



# Full wwPDB X-ray Structure Validation Report ⓘ

May 31, 2016 – 08:01 PM EDT

PDB ID : 4XVW  
Title : Crystal structure of Proteus mirabilis ScsC in a compact conformation  
Authors : Kurth, F.; Furlong, E.J.; Premkumar, L.; Martin, J.L.  
Deposited on : 2015-01-27  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
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/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027674  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027674

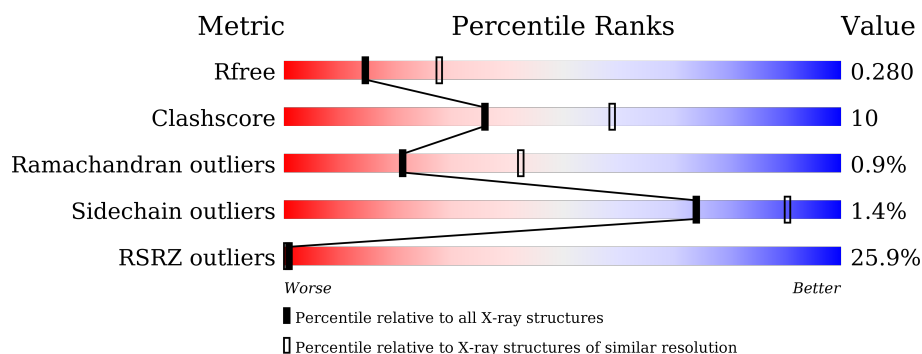
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 91344                       | 2328 (2.60-2.60)                                      |
| Clashscore            | 102246                      | 2679 (2.60-2.60)                                      |
| Ramachandran outliers | 100387                      | 2635 (2.60-2.60)                                      |
| Sidechain outliers    | 100360                      | 2635 (2.60-2.60)                                      |
| RSRZ outliers         | 91569                       | 2334 (2.60-2.60)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                   |
|-----|-------|--------|--|
| 1   | A     | 224    | <div> <div>6%</div> <div>81% 18% .</div> </div>    |
| 1   | B     | 224    | <div> <div>8%</div> <div>84% 14% .</div> </div>    |
| 1   | C     | 224    | <div> <div>8%</div> <div>88% 11% ..</div> </div>   |
| 1   | D     | 224    | <div> <div>7%</div> <div>86% 13% .</div> </div>    |
| 1   | E     | 224    | <div> <div>33%</div> <div>68% 27% . .</div> </div> |
| 1   | F     | 224    | <div> <div>11%</div> <div>81% 17% ..</div> </div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | G     | 224    |                  |
| 1   | H     | 224    |                  |
| 1   | I     | 224    |                  |
| 1   | J     | 224    |                  |
| 1   | K     | 224    |                  |
| 1   | L     | 224    |                  |
| 1   | M     | 224    |                  |
| 1   | N     | 224    |                  |
| 1   | O     | 224    |                  |
| 1   | P     | 224    |                  |
| 1   | Q     | 224    |                  |
| 1   | R     | 224    |                  |
| 1   | T     | 224    |                  |
| 1   | U     | 224    |                  |
| 1   | V     | 224    |                  |
| 1   | W     | 224    |                  |
| 1   | X     | 224    |                  |
| 1   | Y     | 224    |                  |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 83204 atoms, of which 42074 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 DsbA-like protein.

| Mol | Chain | Residues | Atoms |      |      |     |     |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|----|---------|---------|-------|
| 1   | A     | 222      | Total | C    | H    | N   | O   | S | Se | 0       | 3       | 0     |
|     |       |          | 3527  | 1095 | 1790 | 295 | 339 | 4 | 4  |         |         |       |
| 1   | B     | 220      | Total | C    | H    | N   | O   | S | Se | 0       | 5       | 0     |
|     |       |          | 3500  | 1088 | 1774 | 292 | 337 | 4 | 5  |         |         |       |
| 1   | C     | 222      | Total | C    | H    | N   | O   | S | Se | 0       | 3       | 0     |
|     |       |          | 3527  | 1095 | 1790 | 295 | 339 | 4 | 4  |         |         |       |
| 1   | D     | 222      | Total | C    | H    | N   | O   | S | Se | 0       | 3       | 0     |
|     |       |          | 3527  | 1095 | 1790 | 295 | 339 | 4 | 4  |         |         |       |
| 1   | E     | 215      | Total | C    | H    | N   | O   | S | Se | 0       | 3       | 0     |
|     |       |          | 3437  | 1068 | 1745 | 286 | 330 | 4 | 4  |         |         |       |
| 1   | F     | 222      | Total | C    | H    | N   | O   | S | Se | 0       | 3       | 0     |
|     |       |          | 3527  | 1095 | 1790 | 295 | 339 | 4 | 4  |         |         |       |
| 1   | G     | 219      | Total | C    | H    | N   | O   | S | Se | 0       | 3       | 0     |
|     |       |          | 3488  | 1083 | 1769 | 292 | 336 | 4 | 4  |         |         |       |
| 1   | H     | 222      | Total | C    | H    | N   | O   | S | Se | 0       | 3       | 0     |
|     |       |          | 3527  | 1095 | 1790 | 295 | 339 | 4 | 4  |         |         |       |
| 1   | I     | 198      | Total | C    | H    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 3118  | 972  | 1579 | 261 | 300 | 2 | 4  |         |         |       |
| 1   | J     | 219      | Total | C    | H    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 3451  | 1074 | 1750 | 288 | 333 | 2 | 4  |         |         |       |
| 1   | K     | 220      | Total | C    | H    | N   | O   | S | Se | 0       | 5       | 0     |
|     |       |          | 3500  | 1088 | 1774 | 292 | 337 | 4 | 5  |         |         |       |
| 1   | L     | 176      | Total | C    | H    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 2800  | 874  | 1428 | 224 | 268 | 2 | 4  |         |         |       |
| 1   | M     | 220      | Total | C    | H    | N   | O   | S | Se | 0       | 3       | 0     |
|     |       |          | 3482  | 1083 | 1764 | 291 | 336 | 4 | 4  |         |         |       |
| 1   | N     | 220      | Total | C    | H    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 3473  | 1080 | 1763 | 290 | 334 | 2 | 4  |         |         |       |
| 1   | O     | 220      | Total | C    | H    | N   | O   | S | Se | 0       | 3       | 0     |
|     |       |          | 3482  | 1083 | 1764 | 291 | 336 | 4 | 4  |         |         |       |
| 1   | P     | 222      | Total | C    | H    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 3506  | 1089 | 1781 | 293 | 337 | 2 | 4  |         |         |       |

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| Mol | Chain | Residues | Atoms |      |      |     |     |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|----|---------|---------|-------|
| 1   | Q     | 221      | Total | C    | H    | N   | O   | S | Se | 0       | 3       | 0     |
|     |       |          | 3504  | 1089 | 1777 | 293 | 337 | 4 | 4  |         |         |       |
| 1   | R     | 218      | Total | C    | H    | N   | O   | S | Se | 0       | 3       | 0     |
|     |       |          | 3474  | 1079 | 1763 | 290 | 334 | 4 | 4  |         |         |       |
| 1   | T     | 221      | Total | C    | H    | N   | O   | S | Se | 0       | 3       | 0     |
|     |       |          | 3504  | 1089 | 1777 | 293 | 337 | 4 | 4  |         |         |       |
| 1   | U     | 222      | Total | C    | H    | N   | O   | S | Se | 0       | 3       | 0     |
|     |       |          | 3527  | 1095 | 1790 | 295 | 339 | 4 | 4  |         |         |       |
| 1   | V     | 221      | Total | C    | H    | N   | O   | S | Se | 0       | 3       | 0     |
|     |       |          | 3504  | 1089 | 1777 | 293 | 337 | 4 | 4  |         |         |       |
| 1   | W     | 221      | Total | C    | H    | N   | O   | S | Se | 0       | 3       | 0     |
|     |       |          | 3504  | 1089 | 1777 | 293 | 337 | 4 | 4  |         |         |       |
| 1   | X     | 222      | Total | C    | H    | N   | O   | S | Se | 0       | 0       | 0     |
|     |       |          | 3507  | 1089 | 1782 | 293 | 337 | 2 | 4  |         |         |       |
| 1   | Y     | 222      | Total | C    | H    | N   | O   | S | Se | 0       | 3       | 0     |
|     |       |          | 3527  | 1095 | 1790 | 295 | 339 | 4 | 4  |         |         |       |

There are 48 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 1       | SER      | -      | expression tag | UNP C2LPE2 |
| A     | 2       | ASN      | -      | expression tag | UNP C2LPE2 |
| B     | 1       | SER      | -      | expression tag | UNP C2LPE2 |
| B     | 2       | ASN      | -      | expression tag | UNP C2LPE2 |
| C     | 1       | SER      | -      | expression tag | UNP C2LPE2 |
| C     | 2       | ASN      | -      | expression tag | UNP C2LPE2 |
| D     | 1       | SER      | -      | expression tag | UNP C2LPE2 |
| D     | 2       | ASN      | -      | expression tag | UNP C2LPE2 |
| E     | 1       | SER      | -      | expression tag | UNP C2LPE2 |
| E     | 2       | ASN      | -      | expression tag | UNP C2LPE2 |
| F     | 1       | SER      | -      | expression tag | UNP C2LPE2 |
| F     | 2       | ASN      | -      | expression tag | UNP C2LPE2 |
| G     | 1       | SER      | -      | expression tag | UNP C2LPE2 |
| G     | 2       | ASN      | -      | expression tag | UNP C2LPE2 |
| H     | 1       | SER      | -      | expression tag | UNP C2LPE2 |
| H     | 2       | ASN      | -      | expression tag | UNP C2LPE2 |
| I     | 1       | SER      | -      | expression tag | UNP C2LPE2 |
| I     | 2       | ASN      | -      | expression tag | UNP C2LPE2 |
| J     | 1       | SER      | -      | expression tag | UNP C2LPE2 |
| J     | 2       | ASN      | -      | expression tag | UNP C2LPE2 |
| K     | 1       | SER      | -      | expression tag | UNP C2LPE2 |
| K     | 2       | ASN      | -      | expression tag | UNP C2LPE2 |
| L     | 1       | SER      | -      | expression tag | UNP C2LPE2 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| L     | 2       | ASN      | -      | expression tag | UNP C2LPE2 |
| M     | 1       | SER      | -      | expression tag | UNP C2LPE2 |
| M     | 2       | ASN      | -      | expression tag | UNP C2LPE2 |
| N     | 1       | SER      | -      | expression tag | UNP C2LPE2 |
| N     | 2       | ASN      | -      | expression tag | UNP C2LPE2 |
| O     | 1       | SER      | -      | expression tag | UNP C2LPE2 |
| O     | 2       | ASN      | -      | expression tag | UNP C2LPE2 |
| P     | 1       | SER      | -      | expression tag | UNP C2LPE2 |
| P     | 2       | ASN      | -      | expression tag | UNP C2LPE2 |
| Q     | 1       | SER      | -      | expression tag | UNP C2LPE2 |
| Q     | 2       | ASN      | -      | expression tag | UNP C2LPE2 |
| R     | 1       | SER      | -      | expression tag | UNP C2LPE2 |
| R     | 2       | ASN      | -      | expression tag | UNP C2LPE2 |
| T     | 1       | SER      | -      | expression tag | UNP C2LPE2 |
| T     | 2       | ASN      | -      | expression tag | UNP C2LPE2 |
| U     | 1       | SER      | -      | expression tag | UNP C2LPE2 |
| U     | 2       | ASN      | -      | expression tag | UNP C2LPE2 |
| V     | 1       | SER      | -      | expression tag | UNP C2LPE2 |
| V     | 2       | ASN      | -      | expression tag | UNP C2LPE2 |
| W     | 1       | SER      | -      | expression tag | UNP C2LPE2 |
| W     | 2       | ASN      | -      | expression tag | UNP C2LPE2 |
| X     | 1       | SER      | -      | expression tag | UNP C2LPE2 |
| X     | 2       | ASN      | -      | expression tag | UNP C2LPE2 |
| Y     | 1       | SER      | -      | expression tag | UNP C2LPE2 |
| Y     | 2       | ASN      | -      | expression tag | UNP C2LPE2 |

