | 62  | SER  |
| 1   | AE    | 71  | LEU  |
| 1   | AE    | 113 | THR  |
| 1   | AE    | 120 | GLN  |
| 1   | AE    | 150 | ARG  |
| 1   | AE    | 158 | VAL  |
| 1   | AE    | 163 | MET  |
| 1   | AE    | 166 | VAL  |
| 1   | AE    | 187 | LEU  |
| 1   | AE    | 196 | LEU  |
| 1   | AE    | 198 | THR  |
| 1   | AE    | 203 | ASP  |
| 1   | AE    | 209 | LEU  |
| 1   | AE    | 226 | PRO  |
| 1   | AE    | 237 | HIS  |
| 1   | AE    | 246 | GLN  |
| 1   | AF    | 4   | VAL  |
| 1   | AF    | 28  | THR  |
| 1   | AF    | 36  | ARG  |
| 1   | AF    | 39  | ASP  |
| 1   | AF    | 40  | VAL  |
| 1   | AF    | 42  | THR  |
| 1   | AF    | 45  | LEU  |
| 1   | AF    | 49  | THR  |
| 1   | AF    | 62  | SER  |
| 1   | AF    | 71  | LEU  |
| 1   | AF    | 113 | THR  |
| 1   | AF    | 120 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AF    | 150 | ARG  |
| 1   | AF    | 158 | VAL  |
| 1   | AF    | 163 | MET  |
| 1   | AF    | 166 | VAL  |
| 1   | AF    | 187 | LEU  |
| 1   | AF    | 196 | LEU  |
| 1   | AF    | 198 | THR  |
| 1   | AF    | 203 | ASP  |
| 1   | AF    | 209 | LEU  |
| 1   | AF    | 226 | PRO  |
| 1   | AF    | 237 | HIS  |
| 1   | AF    | 246 | GLN  |
| 1   | AG    | 4   | VAL  |
| 1   | AG    | 28  | THR  |
| 1   | AG    | 36  | ARG  |
| 1   | AG    | 39  | ASP  |
| 1   | AG    | 40  | VAL  |
| 1   | AG    | 42  | THR  |
| 1   | AG    | 45  | LEU  |
| 1   | AG    | 49  | THR  |
| 1   | AG    | 62  | SER  |
| 1   | AG    | 71  | LEU  |
| 1   | AG    | 113 | THR  |
| 1   | AG    | 120 | GLN  |
| 1   | AG    | 150 | ARG  |
| 1   | AG    | 158 | VAL  |
| 1   | AG    | 163 | MET  |
| 1   | AG    | 166 | VAL  |
| 1   | AG    | 187 | LEU  |
| 1   | AG    | 196 | LEU  |
| 1   | AG    | 198 | THR  |
| 1   | AG    | 203 | ASP  |
| 1   | AG    | 209 | LEU  |
| 1   | AG    | 226 | PRO  |
| 1   | AG    | 237 | HIS  |
| 1   | AG    | 246 | GLN  |
| 1   | AH    | 4   | VAL  |
| 1   | AH    | 28  | THR  |
| 1   | AH    | 36  | ARG  |
| 1   | AH    | 39  | ASP  |
| 1   | AH    | 40  | VAL  |
| 1   | AH    | 42  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AH    | 45  | LEU  |
| 1   | AH    | 49  | THR  |
| 1   | AH    | 62  | SER  |
| 1   | AH    | 71  | LEU  |
| 1   | AH    | 113 | THR  |
| 1   | AH    | 120 | GLN  |
| 1   | AH    | 150 | ARG  |
| 1   | AH    | 158 | VAL  |
| 1   | AH    | 163 | MET  |
| 1   | AH    | 166 | VAL  |
| 1   | AH    | 187 | LEU  |
| 1   | AH    | 196 | LEU  |
| 1   | AH    | 198 | THR  |
| 1   | AH    | 203 | ASP  |
| 1   | AH    | 209 | LEU  |
| 1   | AH    | 226 | PRO  |
| 1   | AH    | 237 | HIS  |
| 1   | AH    | 246 | GLN  |
| 1   | AI    | 4   | VAL  |
| 1   | AI    | 28  | THR  |
| 1   | AI    | 36  | ARG  |
| 1   | AI    | 39  | ASP  |
| 1   | AI    | 40  | VAL  |
| 1   | AI    | 42  | THR  |
| 1   | AI    | 45  | LEU  |
| 1   | AI    | 49  | THR  |
| 1   | AI    | 62  | SER  |
| 1   | AI    | 71  | LEU  |
| 1   | AI    | 113 | THR  |
| 1   | AI    | 120 | GLN  |
| 1   | AI    | 150 | ARG  |
| 1   | AI    | 158 | VAL  |
| 1   | AI    | 163 | MET  |
| 1   | AI    | 166 | VAL  |
| 1   | AI    | 187 | LEU  |
| 1   | AI    | 196 | LEU  |
| 1   | AI    | 198 | THR  |
| 1   | AI    | 203 | ASP  |
| 1   | AI    | 209 | LEU  |
| 1   | AI    | 226 | PRO  |
| 1   | AI    | 237 | HIS  |
| 1   | AI    | 246 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AJ    | 4   | VAL  |
| 1   | AJ    | 28  | THR  |
| 1   | AJ    | 36  | ARG  |
| 1   | AJ    | 39  | ASP  |
| 1   | AJ    | 40  | VAL  |
| 1   | AJ    | 42  | THR  |
| 1   | AJ    | 45  | LEU  |
| 1   | AJ    | 49  | THR  |
| 1   | AJ    | 62  | SER  |
| 1   | AJ    | 71  | LEU  |
| 1   | AJ    | 113 | THR  |
| 1   | AJ    | 120 | GLN  |
| 1   | AJ    | 150 | ARG  |
| 1   | AJ    | 158 | VAL  |
| 1   | AJ    | 163 | MET  |
| 1   | AJ    | 166 | VAL  |
| 1   | AJ    | 187 | LEU  |
| 1   | AJ    | 196 | LEU  |
| 1   | AJ    | 198 | THR  |
| 1   | AJ    | 203 | ASP  |
| 1   | AJ    | 209 | LEU  |
| 1   | AJ    | 226 | PRO  |
| 1   | AJ    | 237 | HIS  |
| 1   | AJ    | 246 | GLN  |
| 1   | AK    | 4   | VAL  |
| 1   | AK    | 28  | THR  |
| 1   | AK    | 36  | ARG  |
| 1   | AK    | 39  | ASP  |
| 1   | AK    | 40  | VAL  |
| 1   | AK    | 42  | THR  |
| 1   | AK    | 45  | LEU  |
| 1   | AK    | 49  | THR  |
| 1   | AK    | 62  | SER  |
| 1   | AK    | 71  | LEU  |
| 1   | AK    | 113 | THR  |
| 1   | AK    | 120 | GLN  |
| 1   | AK    | 150 | ARG  |
| 1   | AK    | 158 | VAL  |
| 1   | AK    | 163 | MET  |
| 1   | AK    | 166 | VAL  |
| 1   | AK    | 187 | LEU  |
| 1   | AK    | 196 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AK    | 198 | THR  |
| 1   | AK    | 203 | ASP  |
| 1   | AK    | 209 | LEU  |
| 1   | AK    | 226 | PRO  |
| 1   | AK    | 237 | HIS  |
| 1   | AK    | 246 | GLN  |
| 1   | AL    | 4   | VAL  |
| 1   | AL    | 28  | THR  |
| 1   | AL    | 36  | ARG  |
| 1   | AL    | 39  | ASP  |
| 1   | AL    | 40  | VAL  |
| 1   | AL    | 42  | THR  |
| 1   | AL    | 45  | LEU  |
| 1   | AL    | 49  | THR  |
| 1   | AL    | 62  | SER  |
| 1   | AL    | 71  | LEU  |
| 1   | AL    | 113 | THR  |
| 1   | AL    | 120 | GLN  |
| 1   | AL    | 150 | ARG  |
| 1   | AL    | 158 | VAL  |
| 1   | AL    | 163 | MET  |
| 1   | AL    | 166 | VAL  |
| 1   | AL    | 187 | LEU  |
| 1   | AL    | 196 | LEU  |
| 1   | AL    | 198 | THR  |
| 1   | AL    | 203 | ASP  |
| 1   | AL    | 209 | LEU  |
| 1   | AL    | 226 | PRO  |
| 1   | AL    | 237 | HIS  |
| 1   | AL    | 246 | GLN  |
| 1   | AM    | 4   | VAL  |
| 1   | AM    | 28  | THR  |
| 1   | AM    | 36  | ARG  |
| 1   | AM    | 39  | ASP  |
| 1   | AM    | 40  | VAL  |
| 1   | AM    | 42  | THR  |
| 1   | AM    | 45  | LEU  |
| 1   | AM    | 49  | THR  |
| 1   | AM    | 62  | SER  |
| 1   | AM    | 71  | LEU  |
| 1   | AM    | 113 | THR  |
| 1   | AM    | 120 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AM    | 150 | ARG  |
| 1   | AM    | 158 | VAL  |
| 1   | AM    | 163 | MET  |
| 1   | AM    | 166 | VAL  |
| 1   | AM    | 187 | LEU  |
| 1   | AM    | 196 | LEU  |
| 1   | AM    | 198 | THR  |
| 1   | AM    | 203 | ASP  |
| 1   | AM    | 209 | LEU  |
| 1   | AM    | 226 | PRO  |
| 1   | AM    | 237 | HIS  |
| 1   | AM    | 246 | GLN  |
| 1   | AN    | 4   | VAL  |
| 1   | AN    | 28  | THR  |
| 1   | AN    | 36  | ARG  |
| 1   | AN    | 39  | ASP  |
| 1   | AN    | 40  | VAL  |
| 1   | AN    | 42  | THR  |
| 1   | AN    | 45  | LEU  |
| 1   | AN    | 49  | THR  |
| 1   | AN    | 62  | SER  |
| 1   | AN    | 71  | LEU  |
| 1   | AN    | 113 | THR  |
| 1   | AN    | 120 | GLN  |
| 1   | AN    | 150 | ARG  |
| 1   | AN    | 158 | VAL  |
| 1   | AN    | 163 | MET  |
| 1   | AN    | 166 | VAL  |
| 1   | AN    | 187 | LEU  |
| 1   | AN    | 196 | LEU  |
| 1   | AN    | 198 | THR  |
| 1   | AN    | 203 | ASP  |
| 1   | AN    | 209 | LEU  |
| 1   | AN    | 226 | PRO  |
| 1   | AN    | 237 | HIS  |
| 1   | AN    | 246 | GLN  |
| 1   | AO    | 4   | VAL  |
| 1   | AO    | 28  | THR  |
| 1   | AO    | 36  | ARG  |
| 1   | AO    | 39  | ASP  |
| 1   | AO    | 40  | VAL  |
| 1   | AO    | 42  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AO    | 45  | LEU  |
| 1   | AO    | 49  | THR  |
| 1   | AO    | 62  | SER  |
| 1   | AO    | 71  | LEU  |
| 1   | AO    | 113 | THR  |
| 1   | AO    | 120 | GLN  |
| 1   | AO    | 150 | ARG  |
| 1   | AO    | 158 | VAL  |
| 1   | AO    | 163 | MET  |
| 1   | AO    | 166 | VAL  |
| 1   | AO    | 187 | LEU  |
| 1   | AO    | 196 | LEU  |
| 1   | AO    | 198 | THR  |
| 1   | AO    | 203 | ASP  |
| 1   | AO    | 209 | LEU  |
| 1   | AO    | 226 | PRO  |
| 1   | AO    | 237 | HIS  |
| 1   | AO    | 246 | GLN  |
| 1   | AP    | 4   | VAL  |
| 1   | AP    | 28  | THR  |
| 1   | AP    | 36  | ARG  |
| 1   | AP    | 39  | ASP  |
| 1   | AP    | 40  | VAL  |
| 1   | AP    | 42  | THR  |
| 1   | AP    | 45  | LEU  |
| 1   | AP    | 49  | THR  |
| 1   | AP    | 62  | SER  |
| 1   | AP    | 71  | LEU  |
| 1   | AP    | 113 | THR  |
| 1   | AP    | 120 | GLN  |
| 1   | AP    | 150 | ARG  |
| 1   | AP    | 158 | VAL  |
| 1   | AP    | 163 | MET  |
| 1   | AP    | 166 | VAL  |
| 1   | AP    | 187 | LEU  |
| 1   | AP    | 196 | LEU  |
| 1   | AP    | 198 | THR  |
| 1   | AP    | 203 | ASP  |
| 1   | AP    | 209 | LEU  |
| 1   | AP    | 226 | PRO  |
| 1   | AP    | 237 | HIS  |
| 1   | AP    | 246 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AQ    | 4   | VAL  |
| 1   | AQ    | 28  | THR  |
| 1   | AQ    | 36  | ARG  |
| 1   | AQ    | 39  | ASP  |
| 1   | AQ    | 40  | VAL  |
| 1   | AQ    | 42  | THR  |
| 1   | AQ    | 45  | LEU  |
| 1   | AQ    | 49  | THR  |
| 1   | AQ    | 62  | SER  |
| 1   | AQ    | 71  | LEU  |
| 1   | AQ    | 113 | THR  |
| 1   | AQ    | 120 | GLN  |
| 1   | AQ    | 150 | ARG  |
| 1   | AQ    | 158 | VAL  |
| 1   | AQ    | 163 | MET  |
| 1   | AQ    | 166 | VAL  |
| 1   | AQ    | 187 | LEU  |
| 1   | AQ    | 196 | LEU  |
| 1   | AQ    | 198 | THR  |
| 1   | AQ    | 203 | ASP  |
| 1   | AQ    | 209 | LEU  |
| 1   | AQ    | 226 | PRO  |
| 1   | AQ    | 237 | HIS  |
| 1   | AQ    | 246 | GLN  |
| 1   | AR    | 4   | VAL  |
| 1   | AR    | 28  | THR  |
| 1   | AR    | 36  | ARG  |
| 1   | AR    | 39  | ASP  |
| 1   | AR    | 40  | VAL  |
| 1   | AR    | 42  | THR  |
| 1   | AR    | 45  | LEU  |
| 1   | AR    | 49  | THR  |
| 1   | AR    | 62  | SER  |
| 1   | AR    | 71  | LEU  |
| 1   | AR    | 113 | THR  |
| 1   | AR    | 120 | GLN  |
| 1   | AR    | 150 | ARG  |
| 1   | AR    | 158 | VAL  |
| 1   | AR    | 163 | MET  |
| 1   | AR    | 166 | VAL  |
| 1   | AR    | 187 | LEU  |
| 1   | AR    | 196 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AR    | 198 | THR  |
| 1   | AR    | 203 | ASP  |
| 1   | AR    | 209 | LEU  |
| 1   | AR    | 226 | PRO  |
| 1   | AR    | 237 | HIS  |
| 1   | AR    | 246 | GLN  |
| 1   | AS    | 4   | VAL  |
| 1   | AS    | 28  | THR  |
| 1   | AS    | 36  | ARG  |
| 1   | AS    | 39  | ASP  |
| 1   | AS    | 40  | VAL  |
| 1   | AS    | 42  | THR  |
| 1   | AS    | 45  | LEU  |
| 1   | AS    | 49  | THR  |
| 1   | AS    | 62  | SER  |
| 1   | AS    | 71  | LEU  |
| 1   | AS    | 113 | THR  |
| 1   | AS    | 120 | GLN  |
| 1   | AS    | 150 | ARG  |
| 1   | AS    | 158 | VAL  |
| 1   | AS    | 163 | MET  |
| 1   | AS    | 166 | VAL  |
| 1   | AS    | 187 | LEU  |
| 1   | AS    | 196 | LEU  |
| 1   | AS    | 198 | THR  |
| 1   | AS    | 203 | ASP  |
| 1   | AS    | 209 | LEU  |
| 1   | AS    | 226 | PRO  |
| 1   | AS    | 237 | HIS  |
| 1   | AS    | 246 | GLN  |
| 1   | AT    | 4   | VAL  |
| 1   | AT    | 28  | THR  |
| 1   | AT    | 36  | ARG  |
| 1   | AT    | 39  | ASP  |
| 1   | AT    | 40  | VAL  |
| 1   | AT    | 42  | THR  |
| 1   | AT    | 45  | LEU  |
| 1   | AT    | 49  | THR  |
| 1   | AT    | 62  | SER  |
| 1   | AT    | 71  | LEU  |
| 1   | AT    | 113 | THR  |
| 1   | AT    | 120 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AT    | 150 | ARG  |
| 1   | AT    | 158 | VAL  |
| 1   | AT    | 163 | MET  |
| 1   | AT    | 166 | VAL  |
| 1   | AT    | 187 | LEU  |
| 1   | AT    | 196 | LEU  |
| 1   | AT    | 198 | THR  |
| 1   | AT    | 203 | ASP  |
| 1   | AT    | 209 | LEU  |
| 1   | AT    | 226 | PRO  |
| 1   | AT    | 237 | HIS  |
| 1   | AT    | 246 | GLN  |
| 1   | AU    | 4   | VAL  |
| 1   | AU    | 28  | THR  |
| 1   | AU    | 36  | ARG  |
| 1   | AU    | 39  | ASP  |
| 1   | AU    | 40  | VAL  |
| 1   | AU    | 42  | THR  |
| 1   | AU    | 45  | LEU  |
| 1   | AU    | 49  | THR  |
| 1   | AU    | 62  | SER  |
| 1   | AU    | 71  | LEU  |
| 1   | AU    | 113 | THR  |
| 1   | AU    | 120 | GLN  |
| 1   | AU    | 150 | ARG  |
| 1   | AU    | 158 | VAL  |
| 1   | AU    | 163 | MET  |
| 1   | AU    | 166 | VAL  |
| 1   | AU    | 187 | LEU  |
| 1   | AU    | 196 | LEU  |
| 1   | AU    | 198 | THR  |
| 1   | AU    | 203 | ASP  |
| 1   | AU    | 209 | LEU  |
| 1   | AU    | 226 | PRO  |
| 1   | AU    | 237 | HIS  |
| 1   | AU    | 246 | GLN  |
| 1   | AV    | 4   | VAL  |
| 1   | AV    | 28  | THR  |
| 1   | AV    | 36  | ARG  |
| 1   | AV    | 39  | ASP  |
| 1   | AV    | 40  | VAL  |
| 1   | AV    | 42  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AV    | 45  | LEU  |
| 1   | AV    | 49  | THR  |
| 1   | AV    | 62  | SER  |
| 1   | AV    | 71  | LEU  |
| 1   | AV    | 113 | THR  |
| 1   | AV    | 120 | GLN  |
| 1   | AV    | 150 | ARG  |
| 1   | AV    | 158 | VAL  |
| 1   | AV    | 163 | MET  |
| 1   | AV    | 166 | VAL  |
| 1   | AV    | 187 | LEU  |
| 1   | AV    | 196 | LEU  |
| 1   | AV    | 198 | THR  |
| 1   | AV    | 203 | ASP  |
| 1   | AV    | 209 | LEU  |
| 1   | AV    | 226 | PRO  |
| 1   | AV    | 237 | HIS  |
| 1   | AV    | 246 | GLN  |
| 1   | AW    | 4   | VAL  |
| 1   | AW    | 28  | THR  |
| 1   | AW    | 36  | ARG  |
| 1   | AW    | 39  | ASP  |
| 1   | AW    | 40  | VAL  |
| 1   | AW    | 42  | THR  |
| 1   | AW    | 45  | LEU  |
| 1   | AW    | 49  | THR  |
| 1   | AW    | 62  | SER  |
| 1   | AW    | 71  | LEU  |
| 1   | AW    | 113 | THR  |
| 1   | AW    | 120 | GLN  |
| 1   | AW    | 150 | ARG  |
| 1   | AW    | 158 | VAL  |
| 1   | AW    | 163 | MET  |
| 1   | AW    | 166 | VAL  |
| 1   | AW    | 187 | LEU  |
| 1   | AW    | 196 | LEU  |
| 1   | AW    | 198 | THR  |
| 1   | AW    | 203 | ASP  |
| 1   | AW    | 209 | LEU  |
| 1   | AW    | 223 | PRO  |
| 1   | AW    | 226 | PRO  |
| 1   | AW    | 237 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AW    | 246 | GLN  |
| 1   | AX    | 4   | VAL  |
| 1   | AX    | 28  | THR  |
| 1   | AX    | 36  | ARG  |
| 1   | AX    | 39  | ASP  |
| 1   | AX    | 40  | VAL  |
| 1   | AX    | 42  | THR  |
| 1   | AX    | 45  | LEU  |
| 1   | AX    | 49  | THR  |
| 1   | AX    | 62  | SER  |
| 1   | AX    | 71  | LEU  |
| 1   | AX    | 113 | THR  |
| 1   | AX    | 120 | GLN  |
| 1   | AX    | 150 | ARG  |
| 1   | AX    | 158 | VAL  |
| 1   | AX    | 163 | MET  |
| 1   | AX    | 166 | VAL  |
| 1   | AX    | 187 | LEU  |
| 1   | AX    | 196 | LEU  |
| 1   | AX    | 198 | THR  |
| 1   | AX    | 203 | ASP  |
| 1   | AX    | 209 | LEU  |
| 1   | AX    | 226 | PRO  |
| 1   | AX    | 237 | HIS  |
| 1   | AX    | 246 | GLN  |
| 1   | AY    | 4   | VAL  |
| 1   | AY    | 28  | THR  |
| 1   | AY    | 36  | ARG  |
| 1   | AY    | 39  | ASP  |
| 1   | AY    | 40  | VAL  |
| 1   | AY    | 42  | THR  |
| 1   | AY    | 45  | LEU  |
| 1   | AY    | 49  | THR  |
| 1   | AY    | 62  | SER  |
| 1   | AY    | 71  | LEU  |
| 1   | AY    | 113 | THR  |
| 1   | AY    | 120 | GLN  |
| 1   | AY    | 150 | ARG  |
| 1   | AY    | 158 | VAL  |
| 1   | AY    | 163 | MET  |
| 1   | AY    | 166 | VAL  |
| 1   | AY    | 187 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AY    | 196 | LEU  |
| 1   | AY    | 198 | THR  |
| 1   | AY    | 203 | ASP  |
| 1   | AY    | 209 | LEU  |
| 1   | AY    | 226 | PRO  |
| 1   | AY    | 237 | HIS  |
| 1   | AY    | 246 | GLN  |
| 1   | AZ    | 4   | VAL  |
| 1   | AZ    | 28  | THR  |
| 1   | AZ    | 36  | ARG  |
| 1   | AZ    | 39  | ASP  |
| 1   | AZ    | 40  | VAL  |
| 1   | AZ    | 42  | THR  |
| 1   | AZ    | 45  | LEU  |
| 1   | AZ    | 49  | THR  |
| 1   | AZ    | 62  | SER  |
| 1   | AZ    | 71  | LEU  |
| 1   | AZ    | 113 | THR  |
| 1   | AZ    | 120 | GLN  |
| 1   | AZ    | 150 | ARG  |
| 1   | AZ    | 158 | VAL  |
| 1   | AZ    | 163 | MET  |
| 1   | AZ    | 166 | VAL  |
| 1   | AZ    | 187 | LEU  |
| 1   | AZ    | 196 | LEU  |
| 1   | AZ    | 198 | THR  |
| 1   | AZ    | 203 | ASP  |
| 1   | AZ    | 209 | LEU  |
| 1   | AZ    | 226 | PRO  |
| 1   | AZ    | 237 | HIS  |
| 1   | AZ    | 246 | GLN  |
| 1   | A0    | 4   | VAL  |
| 1   | A0    | 28  | THR  |
| 1   | A0    | 36  | ARG  |
| 1   | A0    | 39  | ASP  |
| 1   | A0    | 40  | VAL  |
| 1   | A0    | 42  | THR  |
| 1   | A0    | 45  | LEU  |
| 1   | A0    | 49  | THR  |
| 1   | A0    | 62  | SER  |
| 1   | A0    | 71  | LEU  |
| 1   | A0    | 113 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A0    | 120 | GLN  |
| 1   | A0    | 150 | ARG  |
| 1   | A0    | 158 | VAL  |
| 1   | A0    | 163 | MET  |
| 1   | A0    | 166 | VAL  |
| 1   | A0    | 187 | LEU  |
| 1   | A0    | 196 | LEU  |
| 1   | A0    | 198 | THR  |
| 1   | A0    | 203 | ASP  |
| 1   | A0    | 209 | LEU  |
| 1   | A0    | 226 | PRO  |
| 1   | A0    | 237 | HIS  |
| 1   | A0    | 246 | GLN  |
| 1   | A1    | 4   | VAL  |
| 1   | A1    | 28  | THR  |
| 1   | A1    | 36  | ARG  |
| 1   | A1    | 39  | ASP  |
| 1   | A1    | 40  | VAL  |
| 1   | A1    | 42  | THR  |
| 1   | A1    | 45  | LEU  |
| 1   | A1    | 49  | THR  |
| 1   | A1    | 62  | SER  |
| 1   | A1    | 71  | LEU  |
| 1   | A1    | 113 | THR  |
| 1   | A1    | 120 | GLN  |
| 1   | A1    | 150 | ARG  |
| 1   | A1    | 158 | VAL  |
| 1   | A1    | 163 | MET  |
| 1   | A1    | 166 | VAL  |
| 1   | A1    | 187 | LEU  |
| 1   | A1    | 196 | LEU  |
| 1   | A1    | 198 | THR  |
| 1   | A1    | 203 | ASP  |
| 1   | A1    | 209 | LEU  |
| 1   | A1    | 226 | PRO  |
| 1   | A1    | 237 | HIS  |
| 1   | A1    | 246 | GLN  |
| 1   | A2    | 4   | VAL  |
| 1   | A2    | 28  | THR  |
| 1   | A2    | 36  | ARG  |
| 1   | A2    | 39  | ASP  |
| 1   | A2    | 40  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A2    | 42  | THR  |
| 1   | A2    | 45  | LEU  |
| 1   | A2    | 49  | THR  |
| 1   | A2    | 62  | SER  |
| 1   | A2    | 71  | LEU  |
| 1   | A2    | 113 | THR  |
| 1   | A2    | 120 | GLN  |
| 1   | A2    | 150 | ARG  |
| 1   | A2    | 158 | VAL  |
| 1   | A2    | 163 | MET  |
| 1   | A2    | 166 | VAL  |
| 1   | A2    | 187 | LEU  |
| 1   | A2    | 196 | LEU  |
| 1   | A2    | 198 | THR  |
| 1   | A2    | 203 | ASP  |
| 1   | A2    | 209 | LEU  |
| 1   | A2    | 226 | PRO  |
| 1   | A2    | 237 | HIS  |
| 1   | A2    | 246 | GLN  |
| 1   | A3    | 4   | VAL  |
| 1   | A3    | 28  | THR  |
| 1   | A3    | 36  | ARG  |
| 1   | A3    | 39  | ASP  |
| 1   | A3    | 40  | VAL  |
| 1   | A3    | 42  | THR  |
| 1   | A3    | 45  | LEU  |
| 1   | A3    | 49  | THR  |
| 1   | A3    | 62  | SER  |
| 1   | A3    | 71  | LEU  |
| 1   | A3    | 113 | THR  |
| 1   | A3    | 120 | GLN  |
| 1   | A3    | 150 | ARG  |
| 1   | A3    | 158 | VAL  |
| 1   | A3    | 163 | MET  |
| 1   | A3    | 166 | VAL  |
| 1   | A3    | 187 | LEU  |
| 1   | A3    | 196 | LEU  |
| 1   | A3    | 198 | THR  |
| 1   | A3    | 203 | ASP  |
| 1   | A3    | 209 | LEU  |
| 1   | A3    | 226 | PRO  |
| 1   | A3    | 237 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A3    | 246 | GLN  |
| 1   | A4    | 4   | VAL  |
| 1   | A4    | 28  | THR  |
| 1   | A4    | 36  | ARG  |
| 1   | A4    | 39  | ASP  |
| 1   | A4    | 40  | VAL  |
| 1   | A4    | 42  | THR  |
| 1   | A4    | 45  | LEU  |
| 1   | A4    | 49  | THR  |
| 1   | A4    | 62  | SER  |
| 1   | A4    | 71  | LEU  |
| 1   | A4    | 113 | THR  |
| 1   | A4    | 120 | GLN  |
| 1   | A4    | 150 | ARG  |
| 1   | A4    | 158 | VAL  |
| 1   | A4    | 163 | MET  |
| 1   | A4    | 166 | VAL  |
| 1   | A4    | 187 | LEU  |
| 1   | A4    | 196 | LEU  |
| 1   | A4    | 198 | THR  |
| 1   | A4    | 203 | ASP  |
| 1   | A4    | 209 | LEU  |
| 1   | A4    | 226 | PRO  |
| 1   | A4    | 237 | HIS  |
| 1   | A4    | 246 | GLN  |
| 1   | A5    | 4   | VAL  |
| 1   | A5    | 28  | THR  |
| 1   | A5    | 36  | ARG  |
| 1   | A5    | 39  | ASP  |
| 1   | A5    | 40  | VAL  |
| 1   | A5    | 42  | THR  |
| 1   | A5    | 45  | LEU  |
| 1   | A5    | 49  | THR  |
| 1   | A5    | 62  | SER  |
| 1   | A5    | 71  | LEU  |
| 1   | A5    | 113 | THR  |
| 1   | A5    | 120 | GLN  |
| 1   | A5    | 150 | ARG  |
| 1   | A5    | 158 | VAL  |
| 1   | A5    | 163 | MET  |
| 1   | A5    | 166 | VAL  |
| 1   | A5    | 187 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A5    | 196 | LEU  |
| 1   | A5    | 198 | THR  |
| 1   | A5    | 203 | ASP  |
| 1   | A5    | 209 | LEU  |
| 1   | A5    | 226 | PRO  |
| 1   | A5    | 237 | HIS  |
| 1   | A5    | 246 | GLN  |
| 1   | A6    | 4   | VAL  |
| 1   | A6    | 28  | THR  |
| 1   | A6    | 36  | ARG  |
| 1   | A6    | 39  | ASP  |
| 1   | A6    | 40  | VAL  |
| 1   | A6    | 42  | THR  |
| 1   | A6    | 45  | LEU  |
| 1   | A6    | 49  | THR  |
| 1   | A6    | 62  | SER  |
| 1   | A6    | 71  | LEU  |
| 1   | A6    | 113 | THR  |
| 1   | A6    | 120 | GLN  |
| 1   | A6    | 150 | ARG  |
| 1   | A6    | 158 | VAL  |
| 1   | A6    | 163 | MET  |
| 1   | A6    | 166 | VAL  |
| 1   | A6    | 187 | LEU  |
| 1   | A6    | 196 | LEU  |
| 1   | A6    | 198 | THR  |
| 1   | A6    | 203 | ASP  |
| 1   | A6    | 209 | LEU  |
| 1   | A6    | 226 | PRO  |
| 1   | A6    | 237 | HIS  |
| 1   | A6    | 246 | GLN  |
| 1   | A7    | 4   | VAL  |
| 1   | A7    | 28  | THR  |
| 1   | A7    | 36  | ARG  |
| 1   | A7    | 39  | ASP  |
| 1   | A7    | 40  | VAL  |
| 1   | A7    | 42  | THR  |
| 1   | A7    | 45  | LEU  |
| 1   | A7    | 49  | THR  |
| 1   | A7    | 62  | SER  |
| 1   | A7    | 71  | LEU  |
| 1   | A7    | 113 | THR  |

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*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A7    | 120 | GLN  |
| 1   | A7    | 150 | ARG  |
| 1   | A7    | 158 | VAL  |
| 1   | A7    | 163 | MET  |
| 1   | A7    | 166 | VAL  |
| 1   | A7    | 187 | LEU  |
| 1   | A7    | 196 | LEU  |
| 1   | A7    | 198 | THR  |
| 1   | A7    | 203 | ASP  |
| 1   | A7    | 209 | LEU  |
| 1   | A7    | 226 | PRO  |
| 1   | A7    | 237 | HIS  |
| 1   | A7    | 246 | GLN  |
| 1   | A8    | 4   | VAL  |
| 1   | A8    | 28  | THR  |
| 1   | A8    | 36  | ARG  |
| 1   | A8    | 39  | ASP  |
| 1   | A8    | 40  | VAL  |
| 1   | A8    | 42  | THR  |
| 1   | A8    | 45  | LEU  |
| 1   | A8    | 49  | THR  |
| 1   | A8    | 62  | SER  |
| 1   | A8    | 71  | LEU  |
| 1   | A8    | 113 | THR  |
| 1   | A8    | 120 | GLN  |
| 1   | A8    | 150 | ARG  |
| 1   | A8    | 158 | VAL  |
| 1   | A8    | 163 | MET  |
| 1   | A8    | 166 | VAL  |
| 1   | A8    | 187 | LEU  |
| 1   | A8    | 196 | LEU  |
| 1   | A8    | 198 | THR  |
| 1   | A8    | 203 | ASP  |
| 1   | A8    | 209 | LEU  |
| 1   | A8    | 226 | PRO  |
| 1   | A8    | 237 | HIS  |
| 1   | A8    | 246 | GLN  |
| 1   | A9    | 4   | VAL  |
| 1   | A9    | 28  | THR  |
| 1   | A9    | 36  | ARG  |
| 1   | A9    | 39  | ASP  |
| 1   | A9    | 40  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A9    | 42  | THR  |
| 1   | A9    | 45  | LEU  |
| 1   | A9    | 49  | THR  |
| 1   | A9    | 62  | SER  |
| 1   | A9    | 71  | LEU  |
| 1   | A9    | 113 | THR  |
| 1   | A9    | 120 | GLN  |
| 1   | A9    | 150 | ARG  |
| 1   | A9    | 158 | VAL  |
| 1   | A9    | 163 | MET  |
| 1   | A9    | 166 | VAL  |
| 1   | A9    | 187 | LEU  |
| 1   | A9    | 196 | LEU  |
| 1   | A9    | 198 | THR  |
| 1   | A9    | 203 | ASP  |
| 1   | A9    | 209 | LEU  |
| 1   | A9    | 226 | PRO  |
| 1   | A9    | 237 | HIS  |
| 1   | A9    | 246 | GLN  |
| 1   | Aa    | 4   | VAL  |
| 1   | Aa    | 28  | THR  |
| 1   | Aa    | 36  | ARG  |
| 1   | Aa    | 39  | ASP  |
| 1   | Aa    | 40  | VAL  |
| 1   | Aa    | 42  | THR  |
| 1   | Aa    | 45  | LEU  |
| 1   | Aa    | 49  | THR  |
| 1   | Aa    | 62  | SER  |
| 1   | Aa    | 71  | LEU  |
| 1   | Aa    | 113 | THR  |
| 1   | Aa    | 120 | GLN  |
| 1   | Aa    | 150 | ARG  |
| 1   | Aa    | 158 | VAL  |
| 1   | Aa    | 163 | MET  |
| 1   | Aa    | 166 | VAL  |
| 1   | Aa    | 187 | LEU  |
| 1   | Aa    | 196 | LEU  |
| 1   | Aa    | 198 | THR  |
| 1   | Aa    | 203 | ASP  |
| 1   | Aa    | 209 | LEU  |
| 1   | Aa    | 226 | PRO  |
| 1   | Aa    | 237 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Aa    | 246 | GLN  |
| 1   | Ab    | 4   | VAL  |
| 1   | Ab    | 28  | THR  |
| 1   | Ab    | 36  | ARG  |
| 1   | Ab    | 39  | ASP  |
| 1   | Ab    | 40  | VAL  |
| 1   | Ab    | 42  | THR  |
| 1   | Ab    | 45  | LEU  |
| 1   | Ab    | 49  | THR  |
| 1   | Ab    | 62  | SER  |
| 1   | Ab    | 71  | LEU  |
| 1   | Ab    | 113 | THR  |
| 1   | Ab    | 120 | GLN  |
| 1   | Ab    | 150 | ARG  |
| 1   | Ab    | 158 | VAL  |
| 1   | Ab    | 163 | MET  |
| 1   | Ab    | 166 | VAL  |
| 1   | Ab    | 187 | LEU  |
| 1   | Ab    | 196 | LEU  |
| 1   | Ab    | 198 | THR  |
| 1   | Ab    | 203 | ASP  |
| 1   | Ab    | 209 | LEU  |
| 1   | Ab    | 226 | PRO  |
| 1   | Ab    | 237 | HIS  |
| 1   | Ab    | 246 | GLN  |
| 1   | Ac    | 4   | VAL  |
| 1   | Ac    | 28  | THR  |
| 1   | Ac    | 36  | ARG  |
| 1   | Ac    | 39  | ASP  |
| 1   | Ac    | 40  | VAL  |