- Molecule 2 is water.

| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 2   | A     | 7        | Total O<br>7 7   | 0       | 0       |
| 2   | B     | 10       | Total O<br>10 10 | 0       | 0       |
| 2   | C     | 18       | Total O<br>18 18 | 0       | 0       |
| 2   | D     | 11       | Total O<br>11 11 | 0       | 0       |
| 2   | E     | 14       | Total O<br>14 14 | 0       | 0       |
| 2   | F     | 17       | Total O<br>17 17 | 0       | 0       |
| 2   | G     | 17       | Total O<br>17 17 | 0       | 0       |

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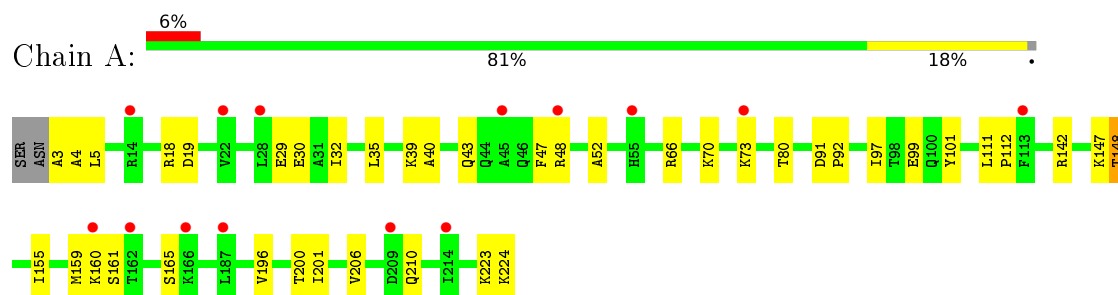
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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 2   | H     | 13       | Total<br>13 | O<br>13 | 0       | 0       |
| 2   | I     | 13       | Total<br>13 | O<br>13 | 0       | 0       |
| 2   | J     | 8        | Total<br>8  | O<br>8  | 0       | 0       |
| 2   | K     | 7        | Total<br>7  | O<br>7  | 0       | 0       |
| 2   | L     | 14       | Total<br>14 | O<br>14 | 0       | 0       |
| 2   | M     | 11       | Total<br>11 | O<br>11 | 0       | 0       |
| 2   | N     | 11       | Total<br>11 | O<br>11 | 0       | 0       |
| 2   | O     | 19       | Total<br>19 | O<br>19 | 0       | 0       |
| 2   | P     | 16       | Total<br>16 | O<br>16 | 0       | 0       |
| 2   | Q     | 17       | Total<br>17 | O<br>17 | 0       | 0       |
| 2   | R     | 9        | Total<br>9  | O<br>9  | 0       | 0       |
| 2   | T     | 10       | Total<br>10 | O<br>10 | 0       | 0       |
| 2   | U     | 6        | Total<br>6  | O<br>6  | 0       | 0       |
| 2   | V     | 9        | Total<br>9  | O<br>9  | 0       | 0       |
| 2   | W     | 6        | Total<br>6  | O<br>6  | 0       | 0       |
| 2   | X     | 9        | Total<br>9  | O<br>9  | 0       | 0       |
| 2   | Y     | 9        | Total<br>9  | O<br>9  | 0       | 0       |

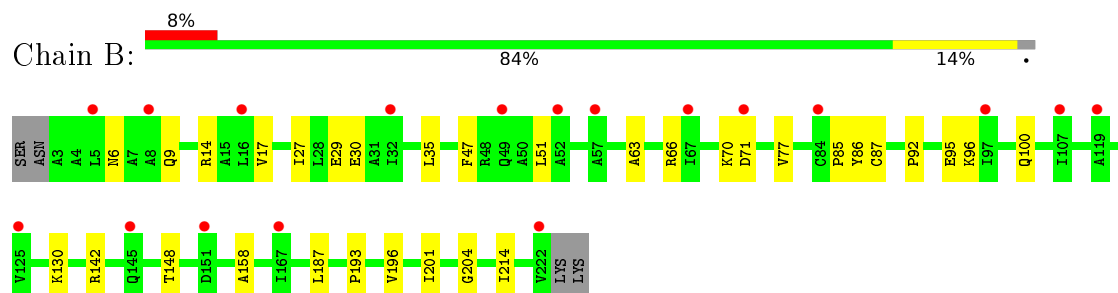
### 3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

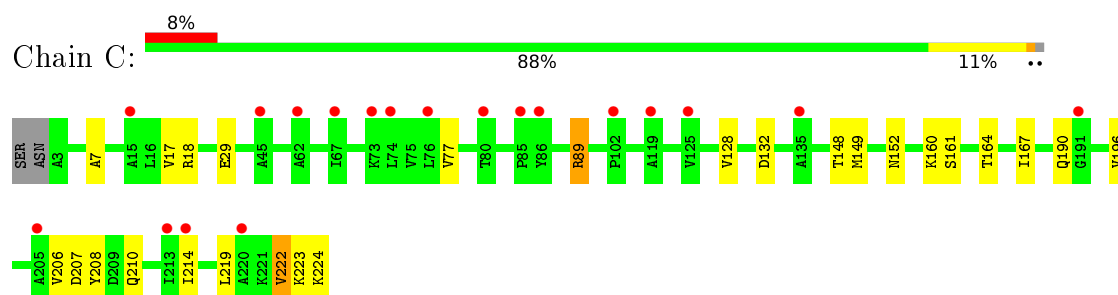
#### • Molecule 1: DsbA-like protein



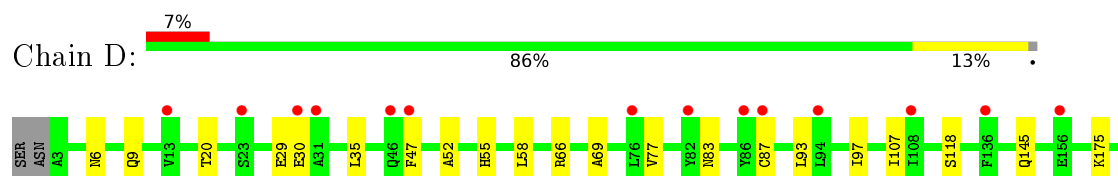
#### • Molecule 1: DsbA-like protein



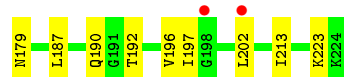
#### • Molecule 1: DsbA-like protein



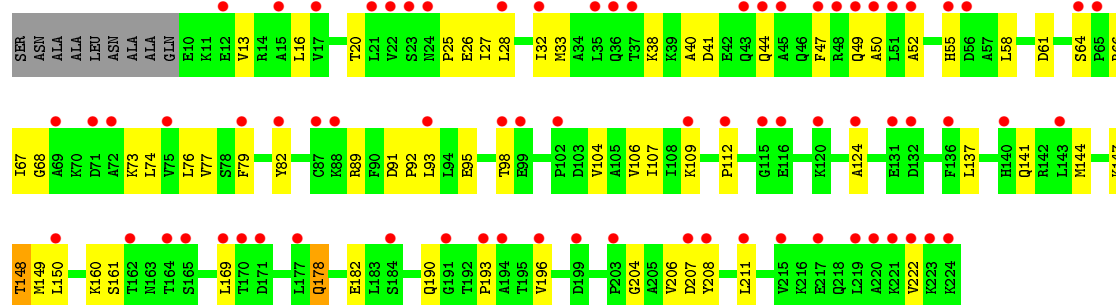
#### • Molecule 1: DsbA-like protein



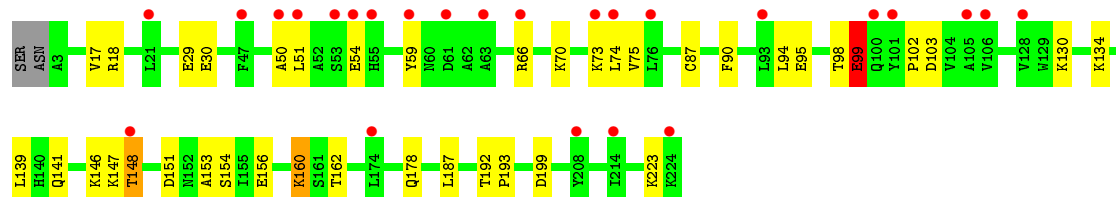
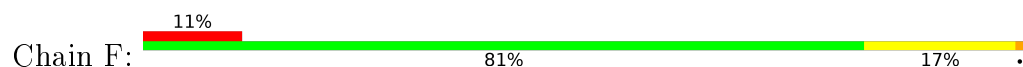




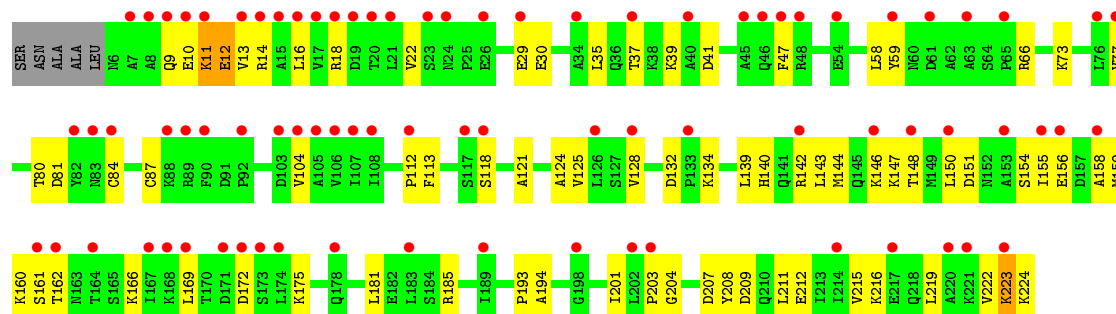
- Molecule 1: DsbA-like protein



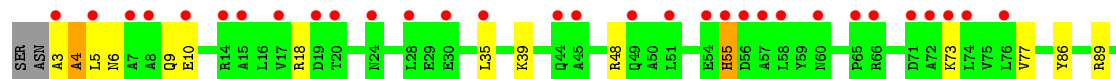
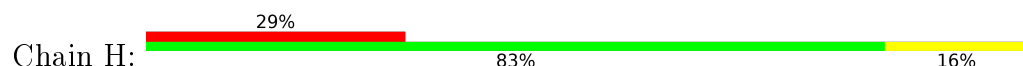
- Molecule 1: DsbA-like protein