| 1   | Ac    | 42  | THR  |
| 1   | Ac    | 45  | LEU  |
| 1   | Ac    | 49  | THR  |
| 1   | Ac    | 62  | SER  |
| 1   | Ac    | 71  | LEU  |
| 1   | Ac    | 113 | THR  |
| 1   | Ac    | 120 | GLN  |
| 1   | Ac    | 150 | ARG  |
| 1   | Ac    | 158 | VAL  |
| 1   | Ac    | 163 | MET  |
| 1   | Ac    | 166 | VAL  |
| 1   | Ac    | 187 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Ac    | 196 | LEU  |
| 1   | Ac    | 198 | THR  |
| 1   | Ac    | 203 | ASP  |
| 1   | Ac    | 209 | LEU  |
| 1   | Ac    | 226 | PRO  |
| 1   | Ac    | 237 | HIS  |
| 1   | Ac    | 246 | GLN  |
| 1   | Ad    | 4   | VAL  |
| 1   | Ad    | 28  | THR  |
| 1   | Ad    | 36  | ARG  |
| 1   | Ad    | 39  | ASP  |
| 1   | Ad    | 40  | VAL  |
| 1   | Ad    | 42  | THR  |
| 1   | Ad    | 45  | LEU  |
| 1   | Ad    | 49  | THR  |
| 1   | Ad    | 62  | SER  |
| 1   | Ad    | 71  | LEU  |
| 1   | Ad    | 113 | THR  |
| 1   | Ad    | 120 | GLN  |
| 1   | Ad    | 150 | ARG  |
| 1   | Ad    | 158 | VAL  |
| 1   | Ad    | 163 | MET  |
| 1   | Ad    | 166 | VAL  |
| 1   | Ad    | 187 | LEU  |
| 1   | Ad    | 196 | LEU  |
| 1   | Ad    | 198 | THR  |
| 1   | Ad    | 203 | ASP  |
| 1   | Ad    | 209 | LEU  |
| 1   | Ad    | 226 | PRO  |
| 1   | Ad    | 237 | HIS  |
| 1   | Ad    | 246 | GLN  |
| 1   | Ae    | 4   | VAL  |
| 1   | Ae    | 28  | THR  |
| 1   | Ae    | 36  | ARG  |
| 1   | Ae    | 39  | ASP  |
| 1   | Ae    | 40  | VAL  |
| 1   | Ae    | 42  | THR  |
| 1   | Ae    | 45  | LEU  |
| 1   | Ae    | 49  | THR  |
| 1   | Ae    | 62  | SER  |
| 1   | Ae    | 71  | LEU  |
| 1   | Ae    | 113 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Ae    | 120 | GLN  |
| 1   | Ae    | 150 | ARG  |
| 1   | Ae    | 158 | VAL  |
| 1   | Ae    | 163 | MET  |
| 1   | Ae    | 166 | VAL  |
| 1   | Ae    | 187 | LEU  |
| 1   | Ae    | 196 | LEU  |
| 1   | Ae    | 198 | THR  |
| 1   | Ae    | 203 | ASP  |
| 1   | Ae    | 209 | LEU  |
| 1   | Ae    | 223 | PRO  |
| 1   | Ae    | 226 | PRO  |
| 1   | Ae    | 237 | HIS  |
| 1   | Ae    | 246 | GLN  |
| 1   | Af    | 4   | VAL  |
| 1   | Af    | 28  | THR  |
| 1   | Af    | 36  | ARG  |
| 1   | Af    | 39  | ASP  |
| 1   | Af    | 40  | VAL  |
| 1   | Af    | 42  | THR  |
| 1   | Af    | 45  | LEU  |
| 1   | Af    | 49  | THR  |
| 1   | Af    | 62  | SER  |
| 1   | Af    | 71  | LEU  |
| 1   | Af    | 113 | THR  |
| 1   | Af    | 120 | GLN  |
| 1   | Af    | 150 | ARG  |
| 1   | Af    | 158 | VAL  |
| 1   | Af    | 163 | MET  |
| 1   | Af    | 166 | VAL  |
| 1   | Af    | 187 | LEU  |
| 1   | Af    | 196 | LEU  |
| 1   | Af    | 198 | THR  |
| 1   | Af    | 203 | ASP  |
| 1   | Af    | 209 | LEU  |
| 1   | Af    | 226 | PRO  |
| 1   | Af    | 237 | HIS  |
| 1   | Af    | 246 | GLN  |
| 1   | Ag    | 4   | VAL  |
| 1   | Ag    | 28  | THR  |
| 1   | Ag    | 36  | ARG  |
| 1   | Ag    | 39  | ASP  |

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*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Ag    | 40  | VAL  |
| 1   | Ag    | 42  | THR  |
| 1   | Ag    | 45  | LEU  |
| 1   | Ag    | 49  | THR  |
| 1   | Ag    | 62  | SER  |
| 1   | Ag    | 71  | LEU  |
| 1   | Ag    | 113 | THR  |
| 1   | Ag    | 120 | GLN  |
| 1   | Ag    | 150 | ARG  |
| 1   | Ag    | 158 | VAL  |
| 1   | Ag    | 163 | MET  |
| 1   | Ag    | 166 | VAL  |
| 1   | Ag    | 187 | LEU  |
| 1   | Ag    | 196 | LEU  |
| 1   | Ag    | 198 | THR  |
| 1   | Ag    | 203 | ASP  |
| 1   | Ag    | 209 | LEU  |
| 1   | Ag    | 226 | PRO  |
| 1   | Ag    | 237 | HIS  |
| 1   | Ag    | 246 | GLN  |
| 1   | Ah    | 4   | VAL  |
| 1   | Ah    | 28  | THR  |
| 1   | Ah    | 36  | ARG  |
| 1   | Ah    | 39  | ASP  |
| 1   | Ah    | 40  | VAL  |
| 1   | Ah    | 42  | THR  |
| 1   | Ah    | 45  | LEU  |
| 1   | Ah    | 49  | THR  |
| 1   | Ah    | 62  | SER  |
| 1   | Ah    | 71  | LEU  |
| 1   | Ah    | 113 | THR  |
| 1   | Ah    | 120 | GLN  |
| 1   | Ah    | 150 | ARG  |
| 1   | Ah    | 158 | VAL  |
| 1   | Ah    | 163 | MET  |
| 1   | Ah    | 166 | VAL  |
| 1   | Ah    | 187 | LEU  |
| 1   | Ah    | 196 | LEU  |
| 1   | Ah    | 198 | THR  |
| 1   | Ah    | 203 | ASP  |
| 1   | Ah    | 209 | LEU  |
| 1   | Ah    | 226 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Ah    | 237 | HIS  |
| 1   | Ah    | 246 | GLN  |
| 1   | Ai    | 4   | VAL  |
| 1   | Ai    | 28  | THR  |
| 1   | Ai    | 36  | ARG  |
| 1   | Ai    | 39  | ASP  |
| 1   | Ai    | 40  | VAL  |
| 1   | Ai    | 42  | THR  |
| 1   | Ai    | 45  | LEU  |
| 1   | Ai    | 49  | THR  |
| 1   | Ai    | 62  | SER  |
| 1   | Ai    | 71  | LEU  |
| 1   | Ai    | 113 | THR  |
| 1   | Ai    | 120 | GLN  |
| 1   | Ai    | 150 | ARG  |
| 1   | Ai    | 158 | VAL  |
| 1   | Ai    | 163 | MET  |
| 1   | Ai    | 166 | VAL  |
| 1   | Ai    | 187 | LEU  |
| 1   | Ai    | 196 | LEU  |
| 1   | Ai    | 198 | THR  |
| 1   | Ai    | 203 | ASP  |
| 1   | Ai    | 209 | LEU  |
| 1   | Ai    | 226 | PRO  |
| 1   | Ai    | 237 | HIS  |
| 1   | Ai    | 246 | GLN  |
| 1   | Aj    | 4   | VAL  |
| 1   | Aj    | 28  | THR  |
| 1   | Aj    | 36  | ARG  |
| 1   | Aj    | 39  | ASP  |
| 1   | Aj    | 40  | VAL  |
| 1   | Aj    | 42  | THR  |
| 1   | Aj    | 45  | LEU  |
| 1   | Aj    | 49  | THR  |
| 1   | Aj    | 62  | SER  |
| 1   | Aj    | 71  | LEU  |
| 1   | Aj    | 113 | THR  |
| 1   | Aj    | 120 | GLN  |
| 1   | Aj    | 150 | ARG  |
| 1   | Aj    | 158 | VAL  |
| 1   | Aj    | 163 | MET  |
| 1   | Aj    | 166 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Aj    | 187 | LEU  |
| 1   | Aj    | 196 | LEU  |
| 1   | Aj    | 198 | THR  |
| 1   | Aj    | 203 | ASP  |
| 1   | Aj    | 209 | LEU  |
| 1   | Aj    | 226 | PRO  |
| 1   | Aj    | 237 | HIS  |
| 1   | Aj    | 246 | GLN  |
| 1   | Ak    | 4   | VAL  |
| 1   | Ak    | 28  | THR  |
| 1   | Ak    | 36  | ARG  |
| 1   | Ak    | 39  | ASP  |
| 1   | Ak    | 40  | VAL  |
| 1   | Ak    | 42  | THR  |
| 1   | Ak    | 45  | LEU  |
| 1   | Ak    | 49  | THR  |
| 1   | Ak    | 62  | SER  |
| 1   | Ak    | 71  | LEU  |
| 1   | Ak    | 113 | THR  |
| 1   | Ak    | 120 | GLN  |
| 1   | Ak    | 150 | ARG  |
| 1   | Ak    | 158 | VAL  |
| 1   | Ak    | 163 | MET  |
| 1   | Ak    | 166 | VAL  |
| 1   | Ak    | 187 | LEU  |
| 1   | Ak    | 196 | LEU  |
| 1   | Ak    | 198 | THR  |
| 1   | Ak    | 203 | ASP  |
| 1   | Ak    | 209 | LEU  |
| 1   | Ak    | 226 | PRO  |
| 1   | Ak    | 237 | HIS  |
| 1   | Ak    | 246 | GLN  |
| 1   | Al    | 4   | VAL  |
| 1   | Al    | 28  | THR  |
| 1   | Al    | 36  | ARG  |
| 1   | Al    | 39  | ASP  |
| 1   | Al    | 40  | VAL  |
| 1   | Al    | 42  | THR  |
| 1   | Al    | 45  | LEU  |
| 1   | Al    | 49  | THR  |
| 1   | Al    | 62  | SER  |
| 1   | Al    | 71  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Al    | 113 | THR  |
| 1   | Al    | 120 | GLN  |
| 1   | Al    | 150 | ARG  |
| 1   | Al    | 158 | VAL  |
| 1   | Al    | 163 | MET  |
| 1   | Al    | 166 | VAL  |
| 1   | Al    | 187 | LEU  |
| 1   | Al    | 196 | LEU  |
| 1   | Al    | 198 | THR  |
| 1   | Al    | 203 | ASP  |
| 1   | Al    | 209 | LEU  |
| 1   | Al    | 226 | PRO  |
| 1   | Al    | 237 | HIS  |
| 1   | Al    | 246 | GLN  |
| 1   | Am    | 4   | VAL  |
| 1   | Am    | 28  | THR  |
| 1   | Am    | 36  | ARG  |
| 1   | Am    | 39  | ASP  |
| 1   | Am    | 40  | VAL  |
| 1   | Am    | 42  | THR  |
| 1   | Am    | 45  | LEU  |
| 1   | Am    | 49  | THR  |
| 1   | Am    | 62  | SER  |
| 1   | Am    | 71  | LEU  |
| 1   | Am    | 113 | THR  |
| 1   | Am    | 120 | GLN  |
| 1   | Am    | 150 | ARG  |
| 1   | Am    | 158 | VAL  |
| 1   | Am    | 163 | MET  |
| 1   | Am    | 166 | VAL  |
| 1   | Am    | 187 | LEU  |
| 1   | Am    | 196 | LEU  |
| 1   | Am    | 198 | THR  |
| 1   | Am    | 203 | ASP  |
| 1   | Am    | 209 | LEU  |
| 1   | Am    | 226 | PRO  |
| 1   | Am    | 237 | HIS  |
| 1   | Am    | 246 | GLN  |
| 1   | An    | 4   | VAL  |
| 1   | An    | 28  | THR  |
| 1   | An    | 36  | ARG  |
| 1   | An    | 39  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | An    | 40  | VAL  |
| 1   | An    | 42  | THR  |
| 1   | An    | 45  | LEU  |
| 1   | An    | 49  | THR  |
| 1   | An    | 62  | SER  |
| 1   | An    | 71  | LEU  |
| 1   | An    | 113 | THR  |
| 1   | An    | 120 | GLN  |
| 1   | An    | 150 | ARG  |
| 1   | An    | 158 | VAL  |
| 1   | An    | 163 | MET  |
| 1   | An    | 166 | VAL  |
| 1   | An    | 187 | LEU  |
| 1   | An    | 196 | LEU  |
| 1   | An    | 198 | THR  |
| 1   | An    | 203 | ASP  |
| 1   | An    | 209 | LEU  |
| 1   | An    | 226 | PRO  |
| 1   | An    | 237 | HIS  |
| 1   | An    | 246 | GLN  |
| 1   | Ao    | 4   | VAL  |
| 1   | Ao    | 28  | THR  |
| 1   | Ao    | 36  | ARG  |
| 1   | Ao    | 39  | ASP  |
| 1   | Ao    | 40  | VAL  |
| 1   | Ao    | 42  | THR  |
| 1   | Ao    | 45  | LEU  |
| 1   | Ao    | 49  | THR  |
| 1   | Ao    | 62  | SER  |
| 1   | Ao    | 71  | LEU  |
| 1   | Ao    | 113 | THR  |
| 1   | Ao    | 120 | GLN  |
| 1   | Ao    | 150 | ARG  |
| 1   | Ao    | 158 | VAL  |
| 1   | Ao    | 163 | MET  |
| 1   | Ao    | 166 | VAL  |
| 1   | Ao    | 187 | LEU  |
| 1   | Ao    | 196 | LEU  |
| 1   | Ao    | 198 | THR  |
| 1   | Ao    | 203 | ASP  |
| 1   | Ao    | 209 | LEU  |
| 1   | Ao    | 226 | PRO  |

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*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Ao    | 237 | HIS  |
| 1   | Ao    | 246 | GLN  |
| 2   | BA    | 45  | SER  |
| 2   | BA    | 49  | ASP  |
| 2   | BA    | 53  | ARG  |
| 2   | BA    | 58  | LEU  |
| 2   | BA    | 70  | PRO  |
| 2   | BA    | 73  | GLN  |
| 2   | BA    | 86  | ASP  |
| 2   | BA    | 88  | LEU  |
| 2   | BA    | 93  | SER  |
| 2   | BA    | 110 | VAL  |
| 2   | BA    | 114 | VAL  |
| 2   | BA    | 126 | VAL  |
| 2   | BA    | 135 | THR  |
| 2   | BA    | 136 | HIS  |
| 2   | BA    | 145 | LEU  |
| 2   | BA    | 146 | GLU  |
| 2   | BA    | 156 | SER  |
| 2   | BA    | 157 | VAL  |
| 2   | BA    | 161 | GLN  |
| 2   | BA    | 166 | ARG  |
| 2   | BA    | 167 | THR  |
| 2   | BA    | 168 | ASN  |
| 2   | BA    | 193 | THR  |
| 2   | BA    | 194 | ILE  |
| 2   | BA    | 197 | LEU  |
| 2   | BA    | 212 | THR  |
| 2   | BB    | 45  | SER  |
| 2   | BB    | 49  | ASP  |
| 2   | BB    | 53  | ARG  |
| 2   | BB    | 58  | LEU  |
| 2   | BB    | 70  | PRO  |
| 2   | BB    | 73  | GLN  |
| 2   | BB    | 86  | ASP  |
| 2   | BB    | 88  | LEU  |
| 2   | BB    | 93  | SER  |
| 2   | BB    | 110 | VAL  |
| 2   | BB    | 114 | VAL  |
| 2   | BB    | 126 | VAL  |
| 2   | BB    | 135 | THR  |
| 2   | BB    | 136 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | BB    | 145 | LEU  |
| 2   | BB    | 146 | GLU  |
| 2   | BB    | 156 | SER  |
| 2   | BB    | 157 | VAL  |
| 2   | BB    | 161 | GLN  |
| 2   | BB    | 166 | ARG  |
| 2   | BB    | 167 | THR  |
| 2   | BB    | 168 | ASN  |
| 2   | BB    | 193 | THR  |
| 2   | BB    | 194 | ILE  |
| 2   | BB    | 197 | LEU  |
| 2   | BB    | 212 | THR  |
| 2   | BC    | 45  | SER  |
| 2   | BC    | 49  | ASP  |
| 2   | BC    | 53  | ARG  |
| 2   | BC    | 58  | LEU  |
| 2   | BC    | 70  | PRO  |
| 2   | BC    | 73  | GLN  |
| 2   | BC    | 86  | ASP  |
| 2   | BC    | 88  | LEU  |
| 2   | BC    | 93  | SER  |
| 2   | BC    | 110 | VAL  |
| 2   | BC    | 114 | VAL  |
| 2   | BC    | 126 | VAL  |
| 2   | BC    | 135 | THR  |
| 2   | BC    | 136 | HIS  |
| 2   | BC    | 145 | LEU  |
| 2   | BC    | 146 | GLU  |
| 2   | BC    | 156 | SER  |
| 2   | BC    | 157 | VAL  |
| 2   | BC    | 161 | GLN  |
| 2   | BC    | 166 | ARG  |
| 2   | BC    | 167 | THR  |
| 2   | BC    | 168 | ASN  |
| 2   | BC    | 193 | THR  |
| 2   | BC    | 194 | ILE  |
| 2   | BC    | 197 | LEU  |
| 2   | BC    | 212 | THR  |
| 2   | BD    | 45  | SER  |
| 2   | BD    | 49  | ASP  |
| 2   | BD    | 53  | ARG  |
| 2   | BD    | 58  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | BD    | 70  | PRO  |
| 2   | BD    | 73  | GLN  |
| 2   | BD    | 86  | ASP  |
| 2   | BD    | 88  | LEU  |
| 2   | BD    | 93  | SER  |
| 2   | BD    | 110 | VAL  |
| 2   | BD    | 114 | VAL  |
| 2   | BD    | 126 | VAL  |
| 2   | BD    | 135 | THR  |
| 2   | BD    | 136 | HIS  |
| 2   | BD    | 145 | LEU  |
| 2   | BD    | 146 | GLU  |
| 2   | BD    | 156 | SER  |
| 2   | BD    | 157 | VAL  |
| 2   | BD    | 161 | GLN  |
| 2   | BD    | 166 | ARG  |
| 2   | BD    | 167 | THR  |
| 2   | BD    | 168 | ASN  |
| 2   | BD    | 193 | THR  |
| 2   | BD    | 194 | ILE  |
| 2   | BD    | 197 | LEU  |
| 2   | BD    | 212 | THR  |
| 2   | BE    | 45  | SER  |
| 2   | BE    | 49  | ASP  |
| 2   | BE    | 53  | ARG  |
| 2   | BE    | 58  | LEU  |
| 2   | BE    | 70  | PRO  |
| 2   | BE    | 73  | GLN  |
| 2   | BE    | 86  | ASP  |
| 2   | BE    | 88  | LEU  |
| 2   | BE    | 93  | SER  |
| 2   | BE    | 110 | VAL  |
| 2   | BE    | 114 | VAL  |
| 2   | BE    | 126 | VAL  |
| 2   | BE    | 135 | THR  |
| 2   | BE    | 136 | HIS  |
| 2   | BE    | 145 | LEU  |
| 2   | BE    | 146 | GLU  |
| 2   | BE    | 156 | SER  |
| 2   | BE    | 157 | VAL  |
| 2   | BE    | 161 | GLN  |
| 2   | BE    | 166 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | BE    | 167 | THR  |
| 2   | BE    | 168 | ASN  |
| 2   | BE    | 193 | THR  |
| 2   | BE    | 194 | ILE  |
| 2   | BE    | 197 | LEU  |
| 2   | BE    | 212 | THR  |
| 2   | BF    | 45  | SER  |
| 2   | BF    | 49  | ASP  |
| 2   | BF    | 53  | ARG  |
| 2   | BF    | 58  | LEU  |
| 2   | BF    | 70  | PRO  |
| 2   | BF    | 73  | GLN  |
| 2   | BF    | 86  | ASP  |
| 2   | BF    | 88  | LEU  |
| 2   | BF    | 93  | SER  |
| 2   | BF    | 110 | VAL  |
| 2   | BF    | 114 | VAL  |
| 2   | BF    | 126 | VAL  |
| 2   | BF    | 135 | THR  |
| 2   | BF    | 136 | HIS  |
| 2   | BF    | 145 | LEU  |
| 2   | BF    | 146 | GLU  |
| 2   | BF    | 156 | SER  |
| 2   | BF    | 157 | VAL  |
| 2   | BF    | 161 | GLN  |
| 2   | BF    | 166 | ARG  |
| 2   | BF    | 167 | THR  |
| 2   | BF    | 168 | ASN  |
| 2   | BF    | 193 | THR  |
| 2   | BF    | 194 | ILE  |
| 2   | BF    | 197 | LEU  |
| 2   | BF    | 212 | THR  |
| 2   | BG    | 45  | SER  |
| 2   | BG    | 49  | ASP  |
| 2   | BG    | 53  | ARG  |
| 2   | BG    | 58  | LEU  |
| 2   | BG    | 70  | PRO  |
| 2   | BG    | 73  | GLN  |
| 2   | BG    | 86  | ASP  |
| 2   | BG    | 88  | LEU  |
| 2   | BG    | 93  | SER  |
| 2   | BG    | 110 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | BG    | 114 | VAL  |
| 2   | BG    | 126 | VAL  |
| 2   | BG    | 135 | THR  |
| 2   | BG    | 136 | HIS  |
| 2   | BG    | 145 | LEU  |
| 2   | BG    | 146 | GLU  |
| 2   | BG    | 156 | SER  |
| 2   | BG    | 157 | VAL  |
| 2   | BG    | 161 | GLN  |
| 2   | BG    | 166 | ARG  |
| 2   | BG    | 167 | THR  |
| 2   | BG    | 168 | ASN  |
| 2   | BG    | 193 | THR  |
| 2   | BG    | 194 | ILE  |
| 2   | BG    | 197 | LEU  |
| 2   | BG    | 212 | THR  |
| 2   | BH    | 45  | SER  |
| 2   | BH    | 49  | ASP  |
| 2   | BH    | 53  | ARG  |
| 2   | BH    | 58  | LEU  |
| 2   | BH    | 70  | PRO  |
| 2   | BH    | 73  | GLN  |
| 2   | BH    | 86  | ASP  |
| 2   | BH    | 88  | LEU  |
| 2   | BH    | 93  | SER  |
| 2   | BH    | 110 | VAL  |
| 2   | BH    | 114 | VAL  |
| 2   | BH    | 126 | VAL  |
| 2   | BH    | 135 | THR  |
| 2   | BH    | 136 | HIS  |
| 2   | BH    | 145 | LEU  |
| 2   | BH    | 146 | GLU  |
| 2   | BH    | 156 | SER  |
| 2   | BH    | 157 | VAL  |
| 2   | BH    | 161 | GLN  |
| 2   | BH    | 166 | ARG  |
| 2   | BH    | 167 | THR  |
| 2   | BH    | 168 | ASN  |
| 2   | BH    | 193 | THR  |
| 2   | BH    | 194 | ILE  |
| 2   | BH    | 197 | LEU  |
| 2   | BH    | 212 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | BI    | 45  | SER  |
| 2   | BI    | 49  | ASP  |
| 2   | BI    | 53  | ARG  |
| 2   | BI    | 58  | LEU  |
| 2   | BI    | 70  | PRO  |
| 2   | BI    | 73  | GLN  |
| 2   | BI    | 86  | ASP  |
| 2   | BI    | 88  | LEU  |
| 2   | BI    | 93  | SER  |
| 2   | BI    | 110 | VAL  |
| 2   | BI    | 114 | VAL  |
| 2   | BI    | 126 | VAL  |
| 2   | BI    | 135 | THR  |
| 2   | BI    | 136 | HIS  |
| 2   | BI    | 145 | LEU  |
| 2   | BI    | 146 | GLU  |
| 2   | BI    | 156 | SER  |
| 2   | BI    | 157 | VAL  |
| 2   | BI    | 161 | GLN  |
| 2   | BI    | 166 | ARG  |
| 2   | BI    | 167 | THR  |
| 2   | BI    | 168 | ASN  |
| 2   | BI    | 193 | THR  |
| 2   | BI    | 194 | ILE  |
| 2   | BI    | 197 | LEU  |
| 2   | BI    | 212 | THR  |
| 2   | BJ    | 45  | SER  |
| 2   | BJ    | 49  | ASP  |
| 2   | BJ    | 53  | ARG  |
| 2   | BJ    | 58  | LEU  |
| 2   | BJ    | 70  | PRO  |
| 2   | BJ    | 73  | GLN  |
| 2   | BJ    | 86  | ASP  |
| 2   | BJ    | 88  | LEU  |
| 2   | BJ    | 93  | SER  |
| 2   | BJ    | 110 | VAL  |
| 2   | BJ    | 114 | VAL  |
| 2   | BJ    | 126 | VAL  |
| 2   | BJ    | 135 | THR  |
| 2   | BJ    | 136 | HIS  |
| 2   | BJ    | 145 | LEU  |
| 2   | BJ    | 146 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | BJ    | 156 | SER  |
| 2   | BJ    | 157 | VAL  |
| 2   | BJ    | 161 | GLN  |
| 2   | BJ    | 166 | ARG  |
| 2   | BJ    | 167 | THR  |
| 2   | BJ    | 168 | ASN  |
| 2   | BJ    | 193 | THR  |
| 2   | BJ    | 194 | ILE  |
| 2   | BJ    | 197 | LEU  |
| 2   | BJ    | 212 | THR  |
| 2   | BK    | 45  | SER  |
| 2   | BK    | 49  | ASP  |
| 2   | BK    | 53  | ARG  |
| 2   | BK    | 58  | LEU  |
| 2   | BK    | 70  | PRO  |
| 2   | BK    | 73  | GLN  |
| 2   | BK    | 86  | ASP  |
| 2   | BK    | 88  | LEU  |
| 2   | BK    | 93  | SER  |
| 2   | BK    | 110 | VAL  |
| 2   | BK    | 114 | VAL  |
| 2   | BK    | 126 | VAL  |
| 2   | BK    | 135 | THR  |
| 2   | BK    | 136 | HIS  |
| 2   | BK    | 145 | LEU  |
| 2   | BK    | 146 | GLU  |
| 2   | BK    | 156 | SER  |
| 2   | BK    | 157 | VAL  |
| 2   | BK    | 161 | GLN  |
| 2   | BK    | 166 | ARG  |
| 2   | BK    | 167 | THR  |
| 2   | BK    | 168 | ASN  |
| 2   | BK    | 193 | THR  |
| 2   | BK    | 194 | ILE  |
| 2   | BK    | 197 | LEU  |
| 2   | BK    | 212 | THR  |
| 2   | BL    | 45  | SER  |
| 2   | BL    | 49  | ASP  |
| 2   | BL    | 53  | ARG  |
| 2   | BL    | 58  | LEU  |
| 2   | BL    | 70  | PRO  |
| 2   | BL    | 73  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | BL    | 86  | ASP  |
| 2   | BL    | 88  | LEU  |
| 2   | BL    | 93  | SER  |
| 2   | BL    | 110 | VAL  |
| 2   | BL    | 114 | VAL  |
| 2   | BL    | 126 | VAL  |
| 2   | BL    | 135 | THR  |
| 2   | BL    | 136 | HIS  |
| 2   | BL    | 145 | LEU  |
| 2   | BL    | 146 | GLU  |
| 2   | BL    | 156 | SER  |
| 2   | BL    | 157 | VAL  |
| 2   | BL    | 161 | GLN  |
| 2   | BL    | 166 | ARG  |
| 2   | BL    | 167 | THR  |
| 2   | BL    | 168 | ASN  |
| 2   | BL    | 193 | THR  |
| 2   | BL    | 194 | ILE  |
| 2   | BL    | 197 | LEU  |
| 2   | BL    | 212 | THR  |
| 2   | BM    | 45  | SER  |
| 2   | BM    | 49  | ASP  |
| 2   | BM    | 53  | ARG  |
| 2   | BM    | 58  | LEU  |
| 2   | BM    | 70  | PRO  |
| 2   | BM    | 73  | GLN  |
| 2   | BM    | 86  | ASP  |
| 2   | BM    | 88  | LEU  |
| 2   | BM    | 93  | SER  |
| 2   | BM    | 110 | VAL  |
| 2   | BM    | 114 | VAL  |
| 2   | BM    | 126 | VAL  |
| 2   | BM    | 135 | THR  |
| 2   | BM    | 136 | HIS  |
| 2   | BM    | 145 | LEU  |
| 2   | BM    | 146 | GLU  |
| 2   | BM    | 156 | SER  |
| 2   | BM    | 157 | VAL  |
| 2   | BM    | 161 | GLN  |
| 2   | BM    | 166 | ARG  |
| 2   | BM    | 167 | THR  |
| 2   | BM    | 168 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | BM    | 193 | THR  |
| 2   | BM    | 194 | ILE  |
| 2   | BM    | 197 | LEU  |
| 2   | BM    | 212 | THR  |
| 2   | BN    | 45  | SER  |
| 2   | BN    | 49  | ASP  |
| 2   | BN    | 53  | ARG  |
| 2   | BN    | 58  | LEU  |
| 2   | BN    | 70  | PRO  |
| 2   | BN    | 73  | GLN  |
| 2   | BN    | 86  | ASP  |
| 2   | BN    | 88  | LEU  |
| 2   | BN    | 93  | SER  |
| 2   | BN    | 110 | VAL  |
| 2   | BN    | 114 | VAL  |
| 2   | BN    | 126 | VAL  |
| 2   | BN    | 135 | THR  |
| 2   | BN    | 136 | HIS  |
| 2   | BN    | 145 | LEU  |
| 2   | BN    | 146 | GLU  |
| 2   | BN    | 156 | SER  |
| 2   | BN    | 157 | VAL  |
| 2   | BN    | 161 | GLN  |
| 2   | BN    | 166 | ARG  |
| 2   | BN    | 167 | THR  |
| 2   | BN    | 168 | ASN  |
| 2   | BN    | 193 | THR  |
| 2   | BN    | 194 | ILE  |
| 2   | BN    | 197 | LEU  |
| 2   | BN    | 212 | THR  |
| 2   | BR    | 45  | SER  |
| 2   | BR    | 49  | ASP  |
| 2   | BR    | 53  | ARG  |
| 2   | BR    | 58  | LEU  |
| 2   | BR    | 70  | PRO  |
| 2   | BR    | 73  | GLN  |
| 2   | BR    | 86  | ASP  |
| 2   | BR    | 88  | LEU  |
| 2   | BR    | 93  | SER  |
| 2   | BR    | 110 | VAL  |
| 2   | BR    | 114 | VAL  |
| 2   | BR    | 126 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | BR    | 135 | THR  |
| 2   | BR    | 136 | HIS  |
| 2   | BR    | 145 | LEU  |
| 2   | BR    | 146 | GLU  |
| 2   | BR    | 156 | SER  |
| 2   | BR    | 157 | VAL  |
| 2   | BR    | 161 | GLN  |
| 2   | BR    | 166 | ARG  |
| 2   | BR    | 167 | THR  |
| 2   | BR    | 168 | ASN  |
| 2   | BR    | 193 | THR  |
| 2   | BR    | 194 | ILE  |
| 2   | BR    | 197 | LEU  |
| 2   | BR    | 212 | THR  |
| 2   | BO    | 45  | SER  |
| 2   | BO    | 49  | ASP  |
| 2   | BO    | 53  | ARG  |
| 2   | BO    | 58  | LEU  |
| 2   | BO    | 70  | PRO  |
| 2   | BO    | 73  | GLN  |
| 2   | BO    | 86  | ASP  |
| 2   | BO    | 88  | LEU  |
| 2   | BO    | 93  | SER  |
| 2   | BO    | 110 | VAL  |
| 2   | BO    | 114 | VAL  |
| 2   | BO    | 126 | VAL  |
| 2   | BO    | 135 | THR  |
| 2   | BO    | 136 | HIS  |
| 2   | BO    | 145 | LEU  |
| 2   | BO    | 146 | GLU  |
| 2   | BO    | 156 | SER  |
| 2   | BO    | 157 | VAL  |
| 2   | BO    | 161 | GLN  |
| 2   | BO    | 166 | ARG  |
| 2   | BO    | 167 | THR  |
| 2   | BO    | 168 | ASN  |
| 2   | BO    | 193 | THR  |
| 2   | BO    | 194 | ILE  |
| 2   | BO    | 197 | LEU  |
| 2   | BO    | 212 | THR  |
| 2   | BS    | 45  | SER  |
| 2   | BS    | 49  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | BS    | 53  | ARG  |
| 2   | BS    | 58  | LEU  |
| 2   | BS    | 70  | PRO  |
| 2   | BS    | 73  | GLN  |
| 2   | BS    | 86  | ASP  |
| 2   | BS    | 88  | LEU  |
| 2   | BS    | 93  | SER  |
| 2   | BS    | 110 | VAL  |
| 2   | BS    | 114 | VAL  |
| 2   | BS    | 126 | VAL  |
| 2   | BS    | 135 | THR  |
| 2   | BS    | 136 | HIS  |
| 2   | BS    | 145 | LEU  |
| 2   | BS    | 146 | GLU  |
| 2   | BS    | 156 | SER  |
| 2   | BS    | 157 | VAL  |
| 2   | BS    | 161 | GLN  |
| 2   | BS    | 166 | ARG  |
| 2   | BS    | 167 | THR  |
| 2   | BS    | 168 | ASN  |
| 2   | BS    | 193 | THR  |
| 2   | BS    | 194 | ILE  |
| 2   | BS    | 197 | LEU  |
| 2   | BS    | 212 | THR  |
| 2   | BP    | 45  | SER  |
| 2   | BP    | 49  | ASP  |
| 2   | BP    | 53  | ARG  |
| 2   | BP    | 58  | LEU  |
| 2   | BP    | 70  | PRO  |
| 2   | BP    | 73  | GLN  |
| 2   | BP    | 86  | ASP  |
| 2   | BP    | 88  | LEU  |
| 2   | BP    | 93  | SER  |
| 2   | BP    | 110 | VAL  |
| 2   | BP    | 114 | VAL  |
| 2   | BP    | 126 | VAL  |
| 2   | BP    | 135 | THR  |
| 2   | BP    | 136 | HIS  |
| 2   | BP    | 145 | LEU  |
| 2   | BP    | 146 | GLU  |
| 2   | BP    | 156 | SER  |
| 2   | BP    | 157 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | BP    | 161 | GLN  |
| 2   | BP    | 166 | ARG  |
| 2   | BP    | 167 | THR  |
| 2   | BP    | 168 | ASN  |
| 2   | BP    | 193 | THR  |
| 2   | BP    | 194 | ILE  |
| 2   | BP    | 197 | LEU  |
| 2   | BP    | 212 | THR  |
| 2   | BQ    | 45  | SER  |
| 2   | BQ    | 49  | ASP  |
| 2   | BQ    | 53  | ARG  |
| 2   | BQ    | 58  | LEU  |
| 2   | BQ    | 70  | PRO  |
| 2   | BQ    | 73  | GLN  |
| 2   | BQ    | 86  | ASP  |
| 2   | BQ    | 88  | LEU  |
| 2   | BQ    | 93  | SER  |
| 2   | BQ    | 110 | VAL  |
| 2   | BQ    | 114 | VAL  |
| 2   | BQ    | 126 | VAL  |
| 2   | BQ    | 135 | THR  |
| 2   | BQ    | 136 | HIS  |
| 2   | BQ    | 145 | LEU  |
| 2   | BQ    | 146 | GLU  |
| 2   | BQ    | 156 | SER  |
| 2   | BQ    | 157 | VAL  |
| 2   | BQ    | 161 | GLN  |
| 2   | BQ    | 166 | ARG  |
| 2   | BQ    | 167 | THR  |
| 2   | BQ    | 168 | ASN  |
| 2   | BQ    | 193 | THR  |
| 2   | BQ    | 194 | ILE  |
| 2   | BQ    | 197 | LEU  |
| 2   | BQ    | 212 | THR  |
| 2   | BT    | 45  | SER  |
| 2   | BT    | 49  | ASP  |
| 2   | BT    | 53  | ARG  |
| 2   | BT    | 58  | LEU  |
| 2   | BT    | 70  | PRO  |
| 2   | BT    | 73  | GLN  |
| 2   | BT    | 86  | ASP  |