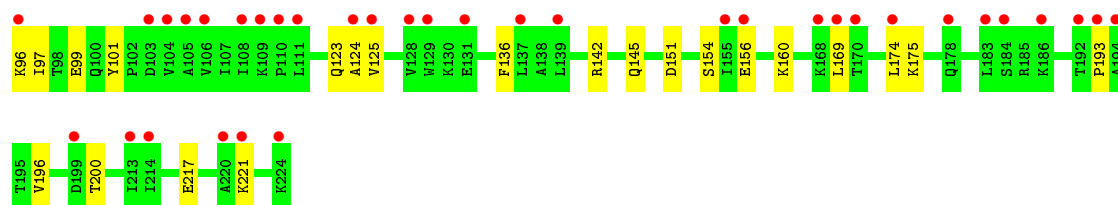


- Molecule 1: DsbA-like protein



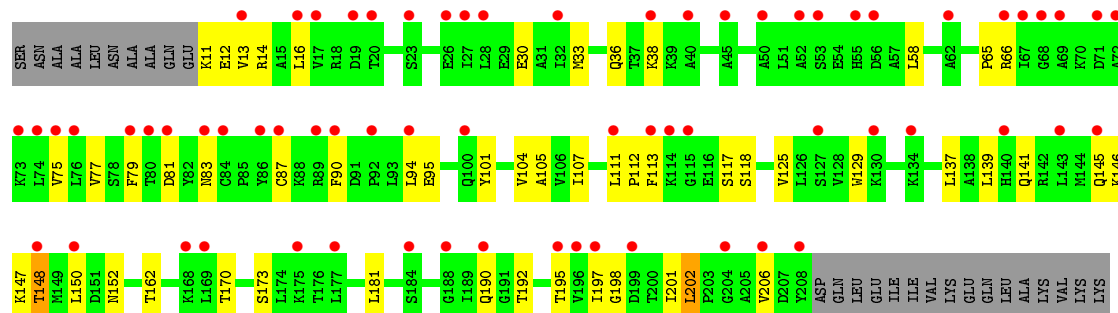
- Molecule 1: DsbA-like protein





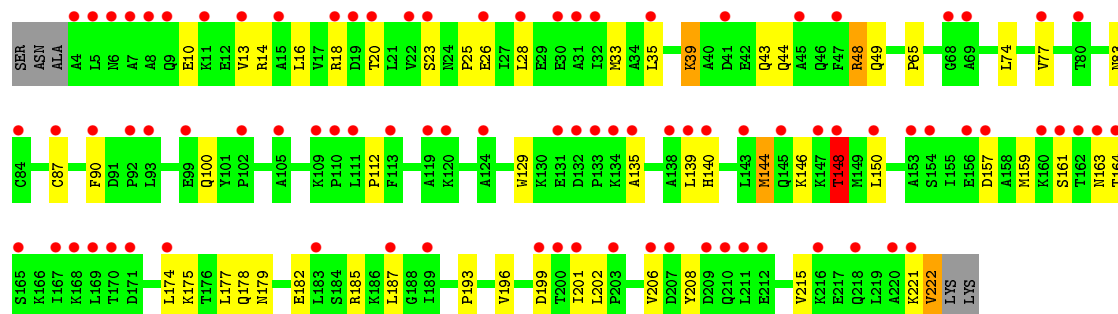
• Molecule 1: DsbA-like protein

Chain I: 30% 65% 23% 12%



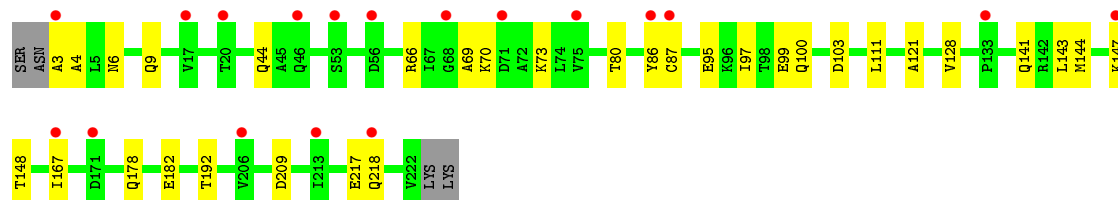
• Molecule 1: DsbA-like protein

Chain J: 39% 73% 23% 4%



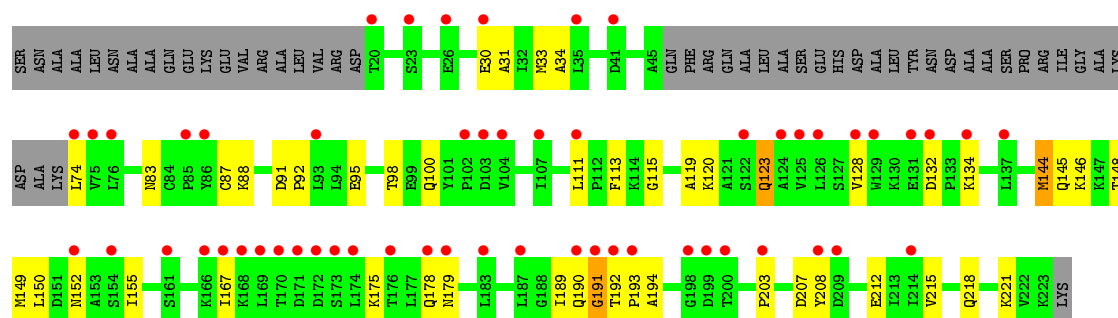
• Molecule 1: DsbA-like protein

Chain K: 8% 84% 14% 2%

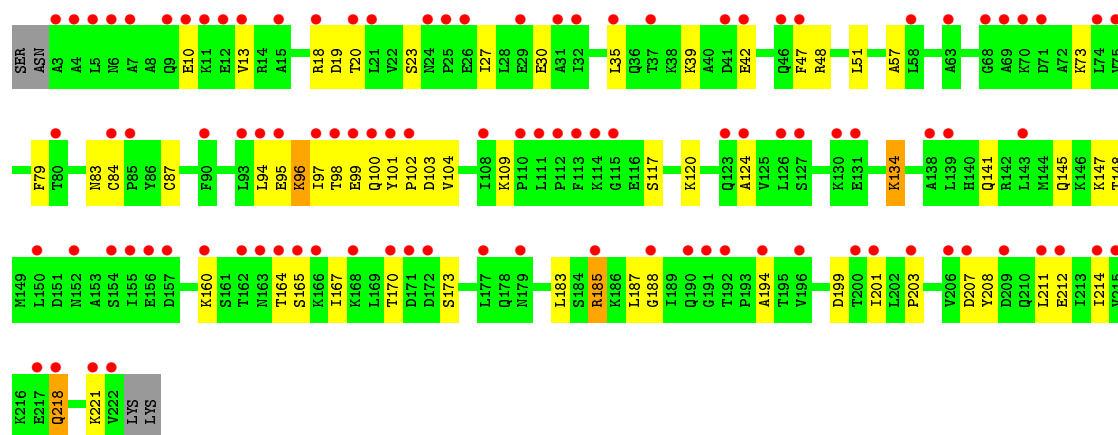
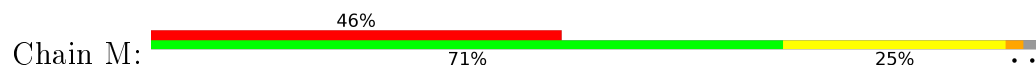


• Molecule 1: DsbA-like protein

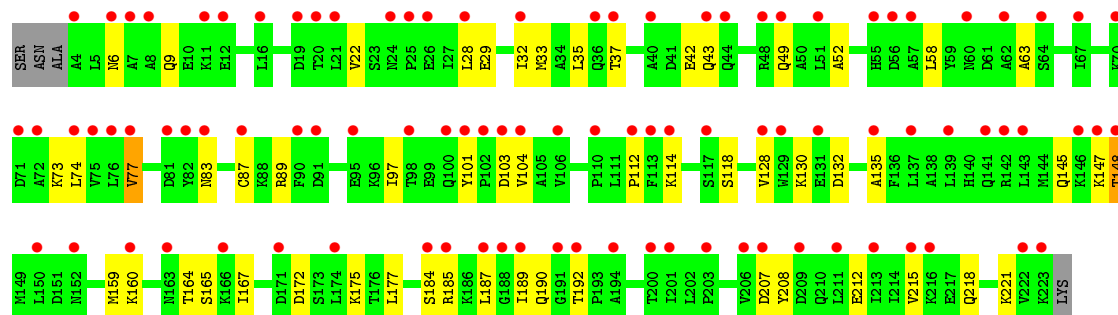
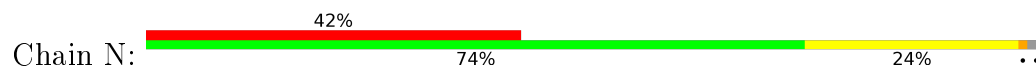
Chain L: 25% 58% 20% 21%



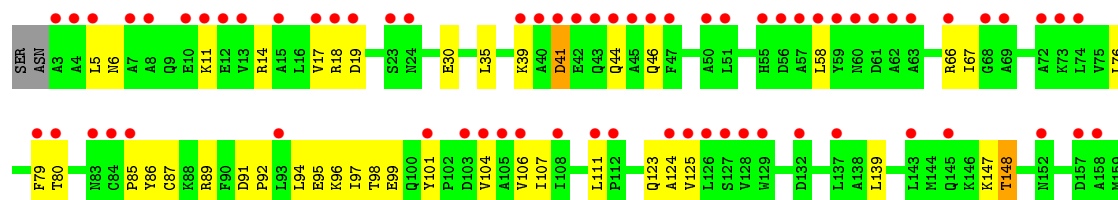
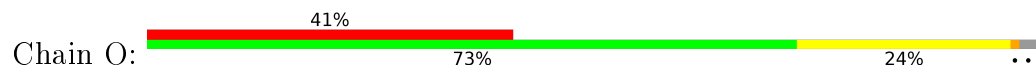
• Molecule 1: DsbA-like protein