| 2   | BT    | 88  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | BT    | 93  | SER  |
| 2   | BT    | 110 | VAL  |
| 2   | BT    | 114 | VAL  |
| 2   | BT    | 126 | VAL  |
| 2   | BT    | 135 | THR  |
| 2   | BT    | 136 | HIS  |
| 2   | BT    | 145 | LEU  |
| 2   | BT    | 146 | GLU  |
| 2   | BT    | 156 | SER  |
| 2   | BT    | 157 | VAL  |
| 2   | BT    | 161 | GLN  |
| 2   | BT    | 166 | ARG  |
| 2   | BT    | 167 | THR  |
| 2   | BT    | 168 | ASN  |
| 2   | BT    | 193 | THR  |
| 2   | BT    | 194 | ILE  |
| 2   | BT    | 197 | LEU  |
| 2   | BT    | 212 | THR  |
| 2   | BU    | 45  | SER  |
| 2   | BU    | 49  | ASP  |
| 2   | BU    | 53  | ARG  |
| 2   | BU    | 58  | LEU  |
| 2   | BU    | 70  | PRO  |
| 2   | BU    | 73  | GLN  |
| 2   | BU    | 86  | ASP  |
| 2   | BU    | 88  | LEU  |
| 2   | BU    | 93  | SER  |
| 2   | BU    | 110 | VAL  |
| 2   | BU    | 114 | VAL  |
| 2   | BU    | 126 | VAL  |
| 2   | BU    | 135 | THR  |
| 2   | BU    | 136 | HIS  |
| 2   | BU    | 145 | LEU  |
| 2   | BU    | 146 | GLU  |
| 2   | BU    | 156 | SER  |
| 2   | BU    | 157 | VAL  |
| 2   | BU    | 161 | GLN  |
| 2   | BU    | 166 | ARG  |
| 2   | BU    | 167 | THR  |
| 2   | BU    | 168 | ASN  |
| 2   | BU    | 193 | THR  |
| 2   | BU    | 194 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | BU    | 197 | LEU  |
| 2   | BU    | 212 | THR  |
| 2   | BV    | 45  | SER  |
| 2   | BV    | 49  | ASP  |
| 2   | BV    | 53  | ARG  |
| 2   | BV    | 58  | LEU  |
| 2   | BV    | 70  | PRO  |
| 2   | BV    | 73  | GLN  |
| 2   | BV    | 86  | ASP  |
| 2   | BV    | 88  | LEU  |
| 2   | BV    | 93  | SER  |
| 2   | BV    | 110 | VAL  |
| 2   | BV    | 114 | VAL  |
| 2   | BV    | 126 | VAL  |
| 2   | BV    | 135 | THR  |
| 2   | BV    | 136 | HIS  |
| 2   | BV    | 145 | LEU  |
| 2   | BV    | 146 | GLU  |
| 2   | BV    | 156 | SER  |
| 2   | BV    | 157 | VAL  |
| 2   | BV    | 161 | GLN  |
| 2   | BV    | 166 | ARG  |
| 2   | BV    | 167 | THR  |
| 2   | BV    | 168 | ASN  |
| 2   | BV    | 193 | THR  |
| 2   | BV    | 194 | ILE  |
| 2   | BV    | 197 | LEU  |
| 2   | BV    | 212 | THR  |
| 2   | BW    | 45  | SER  |
| 2   | BW    | 49  | ASP  |
| 2   | BW    | 53  | ARG  |
| 2   | BW    | 58  | LEU  |
| 2   | BW    | 70  | PRO  |
| 2   | BW    | 73  | GLN  |
| 2   | BW    | 86  | ASP  |
| 2   | BW    | 88  | LEU  |
| 2   | BW    | 93  | SER  |
| 2   | BW    | 110 | VAL  |
| 2   | BW    | 114 | VAL  |
| 2   | BW    | 126 | VAL  |
| 2   | BW    | 135 | THR  |
| 2   | BW    | 136 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | BW    | 145 | LEU  |
| 2   | BW    | 146 | GLU  |
| 2   | BW    | 156 | SER  |
| 2   | BW    | 157 | VAL  |
| 2   | BW    | 161 | GLN  |
| 2   | BW    | 166 | ARG  |
| 2   | BW    | 167 | THR  |
| 2   | BW    | 168 | ASN  |
| 2   | BW    | 193 | THR  |
| 2   | BW    | 194 | ILE  |
| 2   | BW    | 197 | LEU  |
| 2   | BW    | 212 | THR  |
| 2   | BX    | 45  | SER  |
| 2   | BX    | 49  | ASP  |
| 2   | BX    | 53  | ARG  |
| 2   | BX    | 58  | LEU  |
| 2   | BX    | 70  | PRO  |
| 2   | BX    | 73  | GLN  |
| 2   | BX    | 86  | ASP  |
| 2   | BX    | 88  | LEU  |
| 2   | BX    | 93  | SER  |
| 2   | BX    | 110 | VAL  |
| 2   | BX    | 114 | VAL  |
| 2   | BX    | 126 | VAL  |
| 2   | BX    | 135 | THR  |
| 2   | BX    | 136 | HIS  |
| 2   | BX    | 145 | LEU  |
| 2   | BX    | 146 | GLU  |
| 2   | BX    | 156 | SER  |
| 2   | BX    | 157 | VAL  |
| 2   | BX    | 161 | GLN  |
| 2   | BX    | 166 | ARG  |
| 2   | BX    | 167 | THR  |
| 2   | BX    | 168 | ASN  |
| 2   | BX    | 193 | THR  |
| 2   | BX    | 194 | ILE  |
| 2   | BX    | 197 | LEU  |
| 2   | BX    | 212 | THR  |
| 2   | BY    | 45  | SER  |
| 2   | BY    | 49  | ASP  |
| 2   | BY    | 53  | ARG  |
| 2   | BY    | 58  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | BY    | 70  | PRO  |
| 2   | BY    | 73  | GLN  |
| 2   | BY    | 86  | ASP  |
| 2   | BY    | 88  | LEU  |
| 2   | BY    | 93  | SER  |
| 2   | BY    | 110 | VAL  |
| 2   | BY    | 114 | VAL  |
| 2   | BY    | 126 | VAL  |
| 2   | BY    | 135 | THR  |
| 2   | BY    | 136 | HIS  |
| 2   | BY    | 145 | LEU  |
| 2   | BY    | 146 | GLU  |
| 2   | BY    | 156 | SER  |
| 2   | BY    | 157 | VAL  |
| 2   | BY    | 161 | GLN  |
| 2   | BY    | 166 | ARG  |
| 2   | BY    | 167 | THR  |
| 2   | BY    | 168 | ASN  |
| 2   | BY    | 193 | THR  |
| 2   | BY    | 194 | ILE  |
| 2   | BY    | 197 | LEU  |
| 2   | BY    | 212 | THR  |
| 2   | BZ    | 45  | SER  |
| 2   | BZ    | 49  | ASP  |
| 2   | BZ    | 53  | ARG  |
| 2   | BZ    | 58  | LEU  |
| 2   | BZ    | 70  | PRO  |
| 2   | BZ    | 73  | GLN  |
| 2   | BZ    | 86  | ASP  |
| 2   | BZ    | 88  | LEU  |
| 2   | BZ    | 93  | SER  |
| 2   | BZ    | 110 | VAL  |
| 2   | BZ    | 114 | VAL  |
| 2   | BZ    | 126 | VAL  |
| 2   | BZ    | 135 | THR  |
| 2   | BZ    | 136 | HIS  |
| 2   | BZ    | 145 | LEU  |
| 2   | BZ    | 146 | GLU  |
| 2   | BZ    | 156 | SER  |
| 2   | BZ    | 157 | VAL  |
| 2   | BZ    | 161 | GLN  |
| 2   | BZ    | 166 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | BZ    | 167 | THR  |
| 2   | BZ    | 168 | ASN  |
| 2   | BZ    | 193 | THR  |
| 2   | BZ    | 194 | ILE  |
| 2   | BZ    | 197 | LEU  |
| 2   | BZ    | 212 | THR  |
| 2   | B0    | 45  | SER  |
| 2   | B0    | 49  | ASP  |
| 2   | B0    | 53  | ARG  |
| 2   | B0    | 58  | LEU  |
| 2   | B0    | 70  | PRO  |
| 2   | B0    | 73  | GLN  |
| 2   | B0    | 86  | ASP  |
| 2   | B0    | 88  | LEU  |
| 2   | B0    | 93  | SER  |
| 2   | B0    | 110 | VAL  |
| 2   | B0    | 114 | VAL  |
| 2   | B0    | 126 | VAL  |
| 2   | B0    | 135 | THR  |
| 2   | B0    | 136 | HIS  |
| 2   | B0    | 145 | LEU  |
| 2   | B0    | 146 | GLU  |
| 2   | B0    | 156 | SER  |
| 2   | B0    | 157 | VAL  |
| 2   | B0    | 161 | GLN  |
| 2   | B0    | 166 | ARG  |
| 2   | B0    | 167 | THR  |
| 2   | B0    | 168 | ASN  |
| 2   | B0    | 193 | THR  |
| 2   | B0    | 194 | ILE  |
| 2   | B0    | 197 | LEU  |
| 2   | B0    | 212 | THR  |
| 2   | B1    | 45  | SER  |
| 2   | B1    | 49  | ASP  |
| 2   | B1    | 53  | ARG  |
| 2   | B1    | 58  | LEU  |
| 2   | B1    | 70  | PRO  |
| 2   | B1    | 73  | GLN  |
| 2   | B1    | 86  | ASP  |
| 2   | B1    | 88  | LEU  |
| 2   | B1    | 93  | SER  |
| 2   | B1    | 110 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B1    | 114 | VAL  |
| 2   | B1    | 126 | VAL  |
| 2   | B1    | 135 | THR  |
| 2   | B1    | 136 | HIS  |
| 2   | B1    | 145 | LEU  |
| 2   | B1    | 146 | GLU  |
| 2   | B1    | 156 | SER  |
| 2   | B1    | 157 | VAL  |
| 2   | B1    | 161 | GLN  |
| 2   | B1    | 166 | ARG  |
| 2   | B1    | 167 | THR  |
| 2   | B1    | 168 | ASN  |
| 2   | B1    | 193 | THR  |
| 2   | B1    | 194 | ILE  |
| 2   | B1    | 197 | LEU  |
| 2   | B1    | 212 | THR  |
| 2   | B2    | 45  | SER  |
| 2   | B2    | 49  | ASP  |
| 2   | B2    | 53  | ARG  |
| 2   | B2    | 58  | LEU  |
| 2   | B2    | 70  | PRO  |
| 2   | B2    | 73  | GLN  |
| 2   | B2    | 86  | ASP  |
| 2   | B2    | 88  | LEU  |
| 2   | B2    | 93  | SER  |
| 2   | B2    | 110 | VAL  |
| 2   | B2    | 114 | VAL  |
| 2   | B2    | 126 | VAL  |
| 2   | B2    | 135 | THR  |
| 2   | B2    | 136 | HIS  |
| 2   | B2    | 145 | LEU  |
| 2   | B2    | 146 | GLU  |
| 2   | B2    | 156 | SER  |
| 2   | B2    | 157 | VAL  |
| 2   | B2    | 161 | GLN  |
| 2   | B2    | 166 | ARG  |
| 2   | B2    | 167 | THR  |
| 2   | B2    | 168 | ASN  |
| 2   | B2    | 193 | THR  |
| 2   | B2    | 194 | ILE  |
| 2   | B2    | 197 | LEU  |
| 2   | B2    | 212 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B3    | 45  | SER  |
| 2   | B3    | 49  | ASP  |
| 2   | B3    | 53  | ARG  |
| 2   | B3    | 58  | LEU  |
| 2   | B3    | 70  | PRO  |
| 2   | B3    | 73  | GLN  |
| 2   | B3    | 86  | ASP  |
| 2   | B3    | 88  | LEU  |
| 2   | B3    | 93  | SER  |
| 2   | B3    | 110 | VAL  |
| 2   | B3    | 114 | VAL  |
| 2   | B3    | 126 | VAL  |
| 2   | B3    | 135 | THR  |
| 2   | B3    | 136 | HIS  |
| 2   | B3    | 145 | LEU  |
| 2   | B3    | 146 | GLU  |
| 2   | B3    | 156 | SER  |
| 2   | B3    | 157 | VAL  |
| 2   | B3    | 161 | GLN  |
| 2   | B3    | 166 | ARG  |
| 2   | B3    | 167 | THR  |
| 2   | B3    | 168 | ASN  |
| 2   | B3    | 193 | THR  |
| 2   | B3    | 194 | ILE  |
| 2   | B3    | 197 | LEU  |
| 2   | B3    | 212 | THR  |
| 2   | B4    | 45  | SER  |
| 2   | B4    | 49  | ASP  |
| 2   | B4    | 53  | ARG  |
| 2   | B4    | 58  | LEU  |
| 2   | B4    | 70  | PRO  |
| 2   | B4    | 73  | GLN  |
| 2   | B4    | 86  | ASP  |
| 2   | B4    | 88  | LEU  |
| 2   | B4    | 93  | SER  |
| 2   | B4    | 110 | VAL  |
| 2   | B4    | 114 | VAL  |
| 2   | B4    | 126 | VAL  |
| 2   | B4    | 135 | THR  |
| 2   | B4    | 136 | HIS  |
| 2   | B4    | 145 | LEU  |
| 2   | B4    | 146 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B4    | 156 | SER  |
| 2   | B4    | 157 | VAL  |
| 2   | B4    | 161 | GLN  |
| 2   | B4    | 166 | ARG  |
| 2   | B4    | 167 | THR  |
| 2   | B4    | 168 | ASN  |
| 2   | B4    | 193 | THR  |
| 2   | B4    | 194 | ILE  |
| 2   | B4    | 197 | LEU  |
| 2   | B4    | 212 | THR  |
| 2   | B5    | 45  | SER  |
| 2   | B5    | 49  | ASP  |
| 2   | B5    | 53  | ARG  |
| 2   | B5    | 58  | LEU  |
| 2   | B5    | 70  | PRO  |
| 2   | B5    | 73  | GLN  |
| 2   | B5    | 86  | ASP  |
| 2   | B5    | 88  | LEU  |
| 2   | B5    | 93  | SER  |
| 2   | B5    | 110 | VAL  |
| 2   | B5    | 114 | VAL  |
| 2   | B5    | 126 | VAL  |
| 2   | B5    | 135 | THR  |
| 2   | B5    | 136 | HIS  |
| 2   | B5    | 145 | LEU  |
| 2   | B5    | 146 | GLU  |
| 2   | B5    | 156 | SER  |
| 2   | B5    | 157 | VAL  |
| 2   | B5    | 161 | GLN  |
| 2   | B5    | 166 | ARG  |
| 2   | B5    | 167 | THR  |
| 2   | B5    | 168 | ASN  |
| 2   | B5    | 193 | THR  |
| 2   | B5    | 194 | ILE  |
| 2   | B5    | 197 | LEU  |
| 2   | B5    | 212 | THR  |
| 2   | B6    | 45  | SER  |
| 2   | B6    | 49  | ASP  |
| 2   | B6    | 53  | ARG  |
| 2   | B6    | 58  | LEU  |
| 2   | B6    | 70  | PRO  |
| 2   | B6    | 73  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B6    | 86  | ASP  |
| 2   | B6    | 88  | LEU  |
| 2   | B6    | 93  | SER  |
| 2   | B6    | 110 | VAL  |
| 2   | B6    | 114 | VAL  |
| 2   | B6    | 126 | VAL  |
| 2   | B6    | 135 | THR  |
| 2   | B6    | 136 | HIS  |
| 2   | B6    | 145 | LEU  |
| 2   | B6    | 146 | GLU  |
| 2   | B6    | 156 | SER  |
| 2   | B6    | 157 | VAL  |
| 2   | B6    | 161 | GLN  |
| 2   | B6    | 166 | ARG  |
| 2   | B6    | 167 | THR  |
| 2   | B6    | 168 | ASN  |
| 2   | B6    | 193 | THR  |
| 2   | B6    | 194 | ILE  |
| 2   | B6    | 197 | LEU  |
| 2   | B6    | 212 | THR  |
| 2   | B7    | 45  | SER  |
| 2   | B7    | 49  | ASP  |
| 2   | B7    | 53  | ARG  |
| 2   | B7    | 58  | LEU  |
| 2   | B7    | 70  | PRO  |
| 2   | B7    | 73  | GLN  |
| 2   | B7    | 86  | ASP  |
| 2   | B7    | 88  | LEU  |
| 2   | B7    | 93  | SER  |
| 2   | B7    | 110 | VAL  |
| 2   | B7    | 114 | VAL  |
| 2   | B7    | 126 | VAL  |
| 2   | B7    | 135 | THR  |
| 2   | B7    | 136 | HIS  |
| 2   | B7    | 145 | LEU  |
| 2   | B7    | 146 | GLU  |
| 2   | B7    | 156 | SER  |
| 2   | B7    | 157 | VAL  |
| 2   | B7    | 161 | GLN  |
| 2   | B7    | 166 | ARG  |
| 2   | B7    | 167 | THR  |
| 2   | B7    | 168 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B7    | 193 | THR  |
| 2   | B7    | 194 | ILE  |
| 2   | B7    | 197 | LEU  |
| 2   | B7    | 212 | THR  |
| 2   | B8    | 45  | SER  |
| 2   | B8    | 49  | ASP  |
| 2   | B8    | 53  | ARG  |
| 2   | B8    | 58  | LEU  |
| 2   | B8    | 70  | PRO  |
| 2   | B8    | 73  | GLN  |
| 2   | B8    | 86  | ASP  |
| 2   | B8    | 88  | LEU  |
| 2   | B8    | 93  | SER  |
| 2   | B8    | 110 | VAL  |
| 2   | B8    | 114 | VAL  |
| 2   | B8    | 126 | VAL  |
| 2   | B8    | 135 | THR  |
| 2   | B8    | 136 | HIS  |
| 2   | B8    | 145 | LEU  |
| 2   | B8    | 146 | GLU  |
| 2   | B8    | 156 | SER  |
| 2   | B8    | 157 | VAL  |
| 2   | B8    | 161 | GLN  |
| 2   | B8    | 166 | ARG  |
| 2   | B8    | 167 | THR  |
| 2   | B8    | 168 | ASN  |
| 2   | B8    | 193 | THR  |
| 2   | B8    | 194 | ILE  |
| 2   | B8    | 197 | LEU  |
| 2   | B8    | 212 | THR  |
| 2   | B9    | 45  | SER  |
| 2   | B9    | 49  | ASP  |
| 2   | B9    | 53  | ARG  |
| 2   | B9    | 58  | LEU  |
| 2   | B9    | 70  | PRO  |
| 2   | B9    | 73  | GLN  |
| 2   | B9    | 86  | ASP  |
| 2   | B9    | 88  | LEU  |
| 2   | B9    | 93  | SER  |
| 2   | B9    | 110 | VAL  |
| 2   | B9    | 114 | VAL  |
| 2   | B9    | 126 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B9    | 135 | THR  |
| 2   | B9    | 136 | HIS  |
| 2   | B9    | 145 | LEU  |
| 2   | B9    | 146 | GLU  |
| 2   | B9    | 156 | SER  |
| 2   | B9    | 157 | VAL  |
| 2   | B9    | 161 | GLN  |
| 2   | B9    | 166 | ARG  |
| 2   | B9    | 167 | THR  |
| 2   | B9    | 168 | ASN  |
| 2   | B9    | 193 | THR  |
| 2   | B9    | 194 | ILE  |
| 2   | B9    | 197 | LEU  |
| 2   | B9    | 212 | THR  |
| 2   | Ba    | 45  | SER  |
| 2   | Ba    | 49  | ASP  |
| 2   | Ba    | 53  | ARG  |
| 2   | Ba    | 58  | LEU  |
| 2   | Ba    | 70  | PRO  |
| 2   | Ba    | 73  | GLN  |
| 2   | Ba    | 86  | ASP  |
| 2   | Ba    | 88  | LEU  |
| 2   | Ba    | 93  | SER  |
| 2   | Ba    | 110 | VAL  |
| 2   | Ba    | 114 | VAL  |
| 2   | Ba    | 126 | VAL  |
| 2   | Ba    | 135 | THR  |
| 2   | Ba    | 136 | HIS  |
| 2   | Ba    | 145 | LEU  |
| 2   | Ba    | 146 | GLU  |
| 2   | Ba    | 156 | SER  |
| 2   | Ba    | 157 | VAL  |
| 2   | Ba    | 161 | GLN  |
| 2   | Ba    | 166 | ARG  |
| 2   | Ba    | 167 | THR  |
| 2   | Ba    | 168 | ASN  |
| 2   | Ba    | 193 | THR  |
| 2   | Ba    | 194 | ILE  |
| 2   | Ba    | 197 | LEU  |
| 2   | Ba    | 212 | THR  |
| 2   | Bb    | 45  | SER  |
| 2   | Bb    | 49  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Bb    | 53  | ARG  |
| 2   | Bb    | 58  | LEU  |
| 2   | Bb    | 70  | PRO  |
| 2   | Bb    | 73  | GLN  |
| 2   | Bb    | 86  | ASP  |
| 2   | Bb    | 88  | LEU  |
| 2   | Bb    | 93  | SER  |
| 2   | Bb    | 110 | VAL  |
| 2   | Bb    | 114 | VAL  |
| 2   | Bb    | 126 | VAL  |
| 2   | Bb    | 135 | THR  |
| 2   | Bb    | 136 | HIS  |
| 2   | Bb    | 145 | LEU  |
| 2   | Bb    | 146 | GLU  |
| 2   | Bb    | 156 | SER  |
| 2   | Bb    | 157 | VAL  |
| 2   | Bb    | 161 | GLN  |
| 2   | Bb    | 166 | ARG  |
| 2   | Bb    | 167 | THR  |
| 2   | Bb    | 168 | ASN  |
| 2   | Bb    | 193 | THR  |
| 2   | Bb    | 194 | ILE  |
| 2   | Bb    | 197 | LEU  |
| 2   | Bb    | 212 | THR  |
| 2   | Bc    | 45  | SER  |
| 2   | Bc    | 49  | ASP  |
| 2   | Bc    | 53  | ARG  |
| 2   | Bc    | 58  | LEU  |
| 2   | Bc    | 70  | PRO  |
| 2   | Bc    | 73  | GLN  |
| 2   | Bc    | 86  | ASP  |
| 2   | Bc    | 88  | LEU  |
| 2   | Bc    | 93  | SER  |
| 2   | Bc    | 110 | VAL  |
| 2   | Bc    | 114 | VAL  |
| 2   | Bc    | 126 | VAL  |
| 2   | Bc    | 135 | THR  |
| 2   | Bc    | 136 | HIS  |
| 2   | Bc    | 145 | LEU  |
| 2   | Bc    | 146 | GLU  |
| 2   | Bc    | 156 | SER  |
| 2   | Bc    | 157 | VAL  |

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*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Bc    | 161 | GLN  |
| 2   | Bc    | 166 | ARG  |
| 2   | Bc    | 167 | THR  |
| 2   | Bc    | 168 | ASN  |
| 2   | Bc    | 193 | THR  |
| 2   | Bc    | 194 | ILE  |
| 2   | Bc    | 197 | LEU  |
| 2   | Bc    | 212 | THR  |
| 2   | Bd    | 45  | SER  |
| 2   | Bd    | 49  | ASP  |
| 2   | Bd    | 53  | ARG  |
| 2   | Bd    | 58  | LEU  |
| 2   | Bd    | 70  | PRO  |
| 2   | Bd    | 73  | GLN  |
| 2   | Bd    | 86  | ASP  |
| 2   | Bd    | 88  | LEU  |
| 2   | Bd    | 93  | SER  |
| 2   | Bd    | 110 | VAL  |
| 2   | Bd    | 114 | VAL  |
| 2   | Bd    | 126 | VAL  |
| 2   | Bd    | 135 | THR  |
| 2   | Bd    | 136 | HIS  |
| 2   | Bd    | 145 | LEU  |
| 2   | Bd    | 146 | GLU  |
| 2   | Bd    | 156 | SER  |
| 2   | Bd    | 157 | VAL  |
| 2   | Bd    | 161 | GLN  |
| 2   | Bd    | 166 | ARG  |
| 2   | Bd    | 167 | THR  |
| 2   | Bd    | 168 | ASN  |
| 2   | Bd    | 193 | THR  |
| 2   | Bd    | 194 | ILE  |
| 2   | Bd    | 197 | LEU  |
| 2   | Bd    | 212 | THR  |
| 2   | Be    | 45  | SER  |
| 2   | Be    | 49  | ASP  |
| 2   | Be    | 53  | ARG  |
| 2   | Be    | 58  | LEU  |
| 2   | Be    | 70  | PRO  |
| 2   | Be    | 73  | GLN  |
| 2   | Be    | 86  | ASP  |
| 2   | Be    | 88  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Be    | 93  | SER  |
| 2   | Be    | 110 | VAL  |
| 2   | Be    | 114 | VAL  |
| 2   | Be    | 126 | VAL  |
| 2   | Be    | 135 | THR  |
| 2   | Be    | 136 | HIS  |
| 2   | Be    | 145 | LEU  |
| 2   | Be    | 146 | GLU  |
| 2   | Be    | 156 | SER  |
| 2   | Be    | 157 | VAL  |
| 2   | Be    | 161 | GLN  |
| 2   | Be    | 166 | ARG  |
| 2   | Be    | 167 | THR  |
| 2   | Be    | 168 | ASN  |
| 2   | Be    | 193 | THR  |
| 2   | Be    | 194 | ILE  |
| 2   | Be    | 197 | LEU  |
| 2   | Be    | 212 | THR  |
| 2   | Bf    | 45  | SER  |
| 2   | Bf    | 49  | ASP  |
| 2   | Bf    | 53  | ARG  |
| 2   | Bf    | 58  | LEU  |
| 2   | Bf    | 70  | PRO  |
| 2   | Bf    | 73  | GLN  |
| 2   | Bf    | 86  | ASP  |
| 2   | Bf    | 88  | LEU  |
| 2   | Bf    | 93  | SER  |
| 2   | Bf    | 110 | VAL  |
| 2   | Bf    | 114 | VAL  |
| 2   | Bf    | 126 | VAL  |
| 2   | Bf    | 135 | THR  |
| 2   | Bf    | 136 | HIS  |
| 2   | Bf    | 145 | LEU  |
| 2   | Bf    | 146 | GLU  |
| 2   | Bf    | 156 | SER  |
| 2   | Bf    | 157 | VAL  |
| 2   | Bf    | 161 | GLN  |
| 2   | Bf    | 166 | ARG  |
| 2   | Bf    | 167 | THR  |
| 2   | Bf    | 168 | ASN  |
| 2   | Bf    | 193 | THR  |
| 2   | Bf    | 194 | ILE  |

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*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Bf    | 197 | LEU  |
| 2   | Bf    | 212 | THR  |
| 2   | Bg    | 45  | SER  |
| 2   | Bg    | 49  | ASP  |
| 2   | Bg    | 53  | ARG  |
| 2   | Bg    | 58  | LEU  |
| 2   | Bg    | 70  | PRO  |
| 2   | Bg    | 73  | GLN  |
| 2   | Bg    | 86  | ASP  |
| 2   | Bg    | 88  | LEU  |
| 2   | Bg    | 93  | SER  |
| 2   | Bg    | 110 | VAL  |
| 2   | Bg    | 114 | VAL  |
| 2   | Bg    | 126 | VAL  |
| 2   | Bg    | 135 | THR  |
| 2   | Bg    | 136 | HIS  |
| 2   | Bg    | 145 | LEU  |
| 2   | Bg    | 146 | GLU  |
| 2   | Bg    | 156 | SER  |
| 2   | Bg    | 157 | VAL  |
| 2   | Bg    | 161 | GLN  |
| 2   | Bg    | 166 | ARG  |
| 2   | Bg    | 167 | THR  |
| 2   | Bg    | 168 | ASN  |
| 2   | Bg    | 193 | THR  |
| 2   | Bg    | 194 | ILE  |
| 2   | Bg    | 197 | LEU  |
| 2   | Bg    | 212 | THR  |
| 2   | Bh    | 45  | SER  |
| 2   | Bh    | 49  | ASP  |
| 2   | Bh    | 53  | ARG  |
| 2   | Bh    | 58  | LEU  |
| 2   | Bh    | 70  | PRO  |
| 2   | Bh    | 73  | GLN  |
| 2   | Bh    | 86  | ASP  |
| 2   | Bh    | 88  | LEU  |
| 2   | Bh    | 93  | SER  |
| 2   | Bh    | 110 | VAL  |
| 2   | Bh    | 114 | VAL  |
| 2   | Bh    | 126 | VAL  |
| 2   | Bh    | 135 | THR  |
| 2   | Bh    | 136 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Bh    | 145 | LEU  |
| 2   | Bh    | 146 | GLU  |
| 2   | Bh    | 156 | SER  |
| 2   | Bh    | 157 | VAL  |
| 2   | Bh    | 161 | GLN  |
| 2   | Bh    | 166 | ARG  |
| 2   | Bh    | 167 | THR  |
| 2   | Bh    | 168 | ASN  |
| 2   | Bh    | 193 | THR  |
| 2   | Bh    | 194 | ILE  |
| 2   | Bh    | 197 | LEU  |
| 2   | Bh    | 212 | THR  |
| 2   | Bi    | 45  | SER  |
| 2   | Bi    | 49  | ASP  |
| 2   | Bi    | 53  | ARG  |
| 2   | Bi    | 58  | LEU  |
| 2   | Bi    | 70  | PRO  |
| 2   | Bi    | 73  | GLN  |
| 2   | Bi    | 86  | ASP  |
| 2   | Bi    | 88  | LEU  |
| 2   | Bi    | 93  | SER  |
| 2   | Bi    | 110 | VAL  |
| 2   | Bi    | 114 | VAL  |
| 2   | Bi    | 126 | VAL  |
| 2   | Bi    | 135 | THR  |
| 2   | Bi    | 136 | HIS  |
| 2   | Bi    | 145 | LEU  |
| 2   | Bi    | 146 | GLU  |
| 2   | Bi    | 156 | SER  |
| 2   | Bi    | 157 | VAL  |
| 2   | Bi    | 161 | GLN  |
| 2   | Bi    | 166 | ARG  |
| 2   | Bi    | 167 | THR  |
| 2   | Bi    | 168 | ASN  |
| 2   | Bi    | 193 | THR  |
| 2   | Bi    | 194 | ILE  |
| 2   | Bi    | 197 | LEU  |
| 2   | Bi    | 212 | THR  |
| 2   | Bj    | 45  | SER  |
| 2   | Bj    | 49  | ASP  |
| 2   | Bj    | 53  | ARG  |
| 2   | Bj    | 58  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Bj    | 70  | PRO  |
| 2   | Bj    | 73  | GLN  |
| 2   | Bj    | 86  | ASP  |
| 2   | Bj    | 88  | LEU  |
| 2   | Bj    | 93  | SER  |
| 2   | Bj    | 110 | VAL  |
| 2   | Bj    | 114 | VAL  |
| 2   | Bj    | 126 | VAL  |
| 2   | Bj    | 135 | THR  |
| 2   | Bj    | 136 | HIS  |
| 2   | Bj    | 145 | LEU  |
| 2   | Bj    | 146 | GLU  |
| 2   | Bj    | 156 | SER  |
| 2   | Bj    | 157 | VAL  |
| 2   | Bj    | 161 | GLN  |
| 2   | Bj    | 166 | ARG  |
| 2   | Bj    | 167 | THR  |
| 2   | Bj    | 168 | ASN  |
| 2   | Bj    | 193 | THR  |
| 2   | Bj    | 194 | ILE  |
| 2   | Bj    | 197 | LEU  |
| 2   | Bj    | 212 | THR  |
| 2   | Bk    | 45  | SER  |
| 2   | Bk    | 49  | ASP  |
| 2   | Bk    | 53  | ARG  |
| 2   | Bk    | 58  | LEU  |
| 2   | Bk    | 70  | PRO  |
| 2   | Bk    | 73  | GLN  |
| 2   | Bk    | 86  | ASP  |
| 2   | Bk    | 88  | LEU  |
| 2   | Bk    | 93  | SER  |
| 2   | Bk    | 110 | VAL  |
| 2   | Bk    | 114 | VAL  |
| 2   | Bk    | 126 | VAL  |
| 2   | Bk    | 135 | THR  |
| 2   | Bk    | 136 | HIS  |
| 2   | Bk    | 145 | LEU  |
| 2   | Bk    | 146 | GLU  |
| 2   | Bk    | 156 | SER  |
| 2   | Bk    | 157 | VAL  |
| 2   | Bk    | 161 | GLN  |
| 2   | Bk    | 166 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Bk    | 167 | THR  |
| 2   | Bk    | 168 | ASN  |
| 2   | Bk    | 193 | THR  |
| 2   | Bk    | 194 | ILE  |
| 2   | Bk    | 197 | LEU  |
| 2   | Bk    | 212 | THR  |
| 2   | Bl    | 45  | SER  |
| 2   | Bl    | 49  | ASP  |
| 2   | Bl    | 53  | ARG  |
| 2   | Bl    | 58  | LEU  |
| 2   | Bl    | 70  | PRO  |
| 2   | Bl    | 73  | GLN  |
| 2   | Bl    | 86  | ASP  |
| 2   | Bl    | 88  | LEU  |
| 2   | Bl    | 93  | SER  |
| 2   | Bl    | 110 | VAL  |
| 2   | Bl    | 114 | VAL  |
| 2   | Bl    | 126 | VAL  |
| 2   | Bl    | 135 | THR  |
| 2   | Bl    | 136 | HIS  |
| 2   | Bl    | 145 | LEU  |
| 2   | Bl    | 146 | GLU  |
| 2   | Bl    | 156 | SER  |
| 2   | Bl    | 157 | VAL  |
| 2   | Bl    | 161 | GLN  |
| 2   | Bl    | 166 | ARG  |
| 2   | Bl    | 167 | THR  |
| 2   | Bl    | 168 | ASN  |
| 2   | Bl    | 193 | THR  |
| 2   | Bl    | 194 | ILE  |
| 2   | Bl    | 197 | LEU  |
| 2   | Bl    | 212 | THR  |
| 2   | Bm    | 45  | SER  |
| 2   | Bm    | 49  | ASP  |
| 2   | Bm    | 53  | ARG  |
| 2   | Bm    | 58  | LEU  |
| 2   | Bm    | 70  | PRO  |
| 2   | Bm    | 73  | GLN  |
| 2   | Bm    | 86  | ASP  |
| 2   | Bm    | 88  | LEU  |
| 2   | Bm    | 93  | SER  |
| 2   | Bm    | 110 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Bm    | 114 | VAL  |
| 2   | Bm    | 126 | VAL  |
| 2   | Bm    | 135 | THR  |
| 2   | Bm    | 136 | HIS  |
| 2   | Bm    | 145 | LEU  |
| 2   | Bm    | 146 | GLU  |
| 2   | Bm    | 156 | SER  |
| 2   | Bm    | 157 | VAL  |
| 2   | Bm    | 161 | GLN  |
| 2   | Bm    | 166 | ARG  |
| 2   | Bm    | 167 | THR  |
| 2   | Bm    | 168 | ASN  |
| 2   | Bm    | 193 | THR  |
| 2   | Bm    | 194 | ILE  |
| 2   | Bm    | 197 | LEU  |
| 2   | Bm    | 212 | THR  |
| 2   | Bn    | 45  | SER  |
| 2   | Bn    | 49  | ASP  |
| 2   | Bn    | 53  | ARG  |
| 2   | Bn    | 58  | LEU  |
| 2   | Bn    | 70  | PRO  |
| 2   | Bn    | 73  | GLN  |
| 2   | Bn    | 86  | ASP  |
| 2   | Bn    | 88  | LEU  |
| 2   | Bn    | 93  | SER  |
| 2   | Bn    | 110 | VAL  |
| 2   | Bn    | 114 | VAL  |
| 2   | Bn    | 126 | VAL  |
| 2   | Bn    | 135 | THR  |
| 2   | Bn    | 136 | HIS  |
| 2   | Bn    | 145 | LEU  |
| 2   | Bn    | 146 | GLU  |
| 2   | Bn    | 156 | SER  |
| 2   | Bn    | 157 | VAL  |
| 2   | Bn    | 161 | GLN  |
| 2   | Bn    | 166 | ARG  |
| 2   | Bn    | 167 | THR  |
| 2   | Bn    | 168 | ASN  |
| 2   | Bn    | 193 | THR  |
| 2   | Bn    | 194 | ILE  |
| 2   | Bn    | 197 | LEU  |
| 2   | Bn    | 212 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Bo    | 45  | SER  |
| 2   | Bo    | 49  | ASP  |
| 2   | Bo    | 53  | ARG  |
| 2   | Bo    | 58  | LEU  |
| 2   | Bo    | 70  | PRO  |
| 2   | Bo    | 73  | GLN  |
| 2   | Bo    | 86  | ASP  |
| 2   | Bo    | 88  | LEU  |
| 2   | Bo    | 93  | SER  |
| 2   | Bo    | 110 | VAL  |
| 2   | Bo    | 114 | VAL  |
| 2   | Bo    | 126 | VAL  |