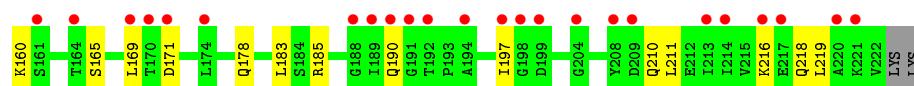


• Molecule 1: DsbA-like protein

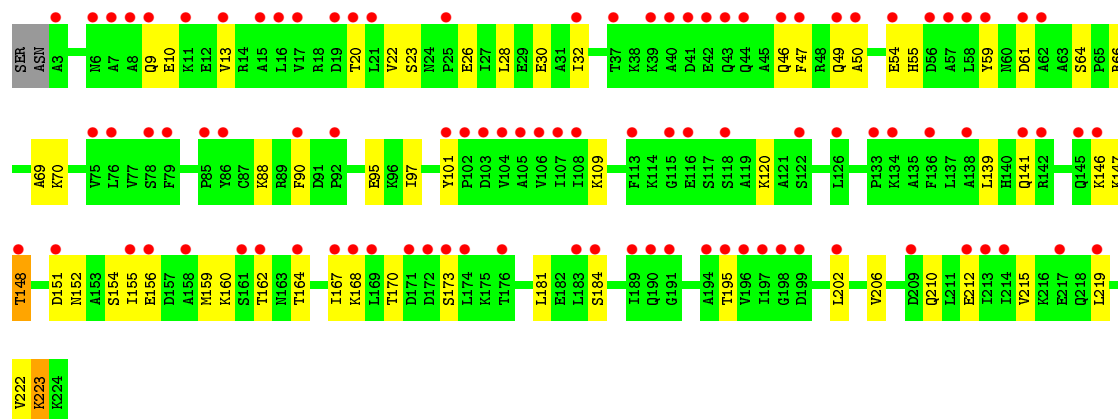
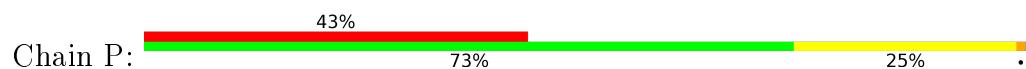


• Molecule 1: DsbA-like protein

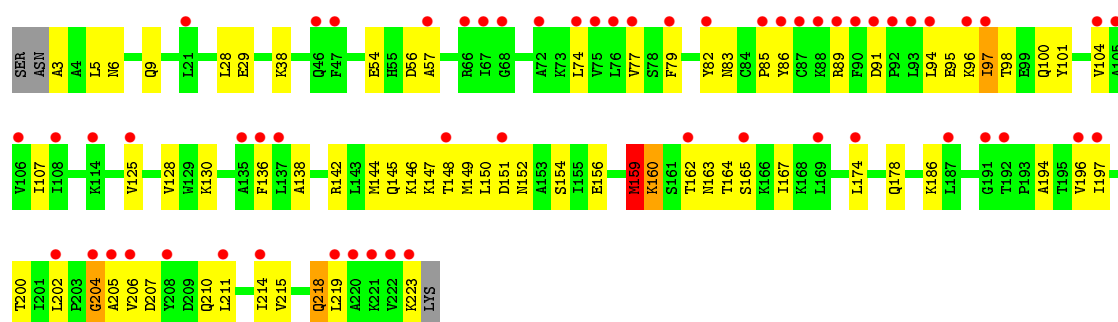




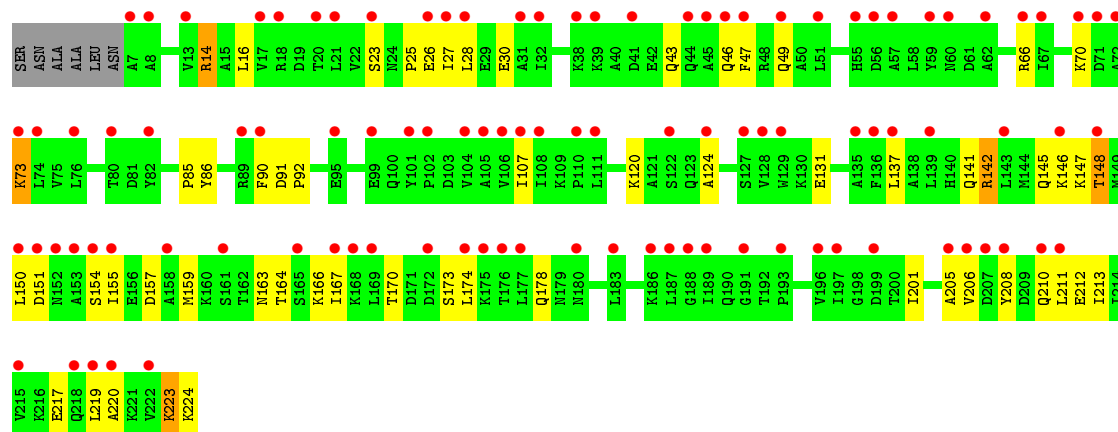
• Molecule 1: DsbA-like protein



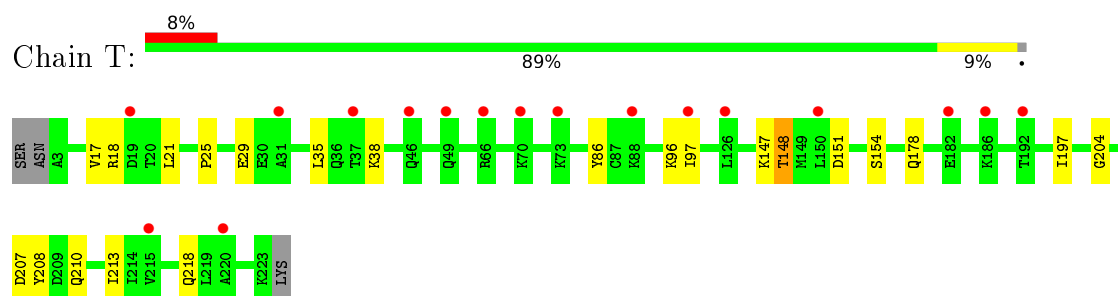
• Molecule 1: DsbA-like protein



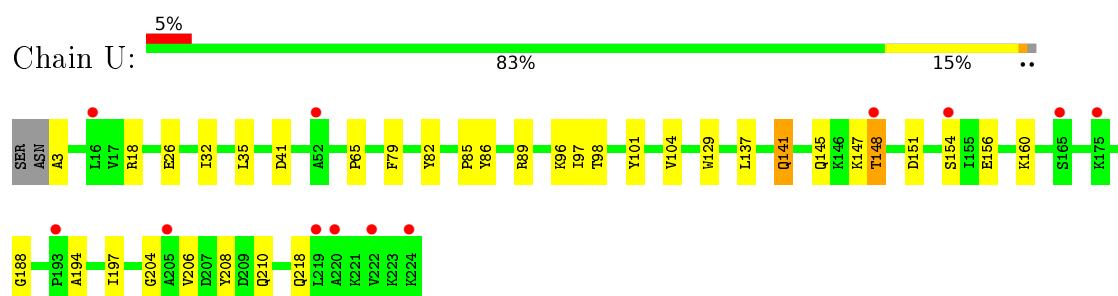
• Molecule 1: DsbA-like protein



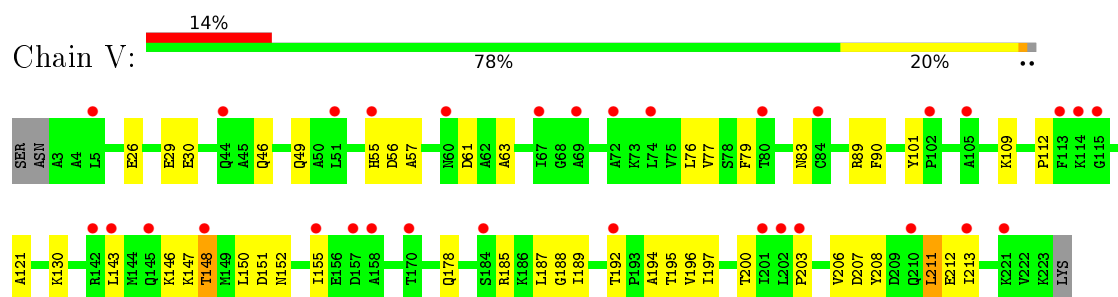
- Molecule 1: DsbA-like protein



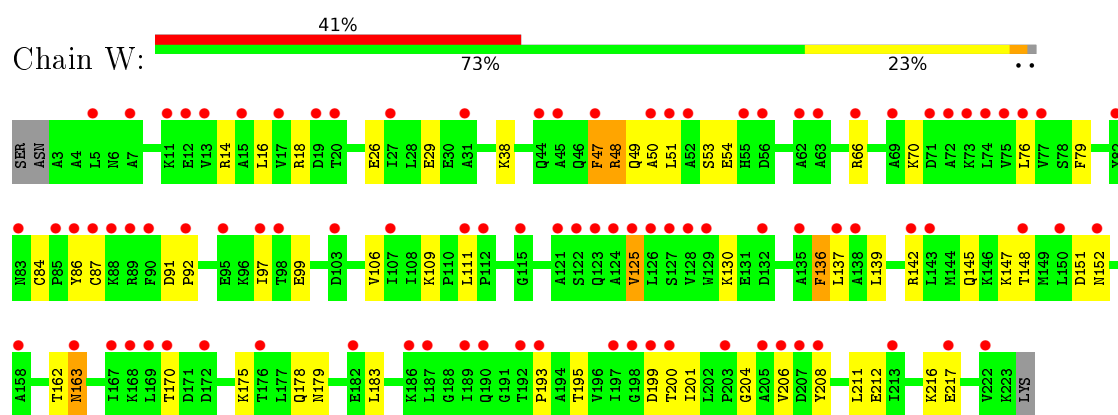
- Molecule 1: DsbA-like protein



- Molecule 1: DsbA-like protein

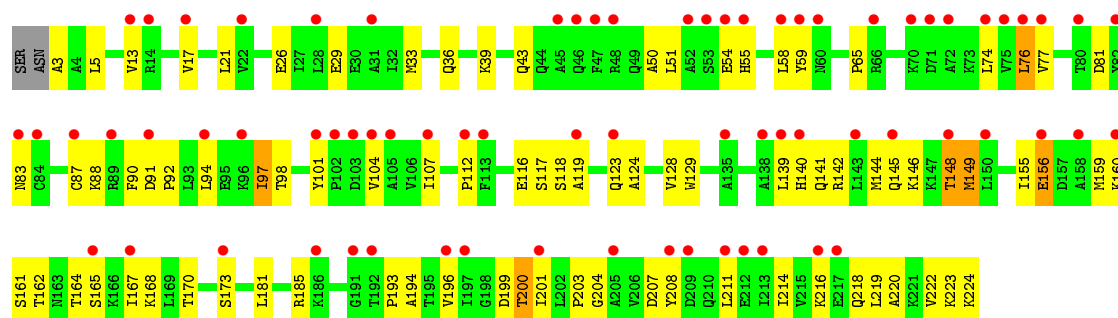


- Molecule 1: DsbA-like protein

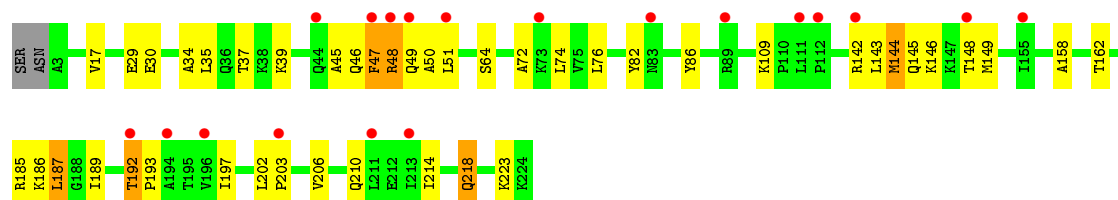
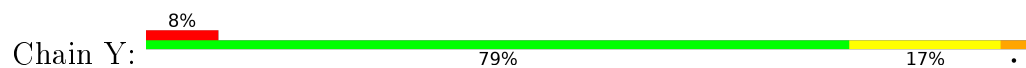


- Molecule 1: DsbA-like protein





• Molecule 1: DsbA-like protein



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 137.47Å 163.88Å 181.94Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 91.15 – 2.60<br>64.30 – 2.60                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.5 (91.15-2.60)<br>98.5 (64.30-2.60)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.07  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.16 (at 2.61Å)   | Xtriage          |
| Refinement program  | PHENIX (phenix.refine: 1.9_1692)                            | Depositor        |
| R, $R_{free}$   | 0.248 , 0.282<br>0.247 , 0.280                              | Depositor<br>DCC |
| $R_{free}$ test set   | 12072 reflections (4.96%)                                   | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 45.0  | Xtriage          |
| Anisotropy  | 0.635   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.41 , 56.3   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$ | Xtriage          |
| Estimated twinning fraction   | 0.467 for h,-k,-l   | Xtriage          |
| Reported twinning fraction  | 0.500 for H, K, L<br>0.500 for H, -K, -L                    | Depositor        |
| Outliers  | 0 of 243406 reflections                                     | Xtriage          |
| $F_o, F_c$ correlation  | 0.79  | EDS              |
| Total number of atoms   | 83204   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 60.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.03 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.1846e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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  >5 | RMSZ        | # Z  >5        |
| 1   | A     | 0.32         | 0/1765  | 0.56        | 0/2377         |
| 1   | B     | 0.27         | 0/1762  | 0.50        | 0/2376         |
| 1   | C     | 0.27         | 0/1765  | 0.53        | 0/2377         |
| 1   | D     | 0.27         | 0/1765  | 0.51        | 0/2377         |
| 1   | E     | 0.30         | 0/1720  | 0.62        | 0/2315         |
| 1   | F     | 0.30         | 0/1765  | 0.55        | 0/2377         |
| 1   | G     | 0.35         | 0/1747  | 0.68        | 0/2352         |
| 1   | H     | 0.30         | 0/1765  | 0.59        | 0/2377         |
| 1   | I     | 0.31         | 0/1558  | 0.65        | 0/2101         |
| 1   | J     | 0.34         | 0/1720  | 0.63        | 0/2320         |
| 1   | K     | 0.28         | 0/1763  | 0.51        | 0/2377         |
| 1   | L     | 0.33         | 0/1386  | 0.59        | 0/1867         |
| 1   | M     | 0.33         | 0/1746  | 0.67        | 0/2355         |
| 1   | N     | 0.32         | 0/1729  | 0.61        | 0/2331         |
| 1   | O     | 0.34         | 0/1746  | 0.63        | 1/2355 (0.0%)  |
| 1   | P     | 0.30         | 0/1744  | 0.62        | 0/2349         |
| 1   | Q     | 0.35         | 0/1755  | 0.70        | 1/2366 (0.0%)  |
| 1   | R     | 0.31         | 0/1739  | 0.61        | 0/2341         |
| 1   | T     | 0.26         | 0/1755  | 0.51        | 0/2366         |
| 1   | U     | 0.29         | 0/1765  | 0.53        | 0/2377         |
| 1   | V     | 0.27         | 0/1755  | 0.57        | 1/2366 (0.0%)  |
| 1   | W     | 0.30         | 0/1755  | 0.64        | 3/2366 (0.1%)  |
| 1   | X     | 0.33         | 0/1744  | 0.71        | 0/2349         |
| 1   | Y     | 0.30         | 0/1765  | 0.62        | 3/2377 (0.1%)  |
| All | All   | 0.31         | 0/41479 | 0.60        | 9/55891 (0.0%) |

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   | E     | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | F     | 0                   | 1                   |
| 1   | J     | 0                   | 2                   |
| 1   | Q     | 0                   | 1                   |
| 1   | X     | 0                   | 1                   |
| All | All   | 0                   | 6                   |

There are no bond length outliers.

All (9) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | W     | 47  | PHE  | N-CA-C    | 6.80  | 129.35      | 111.00   |
| 1   | Y     | 187 | LEU  | CB-CG-CD1 | 6.50  | 122.06      | 111.00   |
| 1   | Y     | 187 | LEU  | CA-CB-CG  | 6.37  | 129.95      | 115.30   |
| 1   | Y     | 51  | LEU  | CA-CB-CG  | 6.15  | 129.45      | 115.30   |
| 1   | O     | 41  | ASP  | CB-CG-OD1 | -5.69 | 113.18      | 118.30   |
| 1   | V     | 211 | LEU  | CA-CB-CG  | 5.43  | 127.78      | 115.30   |
| 1   | W     | 48  | ARG  | NE-CZ-NH2 | -5.21 | 117.69      | 120.30   |
| 1   | W     | 48  | ARG  | NE-CZ-NH1 | 5.14  | 122.87      | 120.30   |
| 1   | Q     | 204 | GLY  | N-CA-C    | 5.13  | 125.92      | 113.10   |

There are no chirality outliers.

All (6) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | E     | 47  | PHE  | Peptide |
| 1   | F     | 99  | GLU  | Peptide |
| 1   | J     | 140 | HIS  | Peptide |
| 1   | J     | 144 | MSE  | Peptide |
| 1   | Q     | 149 | MSE  | Peptide |
| 1   | X     | 156 | GLU  | Peptide |

## 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   | A     | 1737  | 1790     | 1776     | 30      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | B     | 1726  | 1774     | 1748     | 26      | 0            |
| 1   | C     | 1737  | 1790     | 1776     | 18      | 2            |
| 1   | D     | 1737  | 1790     | 1776     | 21      | 0            |
| 1   | E     | 1692  | 1745     | 1731     | 54      | 0            |
| 1   | F     | 1737  | 1790     | 1776     | 31      | 0            |
| 1   | G     | 1719  | 1769     | 1755     | 69      | 2            |
| 1   | H     | 1737  | 1790     | 1776     | 29      | 2            |
| 1   | I     | 1539  | 1579     | 1579     | 36      | 0            |
| 1   | J     | 1701  | 1750     | 1750     | 40      | 2            |
| 1   | K     | 1726  | 1774     | 1751     | 23      | 0            |
| 1   | L     | 1372  | 1428     | 1428     | 32      | 0            |
| 1   | M     | 1718  | 1764     | 1750     | 50      | 1            |
| 1   | N     | 1710  | 1763     | 1763     | 44      | 0            |
| 1   | O     | 1718  | 1764     | 1750     | 51      | 0            |
| 1   | P     | 1725  | 1781     | 1781     | 48      | 0            |
| 1   | Q     | 1727  | 1777     | 1763     | 53      | 0            |
| 1   | R     | 1711  | 1763     | 1749     | 41      | 0            |
| 1   | T     | 1727  | 1777     | 1763     | 20      | 0            |
| 1   | U     | 1737  | 1790     | 1776     | 25      | 1            |
| 1   | V     | 1727  | 1777     | 1763     | 33      | 0            |
| 1   | W     | 1727  | 1777     | 1763     | 38      | 0            |
| 1   | X     | 1725  | 1782     | 1781     | 68      | 0            |
| 1   | Y     | 1737  | 1790     | 1776     | 42      | 0            |
| 2   | A     | 7     | 0        | 0        | 0       | 0            |
| 2   | B     | 10    | 0        | 0        | 0       | 0            |
| 2   | C     | 18    | 0        | 0        | 0       | 0            |
| 2   | D     | 11    | 0        | 0        | 0       | 0            |
| 2   | E     | 14    | 0        | 0        | 0       | 0            |
| 2   | F     | 17    | 0        | 0        | 0       | 0            |
| 2   | G     | 17    | 0        | 0        | 2       | 0            |
| 2   | H     | 13    | 0        | 0        | 0       | 0            |
| 2   | I     | 13    | 0        | 0        | 2       | 0            |
| 2   | J     | 8     | 0        | 0        | 0       | 0            |
| 2   | K     | 7     | 0        | 0        | 0       | 0            |
| 2   | L     | 14    | 0        | 0        | 0       | 0            |
| 2   | M     | 11    | 0        | 0        | 0       | 0            |
| 2   | N     | 11    | 0        | 0        | 1       | 0            |
| 2   | O     | 19    | 0        | 0        | 1       | 0            |
| 2   | P     | 16    | 0        | 0        | 1       | 0            |
| 2   | Q     | 17    | 0        | 0        | 1       | 0            |
| 2   | R     | 9     | 0        | 0        | 1       | 0            |
| 2   | T     | 10    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | U     | 6     | 0        | 0        | 0       | 0            |
| 2   | V     | 9     | 0        | 0        | 0       | 0            |
| 2   | W     | 6     | 0        | 0        | 0       | 0            |
| 2   | X     | 9     | 0        | 0        | 1       | 0            |
| 2   | Y     | 9     | 0        | 0        | 0       | 0            |
| All | All   | 41130 | 42074    | 41800    | 796     | 5            |

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 10.