| 2   | Bo    | 135 | THR  |
| 2   | Bo    | 136 | HIS  |
| 2   | Bo    | 145 | LEU  |
| 2   | Bo    | 146 | GLU  |
| 2   | Bo    | 156 | SER  |
| 2   | Bo    | 157 | VAL  |
| 2   | Bo    | 161 | GLN  |
| 2   | Bo    | 166 | ARG  |
| 2   | Bo    | 167 | THR  |
| 2   | Bo    | 168 | ASN  |
| 2   | Bo    | 193 | THR  |
| 2   | Bo    | 194 | ILE  |
| 2   | Bo    | 197 | LEU  |
| 2   | Bo    | 212 | THR  |
| 2   | Bp    | 45  | SER  |
| 2   | Bp    | 49  | ASP  |
| 2   | Bp    | 53  | ARG  |
| 2   | Bp    | 58  | LEU  |
| 2   | Bp    | 70  | PRO  |
| 2   | Bp    | 73  | GLN  |
| 2   | Bp    | 86  | ASP  |
| 2   | Bp    | 88  | LEU  |
| 2   | Bp    | 93  | SER  |
| 2   | Bp    | 110 | VAL  |
| 2   | Bp    | 114 | VAL  |
| 2   | Bp    | 126 | VAL  |
| 2   | Bp    | 135 | THR  |
| 2   | Bp    | 136 | HIS  |
| 2   | Bp    | 145 | LEU  |
| 2   | Bp    | 146 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Bp    | 156 | SER  |
| 2   | Bp    | 157 | VAL  |
| 2   | Bp    | 161 | GLN  |
| 2   | Bp    | 166 | ARG  |
| 2   | Bp    | 167 | THR  |
| 2   | Bp    | 168 | ASN  |
| 2   | Bp    | 193 | THR  |
| 2   | Bp    | 194 | ILE  |
| 2   | Bp    | 197 | LEU  |
| 2   | Bp    | 212 | THR  |
| 2   | Bq    | 45  | SER  |
| 2   | Bq    | 49  | ASP  |
| 2   | Bq    | 53  | ARG  |
| 2   | Bq    | 58  | LEU  |
| 2   | Bq    | 70  | PRO  |
| 2   | Bq    | 73  | GLN  |
| 2   | Bq    | 86  | ASP  |
| 2   | Bq    | 88  | LEU  |
| 2   | Bq    | 93  | SER  |
| 2   | Bq    | 110 | VAL  |
| 2   | Bq    | 114 | VAL  |
| 2   | Bq    | 126 | VAL  |
| 2   | Bq    | 135 | THR  |
| 2   | Bq    | 136 | HIS  |
| 2   | Bq    | 145 | LEU  |
| 2   | Bq    | 146 | GLU  |
| 2   | Bq    | 156 | SER  |
| 2   | Bq    | 157 | VAL  |
| 2   | Bq    | 161 | GLN  |
| 2   | Bq    | 166 | ARG  |
| 2   | Bq    | 167 | THR  |
| 2   | Bq    | 168 | ASN  |
| 2   | Bq    | 193 | THR  |
| 2   | Bq    | 194 | ILE  |
| 2   | Bq    | 197 | LEU  |
| 2   | Bq    | 212 | THR  |
| 2   | Br    | 45  | SER  |
| 2   | Br    | 49  | ASP  |
| 2   | Br    | 53  | ARG  |
| 2   | Br    | 58  | LEU  |
| 2   | Br    | 70  | PRO  |
| 2   | Br    | 73  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Br    | 86  | ASP  |
| 2   | Br    | 88  | LEU  |
| 2   | Br    | 93  | SER  |
| 2   | Br    | 110 | VAL  |
| 2   | Br    | 114 | VAL  |
| 2   | Br    | 126 | VAL  |
| 2   | Br    | 135 | THR  |
| 2   | Br    | 136 | HIS  |
| 2   | Br    | 145 | LEU  |
| 2   | Br    | 146 | GLU  |
| 2   | Br    | 156 | SER  |
| 2   | Br    | 157 | VAL  |
| 2   | Br    | 161 | GLN  |
| 2   | Br    | 166 | ARG  |
| 2   | Br    | 167 | THR  |
| 2   | Br    | 168 | ASN  |
| 2   | Br    | 193 | THR  |
| 2   | Br    | 194 | ILE  |
| 2   | Br    | 197 | LEU  |
| 2   | Br    | 212 | THR  |
| 2   | Bs    | 45  | SER  |
| 2   | Bs    | 49  | ASP  |
| 2   | Bs    | 53  | ARG  |
| 2   | Bs    | 58  | LEU  |
| 2   | Bs    | 70  | PRO  |
| 2   | Bs    | 73  | GLN  |
| 2   | Bs    | 86  | ASP  |
| 2   | Bs    | 88  | LEU  |
| 2   | Bs    | 93  | SER  |
| 2   | Bs    | 110 | VAL  |
| 2   | Bs    | 114 | VAL  |
| 2   | Bs    | 126 | VAL  |
| 2   | Bs    | 135 | THR  |
| 2   | Bs    | 136 | HIS  |
| 2   | Bs    | 145 | LEU  |
| 2   | Bs    | 146 | GLU  |
| 2   | Bs    | 156 | SER  |
| 2   | Bs    | 157 | VAL  |
| 2   | Bs    | 161 | GLN  |
| 2   | Bs    | 166 | ARG  |
| 2   | Bs    | 167 | THR  |
| 2   | Bs    | 168 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Bs    | 193 | THR  |
| 2   | Bs    | 194 | ILE  |
| 2   | Bs    | 197 | LEU  |
| 2   | Bs    | 212 | THR  |
| 2   | Bt    | 45  | SER  |
| 2   | Bt    | 49  | ASP  |
| 2   | Bt    | 53  | ARG  |
| 2   | Bt    | 58  | LEU  |
| 2   | Bt    | 70  | PRO  |
| 2   | Bt    | 73  | GLN  |
| 2   | Bt    | 86  | ASP  |
| 2   | Bt    | 88  | LEU  |
| 2   | Bt    | 93  | SER  |
| 2   | Bt    | 110 | VAL  |
| 2   | Bt    | 114 | VAL  |
| 2   | Bt    | 126 | VAL  |
| 2   | Bt    | 135 | THR  |
| 2   | Bt    | 136 | HIS  |
| 2   | Bt    | 145 | LEU  |
| 2   | Bt    | 146 | GLU  |
| 2   | Bt    | 156 | SER  |
| 2   | Bt    | 157 | VAL  |
| 2   | Bt    | 161 | GLN  |
| 2   | Bt    | 166 | ARG  |
| 2   | Bt    | 167 | THR  |
| 2   | Bt    | 168 | ASN  |
| 2   | Bt    | 193 | THR  |
| 2   | Bt    | 194 | ILE  |
| 2   | Bt    | 197 | LEU  |
| 2   | Bt    | 212 | THR  |
| 2   | Bu    | 45  | SER  |
| 2   | Bu    | 49  | ASP  |
| 2   | Bu    | 53  | ARG  |
| 2   | Bu    | 58  | LEU  |
| 2   | Bu    | 70  | PRO  |
| 2   | Bu    | 73  | GLN  |
| 2   | Bu    | 86  | ASP  |
| 2   | Bu    | 88  | LEU  |
| 2   | Bu    | 93  | SER  |
| 2   | Bu    | 110 | VAL  |
| 2   | Bu    | 114 | VAL  |
| 2   | Bu    | 126 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Bu    | 135 | THR  |
| 2   | Bu    | 136 | HIS  |
| 2   | Bu    | 145 | LEU  |
| 2   | Bu    | 146 | GLU  |
| 2   | Bu    | 156 | SER  |
| 2   | Bu    | 157 | VAL  |
| 2   | Bu    | 161 | GLN  |
| 2   | Bu    | 166 | ARG  |
| 2   | Bu    | 167 | THR  |
| 2   | Bu    | 168 | ASN  |
| 2   | Bu    | 193 | THR  |
| 2   | Bu    | 194 | ILE  |
| 2   | Bu    | 197 | LEU  |
| 2   | Bu    | 212 | THR  |
| 2   | Bv    | 45  | SER  |
| 2   | Bv    | 49  | ASP  |
| 2   | Bv    | 53  | ARG  |
| 2   | Bv    | 58  | LEU  |
| 2   | Bv    | 70  | PRO  |
| 2   | Bv    | 73  | GLN  |
| 2   | Bv    | 86  | ASP  |
| 2   | Bv    | 88  | LEU  |
| 2   | Bv    | 93  | SER  |
| 2   | Bv    | 110 | VAL  |
| 2   | Bv    | 114 | VAL  |
| 2   | Bv    | 126 | VAL  |
| 2   | Bv    | 135 | THR  |
| 2   | Bv    | 136 | HIS  |
| 2   | Bv    | 145 | LEU  |
| 2   | Bv    | 146 | GLU  |
| 2   | Bv    | 156 | SER  |
| 2   | Bv    | 157 | VAL  |
| 2   | Bv    | 161 | GLN  |
| 2   | Bv    | 166 | ARG  |
| 2   | Bv    | 167 | THR  |
| 2   | Bv    | 168 | ASN  |
| 2   | Bv    | 193 | THR  |
| 2   | Bv    | 194 | ILE  |
| 2   | Bv    | 197 | LEU  |
| 2   | Bv    | 212 | THR  |
| 2   | Bw    | 45  | SER  |
| 2   | Bw    | 49  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Bw    | 53  | ARG  |
| 2   | Bw    | 58  | LEU  |
| 2   | Bw    | 70  | PRO  |
| 2   | Bw    | 73  | GLN  |
| 2   | Bw    | 86  | ASP  |
| 2   | Bw    | 88  | LEU  |
| 2   | Bw    | 93  | SER  |
| 2   | Bw    | 110 | VAL  |
| 2   | Bw    | 114 | VAL  |
| 2   | Bw    | 126 | VAL  |
| 2   | Bw    | 135 | THR  |
| 2   | Bw    | 136 | HIS  |
| 2   | Bw    | 145 | LEU  |
| 2   | Bw    | 146 | GLU  |
| 2   | Bw    | 156 | SER  |
| 2   | Bw    | 157 | VAL  |
| 2   | Bw    | 161 | GLN  |
| 2   | Bw    | 166 | ARG  |
| 2   | Bw    | 167 | THR  |
| 2   | Bw    | 168 | ASN  |
| 2   | Bw    | 193 | THR  |
| 2   | Bw    | 194 | ILE  |
| 2   | Bw    | 197 | LEU  |
| 2   | Bw    | 212 | THR  |
| 2   | Bx    | 45  | SER  |
| 2   | Bx    | 49  | ASP  |
| 2   | Bx    | 53  | ARG  |
| 2   | Bx    | 58  | LEU  |
| 2   | Bx    | 70  | PRO  |
| 2   | Bx    | 73  | GLN  |
| 2   | Bx    | 86  | ASP  |
| 2   | Bx    | 88  | LEU  |
| 2   | Bx    | 93  | SER  |
| 2   | Bx    | 110 | VAL  |
| 2   | Bx    | 114 | VAL  |
| 2   | Bx    | 126 | VAL  |
| 2   | Bx    | 135 | THR  |
| 2   | Bx    | 136 | HIS  |
| 2   | Bx    | 145 | LEU  |
| 2   | Bx    | 146 | GLU  |
| 2   | Bx    | 156 | SER  |
| 2   | Bx    | 157 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Bx    | 161 | GLN  |
| 2   | Bx    | 166 | ARG  |
| 2   | Bx    | 167 | THR  |
| 2   | Bx    | 168 | ASN  |
| 2   | Bx    | 193 | THR  |
| 2   | Bx    | 194 | ILE  |
| 2   | Bx    | 197 | LEU  |
| 2   | Bx    | 212 | THR  |
| 3   | CA    | 5   | VAL  |
| 3   | CA    | 8   | VAL  |
| 3   | CA    | 11  | SER  |
| 3   | CA    | 16  | SER  |
| 3   | CA    | 18  | VAL  |
| 3   | CA    | 23  | THR  |
| 3   | CA    | 31  | VAL  |
| 3   | CA    | 35  | GLN  |
| 3   | CA    | 36  | VAL  |
| 3   | CA    | 42  | ASN  |
| 3   | CA    | 50  | THR  |
| 3   | CA    | 56  | ILE  |
| 3   | CA    | 59  | LYS  |
| 3   | CA    | 64  | VAL  |
| 3   | CA    | 73  | LEU  |
| 3   | CA    | 76  | MET  |
| 3   | CA    | 77  | ASP  |
| 3   | CA    | 80  | LEU  |
| 3   | CA    | 93  | LEU  |
| 3   | CA    | 116 | THR  |
| 3   | CA    | 122 | VAL  |
| 3   | CA    | 129 | SER  |
| 3   | CA    | 135 | ARG  |
| 3   | CA    | 139 | MET  |
| 3   | CA    | 151 | ASN  |
| 3   | CA    | 157 | ASN  |
| 3   | CA    | 161 | SER  |
| 3   | CA    | 175 | THR  |
| 3   | CA    | 176 | VAL  |
| 3   | CA    | 178 | ASN  |
| 3   | CA    | 179 | VAL  |
| 3   | CA    | 183 | LEU  |
| 3   | CA    | 188 | LEU  |
| 3   | CA    | 192 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CA    | 194 | THR  |
| 3   | CA    | 196 | ILE  |
| 3   | CA    | 206 | VAL  |
| 3   | CA    | 208 | VAL  |
| 3   | CA    | 216 | LEU  |
| 3   | CA    | 217 | ARG  |
| 3   | CB    | 5   | VAL  |
| 3   | CB    | 8   | VAL  |
| 3   | CB    | 11  | SER  |
| 3   | CB    | 16  | SER  |
| 3   | CB    | 18  | VAL  |
| 3   | CB    | 23  | THR  |
| 3   | CB    | 31  | VAL  |
| 3   | CB    | 35  | GLN  |
| 3   | CB    | 36  | VAL  |
| 3   | CB    | 42  | ASN  |
| 3   | CB    | 50  | THR  |
| 3   | CB    | 56  | ILE  |
| 3   | CB    | 59  | LYS  |
| 3   | CB    | 64  | VAL  |
| 3   | CB    | 73  | LEU  |
| 3   | CB    | 76  | MET  |
| 3   | CB    | 77  | ASP  |
| 3   | CB    | 80  | LEU  |
| 3   | CB    | 93  | LEU  |
| 3   | CB    | 116 | THR  |
| 3   | CB    | 122 | VAL  |
| 3   | CB    | 129 | SER  |
| 3   | CB    | 135 | ARG  |
| 3   | CB    | 139 | MET  |
| 3   | CB    | 151 | ASN  |
| 3   | CB    | 157 | ASN  |
| 3   | CB    | 161 | SER  |
| 3   | CB    | 175 | THR  |
| 3   | CB    | 176 | VAL  |
| 3   | CB    | 178 | ASN  |
| 3   | CB    | 179 | VAL  |
| 3   | CB    | 183 | LEU  |
| 3   | CB    | 188 | LEU  |
| 3   | CB    | 192 | THR  |
| 3   | CB    | 194 | THR  |
| 3   | CB    | 196 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CB    | 206 | VAL  |
| 3   | CB    | 208 | VAL  |
| 3   | CB    | 216 | LEU  |
| 3   | CB    | 217 | ARG  |
| 3   | CC    | 5   | VAL  |
| 3   | CC    | 8   | VAL  |
| 3   | CC    | 11  | SER  |
| 3   | CC    | 16  | SER  |
| 3   | CC    | 18  | VAL  |
| 3   | CC    | 23  | THR  |
| 3   | CC    | 31  | VAL  |
| 3   | CC    | 35  | GLN  |
| 3   | CC    | 36  | VAL  |
| 3   | CC    | 42  | ASN  |
| 3   | CC    | 50  | THR  |
| 3   | CC    | 56  | ILE  |
| 3   | CC    | 59  | LYS  |
| 3   | CC    | 64  | VAL  |
| 3   | CC    | 73  | LEU  |
| 3   | CC    | 76  | MET  |
| 3   | CC    | 77  | ASP  |
| 3   | CC    | 80  | LEU  |
| 3   | CC    | 93  | LEU  |
| 3   | CC    | 116 | THR  |
| 3   | CC    | 122 | VAL  |
| 3   | CC    | 129 | SER  |
| 3   | CC    | 135 | ARG  |
| 3   | CC    | 139 | MET  |
| 3   | CC    | 151 | ASN  |
| 3   | CC    | 157 | ASN  |
| 3   | CC    | 161 | SER  |
| 3   | CC    | 175 | THR  |
| 3   | CC    | 176 | VAL  |
| 3   | CC    | 178 | ASN  |
| 3   | CC    | 179 | VAL  |
| 3   | CC    | 183 | LEU  |
| 3   | CC    | 188 | LEU  |
| 3   | CC    | 192 | THR  |
| 3   | CC    | 194 | THR  |
| 3   | CC    | 196 | ILE  |
| 3   | CC    | 206 | VAL  |
| 3   | CC    | 208 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CC    | 216 | LEU  |
| 3   | CC    | 217 | ARG  |
| 3   | CD    | 5   | VAL  |
| 3   | CD    | 8   | VAL  |
| 3   | CD    | 11  | SER  |
| 3   | CD    | 16  | SER  |
| 3   | CD    | 18  | VAL  |
| 3   | CD    | 23  | THR  |
| 3   | CD    | 31  | VAL  |
| 3   | CD    | 35  | GLN  |
| 3   | CD    | 36  | VAL  |
| 3   | CD    | 42  | ASN  |
| 3   | CD    | 50  | THR  |
| 3   | CD    | 56  | ILE  |
| 3   | CD    | 59  | LYS  |
| 3   | CD    | 64  | VAL  |
| 3   | CD    | 73  | LEU  |
| 3   | CD    | 76  | MET  |
| 3   | CD    | 77  | ASP  |
| 3   | CD    | 80  | LEU  |
| 3   | CD    | 93  | LEU  |
| 3   | CD    | 116 | THR  |
| 3   | CD    | 122 | VAL  |
| 3   | CD    | 129 | SER  |
| 3   | CD    | 135 | ARG  |
| 3   | CD    | 139 | MET  |
| 3   | CD    | 151 | ASN  |
| 3   | CD    | 157 | ASN  |
| 3   | CD    | 161 | SER  |
| 3   | CD    | 175 | THR  |
| 3   | CD    | 176 | VAL  |
| 3   | CD    | 178 | ASN  |
| 3   | CD    | 179 | VAL  |
| 3   | CD    | 183 | LEU  |
| 3   | CD    | 188 | LEU  |
| 3   | CD    | 192 | THR  |
| 3   | CD    | 194 | THR  |
| 3   | CD    | 196 | ILE  |
| 3   | CD    | 206 | VAL  |
| 3   | CD    | 208 | VAL  |
| 3   | CD    | 216 | LEU  |
| 3   | CD    | 217 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CE    | 5   | VAL  |
| 3   | CE    | 8   | VAL  |
| 3   | CE    | 11  | SER  |
| 3   | CE    | 16  | SER  |
| 3   | CE    | 18  | VAL  |
| 3   | CE    | 23  | THR  |
| 3   | CE    | 31  | VAL  |
| 3   | CE    | 35  | GLN  |
| 3   | CE    | 36  | VAL  |
| 3   | CE    | 42  | ASN  |
| 3   | CE    | 50  | THR  |
| 3   | CE    | 56  | ILE  |
| 3   | CE    | 59  | LYS  |
| 3   | CE    | 64  | VAL  |
| 3   | CE    | 73  | LEU  |
| 3   | CE    | 76  | MET  |
| 3   | CE    | 77  | ASP  |
| 3   | CE    | 80  | LEU  |
| 3   | CE    | 93  | LEU  |
| 3   | CE    | 116 | THR  |
| 3   | CE    | 122 | VAL  |
| 3   | CE    | 129 | SER  |
| 3   | CE    | 135 | ARG  |
| 3   | CE    | 139 | MET  |
| 3   | CE    | 151 | ASN  |
| 3   | CE    | 157 | ASN  |
| 3   | CE    | 161 | SER  |
| 3   | CE    | 175 | THR  |
| 3   | CE    | 176 | VAL  |
| 3   | CE    | 178 | ASN  |
| 3   | CE    | 179 | VAL  |
| 3   | CE    | 183 | LEU  |
| 3   | CE    | 188 | LEU  |
| 3   | CE    | 192 | THR  |
| 3   | CE    | 194 | THR  |
| 3   | CE    | 196 | ILE  |
| 3   | CE    | 206 | VAL  |
| 3   | CE    | 208 | VAL  |
| 3   | CE    | 216 | LEU  |
| 3   | CE    | 217 | ARG  |
| 3   | CF    | 5   | VAL  |
| 3   | CF    | 8   | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CF    | 11  | SER  |
| 3   | CF    | 16  | SER  |
| 3   | CF    | 18  | VAL  |
| 3   | CF    | 23  | THR  |
| 3   | CF    | 31  | VAL  |
| 3   | CF    | 35  | GLN  |
| 3   | CF    | 36  | VAL  |
| 3   | CF    | 42  | ASN  |
| 3   | CF    | 50  | THR  |
| 3   | CF    | 56  | ILE  |
| 3   | CF    | 59  | LYS  |
| 3   | CF    | 64  | VAL  |
| 3   | CF    | 73  | LEU  |
| 3   | CF    | 76  | MET  |
| 3   | CF    | 77  | ASP  |
| 3   | CF    | 80  | LEU  |
| 3   | CF    | 93  | LEU  |
| 3   | CF    | 116 | THR  |
| 3   | CF    | 122 | VAL  |
| 3   | CF    | 129 | SER  |
| 3   | CF    | 135 | ARG  |
| 3   | CF    | 139 | MET  |
| 3   | CF    | 151 | ASN  |
| 3   | CF    | 157 | ASN  |
| 3   | CF    | 161 | SER  |
| 3   | CF    | 175 | THR  |
| 3   | CF    | 176 | VAL  |
| 3   | CF    | 178 | ASN  |
| 3   | CF    | 179 | VAL  |
| 3   | CF    | 183 | LEU  |
| 3   | CF    | 188 | LEU  |
| 3   | CF    | 192 | THR  |
| 3   | CF    | 194 | THR  |
| 3   | CF    | 196 | ILE  |
| 3   | CF    | 206 | VAL  |
| 3   | CF    | 208 | VAL  |
| 3   | CF    | 216 | LEU  |
| 3   | CF    | 217 | ARG  |
| 3   | CG    | 5   | VAL  |
| 3   | CG    | 8   | VAL  |
| 3   | CG    | 11  | SER  |
| 3   | CG    | 16  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CG    | 18  | VAL  |
| 3   | CG    | 23  | THR  |
| 3   | CG    | 31  | VAL  |
| 3   | CG    | 35  | GLN  |
| 3   | CG    | 36  | VAL  |
| 3   | CG    | 42  | ASN  |
| 3   | CG    | 50  | THR  |
| 3   | CG    | 56  | ILE  |
| 3   | CG    | 59  | LYS  |
| 3   | CG    | 64  | VAL  |
| 3   | CG    | 73  | LEU  |
| 3   | CG    | 76  | MET  |
| 3   | CG    | 77  | ASP  |
| 3   | CG    | 80  | LEU  |
| 3   | CG    | 93  | LEU  |
| 3   | CG    | 116 | THR  |
| 3   | CG    | 122 | VAL  |
| 3   | CG    | 129 | SER  |
| 3   | CG    | 135 | ARG  |
| 3   | CG    | 139 | MET  |
| 3   | CG    | 151 | ASN  |
| 3   | CG    | 157 | ASN  |
| 3   | CG    | 161 | SER  |
| 3   | CG    | 175 | THR  |
| 3   | CG    | 176 | VAL  |
| 3   | CG    | 178 | ASN  |
| 3   | CG    | 179 | VAL  |
| 3   | CG    | 183 | LEU  |
| 3   | CG    | 188 | LEU  |
| 3   | CG    | 192 | THR  |
| 3   | CG    | 194 | THR  |
| 3   | CG    | 196 | ILE  |
| 3   | CG    | 206 | VAL  |
| 3   | CG    | 208 | VAL  |
| 3   | CG    | 216 | LEU  |
| 3   | CG    | 217 | ARG  |
| 3   | CH    | 5   | VAL  |
| 3   | CH    | 8   | VAL  |
| 3   | CH    | 11  | SER  |
| 3   | CH    | 16  | SER  |
| 3   | CH    | 18  | VAL  |
| 3   | CH    | 23  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CH    | 31  | VAL  |
| 3   | CH    | 35  | GLN  |
| 3   | CH    | 36  | VAL  |
| 3   | CH    | 42  | ASN  |
| 3   | CH    | 50  | THR  |
| 3   | CH    | 56  | ILE  |
| 3   | CH    | 59  | LYS  |
| 3   | CH    | 64  | VAL  |
| 3   | CH    | 73  | LEU  |
| 3   | CH    | 76  | MET  |
| 3   | CH    | 77  | ASP  |
| 3   | CH    | 80  | LEU  |
| 3   | CH    | 93  | LEU  |
| 3   | CH    | 116 | THR  |
| 3   | CH    | 122 | VAL  |
| 3   | CH    | 129 | SER  |
| 3   | CH    | 135 | ARG  |
| 3   | CH    | 139 | MET  |
| 3   | CH    | 151 | ASN  |
| 3   | CH    | 157 | ASN  |
| 3   | CH    | 161 | SER  |
| 3   | CH    | 175 | THR  |
| 3   | CH    | 176 | VAL  |
| 3   | CH    | 178 | ASN  |
| 3   | CH    | 179 | VAL  |
| 3   | CH    | 183 | LEU  |
| 3   | CH    | 188 | LEU  |
| 3   | CH    | 192 | THR  |
| 3   | CH    | 194 | THR  |
| 3   | CH    | 196 | ILE  |
| 3   | CH    | 206 | VAL  |
| 3   | CH    | 208 | VAL  |
| 3   | CH    | 216 | LEU  |
| 3   | CH    | 217 | ARG  |
| 3   | CI    | 5   | VAL  |
| 3   | CI    | 8   | VAL  |
| 3   | CI    | 11  | SER  |
| 3   | CI    | 16  | SER  |
| 3   | CI    | 18  | VAL  |
| 3   | CI    | 23  | THR  |
| 3   | CI    | 31  | VAL  |
| 3   | CI    | 35  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CI    | 36  | VAL  |
| 3   | CI    | 42  | ASN  |
| 3   | CI    | 50  | THR  |
| 3   | CI    | 56  | ILE  |
| 3   | CI    | 59  | LYS  |
| 3   | CI    | 64  | VAL  |
| 3   | CI    | 73  | LEU  |
| 3   | CI    | 76  | MET  |
| 3   | CI    | 77  | ASP  |
| 3   | CI    | 80  | LEU  |
| 3   | CI    | 93  | LEU  |
| 3   | CI    | 116 | THR  |
| 3   | CI    | 122 | VAL  |
| 3   | CI    | 129 | SER  |
| 3   | CI    | 135 | ARG  |
| 3   | CI    | 139 | MET  |
| 3   | CI    | 151 | ASN  |
| 3   | CI    | 157 | ASN  |
| 3   | CI    | 161 | SER  |
| 3   | CI    | 175 | THR  |
| 3   | CI    | 176 | VAL  |
| 3   | CI    | 178 | ASN  |
| 3   | CI    | 179 | VAL  |
| 3   | CI    | 183 | LEU  |
| 3   | CI    | 188 | LEU  |
| 3   | CI    | 192 | THR  |
| 3   | CI    | 194 | THR  |
| 3   | CI    | 196 | ILE  |
| 3   | CI    | 206 | VAL  |
| 3   | CI    | 208 | VAL  |
| 3   | CI    | 216 | LEU  |
| 3   | CI    | 217 | ARG  |
| 3   | CJ    | 5   | VAL  |
| 3   | CJ    | 8   | VAL  |
| 3   | CJ    | 11  | SER  |
| 3   | CJ    | 16  | SER  |
| 3   | CJ    | 18  | VAL  |
| 3   | CJ    | 23  | THR  |
| 3   | CJ    | 31  | VAL  |
| 3   | CJ    | 35  | GLN  |
| 3   | CJ    | 36  | VAL  |
| 3   | CJ    | 42  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CJ    | 50  | THR  |
| 3   | CJ    | 56  | ILE  |
| 3   | CJ    | 59  | LYS  |
| 3   | CJ    | 64  | VAL  |
| 3   | CJ    | 73  | LEU  |
| 3   | CJ    | 76  | MET  |
| 3   | CJ    | 77  | ASP  |
| 3   | CJ    | 80  | LEU  |
| 3   | CJ    | 93  | LEU  |
| 3   | CJ    | 116 | THR  |
| 3   | CJ    | 122 | VAL  |
| 3   | CJ    | 129 | SER  |
| 3   | CJ    | 135 | ARG  |
| 3   | CJ    | 139 | MET  |
| 3   | CJ    | 151 | ASN  |
| 3   | CJ    | 157 | ASN  |
| 3   | CJ    | 161 | SER  |
| 3   | CJ    | 175 | THR  |
| 3   | CJ    | 176 | VAL  |
| 3   | CJ    | 178 | ASN  |
| 3   | CJ    | 179 | VAL  |
| 3   | CJ    | 183 | LEU  |
| 3   | CJ    | 188 | LEU  |
| 3   | CJ    | 192 | THR  |
| 3   | CJ    | 194 | THR  |
| 3   | CJ    | 196 | ILE  |
| 3   | CJ    | 206 | VAL  |
| 3   | CJ    | 208 | VAL  |
| 3   | CJ    | 216 | LEU  |
| 3   | CJ    | 217 | ARG  |
| 3   | CK    | 5   | VAL  |
| 3   | CK    | 8   | VAL  |
| 3   | CK    | 11  | SER  |
| 3   | CK    | 16  | SER  |
| 3   | CK    | 18  | VAL  |
| 3   | CK    | 23  | THR  |
| 3   | CK    | 31  | VAL  |
| 3   | CK    | 35  | GLN  |
| 3   | CK    | 36  | VAL  |
| 3   | CK    | 42  | ASN  |
| 3   | CK    | 50  | THR  |
| 3   | CK    | 56  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CK    | 59  | LYS  |
| 3   | CK    | 64  | VAL  |
| 3   | CK    | 73  | LEU  |
| 3   | CK    | 76  | MET  |
| 3   | CK    | 77  | ASP  |
| 3   | CK    | 80  | LEU  |
| 3   | CK    | 93  | LEU  |
| 3   | CK    | 116 | THR  |
| 3   | CK    | 122 | VAL  |
| 3   | CK    | 129 | SER  |
| 3   | CK    | 135 | ARG  |
| 3   | CK    | 139 | MET  |
| 3   | CK    | 151 | ASN  |
| 3   | CK    | 157 | ASN  |
| 3   | CK    | 161 | SER  |
| 3   | CK    | 175 | THR  |
| 3   | CK    | 176 | VAL  |
| 3   | CK    | 178 | ASN  |
| 3   | CK    | 179 | VAL  |
| 3   | CK    | 183 | LEU  |
| 3   | CK    | 188 | LEU  |
| 3   | CK    | 192 | THR  |
| 3   | CK    | 194 | THR  |
| 3   | CK    | 196 | ILE  |
| 3   | CK    | 206 | VAL  |
| 3   | CK    | 208 | VAL  |
| 3   | CK    | 216 | LEU  |
| 3   | CK    | 217 | ARG  |
| 3   | CL    | 5   | VAL  |
| 3   | CL    | 8   | VAL  |
| 3   | CL    | 11  | SER  |
| 3   | CL    | 16  | SER  |
| 3   | CL    | 18  | VAL  |
| 3   | CL    | 23  | THR  |
| 3   | CL    | 31  | VAL  |
| 3   | CL    | 35  | GLN  |
| 3   | CL    | 36  | VAL  |
| 3   | CL    | 42  | ASN  |
| 3   | CL    | 50  | THR  |
| 3   | CL    | 56  | ILE  |
| 3   | CL    | 59  | LYS  |
| 3   | CL    | 64  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CL    | 73  | LEU  |
| 3   | CL    | 76  | MET  |
| 3   | CL    | 77  | ASP  |
| 3   | CL    | 80  | LEU  |
| 3   | CL    | 93  | LEU  |
| 3   | CL    | 116 | THR  |
| 3   | CL    | 122 | VAL  |
| 3   | CL    | 129 | SER  |
| 3   | CL    | 135 | ARG  |
| 3   | CL    | 139 | MET  |
| 3   | CL    | 151 | ASN  |
| 3   | CL    | 157 | ASN  |
| 3   | CL    | 161 | SER  |
| 3   | CL    | 175 | THR  |
| 3   | CL    | 176 | VAL  |
| 3   | CL    | 178 | ASN  |
| 3   | CL    | 179 | VAL  |
| 3   | CL    | 183 | LEU  |
| 3   | CL    | 188 | LEU  |
| 3   | CL    | 192 | THR  |
| 3   | CL    | 194 | THR  |
| 3   | CL    | 196 | ILE  |
| 3   | CL    | 206 | VAL  |
| 3   | CL    | 208 | VAL  |
| 3   | CL    | 216 | LEU  |
| 3   | CL    | 217 | ARG  |
| 3   | CM    | 5   | VAL  |
| 3   | CM    | 8   | VAL  |
| 3   | CM    | 11  | SER  |
| 3   | CM    | 16  | SER  |
| 3   | CM    | 18  | VAL  |
| 3   | CM    | 23  | THR  |
| 3   | CM    | 31  | VAL  |
| 3   | CM    | 35  | GLN  |
| 3   | CM    | 36  | VAL  |
| 3   | CM    | 42  | ASN  |
| 3   | CM    | 50  | THR  |
| 3   | CM    | 56  | ILE  |
| 3   | CM    | 59  | LYS  |
| 3   | CM    | 64  | VAL  |
| 3   | CM    | 73  | LEU  |
| 3   | CM    | 76  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CM    | 77  | ASP  |
| 3   | CM    | 80  | LEU  |
| 3   | CM    | 93  | LEU  |
| 3   | CM    | 116 | THR  |
| 3   | CM    | 122 | VAL  |
| 3   | CM    | 129 | SER  |
| 3   | CM    | 135 | ARG  |
| 3   | CM    | 139 | MET  |
| 3   | CM    | 151 | ASN  |
| 3   | CM    | 157 | ASN  |
| 3   | CM    | 161 | SER  |
| 3   | CM    | 175 | THR  |
| 3   | CM    | 176 | VAL  |
| 3   | CM    | 178 | ASN  |
| 3   | CM    | 179 | VAL  |
| 3   | CM    | 183 | LEU  |
| 3   | CM    | 188 | LEU  |
| 3   | CM    | 192 | THR  |
| 3   | CM    | 194 | THR  |
| 3   | CM    | 196 | ILE  |
| 3   | CM    | 206 | VAL  |
| 3   | CM    | 208 | VAL  |
| 3   | CM    | 216 | LEU  |
| 3   | CM    | 217 | ARG  |
| 3   | CN    | 5   | VAL  |
| 3   | CN    | 8   | VAL  |
| 3   | CN    | 11  | SER  |
| 3   | CN    | 16  | SER  |
| 3   | CN    | 18  | VAL  |
| 3   | CN    | 23  | THR  |
| 3   | CN    | 31  | VAL  |
| 3   | CN    | 35  | GLN  |
| 3   | CN    | 36  | VAL  |
| 3   | CN    | 42  | ASN  |
| 3   | CN    | 50  | THR  |
| 3   | CN    | 56  | ILE  |
| 3   | CN    | 59  | LYS  |
| 3   | CN    | 64  | VAL  |
| 3   | CN    | 73  | LEU  |
| 3   | CN    | 76  | MET  |
| 3   | CN    | 77  | ASP  |
| 3   | CN    | 80  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CN    | 93  | LEU  |
| 3   | CN    | 116 | THR  |
| 3   | CN    | 122 | VAL  |
| 3   | CN    | 129 | SER  |
| 3   | CN    | 135 | ARG  |
| 3   | CN    | 139 | MET  |
| 3   | CN    | 151 | ASN  |
| 3   | CN    | 157 | ASN  |
| 3   | CN    | 161 | SER  |
| 3   | CN    | 175 | THR  |
| 3   | CN    | 176 | VAL  |
| 3   | CN    | 178 | ASN  |
| 3   | CN    | 179 | VAL  |
| 3   | CN    | 183 | LEU  |
| 3   | CN    | 188 | LEU  |
| 3   | CN    | 192 | THR  |
| 3   | CN    | 194 | THR  |
| 3   | CN    | 196 | ILE  |
| 3   | CN    | 206 | VAL  |
| 3   | CN    | 208 | VAL  |
| 3   | CN    | 216 | LEU  |
| 3   | CN    | 217 | ARG  |
| 3   | CO    | 5   | VAL  |
| 3   | CO    | 8   | VAL  |
| 3   | CO    | 11  | SER  |
| 3   | CO    | 16  | SER  |
| 3   | CO    | 18  | VAL  |
| 3   | CO    | 23  | THR  |
| 3   | CO    | 31  | VAL  |
| 3   | CO    | 35  | GLN  |
| 3   | CO    | 36  | VAL  |
| 3   | CO    | 42  | ASN  |
| 3   | CO    | 50  | THR  |
| 3   | CO    | 56  | ILE  |
| 3   | CO    | 59  | LYS  |
| 3   | CO    | 64  | VAL  |
| 3   | CO    | 73  | LEU  |
| 3   | CO    | 76  | MET  |
| 3   | CO    | 77  | ASP  |
| 3   | CO    | 80  | LEU  |
| 3   | CO    | 93  | LEU  |
| 3   | CO    | 116 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CO    | 122 | VAL  |
| 3   | CO    | 129 | SER  |
| 3   | CO    | 135 | ARG  |
| 3   | CO    | 139 | MET  |
| 3   | CO    | 151 | ASN  |
| 3   | CO    | 157 | ASN  |
| 3   | CO    | 161 | SER  |
| 3   | CO    | 175 | THR  |
| 3   | CO    | 176 | VAL  |
| 3   | CO    | 178 | ASN  |
| 3   | CO    | 179 | VAL  |
| 3   | CO    | 183 | LEU  |
| 3   | CO    | 188 | LEU  |
| 3   | CO    | 192 | THR  |
| 3   | CO    | 194 | THR  |
| 3   | CO    | 196 | ILE  |
| 3   | CO    | 206 | VAL  |
| 3   | CO    | 208 | VAL  |
| 3   | CO    | 216 | LEU  |
| 3   | CO    | 217 | ARG  |
| 3   | CP    | 5   | VAL  |
| 3   | CP    | 8   | VAL  |
| 3   | CP    | 11  | SER  |
| 3   | CP    | 16  | SER  |
| 3   | CP    | 18  | VAL  |
| 3   | CP    | 23  | THR  |
| 3   | CP    | 31  | VAL  |
| 3   | CP    | 35  | GLN  |
| 3   | CP    | 36  | VAL  |
| 3   | CP    | 42  | ASN  |
| 3   | CP    | 50  | THR  |
| 3   | CP    | 56  | ILE  |
| 3   | CP    | 59  | LYS  |
| 3   | CP    | 64  | VAL  |
| 3   | CP    | 73  | LEU  |
| 3   | CP    | 76  | MET  |
| 3   | CP    | 77  | ASP  |
| 3   | CP    | 80  | LEU  |
| 3   | CP    | 93  | LEU  |
| 3   | CP    | 116 | THR  |
| 3   | CP    | 122 | VAL  |
| 3   | CP    | 129 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CP    | 135 | ARG  |
| 3   | CP    | 139 | MET  |
| 3   | CP    | 151 | ASN  |
| 3   | CP    | 157 | ASN  |
| 3   | CP    | 161 | SER  |
| 3   | CP    | 175 | THR  |
| 3   | CP    | 176 | VAL  |
| 3   | CP    | 178 | ASN  |
| 3   | CP    | 179 | VAL  |
| 3   | CP    | 183 | LEU  |
| 3   | CP    | 188 | LEU  |
| 3   | CP    | 192 | THR  |
| 3   | CP    | 194 | THR  |
| 3   | CP    | 196 | ILE  |
| 3   | CP    | 206 | VAL  |
| 3   | CP    | 208 | VAL  |
| 3   | CP    | 216 | LEU  |
| 3   | CP    | 217 | ARG  |
| 3   | CQ    | 5   | VAL  |
| 3   | CQ    | 8   | VAL  |
| 3   | CQ    | 11  | SER  |
| 3   | CQ    | 16  | SER  |
| 3   | CQ    | 18  | VAL  |
| 3   | CQ    | 23  | THR  |
| 3   | CQ    | 31  | VAL  |
| 3   | CQ    | 35  | GLN  |
| 3   | CQ    | 36  | VAL  |
| 3   | CQ    | 42  | ASN  |
| 3   | CQ    | 50  | THR  |
| 3   | CQ    | 56  | ILE  |
| 3   | CQ    | 59  | LYS  |
| 3   | CQ    | 64  | VAL  |
| 3   | CQ    | 73  | LEU  |
| 3   | CQ    | 76  | MET  |
| 3   | CQ    | 77  | ASP  |
| 3   | CQ    | 80  | LEU  |
| 3   | CQ    | 93  | LEU  |
| 3   | CQ    | 116 | THR  |
| 3   | CQ    | 122 | VAL  |
| 3   | CQ    | 129 | SER  |
| 3   | CQ    | 135 | ARG  |
| 3   | CQ    | 139 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CQ    | 151 | ASN  |
| 3   | CQ    | 157 | ASN  |
| 3   | CQ    | 161 | SER  |
| 3   | CQ    | 175 | THR  |
| 3   | CQ    | 176 | VAL  |
| 3   | CQ    | 178 | ASN  |
| 3   | CQ    | 179 | VAL  |
| 3   | CQ    | 183 | LEU  |
| 3   | CQ    | 188 | LEU  |
| 3   | CQ    | 192 | THR  |
| 3   | CQ    | 194 | THR  |
| 3   | CQ    | 196 | ILE  |
| 3   | CQ    | 206 | VAL  |
| 3   | CQ    | 208 | VAL  |
| 3   | CQ    | 216 | LEU  |
| 3   | CQ    | 217 | ARG  |
| 3   | CR    | 5   | VAL  |
| 3   | CR    | 8   | VAL  |
| 3   | CR    | 11  | SER  |
| 3   | CR    | 16  | SER  |
| 3   | CR    | 18  | VAL  |
| 3   | CR    | 23  | THR  |
| 3   | CR    | 31  | VAL  |
| 3   | CR    | 35  | GLN  |
| 3   | CR    | 36  | VAL  |
| 3   | CR    | 42  | ASN  |
| 3   | CR    | 50  | THR  |
| 3   | CR    | 56  | ILE  |
| 3   | CR    | 59  | LYS  |
| 3   | CR    | 64  | VAL  |
| 3   | CR    | 73  | LEU  |
| 3   | CR    | 76  | MET  |
| 3   | CR    | 77  | ASP  |
| 3   | CR    | 80  | LEU  |
| 3   | CR    | 93  | LEU  |
| 3   | CR    | 116 | THR  |
| 3   | CR    | 122 | VAL  |
| 3   | CR    | 129 | SER  |
| 3   | CR    | 135 | ARG  |
| 3   | CR    | 139 | MET  |
| 3   | CR    | 151 | ASN  |
| 3   | CR    | 157 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CR    | 161 | SER  |
| 3   | CR    | 175 | THR  |
| 3   | CR    | 176 | VAL  |
| 3   | CR    | 178 | ASN  |
| 3   | CR    | 179 | VAL  |
| 3   | CR    | 183 | LEU  |
| 3   | CR    | 188 | LEU  |
| 3   | CR    | 192 | THR  |
| 3   | CR    | 194 | THR  |
| 3   | CR    | 196 | ILE  |
| 3   | CR    | 206 | VAL  |
| 3   | CR    | 208 | VAL  |
| 3   | CR    | 216 | LEU  |
| 3   | CR    | 217 | ARG  |
| 3   | CS    | 5   | VAL  |
| 3   | CS    | 8   | VAL  |
| 3   | CS    | 11  | SER  |
| 3   | CS    | 16  | SER  |
| 3   | CS    | 18  | VAL  |
| 3   | CS    | 23  | THR  |
| 3   | CS    | 31  | VAL  |
| 3   | CS    | 35  | GLN  |
| 3   | CS    | 36  | VAL  |
| 3   | CS    | 42  | ASN  |
| 3   | CS    | 50  | THR  |
| 3   | CS    | 56  | ILE  |
| 3   | CS    | 59  | LYS  |
| 3   | CS    | 64  | VAL  |
| 3   | CS    | 73  | LEU  |
| 3   | CS    | 76  | MET  |
| 3   | CS    | 77  | ASP  |
| 3   | CS    | 80  | LEU  |
| 3   | CS    | 93  | LEU  |
| 3   | CS    | 116 | THR  |
| 3   | CS    | 122 | VAL  |
| 3   | CS    | 129 | SER  |
| 3   | CS    | 135 | ARG  |
| 3   | CS    | 139 | MET  |
| 3   | CS    | 151 | ASN  |
| 3   | CS    | 157 | ASN  |
| 3   | CS    | 161 | SER  |
| 3   | CS    | 175 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CS    | 176 | VAL  |
| 3   | CS    | 178 | ASN  |
| 3   | CS    | 179 | VAL  |
| 3   | CS    | 183 | LEU  |
| 3   | CS    | 188 | LEU  |
| 3   | CS    | 192 | THR  |
| 3   | CS    | 194 | THR  |
| 3   | CS    | 196 | ILE  |
| 3   | CS    | 206 | VAL  |
| 3   | CS    | 208 | VAL  |
| 3   | CS    | 216 | LEU  |
| 3   | CS    | 217 | ARG  |
| 3   | CT    | 5   | VAL  |
| 3   | CT    | 8   | VAL  |
| 3   | CT    | 11  | SER  |
| 3   | CT    | 16  | SER  |
| 3   | CT    | 18  | VAL  |
| 3   | CT    | 23  | THR  |
| 3   | CT    | 31  | VAL  |
| 3   | CT    | 35  | GLN  |
| 3   | CT    | 36  | VAL  |
| 3   | CT    | 42  | ASN  |
| 3   | CT    | 50  | THR  |
| 3   | CT    | 56  | ILE  |
| 3   | CT    | 59  | LYS  |
| 3   | CT    | 64  | VAL  |
| 3   | CT    | 73  | LEU  |
| 3   | CT    | 76  | MET  |
| 3   | CT    | 77  | ASP  |
| 3   | CT    | 80  | LEU  |
| 3   | CT    | 93  | LEU  |
| 3   | CT    | 116 | THR  |
| 3   | CT    | 122 | VAL  |
| 3   | CT    | 129 | SER  |
| 3   | CT    | 135 | ARG  |
| 3   | CT    | 139 | MET  |
| 3   | CT    | 151 | ASN  |
| 3   | CT    | 157 | ASN  |
| 3   | CT    | 161 | SER  |
| 3   | CT    | 175 | THR  |
| 3   | CT    | 176 | VAL  |
| 3   | CT    | 178 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CT    | 179 | VAL  |
| 3   | CT    | 183 | LEU  |
| 3   | CT    | 188 | LEU  |
| 3   | CT    | 192 | THR  |
| 3   | CT    | 194 | THR  |
| 3   | CT    | 196 | ILE  |
| 3   | CT    | 206 | VAL  |
| 3   | CT    | 208 | VAL  |
| 3   | CT    | 216 | LEU  |
| 3   | CT    | 217 | ARG  |
| 3   | CU    | 5   | VAL  |
| 3   | CU    | 8   | VAL  |
| 3   | CU    | 11  | SER  |
| 3   | CU    | 16  | SER  |
| 3   | CU    | 18  | VAL  |
| 3   | CU    | 23  | THR  |
| 3   | CU    | 31  | VAL  |
| 3   | CU    | 35  | GLN  |
| 3   | CU    | 36  | VAL  |
| 3   | CU    | 42  | ASN  |
| 3   | CU    | 50  | THR  |
| 3   | CU    | 56  | ILE  |
| 3   | CU    | 59  | LYS  |
| 3   | CU    | 64  | VAL  |
| 3   | CU    | 73  | LEU  |
| 3   | CU    | 76  | MET  |
| 3   | CU    | 77  | ASP  |
| 3   | CU    | 80  | LEU  |
| 3   | CU    | 93  | LEU  |
| 3   | CU    | 116 | THR  |
| 3   | CU    | 122 | VAL  |
| 3   | CU    | 129 | SER  |
| 3   | CU    | 135 | ARG  |
| 3   | CU    | 139 | MET  |
| 3   | CU    | 151 | ASN  |
| 3   | CU    | 157 | ASN  |
| 3   | CU    | 161 | SER  |
| 3   | CU    | 175 | THR  |
| 3   | CU    | 176 | VAL  |
| 3   | CU    | 178 | ASN  |
| 3   | CU    | 179 | VAL  |
| 3   | CU    | 183 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CU    | 188 | LEU  |
| 3   | CU    | 192 | THR  |
| 3   | CU    | 194 | THR  |
| 3   | CU    | 196 | ILE  |
| 3   | CU    | 206 | VAL  |
| 3   | CU    | 208 | VAL  |
| 3   | CU    | 216 | LEU  |
| 3   | CU    | 217 | ARG  |
| 3   | CV    | 5   | VAL  |
| 3   | CV    | 8   | VAL  |
| 3   | CV    | 11  | SER  |
| 3   | CV    | 16  | SER  |
| 3   | CV    | 18  | VAL  |
| 3   | CV    | 23  | THR  |
| 3   | CV    | 31  | VAL  |
| 3   | CV    | 35  | GLN  |
| 3   | CV    | 36  | VAL  |
| 3   | CV    | 42  | ASN  |
| 3   | CV    | 50  | THR  |
| 3   | CV    | 56  | ILE  |
| 3   | CV    | 59  | LYS  |
| 3   | CV    | 64  | VAL  |
| 3   | CV    | 73  | LEU  |
| 3   | CV    | 76  | MET  |
| 3   | CV    | 77  | ASP  |
| 3   | CV    | 80  | LEU  |
| 3   | CV    | 93  | LEU  |
| 3   | CV    | 116 | THR  |
| 3   | CV    | 122 | VAL  |
| 3   | CV    | 129 | SER  |
| 3   | CV    | 135 | ARG  |
| 3   | CV    | 139 | MET  |
| 3   | CV    | 151 | ASN  |
| 3   | CV    | 157 | ASN  |
| 3   | CV    | 161 | SER  |
| 3   | CV    | 175 | THR  |
| 3   | CV    | 176 | VAL  |
| 3   | CV    | 178 | ASN  |
| 3   | CV    | 179 | VAL  |
| 3   | CV    | 183 | LEU  |
| 3   | CV    | 188 | LEU  |
| 3   | CV    | 192 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CV    | 194 | THR  |
| 3   | CV    | 196 | ILE  |
| 3   | CV    | 206 | VAL  |
| 3   | CV    | 208 | VAL  |
| 3   | CV    | 216 | LEU  |
| 3   | CV    | 217 | ARG  |
| 3   | CW    | 5   | VAL  |
| 3   | CW    | 8   | VAL  |
| 3   | CW    | 11  | SER  |
| 3   | CW    | 16  | SER  |
| 3   | CW    | 18  | VAL  |
| 3   | CW    | 23  | THR  |
| 3   | CW    | 31  | VAL  |
| 3   | CW    | 35  | GLN  |
| 3   | CW    | 36  | VAL  |
| 3   | CW    | 42  | ASN  |
| 3   | CW    | 50  | THR  |
| 3   | CW    | 56  | ILE  |
| 3   | CW    | 59  | LYS  |
| 3   | CW    | 64  | VAL  |
| 3   | CW    | 73  | LEU  |
| 3   | CW    | 76  | MET  |
| 3   | CW    | 77  | ASP  |
| 3   | CW    | 80  | LEU  |
| 3   | CW    | 93  | LEU  |
| 3   | CW    | 116 | THR  |
| 3   | CW    | 122 | VAL  |
| 3   | CW    | 129 | SER  |
| 3   | CW    | 135 | ARG  |
| 3   | CW    | 139 | MET  |
| 3   | CW    | 151 | ASN  |
| 3   | CW    | 157 | ASN  |
| 3   | CW    | 161 | SER  |
| 3   | CW    | 175 | THR  |
| 3   | CW    | 176 | VAL  |
| 3   | CW    | 178 | ASN  |
| 3   | CW    | 179 | VAL  |
| 3   | CW    | 183 | LEU  |
| 3   | CW    | 188 | LEU  |
| 3   | CW    | 192 | THR  |
| 3   | CW    | 194 | THR  |
| 3   | CW    | 196 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CW    | 206 | VAL  |
| 3   | CW    | 208 | VAL  |
| 3   | CW    | 216 | LEU  |
| 3   | CW    | 217 | ARG  |
| 3   | CX    | 5   | VAL  |
| 3   | CX    | 8   | VAL  |
| 3   | CX    | 11  | SER  |
| 3   | CX    | 16  | SER  |
| 3   | CX    | 18  | VAL  |
| 3   | CX    | 23  | THR  |
| 3   | CX    | 31  | VAL  |
| 3   | CX    | 35  | GLN  |
| 3   | CX    | 36  | VAL  |
| 3   | CX    | 42  | ASN  |
| 3   | CX    | 50  | THR  |
| 3   | CX    | 56  | ILE  |
| 3   | CX    | 59  | LYS  |
| 3   | CX    | 64  | VAL  |
| 3   | CX    | 73  | LEU  |
| 3   | CX    | 76  | MET  |
| 3   | CX    | 77  | ASP  |
| 3   | CX    | 80  | LEU  |
| 3   | CX    | 93  | LEU  |
| 3   | CX    | 116 | THR  |
| 3   | CX    | 122 | VAL  |
| 3   | CX    | 129 | SER  |
| 3   | CX    | 135 | ARG  |
| 3   | CX    | 139 | MET  |
| 3   | CX    | 151 | ASN  |
| 3   | CX    | 157 | ASN  |
| 3   | CX    | 161 | SER  |
| 3   | CX    | 175 | THR  |
| 3   | CX    | 176 | VAL  |
| 3   | CX    | 178 | ASN  |
| 3   | CX    | 179 | VAL  |
| 3   | CX    | 183 | LEU  |
| 3   | CX    | 188 | LEU  |
| 3   | CX    | 192 | THR  |
| 3   | CX    | 194 | THR  |
| 3   | CX    | 196 | ILE  |
| 3   | CX    | 206 | VAL  |
| 3   | CX    | 208 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CX    | 216 | LEU  |
| 3   | CX    | 217 | ARG  |
| 3   | CY    | 5   | VAL  |
| 3   | CY    | 8   | VAL  |
| 3   | CY    | 11  | SER  |
| 3   | CY    | 16  | SER  |
| 3   | CY    | 18  | VAL  |
| 3   | CY    | 23  | THR  |
| 3   | CY    | 31  | VAL  |
| 3   | CY    | 35  | GLN  |
| 3   | CY    | 36  | VAL  |
| 3   | CY    | 42  | ASN  |
| 3   | CY    | 50  | THR  |
| 3   | CY    | 56  | ILE  |
| 3   | CY    | 59  | LYS  |
| 3   | CY    | 64  | VAL  |
| 3   | CY    | 73  | LEU  |
| 3   | CY    | 76  | MET  |
| 3   | CY    | 77  | ASP  |
| 3   | CY    | 80  | LEU  |
| 3   | CY    | 93  | LEU  |
| 3   | CY    | 116 | THR  |
| 3   | CY    | 122 | VAL  |
| 3   | CY    | 129 | SER  |
| 3   | CY    | 135 | ARG  |
| 3   | CY    | 139 | MET  |
| 3   | CY    | 151 | ASN  |
| 3   | CY    | 157 | ASN  |
| 3   | CY    | 161 | SER  |
| 3   | CY    | 175 | THR  |
| 3   | CY    | 176 | VAL  |
| 3   | CY    | 178 | ASN  |
| 3   | CY    | 179 | VAL  |
| 3   | CY    | 183 | LEU  |
| 3   | CY    | 188 | LEU  |
| 3   | CY    | 192 | THR  |
| 3   | CY    | 194 | THR  |
| 3   | CY    | 196 | ILE  |
| 3   | CY    | 206 | VAL  |
| 3   | CY    | 208 | VAL  |
| 3   | CY    | 216 | LEU  |
| 3   | CY    | 217 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CZ    | 5   | VAL  |
| 3   | CZ    | 8   | VAL  |
| 3   | CZ    | 11  | SER  |
| 3   | CZ    | 16  | SER  |
| 3   | CZ    | 18  | VAL  |
| 3   | CZ    | 23  | THR  |
| 3   | CZ    | 31  | VAL  |
| 3   | CZ    | 35  | GLN  |
| 3   | CZ    | 36  | VAL  |
| 3   | CZ    | 42  | ASN  |
| 3   | CZ    | 50  | THR  |
| 3   | CZ    | 56  | ILE  |
| 3   | CZ    | 59  | LYS  |
| 3   | CZ    | 64  | VAL  |
| 3   | CZ    | 73  | LEU  |
| 3   | CZ    | 76  | MET  |
| 3   | CZ    | 77  | ASP  |
| 3   | CZ    | 80  | LEU  |
| 3   | CZ    | 93  | LEU  |
| 3   | CZ    | 116 | THR  |
| 3   | CZ    | 122 | VAL  |
| 3   | CZ    | 129 | SER  |
| 3   | CZ    | 135 | ARG  |
| 3   | CZ    | 139 | MET  |
| 3   | CZ    | 151 | ASN  |
| 3   | CZ    | 157 | ASN  |
| 3   | CZ    | 161 | SER  |
| 3   | CZ    | 175 | THR  |
| 3   | CZ    | 176 | VAL  |
| 3   | CZ    | 178 | ASN  |
| 3   | CZ    | 179 | VAL  |
| 3   | CZ    | 183 | LEU  |
| 3   | CZ    | 188 | LEU  |
| 3   | CZ    | 192 | THR  |
| 3   | CZ    | 194 | THR  |
| 3   | CZ    | 196 | ILE  |
| 3   | CZ    | 206 | VAL  |
| 3   | CZ    | 208 | VAL  |
| 3   | CZ    | 216 | LEU  |
| 3   | CZ    | 217 | ARG  |
| 3   | C0    | 5   | VAL  |
| 3   | C0    | 8   | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C0    | 11  | SER  |
| 3   | C0    | 16  | SER  |
| 3   | C0    | 18  | VAL  |
| 3   | C0    | 23  | THR  |
| 3   | C0    | 31  | VAL  |
| 3   | C0    | 35  | GLN  |
| 3   | C0    | 36  | VAL  |
| 3   | C0    | 42  | ASN  |
| 3   | C0    | 50  | THR  |
| 3   | C0    | 56  | ILE  |
| 3   | C0    | 59  | LYS  |
| 3   | C0    | 64  | VAL  |
| 3   | C0    | 73  | LEU  |
| 3   | C0    | 76  | MET  |
| 3   | C0    | 77  | ASP  |
| 3   | C0    | 80  | LEU  |
| 3   | C0    | 93  | LEU  |
| 3   | C0    | 116 | THR  |
| 3   | C0    | 122 | VAL  |
| 3   | C0    | 129 | SER  |
| 3   | C0    | 135 | ARG  |
| 3   | C0    | 139 | MET  |
| 3   | C0    | 151 | ASN  |
| 3   | C0    | 157 | ASN  |
| 3   | C0    | 161 | SER  |
| 3   | C0    | 175 | THR  |
| 3   | C0    | 176 | VAL  |
| 3   | C0    | 178 | ASN  |
| 3   | C0    | 179 | VAL  |
| 3   | C0    | 183 | LEU  |
| 3   | C0    | 188 | LEU  |
| 3   | C0    | 192 | THR  |
| 3   | C0    | 194 | THR  |
| 3   | C0    | 196 | ILE  |
| 3   | C0    | 206 | VAL  |
| 3   | C0    | 208 | VAL  |
| 3   | C0    | 216 | LEU  |
| 3   | C0    | 217 | ARG  |
| 3   | C1    | 5   | VAL  |
| 3   | C1    | 8   | VAL  |
| 3   | C1    | 11  | SER  |
| 3   | C1    | 16  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C1    | 18  | VAL  |
| 3   | C1    | 23  | THR  |
| 3   | C1    | 31  | VAL  |
| 3   | C1    | 35  | GLN  |
| 3   | C1    | 36  | VAL  |
| 3   | C1    | 42  | ASN  |
| 3   | C1    | 50  | THR  |
| 3   | C1    | 56  | ILE  |
| 3   | C1    | 59  | LYS  |
| 3   | C1    | 64  | VAL  |
| 3   | C1    | 73  | LEU  |
| 3   | C1    | 76  | MET  |
| 3   | C1    | 77  | ASP  |
| 3   | C1    | 80  | LEU  |
| 3   | C1    | 93  | LEU  |
| 3   | C1    | 116 | THR  |
| 3   | C1    | 122 | VAL  |
| 3   | C1    | 129 | SER  |
| 3   | C1    | 135 | ARG  |
| 3   | C1    | 139 | MET  |
| 3   | C1    | 151 | ASN  |
| 3   | C1    | 157 | ASN  |
| 3   | C1    | 161 | SER  |
| 3   | C1    | 175 | THR  |
| 3   | C1    | 176 | VAL  |
| 3   | C1    | 178 | ASN  |
| 3   | C1    | 179 | VAL  |
| 3   | C1    | 183 | LEU  |
| 3   | C1    | 188 | LEU  |
| 3   | C1    | 192 | THR  |
| 3   | C1    | 194 | THR  |
| 3   | C1    | 196 | ILE  |
| 3   | C1    | 206 | VAL  |
| 3   | C1    | 208 | VAL  |
| 3   | C1    | 216 | LEU  |
| 3   | C1    | 217 | ARG  |
| 3   | C2    | 5   | VAL  |
| 3   | C2    | 8   | VAL  |
| 3   | C2    | 11  | SER  |
| 3   | C2    | 16  | SER  |
| 3   | C2    | 18  | VAL  |
| 3   | C2    | 23  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C2    | 31  | VAL  |
| 3   | C2    | 35  | GLN  |
| 3   | C2    | 36  | VAL  |
| 3   | C2    | 42  | ASN  |
| 3   | C2    | 50  | THR  |
| 3   | C2    | 56  | ILE  |
| 3   | C2    | 59  | LYS  |
| 3   | C2    | 64  | VAL  |
| 3   | C2    | 73  | LEU  |
| 3   | C2    | 76  | MET  |
| 3   | C2    | 77  | ASP  |
| 3   | C2    | 80  | LEU  |
| 3   | C2    | 93  | LEU  |
| 3   | C2    | 116 | THR  |
| 3   | C2    | 122 | VAL  |
| 3   | C2    | 129 | SER  |
| 3   | C2    | 135 | ARG  |
| 3   | C2    | 139 | MET  |
| 3   | C2    | 151 | ASN  |
| 3   | C2    | 157 | ASN  |
| 3   | C2    | 161 | SER  |
| 3   | C2    | 175 | THR  |
| 3   | C2    | 176 | VAL  |
| 3   | C2    | 178 | ASN  |
| 3   | C2    | 179 | VAL  |
| 3   | C2    | 183 | LEU  |
| 3   | C2    | 188 | LEU  |
| 3   | C2    | 192 | THR  |
| 3   | C2    | 194 | THR  |
| 3   | C2    | 196 | ILE  |
| 3   | C2    | 206 | VAL  |
| 3   | C2    | 208 | VAL  |
| 3   | C2    | 216 | LEU  |
| 3   | C2    | 217 | ARG  |
| 3   | C3    | 5   | VAL  |
| 3   | C3    | 8   | VAL  |
| 3   | C3    | 11  | SER  |
| 3   | C3    | 16  | SER  |
| 3   | C3    | 18  | VAL  |
| 3   | C3    | 23  | THR  |
| 3   | C3    | 31  | VAL  |
| 3   | C3    | 35  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C3    | 36  | VAL  |
| 3   | C3    | 42  | ASN  |
| 3   | C3    | 50  | THR  |
| 3   | C3    | 56  | ILE  |
| 3   | C3    | 59  | LYS  |
| 3   | C3    | 64  | VAL  |
| 3   | C3    | 73  | LEU  |
| 3   | C3    | 76  | MET  |
| 3   | C3    | 77  | ASP  |
| 3   | C3    | 80  | LEU  |
| 3   | C3    | 93  | LEU  |
| 3   | C3    | 116 | THR  |
| 3   | C3    | 122 | VAL  |
| 3   | C3    | 129 | SER  |
| 3   | C3    | 135 | ARG  |
| 3   | C3    | 139 | MET  |
| 3   | C3    | 151 | ASN  |
| 3   | C3    | 157 | ASN  |
| 3   | C3    | 161 | SER  |
| 3   | C3    | 175 | THR  |
| 3   | C3    | 176 | VAL  |
| 3   | C3    | 178 | ASN  |
| 3   | C3    | 179 | VAL  |
| 3   | C3    | 183 | LEU  |
| 3   | C3    | 188 | LEU  |
| 3   | C3    | 192 | THR  |
| 3   | C3    | 194 | THR  |
| 3   | C3    | 196 | ILE  |
| 3   | C3    | 206 | VAL  |
| 3   | C3    | 208 | VAL  |
| 3   | C3    | 216 | LEU  |
| 3   | C3    | 217 | ARG  |
| 3   | C4    | 5   | VAL  |
| 3   | C4    | 8   | VAL  |
| 3   | C4    | 11  | SER  |
| 3   | C4    | 16  | SER  |
| 3   | C4    | 18  | VAL  |
| 3   | C4    | 23  | THR  |
| 3   | C4    | 31  | VAL  |
| 3   | C4    | 35  | GLN  |
| 3   | C4    | 36  | VAL  |
| 3   | C4    | 42  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C4    | 50  | THR  |
| 3   | C4    | 56  | ILE  |
| 3   | C4    | 59  | LYS  |
| 3   | C4    | 64  | VAL  |
| 3   | C4    | 73  | LEU  |
| 3   | C4    | 76  | MET  |
| 3   | C4    | 77  | ASP  |
| 3   | C4    | 80  | LEU  |
| 3   | C4    | 93  | LEU  |
| 3   | C4    | 116 | THR  |
| 3   | C4    | 122 | VAL  |
| 3   | C4    | 129 | SER  |
| 3   | C4    | 135 | ARG  |
| 3   | C4    | 139 | MET  |
| 3   | C4    | 151 | ASN  |
| 3   | C4    | 157 | ASN  |
| 3   | C4    | 161 | SER  |
| 3   | C4    | 175 | THR  |
| 3   | C4    | 176 | VAL  |
| 3   | C4    | 178 | ASN  |
| 3   | C4    | 179 | VAL  |
| 3   | C4    | 183 | LEU  |
| 3   | C4    | 188 | LEU  |
| 3   | C4    | 192 | THR  |
| 3   | C4    | 194 | THR  |
| 3   | C4    | 196 | ILE  |
| 3   | C4    | 206 | VAL  |
| 3   | C4    | 208 | VAL  |
| 3   | C4    | 216 | LEU  |
| 3   | C4    | 217 | ARG  |
| 3   | C5    | 5   | VAL  |
| 3   | C5    | 8   | VAL  |
| 3   | C5    | 11  | SER  |
| 3   | C5    | 16  | SER  |
| 3   | C5    | 18  | VAL  |
| 3   | C5    | 23  | THR  |
| 3   | C5    | 31  | VAL  |
| 3   | C5    | 35  | GLN  |
| 3   | C5    | 36  | VAL  |
| 3   | C5    | 42  | ASN  |
| 3   | C5    | 50  | THR  |
| 3   | C5    | 56  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C5    | 59  | LYS  |
| 3   | C5    | 64  | VAL  |
| 3   | C5    | 73  | LEU  |
| 3   | C5    | 76  | MET  |
| 3   | C5    | 77  | ASP  |
| 3   | C5    | 80  | LEU  |
| 3   | C5    | 93  | LEU  |
| 3   | C5    | 116 | THR  |
| 3   | C5    | 122 | VAL  |
| 3   | C5    | 129 | SER  |
| 3   | C5    | 135 | ARG  |
| 3   | C5    | 139 | MET  |
| 3   | C5    | 151 | ASN  |
| 3   | C5    | 157 | ASN  |
| 3   | C5    | 161 | SER  |
| 3   | C5    | 175 | THR  |
| 3   | C5    | 176 | VAL  |
| 3   | C5    | 178 | ASN  |
| 3   | C5    | 179 | VAL  |
| 3   | C5    | 183 | LEU  |
| 3   | C5    | 188 | LEU  |
| 3   | C5    | 192 | THR  |
| 3   | C5    | 194 | THR  |
| 3   | C5    | 196 | ILE  |
| 3   | C5    | 206 | VAL  |
| 3   | C5    | 208 | VAL  |
| 3   | C5    | 216 | LEU  |
| 3   | C5    | 217 | ARG  |
| 3   | C6    | 5   | VAL  |
| 3   | C6    | 8   | VAL  |
| 3   | C6    | 11  | SER  |
| 3   | C6    | 16  | SER  |
| 3   | C6    | 18  | VAL  |
| 3   | C6    | 23  | THR  |
| 3   | C6    | 31  | VAL  |
| 3   | C6    | 35  | GLN  |
| 3   | C6    | 36  | VAL  |
| 3   | C6    | 42  | ASN  |
| 3   | C6    | 50  | THR  |
| 3   | C6    | 56  | ILE  |
| 3   | C6    | 59  | LYS  |
| 3   | C6    | 64  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C6    | 73  | LEU  |
| 3   | C6    | 76  | MET  |
| 3   | C6    | 77  | ASP  |
| 3   | C6    | 80  | LEU  |
| 3   | C6    | 93  | LEU  |
| 3   | C6    | 116 | THR  |
| 3   | C6    | 122 | VAL  |
| 3   | C6    | 129 | SER  |
| 3   | C6    | 135 | ARG  |
| 3   | C6    | 139 | MET  |
| 3   | C6    | 151 | ASN  |
| 3   | C6    | 157 | ASN  |
| 3   | C6    | 161 | SER  |
| 3   | C6    | 175 | THR  |
| 3   | C6    | 176 | VAL  |
| 3   | C6    | 178 | ASN  |
| 3   | C6    | 179 | VAL  |
| 3   | C6    | 183 | LEU  |
| 3   | C6    | 188 | LEU  |
| 3   | C6    | 192 | THR  |
| 3   | C6    | 194 | THR  |
| 3   | C6    | 196 | ILE  |
| 3   | C6    | 206 | VAL  |
| 3   | C6    | 208 | VAL  |
| 3   | C6    | 216 | LEU  |
| 3   | C6    | 217 | ARG  |
| 3   | C7    | 5   | VAL  |
| 3   | C7    | 8   | VAL  |
| 3   | C7    | 11  | SER  |
| 3   | C7    | 16  | SER  |
| 3   | C7    | 18  | VAL  |
| 3   | C7    | 23  | THR  |
| 3   | C7    | 31  | VAL  |
| 3   | C7    | 35  | GLN  |
| 3   | C7    | 36  | VAL  |
| 3   | C7    | 42  | ASN  |
| 3   | C7    | 50  | THR  |
| 3   | C7    | 56  | ILE  |
| 3   | C7    | 59  | LYS  |
| 3   | C7    | 64  | VAL  |
| 3   | C7    | 73  | LEU  |
| 3   | C7    | 76  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C7    | 77  | ASP  |
| 3   | C7    | 80  | LEU  |
| 3   | C7    | 93  | LEU  |
| 3   | C7    | 116 | THR  |
| 3   | C7    | 122 | VAL  |
| 3   | C7    | 129 | SER  |
| 3   | C7    | 135 | ARG  |
| 3   | C7    | 139 | MET  |
| 3   | C7    | 151 | ASN  |
| 3   | C7    | 157 | ASN  |
| 3   | C7    | 161 | SER  |
| 3   | C7    | 175 | THR  |
| 3   | C7    | 176 | VAL  |
| 3   | C7    | 178 | ASN  |
| 3   | C7    | 179 | VAL  |
| 3   | C7    | 183 | LEU  |
| 3   | C7    | 188 | LEU  |
| 3   | C7    | 192 | THR  |
| 3   | C7    | 194 | THR  |
| 3   | C7    | 196 | ILE  |
| 3   | C7    | 206 | VAL  |
| 3   | C7    | 208 | VAL  |
| 3   | C7    | 216 | LEU  |
| 3   | C7    | 217 | ARG  |
| 3   | C8    | 5   | VAL  |
| 3   | C8    | 8   | VAL  |
| 3   | C8    | 11  | SER  |
| 3   | C8    | 16  | SER  |
| 3   | C8    | 18  | VAL  |
| 3   | C8    | 23  | THR  |
| 3   | C8    | 31  | VAL  |
| 3   | C8    | 35  | GLN  |
| 3   | C8    | 36  | VAL  |
| 3   | C8    | 42  | ASN  |
| 3   | C8    | 50  | THR  |
| 3   | C8    | 56  | ILE  |
| 3   | C8    | 59  | LYS  |
| 3   | C8    | 64  | VAL  |
| 3   | C8    | 73  | LEU  |
| 3   | C8    | 76  | MET  |
| 3   | C8    | 77  | ASP  |
| 3   | C8    | 80  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C8    | 93  | LEU  |
| 3   | C8    | 116 | THR  |
| 3   | C8    | 122 | VAL  |
| 3   | C8    | 129 | SER  |