All (796) 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:O:124:ALA:HA  | 1:O:169:LEU:HD21 | 1.57                     | 0.86              |
| 1:J:100:GLN:OE1 | 1:J:208:TYR:OH   | 1.97                     | 0.83              |
| 1:I:95:GLU:OE2  | 1:I:141:GLN:NE2  | 2.11                     | 0.83              |
| 1:O:14:ARG:NH2  | 1:P:23:SER:OG    | 2.14                     | 0.81              |
| 1:M:57:ALA:O    | 1:M:109:LYS:NZ   | 2.13                     | 0.81              |
| 1:Q:96:LYS:O    | 1:Q:98:THR:N     | 2.14                     | 0.79              |
| 1:I:197:ILE:HB  | 1:I:198:GLY:HA3  | 1.65                     | 0.78              |
| 1:I:87:CYS:SG   | 1:I:192:THR:OG1  | 2.41                     | 0.77              |
| 1:J:178:GLN:NE2 | 1:J:182:GLU:OE2  | 2.18                     | 0.77              |
| 1:G:18:ARG:NH2  | 1:L:30:GLU:OE1   | 2.17                     | 0.77              |
| 1:F:187:LEU:O   | 1:K:86:TYR:OH    | 2.01                     | 0.77              |
| 1:P:61:ASP:OD2  | 1:P:109:LYS:NZ   | 2.18                     | 0.76              |
| 1:B:86:TYR:OH   | 1:D:187:LEU:O    | 2.02                     | 0.76              |
| 1:L:144:MSE:O   | 1:L:146:LYS:N    | 2.20                     | 0.75              |
| 1:T:38:LYS:NZ   | 1:X:26:GLU:OE1   | 2.20                     | 0.75              |
| 1:M:187:LEU:O   | 1:O:86:TYR:OH    | 2.02                     | 0.75              |
| 1:Q:89:ARG:NE   | 1:Q:145:GLN:OE1  | 2.20                     | 0.74              |
| 1:R:43:GLN:O    | 1:W:86:TYR:OH    | 2.08                     | 0.72              |
| 1:G:147:LYS:O   | 1:G:148:THR:OG1  | 2.07                     | 0.71              |
| 1:E:124:ALA:HA  | 1:E:169:LEU:HD22 | 1.73                     | 0.71              |
| 1:Y:142:ARG:NH2 | 1:Y:158:ALA:O    | 2.23                     | 0.71              |
| 1:U:41:ASP:OD1  | 1:V:152:ASN:ND2  | 2.24                     | 0.71              |
| 1:L:128:VAL:O   | 1:L:132:ASP:N    | 2.24                     | 0.70              |
| 1:C:219:LEU:O   | 1:C:224:LYS:NZ   | 2.25                     | 0.70              |
| 1:G:30:GLU:OE1  | 1:H:18:ARG:NH2   | 2.24                     | 0.70              |
| 1:Q:151:ASP:OD1 | 1:Q:152:ASN:N    | 2.24                     | 0.70              |
| 1:E:41:ASP:OD1  | 1:I:152:ASN:ND2  | 2.25                     | 0.69              |
| 1:X:160:LYS:N   | 1:X:165:SER:OG   | 2.26                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:218:GLN:OE1  | 1:K:218:GLN:N    | 2.25                     | 0.69              |
| 1:M:207:ASP:OD1  | 1:M:208:TYR:N    | 2.26                     | 0.69              |
| 1:T:18:ARG:NH2   | 1:Y:30:GLU:OE1   | 2.26                     | 0.68              |
| 1:A:160:LYS:HE3  | 1:A:165:SER:HB2  | 1.75                     | 0.68              |
| 1:O:97:ILE:HG22  | 1:O:104:VAL:HG21 | 1.76                     | 0.67              |
| 1:M:42:GLU:OE1   | 1:M:185:ARG:NH2  | 2.27                     | 0.67              |
| 1:E:124:ALA:HA   | 1:E:169:LEU:CD2  | 2.24                     | 0.67              |
| 1:O:101:TYR:HB2  | 1:O:104:VAL:HG22 | 1.75                     | 0.67              |
| 1:O:18:ARG:NH2   | 1:W:175:LYS:HB2  | 2.09                     | 0.67              |
| 1:M:94:LEU:O     | 1:M:98:THR:OG1   | 2.08                     | 0.67              |
| 1:Y:187:LEU:HB3  | 1:Y:189:ILE:CD1  | 2.25                     | 0.66              |
| 1:P:66:ARG:NH2   | 1:P:69:ALA:O     | 2.28                     | 0.66              |
| 1:G:10:GLU:HA    | 1:G:13:VAL:HG22  | 1.78                     | 0.66              |
| 1:U:156:GLU:O    | 1:U:160:LYS:N    | 2.27                     | 0.66              |
| 1:Q:159:MSE:HE3  | 1:Q:165:SER:HA   | 1.77                     | 0.66              |
| 1:F:95:GLU:O     | 1:F:98:THR:OG1   | 2.13                     | 0.65              |
| 1:H:151:ASP:OD1  | 1:H:154:SER:N    | 2.29                     | 0.65              |
| 1:L:175:LYS:O    | 1:L:179:ASN:ND2  | 2.28                     | 0.65              |
| 1:O:123:GLN:HG2  | 1:O:169:LEU:HD22 | 1.79                     | 0.65              |
| 1:R:205:ALA:O    | 1:W:200:THR:OG1  | 2.15                     | 0.65              |
| 1:P:61:ASP:OD2   | 1:P:64:SER:OG    | 2.15                     | 0.65              |
| 1:J:175:LYS:O    | 1:J:179:ASN:ND2  | 2.29                     | 0.65              |
| 1:P:13:VAL:HG21  | 1:W:16:LEU:HD13  | 1.79                     | 0.65              |
| 1:Q:163:ASN:OD1  | 2:Q:301:HOH:O    | 2.13                     | 0.64              |
| 1:A:19:ASP:OD2   | 1:B:14:ARG:NH2   | 2.30                     | 0.64              |
| 1:X:98:THR:HA    | 1:X:101:TYR:CD2  | 2.33                     | 0.64              |
| 1:F:87[A]:CYS:SG | 1:F:192:THR:HG22 | 2.38                     | 0.64              |
| 1:M:201:ILE:HD11 | 1:O:86:TYR:CZ    | 2.33                     | 0.64              |
| 1:X:159:MSE:O    | 1:X:164:THR:OG1  | 2.15                     | 0.64              |
| 1:R:163:ASN:O    | 1:R:166:LYS:NZ   | 2.31                     | 0.64              |
| 1:Q:147:LYS:O    | 1:Q:148:THR:OG1  | 2.13                     | 0.63              |
| 1:F:160:LYS:HZ1  | 1:J:48:ARG:HB3   | 1.63                     | 0.63              |
| 1:M:100:GLN:NE2  | 1:M:212:GLU:OE1  | 2.30                     | 0.63              |
| 1:R:213:ILE:O    | 1:R:217:GLU:N    | 2.31                     | 0.63              |
| 1:X:168:LYS:NZ   | 2:X:301:HOH:O    | 2.30                     | 0.63              |
| 1:E:38:LYS:HD2   | 1:J:25:PRO:HD2   | 1.80                     | 0.63              |
| 1:Q:200:THR:OG1  | 1:X:207:ASP:OD2  | 2.17                     | 0.63              |
| 1:C:152:ASN:ND2  | 1:K:44:GLN:OE1   | 2.28                     | 0.63              |
| 1:Q:91:ASP:O     | 1:Q:95:GLU:N     | 2.31                     | 0.63              |
| 1:Y:187:LEU:HB3  | 1:Y:189:ILE:HD12 | 1.81                     | 0.63              |
| 1:M:101:TYR:O    | 1:M:103:ASP:N    | 2.31                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:66:ARG:HG2   | 1:D:107:ILE:HD13 | 1.81                     | 0.62              |
| 1:U:26:GLU:OE1   | 1:V:178:GLN:NE2  | 2.32                     | 0.62              |
| 1:G:29:GLU:OE2   | 1:L:178:GLN:NE2  | 2.33                     | 0.62              |
| 1:Q:128:VAL:HG12 | 1:Q:167:ILE:HD11 | 1.82                     | 0.62              |
| 1:A:3:ALA:HA     | 1:A:5:LEU:H      | 1.65                     | 0.62              |
| 1:I:146:LYS:NZ   | 2:I:304:HOH:O    | 2.33                     | 0.62              |
| 1:U:97:ILE:HG22  | 1:U:104:VAL:HG21 | 1.81                     | 0.62              |
| 1:Y:197:ILE:O    | 1:Y:218:GLN:NE2  | 2.33                     | 0.62              |
| 1:G:219:LEU:HA   | 1:G:222:VAL:HG12 | 1.83                     | 0.61              |
| 1:P:170:THR:OG1  | 1:P:173:SER:OG   | 2.16                     | 0.61              |
| 1:K:66:ARG:NH1   | 1:K:70:LYS:O     | 2.33                     | 0.61              |
| 1:N:89:ARG:NH2   | 1:N:207:ASP:OD1  | 2.33                     | 0.61              |
| 1:N:22:VAL:HG13  | 1:R:174:LEU:HD23 | 1.81                     | 0.61              |
| 1:X:193:PRO:O    | 1:X:204:GLY:N    | 2.34                     | 0.61              |
| 1:I:125:VAL:HG12 | 1:I:139:LEU:CD2  | 2.30                     | 0.61              |
| 1:B:63:ALA:O     | 1:B:130:LYS:NZ   | 2.34                     | 0.60              |
| 1:G:37:THR:O     | 1:G:41:ASP:N     | 2.33                     | 0.60              |
| 1:P:46:GLN:HB2   | 1:P:49:GLN:HB3   | 1.83                     | 0.60              |
| 1:U:147:LYS:O    | 1:U:148:THR:OG1  | 2.11                     | 0.60              |
| 1:T:86:TYR:OH    | 1:V:187:LEU:O    | 2.17                     | 0.60              |
| 1:G:142:ARG:HB3  | 1:G:146:LYS:NZ   | 2.16                     | 0.60              |
| 1:J:48:ARG:NH1   | 1:J:199:ASP:OD1  | 2.34                     | 0.60              |
| 1:G:22:VAL:HG13  | 1:L:34:ALA:HB2   | 1.82                     | 0.60              |
| 1:I:201:ILE:O    | 2:I:301:HOH:O    | 2.16                     | 0.60              |
| 1:K:128:VAL:HG22 | 1:K:167:ILE:HD13 | 1.84                     | 0.60              |
| 1:I:112:PRO:HD2  | 1:I:181:LEU:HD13 | 1.83                     | 0.60              |
| 1:D:29:GLU:OE2   | 1:K:178:GLN:NE2  | 2.34                     | 0.59              |
| 1:U:101:TYR:O    | 1:U:104:VAL:HG22 | 2.02                     | 0.59              |
| 1:Q:77:VAL:HG12  | 1:Q:107:ILE:HB   | 1.84                     | 0.59              |
| 1:O:18:ARG:NH2   | 1:P:30:GLU:OE2   | 2.36                     | 0.59              |