| 3   | C8    | 135 | ARG  |
| 3   | C8    | 139 | MET  |
| 3   | C8    | 151 | ASN  |
| 3   | C8    | 157 | ASN  |
| 3   | C8    | 161 | SER  |
| 3   | C8    | 175 | THR  |
| 3   | C8    | 176 | VAL  |
| 3   | C8    | 178 | ASN  |
| 3   | C8    | 179 | VAL  |
| 3   | C8    | 183 | LEU  |
| 3   | C8    | 188 | LEU  |
| 3   | C8    | 192 | THR  |
| 3   | C8    | 194 | THR  |
| 3   | C8    | 196 | ILE  |
| 3   | C8    | 206 | VAL  |
| 3   | C8    | 208 | VAL  |
| 3   | C8    | 216 | LEU  |
| 3   | C8    | 217 | ARG  |
| 3   | C9    | 5   | VAL  |
| 3   | C9    | 8   | VAL  |
| 3   | C9    | 11  | SER  |
| 3   | C9    | 16  | SER  |
| 3   | C9    | 18  | VAL  |
| 3   | C9    | 23  | THR  |
| 3   | C9    | 31  | VAL  |
| 3   | C9    | 35  | GLN  |
| 3   | C9    | 36  | VAL  |
| 3   | C9    | 42  | ASN  |
| 3   | C9    | 50  | THR  |
| 3   | C9    | 56  | ILE  |
| 3   | C9    | 59  | LYS  |
| 3   | C9    | 64  | VAL  |
| 3   | C9    | 73  | LEU  |
| 3   | C9    | 76  | MET  |
| 3   | C9    | 77  | ASP  |
| 3   | C9    | 80  | LEU  |
| 3   | C9    | 93  | LEU  |
| 3   | C9    | 116 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C9    | 122 | VAL  |
| 3   | C9    | 129 | SER  |
| 3   | C9    | 135 | ARG  |
| 3   | C9    | 139 | MET  |
| 3   | C9    | 151 | ASN  |
| 3   | C9    | 157 | ASN  |
| 3   | C9    | 161 | SER  |
| 3   | C9    | 175 | THR  |
| 3   | C9    | 176 | VAL  |
| 3   | C9    | 178 | ASN  |
| 3   | C9    | 179 | VAL  |
| 3   | C9    | 183 | LEU  |
| 3   | C9    | 188 | LEU  |
| 3   | C9    | 192 | THR  |
| 3   | C9    | 194 | THR  |
| 3   | C9    | 196 | ILE  |
| 3   | C9    | 206 | VAL  |
| 3   | C9    | 208 | VAL  |
| 3   | C9    | 216 | LEU  |
| 3   | C9    | 217 | ARG  |
| 3   | Cc    | 5   | VAL  |
| 3   | Cc    | 8   | VAL  |
| 3   | Cc    | 11  | SER  |
| 3   | Cc    | 16  | SER  |
| 3   | Cc    | 18  | VAL  |
| 3   | Cc    | 23  | THR  |
| 3   | Cc    | 31  | VAL  |
| 3   | Cc    | 35  | GLN  |
| 3   | Cc    | 36  | VAL  |
| 3   | Cc    | 42  | ASN  |
| 3   | Cc    | 50  | THR  |
| 3   | Cc    | 56  | ILE  |
| 3   | Cc    | 59  | LYS  |
| 3   | Cc    | 64  | VAL  |
| 3   | Cc    | 73  | LEU  |
| 3   | Cc    | 76  | MET  |
| 3   | Cc    | 77  | ASP  |
| 3   | Cc    | 80  | LEU  |
| 3   | Cc    | 93  | LEU  |
| 3   | Cc    | 116 | THR  |
| 3   | Cc    | 122 | VAL  |
| 3   | Cc    | 129 | SER  |

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*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Cc    | 135 | ARG  |
| 3   | Cc    | 139 | MET  |
| 3   | Cc    | 151 | ASN  |
| 3   | Cc    | 157 | ASN  |
| 3   | Cc    | 161 | SER  |
| 3   | Cc    | 175 | THR  |
| 3   | Cc    | 176 | VAL  |
| 3   | Cc    | 178 | ASN  |
| 3   | Cc    | 179 | VAL  |
| 3   | Cc    | 183 | LEU  |
| 3   | Cc    | 188 | LEU  |
| 3   | Cc    | 192 | THR  |
| 3   | Cc    | 194 | THR  |
| 3   | Cc    | 196 | ILE  |
| 3   | Cc    | 206 | VAL  |
| 3   | Cc    | 208 | VAL  |
| 3   | Cc    | 216 | LEU  |
| 3   | Cc    | 217 | ARG  |
| 3   | Cd    | 5   | VAL  |
| 3   | Cd    | 8   | VAL  |
| 3   | Cd    | 11  | SER  |
| 3   | Cd    | 16  | SER  |
| 3   | Cd    | 18  | VAL  |
| 3   | Cd    | 23  | THR  |
| 3   | Cd    | 31  | VAL  |
| 3   | Cd    | 35  | GLN  |
| 3   | Cd    | 36  | VAL  |
| 3   | Cd    | 42  | ASN  |
| 3   | Cd    | 50  | THR  |
| 3   | Cd    | 56  | ILE  |
| 3   | Cd    | 59  | LYS  |
| 3   | Cd    | 64  | VAL  |
| 3   | Cd    | 73  | LEU  |
| 3   | Cd    | 76  | MET  |
| 3   | Cd    | 77  | ASP  |
| 3   | Cd    | 80  | LEU  |
| 3   | Cd    | 93  | LEU  |
| 3   | Cd    | 116 | THR  |
| 3   | Cd    | 122 | VAL  |
| 3   | Cd    | 129 | SER  |
| 3   | Cd    | 135 | ARG  |
| 3   | Cd    | 139 | MET  |

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*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Cd    | 151 | ASN  |
| 3   | Cd    | 157 | ASN  |
| 3   | Cd    | 161 | SER  |
| 3   | Cd    | 175 | THR  |
| 3   | Cd    | 176 | VAL  |
| 3   | Cd    | 178 | ASN  |
| 3   | Cd    | 179 | VAL  |
| 3   | Cd    | 183 | LEU  |
| 3   | Cd    | 188 | LEU  |
| 3   | Cd    | 192 | THR  |
| 3   | Cd    | 194 | THR  |
| 3   | Cd    | 196 | ILE  |
| 3   | Cd    | 206 | VAL  |
| 3   | Cd    | 208 | VAL  |
| 3   | Cd    | 216 | LEU  |
| 3   | Cd    | 217 | ARG  |
| 3   | Ce    | 5   | VAL  |
| 3   | Ce    | 8   | VAL  |
| 3   | Ce    | 11  | SER  |
| 3   | Ce    | 16  | SER  |
| 3   | Ce    | 18  | VAL  |
| 3   | Ce    | 23  | THR  |
| 3   | Ce    | 31  | VAL  |
| 3   | Ce    | 35  | GLN  |
| 3   | Ce    | 36  | VAL  |
| 3   | Ce    | 42  | ASN  |
| 3   | Ce    | 50  | THR  |
| 3   | Ce    | 56  | ILE  |
| 3   | Ce    | 59  | LYS  |
| 3   | Ce    | 64  | VAL  |
| 3   | Ce    | 73  | LEU  |
| 3   | Ce    | 76  | MET  |
| 3   | Ce    | 77  | ASP  |
| 3   | Ce    | 80  | LEU  |
| 3   | Ce    | 93  | LEU  |
| 3   | Ce    | 116 | THR  |
| 3   | Ce    | 122 | VAL  |
| 3   | Ce    | 129 | SER  |
| 3   | Ce    | 135 | ARG  |
| 3   | Ce    | 139 | MET  |
| 3   | Ce    | 151 | ASN  |
| 3   | Ce    | 157 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Ce    | 161 | SER  |
| 3   | Ce    | 175 | THR  |
| 3   | Ce    | 176 | VAL  |
| 3   | Ce    | 178 | ASN  |
| 3   | Ce    | 179 | VAL  |
| 3   | Ce    | 183 | LEU  |
| 3   | Ce    | 188 | LEU  |
| 3   | Ce    | 192 | THR  |
| 3   | Ce    | 194 | THR  |
| 3   | Ce    | 196 | ILE  |
| 3   | Ce    | 206 | VAL  |
| 3   | Ce    | 208 | VAL  |
| 3   | Ce    | 216 | LEU  |
| 3   | Ce    | 217 | ARG  |
| 3   | Cf    | 5   | VAL  |
| 3   | Cf    | 8   | VAL  |
| 3   | Cf    | 11  | SER  |
| 3   | Cf    | 16  | SER  |
| 3   | Cf    | 18  | VAL  |
| 3   | Cf    | 23  | THR  |
| 3   | Cf    | 31  | VAL  |
| 3   | Cf    | 35  | GLN  |
| 3   | Cf    | 36  | VAL  |
| 3   | Cf    | 42  | ASN  |
| 3   | Cf    | 50  | THR  |
| 3   | Cf    | 56  | ILE  |
| 3   | Cf    | 59  | LYS  |
| 3   | Cf    | 64  | VAL  |
| 3   | Cf    | 73  | LEU  |
| 3   | Cf    | 76  | MET  |
| 3   | Cf    | 77  | ASP  |
| 3   | Cf    | 80  | LEU  |
| 3   | Cf    | 93  | LEU  |
| 3   | Cf    | 116 | THR  |
| 3   | Cf    | 122 | VAL  |
| 3   | Cf    | 129 | SER  |
| 3   | Cf    | 135 | ARG  |
| 3   | Cf    | 139 | MET  |
| 3   | Cf    | 151 | ASN  |
| 3   | Cf    | 157 | ASN  |
| 3   | Cf    | 161 | SER  |
| 3   | Cf    | 175 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Cf    | 176 | VAL  |
| 3   | Cf    | 178 | ASN  |
| 3   | Cf    | 179 | VAL  |
| 3   | Cf    | 183 | LEU  |
| 3   | Cf    | 188 | LEU  |
| 3   | Cf    | 192 | THR  |
| 3   | Cf    | 194 | THR  |
| 3   | Cf    | 196 | ILE  |
| 3   | Cf    | 206 | VAL  |
| 3   | Cf    | 208 | VAL  |
| 3   | Cf    | 216 | LEU  |
| 3   | Cf    | 217 | ARG  |
| 3   | Cg    | 5   | VAL  |
| 3   | Cg    | 8   | VAL  |
| 3   | Cg    | 11  | SER  |
| 3   | Cg    | 16  | SER  |
| 3   | Cg    | 18  | VAL  |
| 3   | Cg    | 23  | THR  |
| 3   | Cg    | 31  | VAL  |
| 3   | Cg    | 35  | GLN  |
| 3   | Cg    | 36  | VAL  |
| 3   | Cg    | 42  | ASN  |
| 3   | Cg    | 50  | THR  |
| 3   | Cg    | 56  | ILE  |
| 3   | Cg    | 59  | LYS  |
| 3   | Cg    | 64  | VAL  |
| 3   | Cg    | 73  | LEU  |
| 3   | Cg    | 76  | MET  |
| 3   | Cg    | 77  | ASP  |
| 3   | Cg    | 80  | LEU  |
| 3   | Cg    | 93  | LEU  |
| 3   | Cg    | 116 | THR  |
| 3   | Cg    | 122 | VAL  |
| 3   | Cg    | 129 | SER  |
| 3   | Cg    | 135 | ARG  |
| 3   | Cg    | 139 | MET  |
| 3   | Cg    | 151 | ASN  |
| 3   | Cg    | 157 | ASN  |
| 3   | Cg    | 161 | SER  |
| 3   | Cg    | 175 | THR  |
| 3   | Cg    | 176 | VAL  |
| 3   | Cg    | 178 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Cg    | 179 | VAL  |
| 3   | Cg    | 183 | LEU  |
| 3   | Cg    | 188 | LEU  |
| 3   | Cg    | 192 | THR  |
| 3   | Cg    | 194 | THR  |
| 3   | Cg    | 196 | ILE  |
| 3   | Cg    | 206 | VAL  |
| 3   | Cg    | 208 | VAL  |
| 3   | Cg    | 216 | LEU  |
| 3   | Cg    | 217 | ARG  |
| 3   | Ch    | 5   | VAL  |
| 3   | Ch    | 8   | VAL  |
| 3   | Ch    | 11  | SER  |
| 3   | Ch    | 16  | SER  |
| 3   | Ch    | 18  | VAL  |
| 3   | Ch    | 23  | THR  |
| 3   | Ch    | 31  | VAL  |
| 3   | Ch    | 35  | GLN  |
| 3   | Ch    | 36  | VAL  |
| 3   | Ch    | 42  | ASN  |
| 3   | Ch    | 50  | THR  |
| 3   | Ch    | 56  | ILE  |
| 3   | Ch    | 59  | LYS  |
| 3   | Ch    | 64  | VAL  |
| 3   | Ch    | 73  | LEU  |
| 3   | Ch    | 76  | MET  |
| 3   | Ch    | 77  | ASP  |
| 3   | Ch    | 80  | LEU  |
| 3   | Ch    | 93  | LEU  |
| 3   | Ch    | 116 | THR  |
| 3   | Ch    | 122 | VAL  |
| 3   | Ch    | 129 | SER  |
| 3   | Ch    | 135 | ARG  |
| 3   | Ch    | 139 | MET  |
| 3   | Ch    | 151 | ASN  |
| 3   | Ch    | 157 | ASN  |
| 3   | Ch    | 161 | SER  |
| 3   | Ch    | 175 | THR  |
| 3   | Ch    | 176 | VAL  |
| 3   | Ch    | 178 | ASN  |
| 3   | Ch    | 179 | VAL  |
| 3   | Ch    | 183 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Ch    | 188 | LEU  |
| 3   | Ch    | 192 | THR  |
| 3   | Ch    | 194 | THR  |
| 3   | Ch    | 196 | ILE  |
| 3   | Ch    | 206 | VAL  |
| 3   | Ch    | 208 | VAL  |
| 3   | Ch    | 216 | LEU  |
| 3   | Ch    | 217 | ARG  |
| 3   | Ci    | 5   | VAL  |
| 3   | Ci    | 8   | VAL  |
| 3   | Ci    | 11  | SER  |
| 3   | Ci    | 16  | SER  |
| 3   | Ci    | 18  | VAL  |
| 3   | Ci    | 23  | THR  |
| 3   | Ci    | 31  | VAL  |
| 3   | Ci    | 35  | GLN  |
| 3   | Ci    | 36  | VAL  |
| 3   | Ci    | 42  | ASN  |
| 3   | Ci    | 50  | THR  |
| 3   | Ci    | 56  | ILE  |
| 3   | Ci    | 59  | LYS  |
| 3   | Ci    | 64  | VAL  |
| 3   | Ci    | 73  | LEU  |
| 3   | Ci    | 76  | MET  |
| 3   | Ci    | 77  | ASP  |
| 3   | Ci    | 80  | LEU  |
| 3   | Ci    | 93  | LEU  |
| 3   | Ci    | 116 | THR  |
| 3   | Ci    | 122 | VAL  |
| 3   | Ci    | 129 | SER  |
| 3   | Ci    | 135 | ARG  |
| 3   | Ci    | 139 | MET  |
| 3   | Ci    | 151 | ASN  |
| 3   | Ci    | 157 | ASN  |
| 3   | Ci    | 161 | SER  |
| 3   | Ci    | 175 | THR  |
| 3   | Ci    | 176 | VAL  |
| 3   | Ci    | 178 | ASN  |
| 3   | Ci    | 179 | VAL  |
| 3   | Ci    | 183 | LEU  |
| 3   | Ci    | 188 | LEU  |
| 3   | Ci    | 192 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Ci    | 194 | THR  |
| 3   | Ci    | 196 | ILE  |
| 3   | Ci    | 206 | VAL  |
| 3   | Ci    | 208 | VAL  |
| 3   | Ci    | 216 | LEU  |
| 3   | Ci    | 217 | ARG  |
| 3   | Cj    | 5   | VAL  |
| 3   | Cj    | 8   | VAL  |
| 3   | Cj    | 11  | SER  |
| 3   | Cj    | 16  | SER  |
| 3   | Cj    | 18  | VAL  |
| 3   | Cj    | 23  | THR  |
| 3   | Cj    | 31  | VAL  |
| 3   | Cj    | 35  | GLN  |
| 3   | Cj    | 36  | VAL  |
| 3   | Cj    | 42  | ASN  |
| 3   | Cj    | 50  | THR  |
| 3   | Cj    | 56  | ILE  |
| 3   | Cj    | 59  | LYS  |
| 3   | Cj    | 64  | VAL  |
| 3   | Cj    | 73  | LEU  |
| 3   | Cj    | 76  | MET  |
| 3   | Cj    | 77  | ASP  |
| 3   | Cj    | 80  | LEU  |
| 3   | Cj    | 93  | LEU  |
| 3   | Cj    | 116 | THR  |
| 3   | Cj    | 122 | VAL  |
| 3   | Cj    | 129 | SER  |
| 3   | Cj    | 135 | ARG  |
| 3   | Cj    | 139 | MET  |
| 3   | Cj    | 151 | ASN  |
| 3   | Cj    | 157 | ASN  |
| 3   | Cj    | 161 | SER  |
| 3   | Cj    | 175 | THR  |
| 3   | Cj    | 176 | VAL  |
| 3   | Cj    | 178 | ASN  |
| 3   | Cj    | 179 | VAL  |
| 3   | Cj    | 183 | LEU  |
| 3   | Cj    | 188 | LEU  |
| 3   | Cj    | 192 | THR  |
| 3   | Cj    | 194 | THR  |
| 3   | Cj    | 196 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Cj    | 206 | VAL  |
| 3   | Cj    | 208 | VAL  |
| 3   | Cj    | 216 | LEU  |
| 3   | Cj    | 217 | ARG  |
| 3   | Ck    | 5   | VAL  |
| 3   | Ck    | 8   | VAL  |
| 3   | Ck    | 11  | SER  |
| 3   | Ck    | 16  | SER  |
| 3   | Ck    | 18  | VAL  |
| 3   | Ck    | 23  | THR  |
| 3   | Ck    | 31  | VAL  |
| 3   | Ck    | 35  | GLN  |
| 3   | Ck    | 36  | VAL  |
| 3   | Ck    | 42  | ASN  |
| 3   | Ck    | 50  | THR  |
| 3   | Ck    | 56  | ILE  |
| 3   | Ck    | 59  | LYS  |
| 3   | Ck    | 64  | VAL  |
| 3   | Ck    | 73  | LEU  |
| 3   | Ck    | 76  | MET  |
| 3   | Ck    | 77  | ASP  |
| 3   | Ck    | 80  | LEU  |
| 3   | Ck    | 93  | LEU  |
| 3   | Ck    | 116 | THR  |
| 3   | Ck    | 122 | VAL  |
| 3   | Ck    | 129 | SER  |
| 3   | Ck    | 135 | ARG  |
| 3   | Ck    | 139 | MET  |
| 3   | Ck    | 151 | ASN  |
| 3   | Ck    | 157 | ASN  |
| 3   | Ck    | 161 | SER  |
| 3   | Ck    | 175 | THR  |
| 3   | Ck    | 176 | VAL  |
| 3   | Ck    | 178 | ASN  |
| 3   | Ck    | 179 | VAL  |
| 3   | Ck    | 183 | LEU  |
| 3   | Ck    | 188 | LEU  |
| 3   | Ck    | 192 | THR  |
| 3   | Ck    | 194 | THR  |
| 3   | Ck    | 196 | ILE  |
| 3   | Ck    | 206 | VAL  |
| 3   | Ck    | 208 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Ck    | 216 | LEU  |
| 3   | Ck    | 217 | ARG  |
| 3   | Cl    | 5   | VAL  |
| 3   | Cl    | 8   | VAL  |
| 3   | Cl    | 11  | SER  |
| 3   | Cl    | 16  | SER  |
| 3   | Cl    | 18  | VAL  |
| 3   | Cl    | 23  | THR  |
| 3   | Cl    | 31  | VAL  |
| 3   | Cl    | 35  | GLN  |
| 3   | Cl    | 36  | VAL  |
| 3   | Cl    | 42  | ASN  |
| 3   | Cl    | 50  | THR  |
| 3   | Cl    | 56  | ILE  |
| 3   | Cl    | 59  | LYS  |
| 3   | Cl    | 64  | VAL  |
| 3   | Cl    | 73  | LEU  |
| 3   | Cl    | 76  | MET  |
| 3   | Cl    | 77  | ASP  |
| 3   | Cl    | 80  | LEU  |
| 3   | Cl    | 93  | LEU  |
| 3   | Cl    | 116 | THR  |
| 3   | Cl    | 122 | VAL  |
| 3   | Cl    | 129 | SER  |
| 3   | Cl    | 135 | ARG  |
| 3   | Cl    | 139 | MET  |
| 3   | Cl    | 151 | ASN  |
| 3   | Cl    | 157 | ASN  |
| 3   | Cl    | 161 | SER  |
| 3   | Cl    | 175 | THR  |
| 3   | Cl    | 176 | VAL  |
| 3   | Cl    | 178 | ASN  |
| 3   | Cl    | 179 | VAL  |
| 3   | Cl    | 183 | LEU  |
| 3   | Cl    | 188 | LEU  |
| 3   | Cl    | 192 | THR  |
| 3   | Cl    | 194 | THR  |
| 3   | Cl    | 196 | ILE  |
| 3   | Cl    | 206 | VAL  |
| 3   | Cl    | 208 | VAL  |
| 3   | Cl    | 216 | LEU  |
| 3   | Cl    | 217 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Cm    | 5   | VAL  |
| 3   | Cm    | 8   | VAL  |
| 3   | Cm    | 11  | SER  |
| 3   | Cm    | 16  | SER  |
| 3   | Cm    | 18  | VAL  |
| 3   | Cm    | 23  | THR  |
| 3   | Cm    | 31  | VAL  |
| 3   | Cm    | 35  | GLN  |
| 3   | Cm    | 36  | VAL  |
| 3   | Cm    | 42  | ASN  |
| 3   | Cm    | 50  | THR  |
| 3   | Cm    | 56  | ILE  |
| 3   | Cm    | 59  | LYS  |
| 3   | Cm    | 64  | VAL  |
| 3   | Cm    | 73  | LEU  |
| 3   | Cm    | 76  | MET  |
| 3   | Cm    | 77  | ASP  |
| 3   | Cm    | 80  | LEU  |
| 3   | Cm    | 93  | LEU  |
| 3   | Cm    | 116 | THR  |
| 3   | Cm    | 122 | VAL  |
| 3   | Cm    | 129 | SER  |
| 3   | Cm    | 135 | ARG  |
| 3   | Cm    | 139 | MET  |
| 3   | Cm    | 151 | ASN  |
| 3   | Cm    | 157 | ASN  |
| 3   | Cm    | 161 | SER  |
| 3   | Cm    | 175 | THR  |
| 3   | Cm    | 176 | VAL  |
| 3   | Cm    | 178 | ASN  |
| 3   | Cm    | 179 | VAL  |
| 3   | Cm    | 183 | LEU  |
| 3   | Cm    | 188 | LEU  |
| 3   | Cm    | 192 | THR  |
| 3   | Cm    | 194 | THR  |
| 3   | Cm    | 196 | ILE  |
| 3   | Cm    | 206 | VAL  |
| 3   | Cm    | 208 | VAL  |
| 3   | Cm    | 216 | LEU  |
| 3   | Cm    | 217 | ARG  |
| 3   | Cn    | 5   | VAL  |
| 3   | Cn    | 8   | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Cn    | 11  | SER  |
| 3   | Cn    | 16  | SER  |
| 3   | Cn    | 18  | VAL  |
| 3   | Cn    | 23  | THR  |
| 3   | Cn    | 31  | VAL  |
| 3   | Cn    | 35  | GLN  |
| 3   | Cn    | 36  | VAL  |
| 3   | Cn    | 42  | ASN  |
| 3   | Cn    | 50  | THR  |
| 3   | Cn    | 56  | ILE  |
| 3   | Cn    | 59  | LYS  |
| 3   | Cn    | 64  | VAL  |
| 3   | Cn    | 73  | LEU  |
| 3   | Cn    | 76  | MET  |
| 3   | Cn    | 77  | ASP  |
| 3   | Cn    | 80  | LEU  |
| 3   | Cn    | 93  | LEU  |
| 3   | Cn    | 116 | THR  |
| 3   | Cn    | 122 | VAL  |
| 3   | Cn    | 129 | SER  |
| 3   | Cn    | 135 | ARG  |
| 3   | Cn    | 139 | MET  |
| 3   | Cn    | 151 | ASN  |
| 3   | Cn    | 157 | ASN  |
| 3   | Cn    | 161 | SER  |
| 3   | Cn    | 175 | THR  |
| 3   | Cn    | 176 | VAL  |
| 3   | Cn    | 178 | ASN  |
| 3   | Cn    | 179 | VAL  |
| 3   | Cn    | 183 | LEU  |
| 3   | Cn    | 188 | LEU  |
| 3   | Cn    | 192 | THR  |
| 3   | Cn    | 194 | THR  |
| 3   | Cn    | 196 | ILE  |
| 3   | Cn    | 206 | VAL  |
| 3   | Cn    | 208 | VAL  |
| 3   | Cn    | 216 | LEU  |
| 3   | Cn    | 217 | ARG  |
| 3   | Co    | 5   | VAL  |
| 3   | Co    | 8   | VAL  |
| 3   | Co    | 11  | SER  |
| 3   | Co    | 16  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Co    | 18  | VAL  |
| 3   | Co    | 23  | THR  |
| 3   | Co    | 31  | VAL  |
| 3   | Co    | 35  | GLN  |
| 3   | Co    | 36  | VAL  |
| 3   | Co    | 42  | ASN  |
| 3   | Co    | 50  | THR  |
| 3   | Co    | 56  | ILE  |
| 3   | Co    | 59  | LYS  |
| 3   | Co    | 64  | VAL  |
| 3   | Co    | 73  | LEU  |
| 3   | Co    | 76  | MET  |
| 3   | Co    | 77  | ASP  |
| 3   | Co    | 80  | LEU  |
| 3   | Co    | 93  | LEU  |
| 3   | Co    | 116 | THR  |
| 3   | Co    | 122 | VAL  |
| 3   | Co    | 129 | SER  |
| 3   | Co    | 135 | ARG  |
| 3   | Co    | 139 | MET  |
| 3   | Co    | 151 | ASN  |
| 3   | Co    | 157 | ASN  |
| 3   | Co    | 161 | SER  |
| 3   | Co    | 175 | THR  |
| 3   | Co    | 176 | VAL  |
| 3   | Co    | 178 | ASN  |
| 3   | Co    | 179 | VAL  |
| 3   | Co    | 183 | LEU  |
| 3   | Co    | 188 | LEU  |
| 3   | Co    | 192 | THR  |
| 3   | Co    | 194 | THR  |
| 3   | Co    | 196 | ILE  |
| 3   | Co    | 206 | VAL  |
| 3   | Co    | 208 | VAL  |
| 3   | Co    | 216 | LEU  |
| 3   | Co    | 217 | ARG  |
| 3   | Cp    | 5   | VAL  |
| 3   | Cp    | 8   | VAL  |
| 3   | Cp    | 11  | SER  |
| 3   | Cp    | 16  | SER  |
| 3   | Cp    | 18  | VAL  |
| 3   | Cp    | 23  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Cp    | 31  | VAL  |
| 3   | Cp    | 35  | GLN  |
| 3   | Cp    | 36  | VAL  |
| 3   | Cp    | 42  | ASN  |
| 3   | Cp    | 50  | THR  |
| 3   | Cp    | 56  | ILE  |
| 3   | Cp    | 59  | LYS  |
| 3   | Cp    | 64  | VAL  |
| 3   | Cp    | 73  | LEU  |
| 3   | Cp    | 76  | MET  |
| 3   | Cp    | 77  | ASP  |
| 3   | Cp    | 80  | LEU  |
| 3   | Cp    | 93  | LEU  |
| 3   | Cp    | 116 | THR  |
| 3   | Cp    | 122 | VAL  |
| 3   | Cp    | 129 | SER  |
| 3   | Cp    | 135 | ARG  |
| 3   | Cp    | 139 | MET  |
| 3   | Cp    | 151 | ASN  |
| 3   | Cp    | 157 | ASN  |
| 3   | Cp    | 161 | SER  |
| 3   | Cp    | 175 | THR  |
| 3   | Cp    | 176 | VAL  |
| 3   | Cp    | 178 | ASN  |
| 3   | Cp    | 179 | VAL  |
| 3   | Cp    | 183 | LEU  |
| 3   | Cp    | 188 | LEU  |
| 3   | Cp    | 192 | THR  |
| 3   | Cp    | 194 | THR  |
| 3   | Cp    | 196 | ILE  |
| 3   | Cp    | 206 | VAL  |
| 3   | Cp    | 208 | VAL  |
| 3   | Cp    | 216 | LEU  |
| 3   | Cp    | 217 | ARG  |
| 3   | Cq    | 5   | VAL  |
| 3   | Cq    | 8   | VAL  |
| 3   | Cq    | 11  | SER  |
| 3   | Cq    | 16  | SER  |
| 3   | Cq    | 18  | VAL  |
| 3   | Cq    | 23  | THR  |
| 3   | Cq    | 31  | VAL  |
| 3   | Cq    | 35  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Cq    | 36  | VAL  |
| 3   | Cq    | 42  | ASN  |
| 3   | Cq    | 50  | THR  |
| 3   | Cq    | 56  | ILE  |
| 3   | Cq    | 59  | LYS  |
| 3   | Cq    | 64  | VAL  |
| 3   | Cq    | 73  | LEU  |
| 3   | Cq    | 76  | MET  |
| 3   | Cq    | 77  | ASP  |
| 3   | Cq    | 80  | LEU  |
| 3   | Cq    | 93  | LEU  |
| 3   | Cq    | 116 | THR  |
| 3   | Cq    | 122 | VAL  |
| 3   | Cq    | 129 | SER  |
| 3   | Cq    | 135 | ARG  |
| 3   | Cq    | 139 | MET  |
| 3   | Cq    | 151 | ASN  |
| 3   | Cq    | 157 | ASN  |
| 3   | Cq    | 161 | SER  |
| 3   | Cq    | 175 | THR  |
| 3   | Cq    | 176 | VAL  |
| 3   | Cq    | 178 | ASN  |
| 3   | Cq    | 179 | VAL  |
| 3   | Cq    | 183 | LEU  |
| 3   | Cq    | 188 | LEU  |
| 3   | Cq    | 192 | THR  |
| 3   | Cq    | 194 | THR  |
| 3   | Cq    | 196 | ILE  |
| 3   | Cq    | 206 | VAL  |
| 3   | Cq    | 208 | VAL  |
| 3   | Cq    | 216 | LEU  |
| 3   | Cq    | 217 | ARG  |
| 3   | Cr    | 5   | VAL  |
| 3   | Cr    | 8   | VAL  |
| 3   | Cr    | 11  | SER  |
| 3   | Cr    | 16  | SER  |
| 3   | Cr    | 18  | VAL  |
| 3   | Cr    | 23  | THR  |
| 3   | Cr    | 31  | VAL  |
| 3   | Cr    | 35  | GLN  |
| 3   | Cr    | 36  | VAL  |
| 3   | Cr    | 42  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Cr    | 50  | THR  |
| 3   | Cr    | 56  | ILE  |
| 3   | Cr    | 59  | LYS  |
| 3   | Cr    | 64  | VAL  |
| 3   | Cr    | 73  | LEU  |
| 3   | Cr    | 76  | MET  |
| 3   | Cr    | 77  | ASP  |
| 3   | Cr    | 80  | LEU  |
| 3   | Cr    | 93  | LEU  |
| 3   | Cr    | 116 | THR  |
| 3   | Cr    | 122 | VAL  |
| 3   | Cr    | 129 | SER  |
| 3   | Cr    | 135 | ARG  |
| 3   | Cr    | 139 | MET  |
| 3   | Cr    | 151 | ASN  |
| 3   | Cr    | 157 | ASN  |
| 3   | Cr    | 161 | SER  |
| 3   | Cr    | 175 | THR  |
| 3   | Cr    | 176 | VAL  |
| 3   | Cr    | 178 | ASN  |
| 3   | Cr    | 179 | VAL  |
| 3   | Cr    | 183 | LEU  |
| 3   | Cr    | 188 | LEU  |
| 3   | Cr    | 192 | THR  |
| 3   | Cr    | 194 | THR  |
| 3   | Cr    | 196 | ILE  |
| 3   | Cr    | 206 | VAL  |
| 3   | Cr    | 208 | VAL  |
| 3   | Cr    | 216 | LEU  |
| 3   | Cr    | 217 | ARG  |
| 3   | Cs    | 5   | VAL  |
| 3   | Cs    | 8   | VAL  |
| 3   | Cs    | 11  | SER  |
| 3   | Cs    | 16  | SER  |
| 3   | Cs    | 18  | VAL  |
| 3   | Cs    | 23  | THR  |
| 3   | Cs    | 31  | VAL  |
| 3   | Cs    | 35  | GLN  |
| 3   | Cs    | 36  | VAL  |
| 3   | Cs    | 42  | ASN  |
| 3   | Cs    | 50  | THR  |
| 3   | Cs    | 56  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Cs    | 59  | LYS  |
| 3   | Cs    | 64  | VAL  |
| 3   | Cs    | 73  | LEU  |
| 3   | Cs    | 76  | MET  |
| 3   | Cs    | 77  | ASP  |
| 3   | Cs    | 80  | LEU  |
| 3   | Cs    | 93  | LEU  |
| 3   | Cs    | 116 | THR  |
| 3   | Cs    | 122 | VAL  |
| 3   | Cs    | 129 | SER  |
| 3   | Cs    | 135 | ARG  |
| 3   | Cs    | 139 | MET  |
| 3   | Cs    | 151 | ASN  |
| 3   | Cs    | 157 | ASN  |
| 3   | Cs    | 161 | SER  |
| 3   | Cs    | 175 | THR  |
| 3   | Cs    | 176 | VAL  |
| 3   | Cs    | 178 | ASN  |
| 3   | Cs    | 179 | VAL  |
| 3   | Cs    | 183 | LEU  |
| 3   | Cs    | 188 | LEU  |
| 3   | Cs    | 192 | THR  |
| 3   | Cs    | 194 | THR  |
| 3   | Cs    | 196 | ILE  |
| 3   | Cs    | 206 | VAL  |
| 3   | Cs    | 208 | VAL  |
| 3   | Cs    | 216 | LEU  |
| 3   | Cs    | 217 | ARG  |
| 3   | Ct    | 5   | VAL  |
| 3   | Ct    | 8   | VAL  |
| 3   | Ct    | 11  | SER  |
| 3   | Ct    | 16  | SER  |
| 3   | Ct    | 18  | VAL  |
| 3   | Ct    | 23  | THR  |
| 3   | Ct    | 31  | VAL  |
| 3   | Ct    | 35  | GLN  |
| 3   | Ct    | 36  | VAL  |
| 3   | Ct    | 42  | ASN  |
| 3   | Ct    | 50  | THR  |
| 3   | Ct    | 56  | ILE  |
| 3   | Ct    | 59  | LYS  |
| 3   | Ct    | 64  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Ct    | 73  | LEU  |
| 3   | Ct    | 76  | MET  |
| 3   | Ct    | 77  | ASP  |
| 3   | Ct    | 80  | LEU  |
| 3   | Ct    | 93  | LEU  |
| 3   | Ct    | 116 | THR  |
| 3   | Ct    | 122 | VAL  |
| 3   | Ct    | 129 | SER  |
| 3   | Ct    | 135 | ARG  |
| 3   | Ct    | 139 | MET  |
| 3   | Ct    | 151 | ASN  |
| 3   | Ct    | 157 | ASN  |
| 3   | Ct    | 161 | SER  |
| 3   | Ct    | 175 | THR  |
| 3   | Ct    | 176 | VAL  |
| 3   | Ct    | 178 | ASN  |
| 3   | Ct    | 179 | VAL  |
| 3   | Ct    | 183 | LEU  |
| 3   | Ct    | 188 | LEU  |
| 3   | Ct    | 192 | THR  |
| 3   | Ct    | 194 | THR  |
| 3   | Ct    | 196 | ILE  |
| 3   | Ct    | 206 | VAL  |
| 3   | Ct    | 208 | VAL  |
| 3   | Ct    | 216 | LEU  |
| 3   | Ct    | 217 | ARG  |
| 3   | Cu    | 5   | VAL  |
| 3   | Cu    | 8   | VAL  |
| 3   | Cu    | 11  | SER  |
| 3   | Cu    | 16  | SER  |
| 3   | Cu    | 18  | VAL  |
| 3   | Cu    | 23  | THR  |
| 3   | Cu    | 31  | VAL  |
| 3   | Cu    | 35  | GLN  |
| 3   | Cu    | 36  | VAL  |
| 3   | Cu    | 42  | ASN  |
| 3   | Cu    | 50  | THR  |
| 3   | Cu    | 56  | ILE  |
| 3   | Cu    | 59  | LYS  |
| 3   | Cu    | 64  | VAL  |
| 3   | Cu    | 73  | LEU  |
| 3   | Cu    | 76  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Cu    | 77  | ASP  |
| 3   | Cu    | 80  | LEU  |
| 3   | Cu    | 93  | LEU  |
| 3   | Cu    | 116 | THR  |
| 3   | Cu    | 122 | VAL  |
| 3   | Cu    | 129 | SER  |
| 3   | Cu    | 135 | ARG  |
| 3   | Cu    | 139 | MET  |
| 3   | Cu    | 151 | ASN  |
| 3   | Cu    | 157 | ASN  |
| 3   | Cu    | 161 | SER  |
| 3   | Cu    | 175 | THR  |
| 3   | Cu    | 176 | VAL  |
| 3   | Cu    | 178 | ASN  |
| 3   | Cu    | 179 | VAL  |
| 3   | Cu    | 183 | LEU  |
| 3   | Cu    | 188 | LEU  |
| 3   | Cu    | 192 | THR  |
| 3   | Cu    | 194 | THR  |
| 3   | Cu    | 196 | ILE  |
| 3   | Cu    | 206 | VAL  |
| 3   | Cu    | 208 | VAL  |
| 3   | Cu    | 216 | LEU  |
| 3   | Cu    | 217 | ARG  |
| 3   | Cv    | 5   | VAL  |
| 3   | Cv    | 8   | VAL  |
| 3   | Cv    | 11  | SER  |
| 3   | Cv    | 16  | SER  |
| 3   | Cv    | 18  | VAL  |
| 3   | Cv    | 23  | THR  |
| 3   | Cv    | 31  | VAL  |
| 3   | Cv    | 35  | GLN  |
| 3   | Cv    | 36  | VAL  |
| 3   | Cv    | 42  | ASN  |
| 3   | Cv    | 50  | THR  |
| 3   | Cv    | 56  | ILE  |
| 3   | Cv    | 59  | LYS  |
| 3   | Cv    | 64  | VAL  |
| 3   | Cv    | 73  | LEU  |
| 3   | Cv    | 76  | MET  |
| 3   | Cv    | 77  | ASP  |
| 3   | Cv    | 80  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Cv    | 93  | LEU  |
| 3   | Cv    | 116 | THR  |
| 3   | Cv    | 122 | VAL  |
| 3   | Cv    | 129 | SER  |
| 3   | Cv    | 135 | ARG  |
| 3   | Cv    | 139 | MET  |
| 3   | Cv    | 151 | ASN  |
| 3   | Cv    | 157 | ASN  |
| 3   | Cv    | 161 | SER  |
| 3   | Cv    | 175 | THR  |
| 3   | Cv    | 176 | VAL  |
| 3   | Cv    | 178 | ASN  |
| 3   | Cv    | 179 | VAL  |
| 3   | Cv    | 183 | LEU  |
| 3   | Cv    | 188 | LEU  |
| 3   | Cv    | 192 | THR  |
| 3   | Cv    | 194 | THR  |
| 3   | Cv    | 196 | ILE  |
| 3   | Cv    | 206 | VAL  |
| 3   | Cv    | 208 | VAL  |
| 3   | Cv    | 216 | LEU  |
| 3   | Cv    | 217 | ARG  |
| 3   | Cw    | 5   | VAL  |
| 3   | Cw    | 8   | VAL  |
| 3   | Cw    | 11  | SER  |
| 3   | Cw    | 16  | SER  |
| 3   | Cw    | 18  | VAL  |
| 3   | Cw    | 23  | THR  |
| 3   | Cw    | 31  | VAL  |
| 3   | Cw    | 35  | GLN  |
| 3   | Cw    | 36  | VAL  |
| 3   | Cw    | 42  | ASN  |
| 3   | Cw    | 50  | THR  |
| 3   | Cw    | 56  | ILE  |
| 3   | Cw    | 59  | LYS  |
| 3   | Cw    | 64  | VAL  |
| 3   | Cw    | 73  | LEU  |
| 3   | Cw    | 76  | MET  |
| 3   | Cw    | 77  | ASP  |
| 3   | Cw    | 80  | LEU  |
| 3   | Cw    | 93  | LEU  |
| 3   | Cw    | 116 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Cw    | 122 | VAL  |
| 3   | Cw    | 129 | SER  |
| 3   | Cw    | 135 | ARG  |
| 3   | Cw    | 139 | MET  |
| 3   | Cw    | 151 | ASN  |
| 3   | Cw    | 157 | ASN  |
| 3   | Cw    | 161 | SER  |
| 3   | Cw    | 175 | THR  |
| 3   | Cw    | 176 | VAL  |
| 3   | Cw    | 178 | ASN  |
| 3   | Cw    | 179 | VAL  |
| 3   | Cw    | 183 | LEU  |
| 3   | Cw    | 188 | LEU  |
| 3   | Cw    | 192 | THR  |
| 3   | Cw    | 194 | THR  |
| 3   | Cw    | 196 | ILE  |
| 3   | Cw    | 206 | VAL  |
| 3   | Cw    | 208 | VAL  |
| 3   | Cw    | 216 | LEU  |
| 3   | Cw    | 217 | ARG  |
| 3   | Cx    | 5   | VAL  |
| 3   | Cx    | 8   | VAL  |
| 3   | Cx    | 11  | SER  |
| 3   | Cx    | 16  | SER  |
| 3   | Cx    | 18  | VAL  |
| 3   | Cx    | 23  | THR  |
| 3   | Cx    | 31  | VAL  |
| 3   | Cx    | 35  | GLN  |
| 3   | Cx    | 36  | VAL  |
| 3   | Cx    | 42  | ASN  |
| 3   | Cx    | 50  | THR  |
| 3   | Cx    | 56  | ILE  |
| 3   | Cx    | 59  | LYS  |
| 3   | Cx    | 64  | VAL  |
| 3   | Cx    | 73  | LEU  |
| 3   | Cx    | 76  | MET  |
| 3   | Cx    | 77  | ASP  |
| 3   | Cx    | 80  | LEU  |
| 3   | Cx    | 93  | LEU  |
| 3   | Cx    | 116 | THR  |
| 3   | Cx    | 122 | VAL  |
| 3   | Cx    | 129 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Cx    | 135 | ARG  |
| 3   | Cx    | 139 | MET  |
| 3   | Cx    | 151 | ASN  |
| 3   | Cx    | 157 | ASN  |
| 3   | Cx    | 161 | SER  |
| 3   | Cx    | 175 | THR  |
| 3   | Cx    | 176 | VAL  |
| 3   | Cx    | 178 | ASN  |
| 3   | Cx    | 179 | VAL  |
| 3   | Cx    | 183 | LEU  |
| 3   | Cx    | 188 | LEU  |
| 3   | Cx    | 192 | THR  |
| 3   | Cx    | 194 | THR  |
| 3   | Cx    | 196 | ILE  |
| 3   | Cx    | 206 | VAL  |
| 3   | Cx    | 208 | VAL  |
| 3   | Cx    | 216 | LEU  |
| 3   | Cx    | 217 | ARG  |
| 3   | DA    | 5   | VAL  |
| 3   | DA    | 8   | VAL  |
| 3   | DA    | 11  | SER  |
| 3   | DA    | 16  | SER  |
| 3   | DA    | 18  | VAL  |
| 3   | DA    | 23  | THR  |
| 3   | DA    | 31  | VAL  |
| 3   | DA    | 35  | GLN  |
| 3   | DA    | 36  | VAL  |
| 3   | DA    | 42  | ASN  |
| 3   | DA    | 50  | THR  |
| 3   | DA    | 56  | ILE  |
| 3   | DA    | 59  | LYS  |
| 3   | DA    | 64  | VAL  |
| 3   | DA    | 73  | LEU  |
| 3   | DA    | 76  | MET  |
| 3   | DA    | 77  | ASP  |
| 3   | DA    | 80  | LEU  |
| 3   | DA    | 93  | LEU  |
| 3   | DA    | 116 | THR  |
| 3   | DA    | 122 | VAL  |
| 3   | DA    | 129 | SER  |
| 3   | DA    | 135 | ARG  |
| 3   | DA    | 139 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | DA    | 151 | ASN  |
| 3   | DA    | 157 | ASN  |
| 3   | DA    | 161 | SER  |
| 3   | DA    | 175 | THR  |
| 3   | DA    | 176 | VAL  |
| 3   | DA    | 178 | ASN  |
| 3   | DA    | 179 | VAL  |
| 3   | DA    | 183 | LEU  |
| 3   | DA    | 188 | LEU  |
| 3   | DA    | 192 | THR  |
| 3   | DA    | 194 | THR  |
| 3   | DA    | 196 | ILE  |
| 3   | DA    | 206 | VAL  |
| 3   | DA    | 208 | VAL  |
| 3   | DA    | 216 | LEU  |
| 3   | DA    | 217 | ARG  |
| 3   | DB    | 5   | VAL  |
| 3   | DB    | 8   | VAL  |
| 3   | DB    | 11  | SER  |
| 3   | DB    | 16  | SER  |
| 3   | DB    | 18  | VAL  |
| 3   | DB    | 23  | THR  |
| 3   | DB    | 31  | VAL  |
| 3   | DB    | 35  | GLN  |
| 3   | DB    | 36  | VAL  |
| 3   | DB    | 42  | ASN  |
| 3   | DB    | 50  | THR  |
| 3   | DB    | 56  | ILE  |
| 3   | DB    | 59  | LYS  |
| 3   | DB    | 64  | VAL  |
| 3   | DB    | 73  | LEU  |
| 3   | DB    | 76  | MET  |
| 3   | DB    | 77  | ASP  |
| 3   | DB    | 80  | LEU  |
| 3   | DB    | 93  | LEU  |
| 3   | DB    | 116 | THR  |
| 3   | DB    | 122 | VAL  |
| 3   | DB    | 129 | SER  |
| 3   | DB    | 135 | ARG  |
| 3   | DB    | 139 | MET  |
| 3   | DB    | 151 | ASN  |
| 3   | DB    | 157 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | DB    | 161 | SER  |
| 3   | DB    | 175 | THR  |
| 3   | DB    | 176 | VAL  |
| 3   | DB    | 178 | ASN  |
| 3   | DB    | 179 | VAL  |
| 3   | DB    | 183 | LEU  |
| 3   | DB    | 188 | LEU  |
| 3   | DB    | 192 | THR  |
| 3   | DB    | 194 | THR  |
| 3   | DB    | 196 | ILE  |
| 3   | DB    | 206 | VAL  |
| 3   | DB    | 208 | VAL  |
| 3   | DB    | 216 | LEU  |
| 3   | DB    | 217 | ARG  |
| 1   | DC    | 4   | VAL  |
| 1   | DC    | 28  | THR  |
| 1   | DC    | 36  | ARG  |
| 1   | DC    | 39  | ASP  |
| 1   | DC    | 40  | VAL  |
| 1   | DC    | 42  | THR  |
| 1   | DC    | 45  | LEU  |
| 1   | DC    | 49  | THR  |
| 1   | DC    | 62  | SER  |
| 1   | DC    | 71  | LEU  |
| 1   | DC    | 113 | THR  |
| 1   | DC    | 120 | GLN  |
| 1   | DC    | 150 | ARG  |
| 1   | DC    | 158 | VAL  |
| 1   | DC    | 163 | MET  |
| 1   | DC    | 166 | VAL  |
| 1   | DC    | 187 | LEU  |
| 1   | DC    | 196 | LEU  |
| 1   | DC    | 198 | THR  |
| 1   | DC    | 203 | ASP  |
| 1   | DC    | 209 | LEU  |
| 1   | DC    | 226 | PRO  |
| 1   | DC    | 237 | HIS  |
| 1   | DC    | 246 | GLN  |
| 1   | DD    | 4   | VAL  |
| 1   | DD    | 28  | THR  |
| 1   | DD    | 36  | ARG  |
| 1   | DD    | 39  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | DD    | 40  | VAL  |
| 1   | DD    | 42  | THR  |
| 1   | DD    | 45  | LEU  |
| 1   | DD    | 49  | THR  |
| 1   | DD    | 62  | SER  |
| 1   | DD    | 71  | LEU  |
| 1   | DD    | 113 | THR  |
| 1   | DD    | 120 | GLN  |
| 1   | DD    | 150 | ARG  |
| 1   | DD    | 158 | VAL  |
| 1   | DD    | 163 | MET  |
| 1   | DD    | 166 | VAL  |
| 1   | DD    | 187 | LEU  |
| 1   | DD    | 196 | LEU  |
| 1   | DD    | 198 | THR  |
| 1   | DD    | 203 | ASP  |
| 1   | DD    | 209 | LEU  |
| 1   | DD    | 226 | PRO  |
| 1   | DD    | 237 | HIS  |
| 1   | DD    | 246 | GLN  |
| 1   | DE    | 4   | VAL  |
| 1   | DE    | 28  | THR  |
| 1   | DE    | 36  | ARG  |
| 1   | DE    | 39  | ASP  |
| 1   | DE    | 40  | VAL  |
| 1   | DE    | 42  | THR  |
| 1   | DE    | 45  | LEU  |
| 1   | DE    | 49  | THR  |
| 1   | DE    | 62  | SER  |
| 1   | DE    | 71  | LEU  |
| 1   | DE    | 113 | THR  |
| 1   | DE    | 120 | GLN  |
| 1   | DE    | 150 | ARG  |
| 1   | DE    | 158 | VAL  |
| 1   | DE    | 163 | MET  |
| 1   | DE    | 166 | VAL  |
| 1   | DE    | 187 | LEU  |
| 1   | DE    | 196 | LEU  |
| 1   | DE    | 198 | THR  |
| 1   | DE    | 203 | ASP  |
| 1   | DE    | 209 | LEU  |
| 1   | DE    | 226 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | DE    | 237 | HIS  |
| 1   | DE    | 246 | GLN  |
| 1   | DF    | 4   | VAL  |
| 1   | DF    | 28  | THR  |
| 1   | DF    | 36  | ARG  |
| 1   | DF    | 39  | ASP  |
| 1   | DF    | 40  | VAL  |
| 1   | DF    | 42  | THR  |
| 1   | DF    | 45  | LEU  |
| 1   | DF    | 49  | THR  |
| 1   | DF    | 62  | SER  |
| 1   | DF    | 71  | LEU  |
| 1   | DF    | 113 | THR  |
| 1   | DF    | 120 | GLN  |
| 1   | DF    | 150 | ARG  |
| 1   | DF    | 158 | VAL  |
| 1   | DF    | 163 | MET  |
| 1   | DF    | 166 | VAL  |
| 1   | DF    | 187 | LEU  |
| 1   | DF    | 196 | LEU  |
| 1   | DF    | 198 | THR  |
| 1   | DF    | 203 | ASP  |
| 1   | DF    | 209 | LEU  |
| 1   | DF    | 226 | PRO  |
| 1   | DF    | 237 | HIS  |
| 1   | DF    | 246 | GLN  |
| 1   | DG    | 4   | VAL  |
| 1   | DG    | 28  | THR  |
| 1   | DG    | 36  | ARG  |
| 1   | DG    | 39  | ASP  |
| 1   | DG    | 40  | VAL  |
| 1   | DG    | 42  | THR  |
| 1   | DG    | 45  | LEU  |
| 1   | DG    | 49  | THR  |
| 1   | DG    | 62  | SER  |
| 1   | DG    | 71  | LEU  |
| 1   | DG    | 113 | THR  |
| 1   | DG    | 120 | GLN  |
| 1   | DG    | 150 | ARG  |
| 1   | DG    | 158 | VAL  |
| 1   | DG    | 163 | MET  |
| 1   | DG    | 166 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | DG    | 187 | LEU  |
| 1   | DG    | 196 | LEU  |
| 1   | DG    | 198 | THR  |
| 1   | DG    | 203 | ASP  |
| 1   | DG    | 209 | LEU  |
| 1   | DG    | 223 | PRO  |
| 1   | DG    | 226 | PRO  |
| 1   | DG    | 237 | HIS  |
| 1   | DG    | 246 | GLN  |
| 1   | DH    | 4   | VAL  |
| 1   | DH    | 28  | THR  |
| 1   | DH    | 36  | ARG  |
| 1   | DH    | 39  | ASP  |
| 1   | DH    | 40  | VAL  |
| 1   | DH    | 42  | THR  |
| 1   | DH    | 45  | LEU  |
| 1   | DH    | 49  | THR  |
| 1   | DH    | 62  | SER  |
| 1   | DH    | 71  | LEU  |
| 1   | DH    | 113 | THR  |
| 1   | DH    | 120 | GLN  |
| 1   | DH    | 150 | ARG  |
| 1   | DH    | 158 | VAL  |
| 1   | DH    | 163 | MET  |
| 1   | DH    | 166 | VAL  |
| 1   | DH    | 187 | LEU  |
| 1   | DH    | 196 | LEU  |
| 1   | DH    | 198 | THR  |
| 1   | DH    | 203 | ASP  |
| 1   | DH    | 209 | LEU  |
| 1   | DH    | 226 | PRO  |
| 1   | DH    | 237 | HIS  |
| 1   | DH    | 246 | GLN  |
| 1   | DI    | 4   | VAL  |
| 1   | DI    | 28  | THR  |
| 1   | DI    | 36  | ARG  |
| 1   | DI    | 39  | ASP  |
| 1   | DI    | 40  | VAL  |
| 1   | DI    | 42  | THR  |
| 1   | DI    | 45  | LEU  |
| 1   | DI    | 49  | THR  |
| 1   | DI    | 62  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | DI    | 71  | LEU  |
| 1   | DI    | 113 | THR  |
| 1   | DI    | 120 | GLN  |
| 1   | DI    | 150 | ARG  |
| 1   | DI    | 158 | VAL  |
| 1   | DI    | 163 | MET  |
| 1   | DI    | 166 | VAL  |
| 1   | DI    | 187 | LEU  |
| 1   | DI    | 196 | LEU  |
| 1   | DI    | 198 | THR  |
| 1   | DI    | 203 | ASP  |
| 1   | DI    | 209 | LEU  |
| 1   | DI    | 226 | PRO  |
| 1   | DI    | 237 | HIS  |
| 1   | DI    | 246 | GLN  |
| 1   | DJ    | 4   | VAL  |
| 1   | DJ    | 28  | THR  |
| 1   | DJ    | 36  | ARG  |
| 1   | DJ    | 39  | ASP  |
| 1   | DJ    | 40  | VAL  |
| 1   | DJ    | 42  | THR  |
| 1   | DJ    | 45  | LEU  |
| 1   | DJ    | 49  | THR  |
| 1   | DJ    | 62  | SER  |
| 1   | DJ    | 71  | LEU  |
| 1   | DJ    | 113 | THR  |
| 1   | DJ    | 120 | GLN  |
| 1   | DJ    | 150 | ARG  |
| 1   | DJ    | 158 | VAL  |
| 1   | DJ    | 163 | MET  |
| 1   | DJ    | 166 | VAL  |
| 1   | DJ    | 187 | LEU  |
| 1   | DJ    | 196 | LEU  |
| 1   | DJ    | 198 | THR  |
| 1   | DJ    | 203 | ASP  |
| 1   | DJ    | 209 | LEU  |
| 1   | DJ    | 226 | PRO  |
| 1   | DJ    | 237 | HIS  |
| 1   | DJ    | 246 | GLN  |
| 1   | DK    | 4   | VAL  |
| 1   | DK    | 28  | THR  |
| 1   | DK    | 36  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | DK    | 39  | ASP  |
| 1   | DK    | 40  | VAL  |
| 1   | DK    | 42  | THR  |
| 1   | DK    | 45  | LEU  |
| 1   | DK    | 49  | THR  |
| 1   | DK    | 62  | SER  |
| 1   | DK    | 71  | LEU  |
| 1   | DK    | 113 | THR  |
| 1   | DK    | 120 | GLN  |
| 1   | DK    | 150 | ARG  |
| 1   | DK    | 158 | VAL  |
| 1   | DK    | 163 | MET  |
| 1   | DK    | 166 | VAL  |
| 1   | DK    | 187 | LEU  |
| 1   | DK    | 196 | LEU  |
| 1   | DK    | 198 | THR  |
| 1   | DK    | 203 | ASP  |
| 1   | DK    | 209 | LEU  |
| 1   | DK    | 226 | PRO  |
| 1   | DK    | 237 | HIS  |
| 1   | DK    | 246 | GLN  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1200) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 47  | ASN  |
| 1   | AA    | 87  | GLN  |
| 1   | AA    | 191 | HIS  |
| 1   | AA    | 217 | ASN  |
| 1   | AA    | 242 | ASN  |
| 1   | AA    | 246 | GLN  |
| 1   | AB    | 47  | ASN  |
| 1   | AB    | 87  | GLN  |
| 1   | AB    | 191 | HIS  |
| 1   | AB    | 217 | ASN  |
| 1   | AB    | 242 | ASN  |
| 1   | AB    | 246 | GLN  |
| 1   | AC    | 47  | ASN  |
| 1   | AC    | 87  | GLN  |
| 1   | AC    | 191 | HIS  |
| 1   | AC    | 217 | ASN  |
| 1   | AC    | 242 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AC    | 246 | GLN  |
| 1   | AD    | 47  | ASN  |
| 1   | AD    | 87  | GLN  |
| 1   | AD    | 191 | HIS  |
| 1   | AD    | 217 | ASN  |
| 1   | AD    | 242 | ASN  |
| 1   | AD    | 246 | GLN  |
| 1   | AE    | 47  | ASN  |
| 1   | AE    | 87  | GLN  |
| 1   | AE    | 191 | HIS  |
| 1   | AE    | 217 | ASN  |
| 1   | AE    | 242 | ASN  |
| 1   | AE    | 246 | GLN  |
| 1   | AF    | 47  | ASN  |
| 1   | AF    | 87  | GLN  |
| 1   | AF    | 191 | HIS  |
| 1   | AF    | 217 | ASN  |
| 1   | AF    | 242 | ASN  |
| 1   | AF    | 246 | GLN  |
| 1   | AG    | 47  | ASN  |
| 1   | AG    | 87  | GLN  |
| 1   | AG    | 191 | HIS  |
| 1   | AG    | 217 | ASN  |
| 1   | AG    | 242 | ASN  |
| 1   | AG    | 246 | GLN  |
| 1   | AH    | 47  | ASN  |
| 1   | AH    | 87  | GLN  |
| 1   | AH    | 191 | HIS  |
| 1   | AH    | 217 | ASN  |
| 1   | AH    | 242 | ASN  |
| 1   | AH    | 246 | GLN  |
| 1   | AI    | 47  | ASN  |
| 1   | AI    | 87  | GLN  |
| 1   | AI    | 191 | HIS  |
| 1   | AI    | 217 | ASN  |
| 1   | AI    | 242 | ASN  |
| 1   | AI    | 246 | GLN  |
| 1   | AJ    | 47  | ASN  |
| 1   | AJ    | 87  | GLN  |
| 1   | AJ    | 191 | HIS  |
| 1   | AJ    | 217 | ASN  |
| 1   | AJ    | 242 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AJ    | 246 | GLN  |
| 1   | AK    | 47  | ASN  |
| 1   | AK    | 87  | GLN  |
| 1   | AK    | 191 | HIS  |
| 1   | AK    | 217 | ASN  |
| 1   | AK    | 242 | ASN  |
| 1   | AK    | 246 | GLN  |
| 1   | AL    | 47  | ASN  |
| 1   | AL    | 87  | GLN  |
| 1   | AL    | 191 | HIS  |
| 1   | AL    | 217 | ASN  |
| 1   | AL    | 242 | ASN  |
| 1   | AL    | 246 | GLN  |
| 1   | AM    | 47  | ASN  |
| 1   | AM    | 87  | GLN  |
| 1   | AM    | 191 | HIS  |
| 1   | AM    | 217 | ASN  |
| 1   | AM    | 242 | ASN  |
| 1   | AM    | 246 | GLN  |
| 1   | AN    | 47  | ASN  |
| 1   | AN    | 87  | GLN  |
| 1   | AN    | 191 | HIS  |
| 1   | AN    | 217 | ASN  |
| 1   | AN    | 242 | ASN  |
| 1   | AN    | 246 | GLN  |
| 1   | AO    | 47  | ASN  |
| 1   | AO    | 87  | GLN  |
| 1   | AO    | 191 | HIS  |
| 1   | AO    | 217 | ASN  |
| 1   | AO    | 242 | ASN  |
| 1   | AO    | 246 | GLN  |
| 1   | AP    | 47  | ASN  |
| 1   | AP    | 87  | GLN  |
| 1   | AP    | 191 | HIS  |
| 1   | AP    | 217 | ASN  |
| 1   | AP    | 242 | ASN  |
| 1   | AP    | 246 | GLN  |
| 1   | AQ    | 47  | ASN  |
| 1   | AQ    | 87  | GLN  |
| 1   | AQ    | 191 | HIS  |
| 1   | AQ    | 217 | ASN  |
| 1   | AQ    | 242 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AQ    | 246 | GLN  |
| 1   | AR    | 47  | ASN  |
| 1   | AR    | 87  | GLN  |
| 1   | AR    | 191 | HIS  |
| 1   | AR    | 217 | ASN  |
| 1   | AR    | 242 | ASN  |
| 1   | AR    | 246 | GLN  |
| 1   | AS    | 47  | ASN  |
| 1   | AS    | 87  | GLN  |
| 1   | AS    | 191 | HIS  |
| 1   | AS    | 217 | ASN  |
| 1   | AS    | 242 | ASN  |
| 1   | AS    | 246 | GLN  |
| 1   | AT    | 47  | ASN  |
| 1   | AT    | 87  | GLN  |
| 1   | AT    | 191 | HIS  |
| 1   | AT    | 217 | ASN  |
| 1   | AT    | 242 | ASN  |
| 1   | AT    | 246 | GLN  |
| 1   | AU    | 47  | ASN  |
| 1   | AU    | 87  | GLN  |
| 1   | AU    | 191 | HIS  |
| 1   | AU    | 217 | ASN  |
| 1   | AU    | 242 | ASN  |
| 1   | AU    | 246 | GLN  |
| 1   | AV    | 47  | ASN  |
| 1   | AV    | 87  | GLN  |
| 1   | AV    | 191 | HIS  |
| 1   | AV    | 217 | ASN  |
| 1   | AV    | 242 | ASN  |
| 1   | AV    | 246 | GLN  |
| 1   | AW    | 47  | ASN  |
| 1   | AW    | 87  | GLN  |
| 1   | AW    | 191 | HIS  |
| 1   | AW    | 217 | ASN  |
| 1   | AW    | 242 | ASN  |
| 1   | AW    | 246 | GLN  |
| 1   | AX    | 47  | ASN  |
| 1   | AX    | 87  | GLN  |
| 1   | AX    | 191 | HIS  |
| 1   | AX    | 217 | ASN  |
| 1   | AX    | 242 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AX    | 246 | GLN  |
| 1   | AY    | 47  | ASN  |
| 1   | AY    | 87  | GLN  |
| 1   | AY    | 191 | HIS  |
| 1   | AY    | 217 | ASN  |
| 1   | AY    | 242 | ASN  |
| 1   | AY    | 246 | GLN  |
| 1   | AZ    | 47  | ASN  |
| 1   | AZ    | 87  | GLN  |
| 1   | AZ    | 191 | HIS  |
| 1   | AZ    | 217 | ASN  |
| 1   | AZ    | 242 | ASN  |
| 1   | AZ    | 246 | GLN  |
| 1   | A0    | 47  | ASN  |
| 1   | A0    | 87  | GLN  |
| 1   | A0    | 191 | HIS  |
| 1   | A0    | 217 | ASN  |
| 1   | A0    | 242 | ASN  |
| 1   | A0    | 246 | GLN  |
| 1   | A1    | 47  | ASN  |
| 1   | A1    | 87  | GLN  |
| 1   | A1    | 191 | HIS  |
| 1   | A1    | 217 | ASN  |
| 1   | A1    | 242 | ASN  |
| 1   | A1    | 246 | GLN  |
| 1   | A2    | 47  | ASN  |
| 1   | A2    | 87  | GLN  |
| 1   | A2    | 191 | HIS  |
| 1   | A2    | 217 | ASN  |
| 1   | A2    | 242 | ASN  |
| 1   | A2    | 246 | GLN  |
| 1   | A3    | 47  | ASN  |
| 1   | A3    | 87  | GLN  |
| 1   | A3    | 191 | HIS  |
| 1   | A3    | 217 | ASN  |
| 1   | A3    | 242 | ASN  |
| 1   | A3    | 246 | GLN  |
| 1   | A4    | 47  | ASN  |
| 1   | A4    | 87  | GLN  |
| 1   | A4    | 191 | HIS  |
| 1   | A4    | 217 | ASN  |
| 1   | A4    | 242 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A4    | 246 | GLN  |
| 1   | A5    | 47  | ASN  |
| 1   | A5    | 87  | GLN  |
| 1   | A5    | 191 | HIS  |
| 1   | A5    | 217 | ASN  |
| 1   | A5    | 242 | ASN  |
| 1   | A5    | 246 | GLN  |
| 1   | A6    | 47  | ASN  |
| 1   | A6    | 87  | GLN  |
| 1   | A6    | 191 | HIS  |
| 1   | A6    | 217 | ASN  |
| 1   | A6    | 242 | ASN  |
| 1   | A6    | 246 | GLN  |
| 1   | A7    | 47  | ASN  |
| 1   | A7    | 87  | GLN  |
| 1   | A7    | 191 | HIS  |
| 1   | A7    | 217 | ASN  |
| 1   | A7    | 242 | ASN  |
| 1   | A7    | 246 | GLN  |
| 1   | A8    | 47  | ASN  |
| 1   | A8    | 87  | GLN  |
| 1   | A8    | 191 | HIS  |
| 1   | A8    | 217 | ASN  |
| 1   | A8    | 242 | ASN  |
| 1   | A8    | 246 | GLN  |
| 1   | A9    | 47  | ASN  |
| 1   | A9    | 87  | GLN  |
| 1   | A9    | 191 | HIS  |
| 1   | A9    | 217 | ASN  |
| 1   | A9    | 242 | ASN  |
| 1   | A9    | 246 | GLN  |
| 1   | Aa    | 47  | ASN  |
| 1   | Aa    | 87  | GLN  |
| 1   | Aa    | 191 | HIS  |
| 1   | Aa    | 217 | ASN  |
| 1   | Aa    | 242 | ASN  |
| 1   | Aa    | 246 | GLN  |
| 1   | Ab    | 47  | ASN  |
| 1   | Ab    | 87  | GLN  |
| 1   | Ab    | 191 | HIS  |
| 1   | Ab    | 217 | ASN  |
| 1   | Ab    | 242 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Ab    | 246 | GLN  |
| 1   | Ac    | 47  | ASN  |
| 1   | Ac    | 87  | GLN  |
| 1   | Ac    | 191 | HIS  |
| 1   | Ac    | 217 | ASN  |
| 1   | Ac    | 242 | ASN  |
| 1   | Ac    | 246 | GLN  |
| 1   | Ad    | 47  | ASN  |
| 1   | Ad    | 87  | GLN  |
| 1   | Ad    | 191 | HIS  |
| 1   | Ad    | 217 | ASN  |
| 1   | Ad    | 242 | ASN  |
| 1   | Ad    | 246 | GLN  |
| 1   | Ae    | 47  | ASN  |
| 1   | Ae    | 87  | GLN  |
| 1   | Ae    | 191 | HIS  |
| 1   | Ae    | 217 | ASN  |
| 1   | Ae    | 242 | ASN  |
| 1   | Ae    | 246 | GLN  |
| 1   | Af    | 47  | ASN  |
| 1   | Af    | 87  | GLN  |
| 1   | Af    | 191 | HIS  |
| 1   | Af    | 217 | ASN  |
| 1   | Af    | 242 | ASN  |
| 1   | Af    | 246 | GLN  |
| 1   | Ag    | 47  | ASN  |
| 1   | Ag    | 87  | GLN  |
| 1   | Ag    | 191 | HIS  |
| 1   | Ag    | 217 | ASN  |
| 1   | Ag    | 242 | ASN  |
| 1   | Ag    | 246 | GLN  |
| 1   | Ah    | 47  | ASN  |
| 1   | Ah    | 87  | GLN  |
| 1   | Ah    | 191 | HIS  |
| 1   | Ah    | 217 | ASN  |
| 1   | Ah    | 242 | ASN  |
| 1   | Ah    | 246 | GLN  |
| 1   | Ai    | 47  | ASN  |
| 1   | Ai    | 87  | GLN  |
| 1   | Ai    | 191 | HIS  |
| 1   | Ai    | 217 | ASN  |
| 1   | Ai    | 242 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Ai    | 246 | GLN  |
| 1   | Aj    | 47  | ASN  |
| 1   | Aj    | 87  | GLN  |
| 1   | Aj    | 191 | HIS  |
| 1   | Aj    | 217 | ASN  |
| 1   | Aj    | 242 | ASN  |
| 1   | Aj    | 246 | GLN  |
| 1   | Ak    | 47  | ASN  |
| 1   | Ak    | 87  | GLN  |
| 1   | Ak    | 191 | HIS  |
| 1   | Ak    | 217 | ASN  |
| 1   | Ak    | 242 | ASN  |
| 1   | Ak    | 246 | GLN  |
| 1   | Al    | 47  | ASN  |
| 1   | Al    | 87  | GLN  |
| 1   | Al    | 191 | HIS  |
| 1   | Al    | 217 | ASN  |
| 1   | Al    | 242 | ASN  |
| 1   | Al    | 246 | GLN  |
| 1   | Am    | 47  | ASN  |
| 1   | Am    | 87  | GLN  |
| 1   | Am    | 191 | HIS  |
| 1   | Am    | 217 | ASN  |
| 1   | Am    | 242 | ASN  |
| 1   | Am    | 246 | GLN  |
| 1   | An    | 47  | ASN  |
| 1   | An    | 87  | GLN  |
| 1   | An    | 191 | HIS  |
| 1   | An    | 217 | ASN  |
| 1   | An    | 242 | ASN  |
| 1   | An    | 246 | GLN  |
| 1   | Ao    | 47  | ASN  |
| 1   | Ao    | 87  | GLN  |
| 1   | Ao    | 191 | HIS  |
| 1   | Ao    | 217 | ASN  |
| 1   | Ao    | 242 | ASN  |
| 1   | Ao    | 246 | GLN  |
| 2   | BA    | 73  | GLN  |
| 2   | BA    | 77  | HIS  |
| 2   | BA    | 95  | HIS  |
| 2   | BA    | 101 | HIS  |
| 2   | BA    | 134 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | BA    | 136 | HIS  |
| 2   | BA    | 168 | ASN  |
| 2   | BA    | 190 | ASN  |
| 2   | BB    | 73  | GLN  |
| 2   | BB    | 77  | HIS  |
| 2   | BB    | 95  | HIS  |
| 2   | BB    | 101 | HIS  |
| 2   | BB    | 134 | HIS  |
| 2   | BB    | 136 | HIS  |
| 2   | BB    | 168 | ASN  |
| 2   | BB    | 190 | ASN  |
| 2   | BC    | 73  | GLN  |
| 2   | BC    | 77  | HIS  |
| 2   | BC    | 95  | HIS  |
| 2   | BC    | 101 | HIS  |
| 2   | BC    | 134 | HIS  |
| 2   | BC    | 136 | HIS  |
| 2   | BC    | 168 | ASN  |
| 2   | BC    | 190 | ASN  |
| 2   | BD    | 73  | GLN  |
| 2   | BD    | 77  | HIS  |
| 2   | BD    | 95  | HIS  |
| 2   | BD    | 101 | HIS  |
| 2   | BD    | 134 | HIS  |
| 2   | BD    | 136 | HIS  |
| 2   | BD    | 168 | ASN  |
| 2   | BD    | 190 | ASN  |
| 2   | BE    | 73  | GLN  |
| 2   | BE    | 77  | HIS  |
| 2   | BE    | 95  | HIS  |
| 2   | BE    | 101 | HIS  |
| 2   | BE    | 134 | HIS  |
| 2   | BE    | 136 | HIS  |
| 2   | BE    | 168 | ASN  |
| 2   | BE    | 190 | ASN  |
| 2   | BF    | 73  | GLN  |
| 2   | BF    | 77  | HIS  |
| 2   | BF    | 95  | HIS  |
| 2   | BF    | 101 | HIS  |
| 2   | BF    | 134 | HIS  |
| 2   | BF    | 136 | HIS  |
| 2   | BF    | 168 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | BF    | 190 | ASN  |
| 2   | BG    | 73  | GLN  |
| 2   | BG    | 77  | HIS  |
| 2   | BG    | 95  | HIS  |
| 2   | BG    | 101 | HIS  |
| 2   | BG    | 134 | HIS  |
| 2   | BG    | 136 | HIS  |
| 2   | BG    | 168 | ASN  |
| 2   | BG    | 190 | ASN  |
| 2   | BH    | 73  | GLN  |
| 2   | BH    | 77  | HIS  |
| 2   | BH    | 95  | HIS  |
| 2   | BH    | 101 | HIS  |
| 2   | BH    | 134 | HIS  |
| 2   | BH    | 136 | HIS  |
| 2   | BH    | 168 | ASN  |
| 2   | BH    | 190 | ASN  |
| 2   | BI    | 73  | GLN  |
| 2   | BI    | 77  | HIS  |
| 2   | BI    | 95  | HIS  |
| 2   | BI    | 101 | HIS  |
| 2   | BI    | 134 | HIS  |
| 2   | BI    | 136 | HIS  |
| 2   | BI    | 168 | ASN  |
| 2   | BI    | 190 | ASN  |
| 2   | BJ    | 73  | GLN  |
| 2   | BJ    | 77  | HIS  |
| 2   | BJ    | 95  | HIS  |
| 2   | BJ    | 101 | HIS  |
| 2   | BJ    | 134 | HIS  |
| 2   | BJ    | 136 | HIS  |
| 2   | BJ    | 168 | ASN  |
| 2   | BJ    | 190 | ASN  |
| 2   | BK    | 73  | GLN  |
| 2   | BK    | 77  | HIS  |