| 1:A:18:ARG:NH1   | 1:F:30:GLU:OE2   | 2.34                     | 0.59              |
| 1:E:28:LEU:O     | 1:E:32:ILE:N     | 2.34                     | 0.59              |
| 1:G:22:VAL:HG22  | 1:L:31:ALA:HA    | 1.85                     | 0.59              |
| 1:O:5:LEU:CD1    | 1:P:9:GLN:HG2    | 2.32                     | 0.59              |
| 1:Q:174:LEU:CD2  | 1:V:30:GLU:HG3   | 2.32                     | 0.59              |
| 1:X:185:ARG:NH1  | 1:Y:29:GLU:OE2   | 2.34                     | 0.59              |
| 1:R:142:ARG:HA   | 1:R:145:GLN:HG2  | 1.84                     | 0.59              |
| 1:G:13:VAL:HG23  | 1:G:14:ARG:N     | 2.17                     | 0.59              |
| 1:X:148:THR:HG22 | 1:X:149:MSE:H    | 1.68                     | 0.59              |
| 1:H:96:LYS:HA    | 1:H:99:GLU:HG2   | 1.84                     | 0.59              |
| 1:M:94:LEU:HA    | 1:M:97:ILE:HG12  | 1.85                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:87[A]:CYS:SG | 1:D:192:THR:OG1  | 2.59                     | 0.59              |
| 1:G:146:LYS:NZ   | 1:G:158:ALA:HB2  | 2.17                     | 0.59              |
| 1:G:58:LEU:CD2   | 1:G:77:VAL:HG21  | 2.33                     | 0.59              |
| 1:J:39:LYS:HD3   | 1:J:39:LYS:N     | 2.17                     | 0.59              |
| 1:P:46:GLN:O     | 1:P:50:ALA:N     | 2.36                     | 0.59              |
| 1:Q:160:LYS:HA   | 1:Q:164:THR:H    | 1.68                     | 0.59              |
| 1:A:48:ARG:NH2   | 1:E:161:SER:OG   | 2.36                     | 0.58              |
| 1:I:30:GLU:HG3   | 1:J:174:LEU:HD22 | 1.85                     | 0.58              |
| 1:J:35:LEU:HG    | 1:J:39:LYS:HE2   | 1.85                     | 0.58              |
| 1:B:47:PHE:CE1   | 1:B:201:ILE:HG12 | 2.38                     | 0.58              |
| 1:H:124:ALA:HA   | 1:H:169:LEU:CD2  | 2.33                     | 0.58              |
| 1:R:147:LYS:O    | 1:R:148:THR:OG1  | 2.11                     | 0.58              |
| 1:E:50:ALA:O     | 1:E:55:HIS:N     | 2.36                     | 0.58              |
| 1:O:19:ASP:OD2   | 1:W:14:ARG:NH1   | 2.35                     | 0.58              |
| 1:L:87:CYS:SG    | 1:L:192:THR:CG2  | 2.92                     | 0.58              |
| 1:U:98:THR:HA    | 1:U:104:VAL:HG23 | 1.84                     | 0.57              |
| 1:A:35:LEU:HD21  | 1:A:39:LYS:HE3   | 1.84                     | 0.57              |
| 1:K:128:VAL:HG22 | 1:K:167:ILE:CD1  | 2.34                     | 0.57              |
| 1:O:125:VAL:HG12 | 1:O:139:LEU:HD22 | 1.87                     | 0.57              |
| 1:Q:74:LEU:HB2   | 1:Q:219:LEU:HD21 | 1.86                     | 0.57              |
| 1:U:156:GLU:O    | 1:U:160:LYS:HG3  | 2.04                     | 0.57              |
| 1:M:214:ILE:O    | 1:M:218:GLN:NE2  | 2.38                     | 0.57              |
| 1:E:74:LEU:HD21  | 1:E:76:LEU:HD11  | 1.85                     | 0.57              |
| 1:O:67:ILE:HB    | 1:O:106:VAL:CG2  | 2.35                     | 0.57              |
| 1:A:147:LYS:O    | 1:A:148:THR:OG1  | 2.14                     | 0.57              |
| 1:W:193:PRO:O    | 1:W:204:GLY:N    | 2.37                     | 0.57              |
| 1:N:32:ILE:HD13  | 1:R:28:LEU:HD21  | 1.87                     | 0.56              |
| 1:U:18:ARG:NH2   | 1:V:30:GLU:OE1   | 2.38                     | 0.56              |
| 1:Y:144:MSE:O    | 1:Y:146:LYS:N    | 2.39                     | 0.56              |
| 1:G:66:ARG:NH2   | 2:G:301:HOH:O    | 2.39                     | 0.56              |
| 1:M:147:LYS:O    | 1:M:148:THR:OG1  | 2.17                     | 0.56              |
| 1:X:50:ALA:O     | 1:X:54:GLU:HB2   | 2.05                     | 0.56              |
| 1:G:22:VAL:HG13  | 1:L:34:ALA:CB    | 2.36                     | 0.56              |
| 1:M:47:PHE:CE2   | 1:O:85:PRO:HB2   | 2.39                     | 0.56              |
| 1:K:147:LYS:O    | 1:K:148:THR:OG1  | 2.22                     | 0.56              |
| 1:Q:156:GLU:HA   | 1:Q:159:MSE:SE   | 2.56                     | 0.56              |
| 1:C:207:ASP:OD1  | 1:C:208:TYR:N    | 2.38                     | 0.56              |
| 1:O:11:LYS:HA    | 1:O:14:ARG:HB2   | 1.88                     | 0.56              |
| 1:Y:35:LEU:CD2   | 1:Y:39:LYS:HE3   | 2.35                     | 0.56              |
| 1:G:222:VAL:HG13 | 1:G:223:LYS:H    | 1.71                     | 0.56              |
| 1:D:66:ARG:HG2   | 1:D:107:ILE:CD1  | 2.36                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:79:PHE:HB3   | 1:O:111:LEU:HD11 | 1.89                     | 0.55              |
| 1:J:10:GLU:HA    | 1:J:13:VAL:HG22  | 1.88                     | 0.55              |
| 1:R:66:ARG:HE    | 1:R:107:ILE:HD11 | 1.70                     | 0.55              |
| 1:V:56:ASP:OD1   | 1:V:57:ALA:N     | 2.38                     | 0.55              |
| 1:C:210:GLN:O    | 1:C:214:ILE:HD12 | 2.06                     | 0.55              |
| 1:F:146:LYS:NZ   | 1:F:154:SER:O    | 2.40                     | 0.55              |
| 1:G:142:ARG:NH2  | 1:G:161:SER:OG   | 2.39                     | 0.55              |
| 1:G:58:LEU:HD22  | 1:G:59:TYR:CE2   | 2.42                     | 0.55              |
| 1:U:197:ILE:O    | 1:U:218:GLN:NE2  | 2.40                     | 0.55              |
| 1:E:73:LYS:HE3   | 1:E:222:VAL:HG22 | 1.89                     | 0.55              |
| 1:P:26:GLU:OE2   | 2:P:301:HOH:O    | 2.18                     | 0.55              |
| 1:G:11:LYS:HE2   | 1:H:4:ALA:HB2    | 1.89                     | 0.55              |
| 1:X:216:LYS:HA   | 1:X:219:LEU:HD12 | 1.89                     | 0.55              |
| 1:D:52:ALA:O     | 1:D:55:HIS:ND1   | 2.40                     | 0.55              |
| 1:N:97:ILE:HD12  | 1:N:215:VAL:HG21 | 1.88                     | 0.55              |
| 1:Q:207:ASP:H    | 1:X:200:THR:HG21 | 1.72                     | 0.55              |
| 1:Q:206:VAL:HG22 | 1:Q:210:GLN:HB2  | 1.88                     | 0.54              |
| 1:X:156:GLU:HA   | 1:X:159:MSE:CG   | 2.37                     | 0.54              |
| 1:E:13:VAL:HG21  | 1:I:16:LEU:HD13  | 1.89                     | 0.54              |
| 1:U:85:PRO:O     | 1:U:89:ARG:NH1   | 2.40                     | 0.54              |
| 1:M:95:GLU:OE1   | 1:M:141:GLN:NE2  | 2.36                     | 0.54              |
| 1:D:66:ARG:NH2   | 1:D:69:ALA:O     | 2.40                     | 0.54              |
| 1:A:196:VAL:HG22 | 1:A:201:ILE:HD12 | 1.89                     | 0.54              |
| 1:M:10:GLU:O     | 1:M:13:VAL:HG22  | 2.07                     | 0.54              |
| 1:W:130:LYS:NZ   | 1:W:170:THR:OG1  | 2.39                     | 0.54              |
| 1:A:73:LYS:HE2   | 1:A:224:LYS:HD3  | 1.89                     | 0.54              |
| 1:P:147:LYS:O    | 1:P:148:THR:OG1  | 2.25                     | 0.54              |
| 1:E:58:LEU:HD22  | 1:E:77:VAL:HG11  | 1.89                     | 0.54              |
| 1:B:30:GLU:OE1   | 1:F:18:ARG:NH2   | 2.41                     | 0.54              |
| 1:G:73:LYS:HD2   | 1:G:223:LYS:HD3  | 1.89                     | 0.54              |
| 1:L:88:LYS:HE3   | 1:L:144:MSE:O    | 2.08                     | 0.54              |
| 1:M:120:LYS:HD3  | 1:N:37:THR:HG21  | 1.90                     | 0.54              |
| 1:Q:160:LYS:HG3  | 1:Q:160:LYS:O    | 2.06                     | 0.54              |
| 1:A:66:ARG:NH1   | 1:A:70:LYS:O     | 2.41                     | 0.53              |
| 1:X:101:TYR:CD2  | 1:X:104:VAL:HG23 | 2.43                     | 0.53              |
| 1:M:30:GLU:HB3   | 1:R:178:GLN:HG3  | 1.89                     | 0.53              |
| 1:O:67:ILE:HG21  | 1:O:95:GLU:HG3   | 1.89                     | 0.53              |
| 1:A:160:LYS:HG3  | 1:A:165:SER:HB2  | 1.91                     | 0.53              |
| 1:K:95:GLU:OE1   | 1:K:141:GLN:NE2  | 2.40                     | 0.53              |
| 1:Q:204:GLY:HA3  | 1:X:203:PRO:HD2  | 1.89                     | 0.53              |
| 1:A:35:LEU:CD2   | 1:A:39:LYS:HE3   | 2.38                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:211:LEU:O    | 1:G:215:VAL:HG22 | 2.09                     | 0.53              |
| 1:K:66:ARG:NH2   | 1:K:69:ALA:O     | 2.42                     | 0.53              |
| 1:X:88:LYS:O     | 1:X:144:MSE:HE1  | 2.09                     | 0.53              |
| 1:L:128:VAL:HG12 | 1:L:167:ILE:HD13 | 1.91                     | 0.53              |
| 1:B:196:VAL:HG22 | 1:B:201:ILE:CD1  | 2.38                     | 0.53              |
| 1:F:147:LYS:O    | 1:F:148:THR:OG1  | 2.19                     | 0.53              |