| 2   | BK    | 95  | HIS  |
| 2   | BK    | 101 | HIS  |
| 2   | BK    | 134 | HIS  |
| 2   | BK    | 136 | HIS  |
| 2   | BK    | 168 | ASN  |
| 2   | BK    | 190 | ASN  |
| 2   | BL    | 73  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | BL    | 77  | HIS  |
| 2   | BL    | 95  | HIS  |
| 2   | BL    | 101 | HIS  |
| 2   | BL    | 134 | HIS  |
| 2   | BL    | 136 | HIS  |
| 2   | BL    | 168 | ASN  |
| 2   | BL    | 190 | ASN  |
| 2   | BM    | 73  | GLN  |
| 2   | BM    | 77  | HIS  |
| 2   | BM    | 95  | HIS  |
| 2   | BM    | 101 | HIS  |
| 2   | BM    | 134 | HIS  |
| 2   | BM    | 136 | HIS  |
| 2   | BM    | 168 | ASN  |
| 2   | BM    | 190 | ASN  |
| 2   | BN    | 73  | GLN  |
| 2   | BN    | 77  | HIS  |
| 2   | BN    | 95  | HIS  |
| 2   | BN    | 101 | HIS  |
| 2   | BN    | 134 | HIS  |
| 2   | BN    | 136 | HIS  |
| 2   | BN    | 168 | ASN  |
| 2   | BN    | 190 | ASN  |
| 2   | BR    | 73  | GLN  |
| 2   | BR    | 77  | HIS  |
| 2   | BR    | 95  | HIS  |
| 2   | BR    | 101 | HIS  |
| 2   | BR    | 134 | HIS  |
| 2   | BR    | 136 | HIS  |
| 2   | BR    | 168 | ASN  |
| 2   | BR    | 190 | ASN  |
| 2   | BO    | 73  | GLN  |
| 2   | BO    | 77  | HIS  |
| 2   | BO    | 95  | HIS  |
| 2   | BO    | 101 | HIS  |
| 2   | BO    | 134 | HIS  |
| 2   | BO    | 136 | HIS  |
| 2   | BO    | 168 | ASN  |
| 2   | BO    | 190 | ASN  |
| 2   | BS    | 73  | GLN  |
| 2   | BS    | 77  | HIS  |
| 2   | BS    | 95  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | BS    | 101 | HIS  |
| 2   | BS    | 134 | HIS  |
| 2   | BS    | 136 | HIS  |
| 2   | BS    | 168 | ASN  |
| 2   | BS    | 190 | ASN  |
| 2   | BP    | 73  | GLN  |
| 2   | BP    | 77  | HIS  |
| 2   | BP    | 95  | HIS  |
| 2   | BP    | 101 | HIS  |
| 2   | BP    | 134 | HIS  |
| 2   | BP    | 136 | HIS  |
| 2   | BP    | 168 | ASN  |
| 2   | BP    | 190 | ASN  |
| 2   | BQ    | 73  | GLN  |
| 2   | BQ    | 77  | HIS  |
| 2   | BQ    | 95  | HIS  |
| 2   | BQ    | 101 | HIS  |
| 2   | BQ    | 134 | HIS  |
| 2   | BQ    | 136 | HIS  |
| 2   | BQ    | 168 | ASN  |
| 2   | BQ    | 190 | ASN  |
| 2   | BT    | 73  | GLN  |
| 2   | BT    | 77  | HIS  |
| 2   | BT    | 95  | HIS  |
| 2   | BT    | 101 | HIS  |
| 2   | BT    | 134 | HIS  |
| 2   | BT    | 136 | HIS  |
| 2   | BT    | 168 | ASN  |
| 2   | BT    | 190 | ASN  |
| 2   | BU    | 73  | GLN  |
| 2   | BU    | 77  | HIS  |
| 2   | BU    | 95  | HIS  |
| 2   | BU    | 101 | HIS  |
| 2   | BU    | 134 | HIS  |
| 2   | BU    | 136 | HIS  |
| 2   | BU    | 168 | ASN  |
| 2   | BU    | 190 | ASN  |
| 2   | BV    | 73  | GLN  |
| 2   | BV    | 77  | HIS  |
| 2   | BV    | 95  | HIS  |
| 2   | BV    | 101 | HIS  |
| 2   | BV    | 134 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | BV    | 136 | HIS  |
| 2   | BV    | 168 | ASN  |
| 2   | BV    | 190 | ASN  |
| 2   | BW    | 73  | GLN  |
| 2   | BW    | 77  | HIS  |
| 2   | BW    | 95  | HIS  |
| 2   | BW    | 101 | HIS  |
| 2   | BW    | 134 | HIS  |
| 2   | BW    | 136 | HIS  |
| 2   | BW    | 168 | ASN  |
| 2   | BW    | 190 | ASN  |
| 2   | BX    | 73  | GLN  |
| 2   | BX    | 77  | HIS  |
| 2   | BX    | 95  | HIS  |
| 2   | BX    | 101 | HIS  |
| 2   | BX    | 134 | HIS  |
| 2   | BX    | 136 | HIS  |
| 2   | BX    | 168 | ASN  |
| 2   | BX    | 190 | ASN  |
| 2   | BY    | 73  | GLN  |
| 2   | BY    | 77  | HIS  |
| 2   | BY    | 95  | HIS  |
| 2   | BY    | 101 | HIS  |
| 2   | BY    | 134 | HIS  |
| 2   | BY    | 136 | HIS  |
| 2   | BY    | 168 | ASN  |
| 2   | BY    | 190 | ASN  |
| 2   | BZ    | 73  | GLN  |
| 2   | BZ    | 77  | HIS  |
| 2   | BZ    | 95  | HIS  |
| 2   | BZ    | 101 | HIS  |
| 2   | BZ    | 134 | HIS  |
| 2   | BZ    | 136 | HIS  |
| 2   | BZ    | 168 | ASN  |
| 2   | BZ    | 190 | ASN  |
| 2   | B0    | 73  | GLN  |
| 2   | B0    | 77  | HIS  |
| 2   | B0    | 95  | HIS  |
| 2   | B0    | 101 | HIS  |
| 2   | B0    | 134 | HIS  |
| 2   | B0    | 136 | HIS  |
| 2   | B0    | 168 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B0    | 190 | ASN  |
| 2   | B1    | 73  | GLN  |
| 2   | B1    | 77  | HIS  |
| 2   | B1    | 95  | HIS  |
| 2   | B1    | 101 | HIS  |
| 2   | B1    | 134 | HIS  |
| 2   | B1    | 136 | HIS  |
| 2   | B1    | 168 | ASN  |
| 2   | B1    | 190 | ASN  |
| 2   | B2    | 73  | GLN  |
| 2   | B2    | 77  | HIS  |
| 2   | B2    | 95  | HIS  |
| 2   | B2    | 101 | HIS  |
| 2   | B2    | 134 | HIS  |
| 2   | B2    | 136 | HIS  |
| 2   | B2    | 168 | ASN  |
| 2   | B2    | 190 | ASN  |
| 2   | B3    | 73  | GLN  |
| 2   | B3    | 77  | HIS  |
| 2   | B3    | 95  | HIS  |
| 2   | B3    | 101 | HIS  |
| 2   | B3    | 134 | HIS  |
| 2   | B3    | 136 | HIS  |
| 2   | B3    | 168 | ASN  |
| 2   | B3    | 190 | ASN  |
| 2   | B4    | 73  | GLN  |
| 2   | B4    | 77  | HIS  |
| 2   | B4    | 95  | HIS  |
| 2   | B4    | 101 | HIS  |
| 2   | B4    | 134 | HIS  |
| 2   | B4    | 136 | HIS  |
| 2   | B4    | 168 | ASN  |
| 2   | B4    | 190 | ASN  |
| 2   | B5    | 73  | GLN  |
| 2   | B5    | 77  | HIS  |
| 2   | B5    | 95  | HIS  |
| 2   | B5    | 101 | HIS  |
| 2   | B5    | 134 | HIS  |
| 2   | B5    | 136 | HIS  |
| 2   | B5    | 168 | ASN  |
| 2   | B5    | 190 | ASN  |
| 2   | B6    | 73  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B6    | 77  | HIS  |
| 2   | B6    | 95  | HIS  |
| 2   | B6    | 101 | HIS  |
| 2   | B6    | 134 | HIS  |
| 2   | B6    | 136 | HIS  |
| 2   | B6    | 168 | ASN  |
| 2   | B6    | 190 | ASN  |
| 2   | B7    | 73  | GLN  |
| 2   | B7    | 77  | HIS  |
| 2   | B7    | 95  | HIS  |
| 2   | B7    | 101 | HIS  |
| 2   | B7    | 134 | HIS  |
| 2   | B7    | 136 | HIS  |
| 2   | B7    | 168 | ASN  |
| 2   | B7    | 190 | ASN  |
| 2   | B8    | 73  | GLN  |
| 2   | B8    | 77  | HIS  |
| 2   | B8    | 95  | HIS  |
| 2   | B8    | 101 | HIS  |
| 2   | B8    | 134 | HIS  |
| 2   | B8    | 136 | HIS  |
| 2   | B8    | 168 | ASN  |
| 2   | B8    | 190 | ASN  |
| 2   | B9    | 73  | GLN  |
| 2   | B9    | 77  | HIS  |
| 2   | B9    | 95  | HIS  |
| 2   | B9    | 101 | HIS  |
| 2   | B9    | 134 | HIS  |
| 2   | B9    | 136 | HIS  |
| 2   | B9    | 168 | ASN  |
| 2   | B9    | 190 | ASN  |
| 2   | Ba    | 73  | GLN  |
| 2   | Ba    | 77  | HIS  |
| 2   | Ba    | 95  | HIS  |
| 2   | Ba    | 101 | HIS  |
| 2   | Ba    | 134 | HIS  |
| 2   | Ba    | 136 | HIS  |
| 2   | Ba    | 168 | ASN  |
| 2   | Ba    | 190 | ASN  |
| 2   | Bb    | 73  | GLN  |
| 2   | Bb    | 77  | HIS  |
| 2   | Bb    | 95  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Bb    | 101 | HIS  |
| 2   | Bb    | 134 | HIS  |
| 2   | Bb    | 136 | HIS  |
| 2   | Bb    | 168 | ASN  |
| 2   | Bb    | 190 | ASN  |
| 2   | Bc    | 73  | GLN  |
| 2   | Bc    | 77  | HIS  |
| 2   | Bc    | 95  | HIS  |
| 2   | Bc    | 101 | HIS  |
| 2   | Bc    | 134 | HIS  |
| 2   | Bc    | 136 | HIS  |
| 2   | Bc    | 168 | ASN  |
| 2   | Bc    | 190 | ASN  |
| 2   | Bd    | 73  | GLN  |
| 2   | Bd    | 77  | HIS  |
| 2   | Bd    | 95  | HIS  |
| 2   | Bd    | 101 | HIS  |
| 2   | Bd    | 134 | HIS  |
| 2   | Bd    | 136 | HIS  |
| 2   | Bd    | 168 | ASN  |
| 2   | Bd    | 190 | ASN  |
| 2   | Be    | 73  | GLN  |
| 2   | Be    | 77  | HIS  |
| 2   | Be    | 95  | HIS  |
| 2   | Be    | 101 | HIS  |
| 2   | Be    | 134 | HIS  |
| 2   | Be    | 136 | HIS  |
| 2   | Be    | 168 | ASN  |
| 2   | Be    | 190 | ASN  |
| 2   | Bf    | 73  | GLN  |
| 2   | Bf    | 77  | HIS  |
| 2   | Bf    | 95  | HIS  |
| 2   | Bf    | 101 | HIS  |
| 2   | Bf    | 134 | HIS  |
| 2   | Bf    | 136 | HIS  |
| 2   | Bf    | 168 | ASN  |
| 2   | Bf    | 190 | ASN  |
| 2   | Bg    | 73  | GLN  |
| 2   | Bg    | 77  | HIS  |
| 2   | Bg    | 95  | HIS  |
| 2   | Bg    | 101 | HIS  |
| 2   | Bg    | 134 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Bg    | 136 | HIS  |
| 2   | Bg    | 168 | ASN  |
| 2   | Bg    | 190 | ASN  |
| 2   | Bh    | 73  | GLN  |
| 2   | Bh    | 77  | HIS  |
| 2   | Bh    | 95  | HIS  |
| 2   | Bh    | 101 | HIS  |
| 2   | Bh    | 134 | HIS  |
| 2   | Bh    | 136 | HIS  |
| 2   | Bh    | 168 | ASN  |
| 2   | Bh    | 190 | ASN  |
| 2   | Bi    | 73  | GLN  |
| 2   | Bi    | 77  | HIS  |
| 2   | Bi    | 95  | HIS  |
| 2   | Bi    | 101 | HIS  |
| 2   | Bi    | 134 | HIS  |
| 2   | Bi    | 136 | HIS  |
| 2   | Bi    | 168 | ASN  |
| 2   | Bi    | 190 | ASN  |
| 2   | Bj    | 73  | GLN  |
| 2   | Bj    | 77  | HIS  |
| 2   | Bj    | 95  | HIS  |
| 2   | Bj    | 101 | HIS  |
| 2   | Bj    | 134 | HIS  |
| 2   | Bj    | 136 | HIS  |
| 2   | Bj    | 168 | ASN  |
| 2   | Bj    | 190 | ASN  |
| 2   | Bk    | 73  | GLN  |
| 2   | Bk    | 77  | HIS  |
| 2   | Bk    | 95  | HIS  |
| 2   | Bk    | 101 | HIS  |
| 2   | Bk    | 134 | HIS  |
| 2   | Bk    | 136 | HIS  |
| 2   | Bk    | 168 | ASN  |
| 2   | Bk    | 190 | ASN  |
| 2   | Bl    | 73  | GLN  |
| 2   | Bl    | 77  | HIS  |
| 2   | Bl    | 95  | HIS  |
| 2   | Bl    | 101 | HIS  |
| 2   | Bl    | 134 | HIS  |
| 2   | Bl    | 136 | HIS  |
| 2   | Bl    | 168 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B1    | 190 | ASN  |
| 2   | Bm    | 73  | GLN  |
| 2   | Bm    | 77  | HIS  |
| 2   | Bm    | 95  | HIS  |
| 2   | Bm    | 101 | HIS  |
| 2   | Bm    | 134 | HIS  |
| 2   | Bm    | 136 | HIS  |
| 2   | Bm    | 168 | ASN  |
| 2   | Bm    | 190 | ASN  |
| 2   | Bn    | 73  | GLN  |
| 2   | Bn    | 77  | HIS  |
| 2   | Bn    | 95  | HIS  |
| 2   | Bn    | 101 | HIS  |
| 2   | Bn    | 134 | HIS  |
| 2   | Bn    | 136 | HIS  |
| 2   | Bn    | 168 | ASN  |
| 2   | Bn    | 190 | ASN  |
| 2   | Bo    | 73  | GLN  |
| 2   | Bo    | 77  | HIS  |
| 2   | Bo    | 95  | HIS  |
| 2   | Bo    | 101 | HIS  |
| 2   | Bo    | 134 | HIS  |
| 2   | Bo    | 136 | HIS  |
| 2   | Bo    | 168 | ASN  |
| 2   | Bo    | 190 | ASN  |
| 2   | Bp    | 73  | GLN  |
| 2   | Bp    | 77  | HIS  |
| 2   | Bp    | 95  | HIS  |
| 2   | Bp    | 101 | HIS  |
| 2   | Bp    | 134 | HIS  |
| 2   | Bp    | 136 | HIS  |
| 2   | Bp    | 168 | ASN  |
| 2   | Bp    | 190 | ASN  |
| 2   | Bq    | 73  | GLN  |
| 2   | Bq    | 77  | HIS  |
| 2   | Bq    | 95  | HIS  |
| 2   | Bq    | 101 | HIS  |
| 2   | Bq    | 134 | HIS  |
| 2   | Bq    | 136 | HIS  |
| 2   | Bq    | 168 | ASN  |
| 2   | Bq    | 190 | ASN  |
| 2   | Br    | 73  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Br    | 77  | HIS  |
| 2   | Br    | 95  | HIS  |
| 2   | Br    | 101 | HIS  |
| 2   | Br    | 134 | HIS  |
| 2   | Br    | 136 | HIS  |
| 2   | Br    | 168 | ASN  |
| 2   | Br    | 190 | ASN  |
| 2   | Bs    | 73  | GLN  |
| 2   | Bs    | 77  | HIS  |
| 2   | Bs    | 95  | HIS  |
| 2   | Bs    | 101 | HIS  |
| 2   | Bs    | 134 | HIS  |
| 2   | Bs    | 136 | HIS  |
| 2   | Bs    | 168 | ASN  |
| 2   | Bs    | 190 | ASN  |
| 2   | Bt    | 73  | GLN  |
| 2   | Bt    | 77  | HIS  |
| 2   | Bt    | 95  | HIS  |
| 2   | Bt    | 101 | HIS  |
| 2   | Bt    | 134 | HIS  |
| 2   | Bt    | 136 | HIS  |
| 2   | Bt    | 168 | ASN  |
| 2   | Bt    | 190 | ASN  |
| 2   | Bu    | 73  | GLN  |
| 2   | Bu    | 77  | HIS  |
| 2   | Bu    | 95  | HIS  |
| 2   | Bu    | 101 | HIS  |
| 2   | Bu    | 134 | HIS  |
| 2   | Bu    | 136 | HIS  |
| 2   | Bu    | 168 | ASN  |
| 2   | Bu    | 190 | ASN  |
| 2   | Bv    | 73  | GLN  |
| 2   | Bv    | 77  | HIS  |
| 2   | Bv    | 95  | HIS  |
| 2   | Bv    | 101 | HIS  |
| 2   | Bv    | 134 | HIS  |
| 2   | Bv    | 136 | HIS  |
| 2   | Bv    | 168 | ASN  |
| 2   | Bv    | 190 | ASN  |
| 2   | Bw    | 73  | GLN  |
| 2   | Bw    | 77  | HIS  |
| 2   | Bw    | 95  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Bw    | 101 | HIS  |
| 2   | Bw    | 134 | HIS  |
| 2   | Bw    | 136 | HIS  |
| 2   | Bw    | 168 | ASN  |
| 2   | Bw    | 190 | ASN  |
| 2   | Bx    | 73  | GLN  |
| 2   | Bx    | 77  | HIS  |
| 2   | Bx    | 95  | HIS  |
| 2   | Bx    | 101 | HIS  |
| 2   | Bx    | 134 | HIS  |
| 2   | Bx    | 136 | HIS  |
| 2   | Bx    | 168 | ASN  |
| 2   | Bx    | 190 | ASN  |
| 3   | CA    | 35  | GLN  |
| 3   | CA    | 42  | ASN  |
| 3   | CA    | 75  | GLN  |
| 3   | CA    | 157 | ASN  |
| 3   | CA    | 178 | ASN  |
| 3   | CA    | 184 | GLN  |
| 3   | CB    | 35  | GLN  |
| 3   | CB    | 42  | ASN  |
| 3   | CB    | 75  | GLN  |
| 3   | CB    | 157 | ASN  |
| 3   | CB    | 178 | ASN  |
| 3   | CB    | 184 | GLN  |
| 3   | CC    | 35  | GLN  |
| 3   | CC    | 42  | ASN  |
| 3   | CC    | 75  | GLN  |
| 3   | CC    | 157 | ASN  |
| 3   | CC    | 178 | ASN  |
| 3   | CC    | 184 | GLN  |
| 3   | CD    | 35  | GLN  |
| 3   | CD    | 42  | ASN  |
| 3   | CD    | 75  | GLN  |
| 3   | CD    | 157 | ASN  |
| 3   | CD    | 178 | ASN  |
| 3   | CD    | 184 | GLN  |
| 3   | CE    | 35  | GLN  |
| 3   | CE    | 42  | ASN  |
| 3   | CE    | 75  | GLN  |
| 3   | CE    | 157 | ASN  |
| 3   | CE    | 178 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CE    | 184 | GLN  |
| 3   | CF    | 35  | GLN  |
| 3   | CF    | 42  | ASN  |
| 3   | CF    | 75  | GLN  |
| 3   | CF    | 157 | ASN  |
| 3   | CF    | 178 | ASN  |
| 3   | CF    | 184 | GLN  |
| 3   | CG    | 35  | GLN  |
| 3   | CG    | 42  | ASN  |
| 3   | CG    | 75  | GLN  |
| 3   | CG    | 157 | ASN  |
| 3   | CG    | 178 | ASN  |
| 3   | CG    | 184 | GLN  |
| 3   | CH    | 35  | GLN  |
| 3   | CH    | 42  | ASN  |
| 3   | CH    | 75  | GLN  |
| 3   | CH    | 157 | ASN  |
| 3   | CH    | 178 | ASN  |
| 3   | CH    | 184 | GLN  |
| 3   | CI    | 35  | GLN  |
| 3   | CI    | 42  | ASN  |
| 3   | CI    | 75  | GLN  |
| 3   | CI    | 157 | ASN  |
| 3   | CI    | 178 | ASN  |
| 3   | CI    | 184 | GLN  |
| 3   | CJ    | 35  | GLN  |
| 3   | CJ    | 42  | ASN  |
| 3   | CJ    | 75  | GLN  |
| 3   | CJ    | 157 | ASN  |
| 3   | CJ    | 178 | ASN  |
| 3   | CJ    | 184 | GLN  |
| 3   | CK    | 35  | GLN  |
| 3   | CK    | 42  | ASN  |
| 3   | CK    | 75  | GLN  |
| 3   | CK    | 157 | ASN  |
| 3   | CK    | 178 | ASN  |
| 3   | CK    | 184 | GLN  |
| 3   | CL    | 35  | GLN  |
| 3   | CL    | 42  | ASN  |
| 3   | CL    | 75  | GLN  |
| 3   | CL    | 157 | ASN  |
| 3   | CL    | 178 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CL    | 184 | GLN  |
| 3   | CM    | 35  | GLN  |
| 3   | CM    | 42  | ASN  |
| 3   | CM    | 75  | GLN  |
| 3   | CM    | 157 | ASN  |
| 3   | CM    | 178 | ASN  |
| 3   | CM    | 184 | GLN  |
| 3   | CN    | 35  | GLN  |
| 3   | CN    | 42  | ASN  |
| 3   | CN    | 75  | GLN  |
| 3   | CN    | 157 | ASN  |
| 3   | CN    | 178 | ASN  |
| 3   | CN    | 184 | GLN  |
| 3   | CO    | 35  | GLN  |
| 3   | CO    | 42  | ASN  |
| 3   | CO    | 75  | GLN  |
| 3   | CO    | 157 | ASN  |
| 3   | CO    | 178 | ASN  |
| 3   | CO    | 184 | GLN  |
| 3   | CP    | 35  | GLN  |
| 3   | CP    | 42  | ASN  |
| 3   | CP    | 75  | GLN  |
| 3   | CP    | 157 | ASN  |
| 3   | CP    | 178 | ASN  |
| 3   | CP    | 184 | GLN  |
| 3   | CQ    | 35  | GLN  |
| 3   | CQ    | 42  | ASN  |
| 3   | CQ    | 75  | GLN  |
| 3   | CQ    | 157 | ASN  |
| 3   | CQ    | 178 | ASN  |
| 3   | CQ    | 184 | GLN  |
| 3   | CR    | 35  | GLN  |
| 3   | CR    | 42  | ASN  |
| 3   | CR    | 75  | GLN  |
| 3   | CR    | 157 | ASN  |
| 3   | CR    | 178 | ASN  |
| 3   | CR    | 184 | GLN  |
| 3   | CS    | 35  | GLN  |
| 3   | CS    | 42  | ASN  |
| 3   | CS    | 75  | GLN  |
| 3   | CS    | 157 | ASN  |
| 3   | CS    | 178 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CS    | 184 | GLN  |
| 3   | CT    | 35  | GLN  |
| 3   | CT    | 42  | ASN  |
| 3   | CT    | 75  | GLN  |
| 3   | CT    | 157 | ASN  |
| 3   | CT    | 178 | ASN  |
| 3   | CT    | 184 | GLN  |
| 3   | CU    | 35  | GLN  |
| 3   | CU    | 42  | ASN  |
| 3   | CU    | 75  | GLN  |
| 3   | CU    | 157 | ASN  |
| 3   | CU    | 178 | ASN  |
| 3   | CU    | 184 | GLN  |
| 3   | CV    | 35  | GLN  |
| 3   | CV    | 42  | ASN  |
| 3   | CV    | 75  | GLN  |
| 3   | CV    | 157 | ASN  |
| 3   | CV    | 178 | ASN  |
| 3   | CV    | 184 | GLN  |
| 3   | CW    | 35  | GLN  |
| 3   | CW    | 42  | ASN  |
| 3   | CW    | 75  | GLN  |
| 3   | CW    | 157 | ASN  |
| 3   | CW    | 178 | ASN  |
| 3   | CW    | 184 | GLN  |
| 3   | CX    | 35  | GLN  |
| 3   | CX    | 42  | ASN  |
| 3   | CX    | 75  | GLN  |
| 3   | CX    | 157 | ASN  |
| 3   | CX    | 178 | ASN  |
| 3   | CX    | 184 | GLN  |
| 3   | CY    | 35  | GLN  |
| 3   | CY    | 42  | ASN  |
| 3   | CY    | 75  | GLN  |
| 3   | CY    | 157 | ASN  |
| 3   | CY    | 178 | ASN  |
| 3   | CY    | 184 | GLN  |
| 3   | CZ    | 35  | GLN  |
| 3   | CZ    | 42  | ASN  |
| 3   | CZ    | 75  | GLN  |
| 3   | CZ    | 157 | ASN  |
| 3   | CZ    | 178 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CZ    | 184 | GLN  |
| 3   | C0    | 35  | GLN  |
| 3   | C0    | 42  | ASN  |
| 3   | C0    | 75  | GLN  |
| 3   | C0    | 157 | ASN  |
| 3   | C0    | 178 | ASN  |
| 3   | C0    | 184 | GLN  |
| 3   | C1    | 35  | GLN  |
| 3   | C1    | 42  | ASN  |
| 3   | C1    | 75  | GLN  |
| 3   | C1    | 157 | ASN  |
| 3   | C1    | 178 | ASN  |
| 3   | C1    | 184 | GLN  |
| 3   | C2    | 35  | GLN  |
| 3   | C2    | 42  | ASN  |
| 3   | C2    | 75  | GLN  |
| 3   | C2    | 157 | ASN  |
| 3   | C2    | 178 | ASN  |
| 3   | C2    | 184 | GLN  |
| 3   | C3    | 35  | GLN  |
| 3   | C3    | 42  | ASN  |
| 3   | C3    | 75  | GLN  |
| 3   | C3    | 157 | ASN  |
| 3   | C3    | 178 | ASN  |
| 3   | C3    | 184 | GLN  |
| 3   | C4    | 35  | GLN  |
| 3   | C4    | 42  | ASN  |
| 3   | C4    | 75  | GLN  |
| 3   | C4    | 157 | ASN  |
| 3   | C4    | 178 | ASN  |
| 3   | C4    | 184 | GLN  |
| 3   | C5    | 35  | GLN  |
| 3   | C5    | 42  | ASN  |
| 3   | C5    | 75  | GLN  |
| 3   | C5    | 157 | ASN  |
| 3   | C5    | 178 | ASN  |
| 3   | C5    | 184 | GLN  |
| 3   | C6    | 35  | GLN  |
| 3   | C6    | 42  | ASN  |
| 3   | C6    | 75  | GLN  |
| 3   | C6    | 157 | ASN  |
| 3   | C6    | 178 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C6    | 184 | GLN  |
| 3   | C7    | 35  | GLN  |
| 3   | C7    | 42  | ASN  |
| 3   | C7    | 75  | GLN  |
| 3   | C7    | 157 | ASN  |
| 3   | C7    | 178 | ASN  |
| 3   | C7    | 184 | GLN  |
| 3   | C8    | 35  | GLN  |
| 3   | C8    | 42  | ASN  |
| 3   | C8    | 75  | GLN  |
| 3   | C8    | 157 | ASN  |
| 3   | C8    | 178 | ASN  |
| 3   | C8    | 184 | GLN  |
| 3   | C9    | 35  | GLN  |
| 3   | C9    | 42  | ASN  |
| 3   | C9    | 75  | GLN  |
| 3   | C9    | 157 | ASN  |
| 3   | C9    | 178 | ASN  |
| 3   | C9    | 184 | GLN  |
| 3   | Cc    | 35  | GLN  |
| 3   | Cc    | 42  | ASN  |
| 3   | Cc    | 75  | GLN  |
| 3   | Cc    | 157 | ASN  |
| 3   | Cc    | 178 | ASN  |
| 3   | Cc    | 184 | GLN  |
| 3   | Cd    | 35  | GLN  |
| 3   | Cd    | 42  | ASN  |
| 3   | Cd    | 75  | GLN  |
| 3   | Cd    | 157 | ASN  |
| 3   | Cd    | 178 | ASN  |
| 3   | Cd    | 184 | GLN  |
| 3   | Ce    | 35  | GLN  |
| 3   | Ce    | 42  | ASN  |
| 3   | Ce    | 75  | GLN  |
| 3   | Ce    | 157 | ASN  |
| 3   | Ce    | 178 | ASN  |
| 3   | Ce    | 184 | GLN  |
| 3   | Cf    | 35  | GLN  |
| 3   | Cf    | 42  | ASN  |
| 3   | Cf    | 75  | GLN  |
| 3   | Cf    | 157 | ASN  |
| 3   | Cf    | 178 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Cf    | 184 | GLN  |
| 3   | Cg    | 35  | GLN  |
| 3   | Cg    | 42  | ASN  |
| 3   | Cg    | 75  | GLN  |
| 3   | Cg    | 157 | ASN  |
| 3   | Cg    | 178 | ASN  |
| 3   | Cg    | 184 | GLN  |
| 3   | Ch    | 35  | GLN  |
| 3   | Ch    | 42  | ASN  |
| 3   | Ch    | 75  | GLN  |
| 3   | Ch    | 157 | ASN  |
| 3   | Ch    | 178 | ASN  |
| 3   | Ch    | 184 | GLN  |
| 3   | Ci    | 35  | GLN  |
| 3   | Ci    | 42  | ASN  |
| 3   | Ci    | 75  | GLN  |
| 3   | Ci    | 157 | ASN  |
| 3   | Ci    | 178 | ASN  |
| 3   | Ci    | 184 | GLN  |
| 3   | Cj    | 35  | GLN  |
| 3   | Cj    | 42  | ASN  |
| 3   | Cj    | 75  | GLN  |
| 3   | Cj    | 157 | ASN  |
| 3   | Cj    | 178 | ASN  |
| 3   | Cj    | 184 | GLN  |
| 3   | Ck    | 35  | GLN  |
| 3   | Ck    | 42  | ASN  |
| 3   | Ck    | 75  | GLN  |
| 3   | Ck    | 157 | ASN  |
| 3   | Ck    | 178 | ASN  |
| 3   | Ck    | 184 | GLN  |
| 3   | Cl    | 35  | GLN  |
| 3   | Cl    | 42  | ASN  |
| 3   | Cl    | 75  | GLN  |
| 3   | Cl    | 157 | ASN  |
| 3   | Cl    | 178 | ASN  |
| 3   | Cl    | 184 | GLN  |
| 3   | Cm    | 35  | GLN  |
| 3   | Cm    | 42  | ASN  |
| 3   | Cm    | 75  | GLN  |
| 3   | Cm    | 157 | ASN  |
| 3   | Cm    | 178 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Cm    | 184 | GLN  |
| 3   | Cn    | 35  | GLN  |
| 3   | Cn    | 42  | ASN  |
| 3   | Cn    | 75  | GLN  |
| 3   | Cn    | 157 | ASN  |
| 3   | Cn    | 178 | ASN  |
| 3   | Cn    | 184 | GLN  |
| 3   | Co    | 35  | GLN  |
| 3   | Co    | 42  | ASN  |
| 3   | Co    | 75  | GLN  |
| 3   | Co    | 157 | ASN  |
| 3   | Co    | 178 | ASN  |
| 3   | Co    | 184 | GLN  |
| 3   | Cp    | 35  | GLN  |
| 3   | Cp    | 42  | ASN  |
| 3   | Cp    | 75  | GLN  |
| 3   | Cp    | 157 | ASN  |
| 3   | Cp    | 178 | ASN  |
| 3   | Cp    | 184 | GLN  |
| 3   | Cq    | 35  | GLN  |
| 3   | Cq    | 42  | ASN  |
| 3   | Cq    | 75  | GLN  |
| 3   | Cq    | 157 | ASN  |
| 3   | Cq    | 178 | ASN  |
| 3   | Cq    | 184 | GLN  |
| 3   | Cr    | 35  | GLN  |
| 3   | Cr    | 42  | ASN  |
| 3   | Cr    | 75  | GLN  |
| 3   | Cr    | 157 | ASN  |
| 3   | Cr    | 178 | ASN  |
| 3   | Cr    | 184 | GLN  |
| 3   | Cs    | 35  | GLN  |
| 3   | Cs    | 42  | ASN  |
| 3   | Cs    | 75  | GLN  |
| 3   | Cs    | 157 | ASN  |
| 3   | Cs    | 178 | ASN  |
| 3   | Cs    | 184 | GLN  |
| 3   | Ct    | 35  | GLN  |
| 3   | Ct    | 42  | ASN  |
| 3   | Ct    | 75  | GLN  |
| 3   | Ct    | 157 | ASN  |
| 3   | Ct    | 178 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | Ct    | 184 | GLN  |
| 3   | Cu    | 35  | GLN  |
| 3   | Cu    | 42  | ASN  |
| 3   | Cu    | 75  | GLN  |
| 3   | Cu    | 157 | ASN  |
| 3   | Cu    | 178 | ASN  |
| 3   | Cu    | 184 | GLN  |
| 3   | Cv    | 35  | GLN  |
| 3   | Cv    | 42  | ASN  |
| 3   | Cv    | 75  | GLN  |
| 3   | Cv    | 157 | ASN  |
| 3   | Cv    | 178 | ASN  |
| 3   | Cv    | 184 | GLN  |
| 3   | Cw    | 35  | GLN  |
| 3   | Cw    | 42  | ASN  |
| 3   | Cw    | 75  | GLN  |
| 3   | Cw    | 157 | ASN  |
| 3   | Cw    | 178 | ASN  |
| 3   | Cw    | 184 | GLN  |
| 3   | Cx    | 35  | GLN  |
| 3   | Cx    | 42  | ASN  |
| 3   | Cx    | 75  | GLN  |
| 3   | Cx    | 157 | ASN  |
| 3   | Cx    | 178 | ASN  |
| 3   | Cx    | 184 | GLN  |
| 3   | DA    | 35  | GLN  |
| 3   | DA    | 42  | ASN  |
| 3   | DA    | 75  | GLN  |
| 3   | DA    | 157 | ASN  |
| 3   | DA    | 178 | ASN  |
| 3   | DA    | 184 | GLN  |
| 3   | DB    | 35  | GLN  |
| 3   | DB    | 42  | ASN  |
| 3   | DB    | 75  | GLN  |
| 3   | DB    | 157 | ASN  |
| 3   | DB    | 178 | ASN  |
| 3   | DB    | 184 | GLN  |
| 1   | DC    | 47  | ASN  |
| 1   | DC    | 87  | GLN  |
| 1   | DC    | 191 | HIS  |
| 1   | DC    | 217 | ASN  |
| 1   | DC    | 242 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | DC    | 246 | GLN  |
| 1   | DD    | 47  | ASN  |
| 1   | DD    | 87  | GLN  |
| 1   | DD    | 191 | HIS  |
| 1   | DD    | 217 | ASN  |
| 1   | DD    | 242 | ASN  |
| 1   | DD    | 246 | GLN  |
| 1   | DE    | 47  | ASN  |
| 1   | DE    | 87  | GLN  |
| 1   | DE    | 191 | HIS  |
| 1   | DE    | 217 | ASN  |
| 1   | DE    | 242 | ASN  |
| 1   | DE    | 246 | GLN  |
| 1   | DF    | 47  | ASN  |
| 1   | DF    | 87  | GLN  |
| 1   | DF    | 191 | HIS  |
| 1   | DF    | 217 | ASN  |
| 1   | DF    | 242 | ASN  |
| 1   | DF    | 246 | GLN  |
| 1   | DG    | 47  | ASN  |
| 1   | DG    | 87  | GLN  |
| 1   | DG    | 191 | HIS  |
| 1   | DG    | 217 | ASN  |
| 1   | DG    | 242 | ASN  |
| 1   | DG    | 246 | GLN  |
| 1   | DH    | 47  | ASN  |
| 1   | DH    | 87  | GLN  |
| 1   | DH    | 191 | HIS  |
| 1   | DH    | 217 | ASN  |
| 1   | DH    | 242 | ASN  |
| 1   | DH    | 246 | GLN  |
| 1   | DI    | 47  | ASN  |
| 1   | DI    | 87  | GLN  |
| 1   | DI    | 191 | HIS  |
| 1   | DI    | 217 | ASN  |
| 1   | DI    | 242 | ASN  |
| 1   | DI    | 246 | GLN  |
| 1   | DJ    | 47  | ASN  |
| 1   | DJ    | 87  | GLN  |
| 1   | DJ    | 191 | HIS  |
| 1   | DJ    | 217 | ASN  |
| 1   | DJ    | 242 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | DJ    | 246 | GLN  |
| 1   | DK    | 47  | ASN  |
| 1   | DK    | 87  | GLN  |
| 1   | DK    | 191 | HIS  |
| 1   | DK    | 217 | ASN  |
| 1   | DK    | 242 | ASN  |
| 1   | DK    | 246 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.