| 1:O:30:GLU:OE1   | 1:W:18:ARG:NH1   | 2.42                     | 0.53              |
| 1:U:86:TYR:OH    | 1:Y:187:LEU:O    | 2.27                     | 0.53              |
| 1:Y:192:THR:HG22 | 1:Y:193:PRO:HA   | 1.90                     | 0.53              |
| 1:J:90:PHE:HE1   | 1:J:206:VAL:HG22 | 1.74                     | 0.52              |
| 1:M:96:LYS:HE3   | 1:M:208:TYR:CE1  | 2.44                     | 0.52              |
| 1:M:218:GLN:OE1  | 1:O:210:GLN:NE2  | 2.42                     | 0.52              |
| 1:Y:142:ARG:NH2  | 1:Y:162:THR:HG23 | 2.24                     | 0.52              |
| 1:P:164:THR:O    | 1:P:167:ILE:HG22 | 2.09                     | 0.52              |
| 1:R:157:ASP:OD1  | 2:R:301:HOH:O    | 2.19                     | 0.52              |
| 1:A:3:ALA:HA     | 1:A:4:ALA:HB3    | 1.91                     | 0.52              |
| 1:G:18:ARG:HH21  | 1:H:175:LYS:HG3  | 1.75                     | 0.52              |
| 1:G:194:ALA:HA   | 1:G:203:PRO:HA   | 1.92                     | 0.52              |
| 1:M:120:LYS:O    | 1:M:124:ALA:N    | 2.41                     | 0.52              |
| 1:Q:86:TYR:CD2   | 1:Q:205:ALA:HB1  | 2.44                     | 0.52              |
| 1:X:222:VAL:O    | 1:X:224:LYS:N    | 2.42                     | 0.52              |
| 1:Q:142:ARG:O    | 1:Q:146:LYS:HE2  | 2.09                     | 0.52              |
| 1:X:141:GLN:O    | 1:X:145:GLN:N    | 2.42                     | 0.52              |
| 1:X:58:LEU:HB3   | 1:X:59:TYR:CD1   | 2.45                     | 0.52              |
| 1:I:66:ARG:HB3   | 1:I:107:ILE:HD13 | 1.91                     | 0.52              |
| 1:T:178:GLN:NE2  | 1:X:29:GLU:OE2   | 2.39                     | 0.52              |
| 1:Y:64:SER:OG    | 1:Y:109:LYS:NZ   | 2.40                     | 0.52              |
| 1:G:16:LEU:HD11  | 1:H:10:GLU:HG3   | 1.90                     | 0.52              |
| 1:G:207:ASP:OD1  | 1:G:208:TYR:N    | 2.43                     | 0.52              |
| 1:L:115:GLY:HA3  | 1:L:149:MSE:HE1  | 1.91                     | 0.52              |
| 1:O:178:GLN:NE2  | 1:W:26:GLU:OE1   | 2.42                     | 0.52              |
| 1:X:208:TYR:HA   | 1:X:211:LEU:HD13 | 1.91                     | 0.52              |
| 1:J:83:ASN:HA    | 1:J:144:MSE:HG3  | 1.92                     | 0.52              |
| 1:J:157:ASP:O    | 1:J:161:SER:N    | 2.41                     | 0.52              |
| 1:C:17:VAL:HG11  | 1:D:20:THR:HG21  | 1.91                     | 0.51              |
| 1:G:9:GLN:C      | 1:G:11:LYS:N     | 2.62                     | 0.51              |
| 1:N:63:ALA:O     | 1:N:130:LYS:NZ   | 2.32                     | 0.51              |
| 1:O:41:ASP:HA    | 1:O:44:GLN:HB2   | 1.91                     | 0.51              |
| 1:X:142:ARG:HH21 | 1:X:162:THR:HG23 | 1.75                     | 0.51              |
| 1:E:25:PRO:HD2   | 1:I:38:LYS:HD2   | 1.93                     | 0.51              |
| 1:G:143:LEU:HD22 | 1:G:150:LEU:HD13 | 1.91                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:16:LEU:O     | 1:J:20:THR:OG1   | 2.23                     | 0.51              |
| 1:J:196:VAL:HG12 | 1:J:201:ILE:HD12 | 1.92                     | 0.51              |
| 1:N:58:LEU:HD22  | 1:N:77:VAL:HG21  | 1.91                     | 0.51              |
| 1:X:194:ALA:HB1  | 1:X:201:ILE:HD11 | 1.92                     | 0.51              |
| 1:D:93:LEU:O     | 1:D:97:ILE:HD12  | 2.09                     | 0.51              |
| 1:L:128:VAL:HG12 | 1:L:167:ILE:HG21 | 1.92                     | 0.51              |
| 1:Q:215:VAL:O    | 1:Q:218:GLN:NE2  | 2.43                     | 0.51              |
| 1:W:142:ARG:HA   | 1:W:145:GLN:HB2  | 1.92                     | 0.51              |
| 1:W:84[B]:CYS:SG | 1:W:87[B]:CYS:N  | 2.83                     | 0.51              |
| 1:E:178:GLN:NE2  | 1:J:26:GLU:O     | 2.44                     | 0.51              |
| 1:N:184:SER:OG   | 1:N:189:ILE:O    | 2.28                     | 0.51              |
| 1:X:50:ALA:O     | 1:X:54:GLU:N     | 2.43                     | 0.51              |
| 1:G:151:ASP:H    | 1:G:154:SER:HB2  | 1.75                     | 0.51              |
| 1:Q:160:LYS:HB3  | 1:Q:165:SER:OG   | 2.11                     | 0.51              |
| 1:R:46:GLN:HB2   | 1:R:49:GLN:HE22  | 1.75                     | 0.51              |
| 1:M:84[B]:CYS:SG | 1:M:87[B]:CYS:N  | 2.83                     | 0.51              |
| 1:G:11:LYS:HE2   | 1:H:4:ALA:CB     | 2.39                     | 0.51              |
| 1:N:97:ILE:HG22  | 1:N:104:VAL:HG11 | 1.93                     | 0.51              |
| 1:Y:47:PHE:O     | 1:Y:48:ARG:NH1   | 2.44                     | 0.51              |
| 1:A:35:LEU:HD11  | 1:B:29:GLU:HB2   | 1.93                     | 0.51              |
| 1:K:66:ARG:CZ    | 1:K:69:ALA:O     | 2.59                     | 0.51              |
| 1:O:147:LYS:O    | 1:O:148:THR:OG1  | 2.29                     | 0.51              |
| 1:E:95:GLU:O     | 1:E:98:THR:OG1   | 2.24                     | 0.51              |
| 1:H:55:HIS:C     | 1:H:55:HIS:ND1   | 2.64                     | 0.51              |
| 1:O:18:ARG:NH2   | 1:P:30:GLU:OE1   | 2.45                     | 0.51              |
| 1:Q:138:ALA:HB3  | 1:Q:162:THR:HG23 | 1.92                     | 0.51              |
| 1:X:160:LYS:HA   | 1:X:164:THR:H    | 1.75                     | 0.51              |
| 1:C:89:ARG:O     | 1:C:89:ARG:HG3   | 2.10                     | 0.50              |
| 1:M:47:PHE:CD2   | 1:O:86:TYR:CE1   | 2.99                     | 0.50              |
| 1:V:63:ALA:O     | 1:V:130:LYS:NZ   | 2.42                     | 0.50              |
| 1:F:51:LEU:HD22  | 1:F:199:ASP:HA   | 1.93                     | 0.50              |
| 1:E:49:GLN:HG2   | 1:E:49:GLN:O     | 2.11                     | 0.50              |
| 1:W:50:ALA:O     | 1:W:54:GLU:N     | 2.42                     | 0.50              |
| 1:N:187:LEU:HB3  | 1:N:189:ILE:CD1  | 2.42                     | 0.50              |
| 1:X:160:LYS:HB2  | 1:X:165:SER:HB2  | 1.94                     | 0.50              |
| 1:F:73:LYS:HG3   | 1:F:74:LEU:N     | 2.26                     | 0.50              |
| 1:L:87:CYS:SG    | 1:L:192:THR:HG22 | 2.52                     | 0.50              |
| 1:G:142:ARG:HB3  | 1:G:146:LYS:HZ1  | 1.77                     | 0.50              |
| 1:E:20:THR:CG2   | 1:J:14:ARG:HG2   | 2.42                     | 0.50              |
| 1:P:139:LEU:HA   | 1:P:162:THR:HG21 | 1.93                     | 0.50              |
| 1:C:18:ARG:NH2   | 1:D:30:GLU:OE2   | 2.44                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:208:TYR:CG   | 1:G:209:ASP:N    | 2.80                     | 0.50              |
| 1:H:156:GLU:HB2  | 1:H:160:LYS:NZ   | 2.26                     | 0.50              |
| 1:R:137:LEU:O    | 1:R:141:GLN:HG3  | 2.12                     | 0.50              |
| 1:V:150:LEU:HD23 | 1:V:155:ILE:HD13 | 1.93                     | 0.50              |
| 1:X:59:TYR:CE1   | 1:X:77:VAL:HG13  | 2.47                     | 0.50              |
| 1:A:200:THR:HG21 | 1:C:207:ASP:HB2  | 1.94                     | 0.50              |
| 1:G:10:GLU:HA    | 1:G:13:VAL:CG2   | 2.41                     | 0.50              |
| 1:M:18:ARG:NH1   | 1:R:30:GLU:OE2   | 2.45                     | 0.50              |
| 1:B:214:ILE:HG12 | 1:D:213:ILE:HD11 | 1.93                     | 0.49              |
| 1:H:55:HIS:C     | 1:H:55:HIS:HD1   | 2.15                     | 0.49              |
| 1:K:66:ARG:NE    | 1:K:69:ALA:O     | 2.44                     | 0.49              |
| 1:O:197:ILE:HG22 | 1:O:218:GLN:HG3  | 1.94                     | 0.49              |
| 1:Q:178:GLN:NE2  | 1:V:29:GLU:OE2   | 2.45                     | 0.49              |
| 1:T:207:ASP:OD1  | 1:V:200:THR:OG1  | 2.29                     | 0.49              |
| 1:X:51:LEU:O     | 1:X:55:HIS:NE2   | 2.44                     | 0.49              |
| 1:P:66:ARG:NH1   | 1:P:70:LYS:O     | 2.44                     | 0.49              |
| 1:X:139:LEU:HD11 | 1:X:159:MSE:SE   | 2.62                     | 0.49              |
| 1:M:47:PHE:CE2   | 1:O:86:TYR:CE1   | 3.00                     | 0.49              |
| 1:H:124:ALA:HA   | 1:H:169:LEU:HD21 | 1.93                     | 0.49              |
| 1:A:30:GLU:HB2   | 1:F:178:GLN:HG3  | 1.93                     | 0.49              |
| 1:X:98:THR:HA    | 1:X:101:TYR:CE2  | 2.48                     | 0.49              |
| 1:Q:54:GLU:OE1   | 1:Q:186:LYS:NZ   | 2.46                     | 0.49              |
| 1:B:196:VAL:HG22 | 1:B:201:ILE:HD12 | 1.94                     | 0.49              |
| 1:L:100:GLN:NE2  | 1:L:212:GLU:OE2  | 2.38                     | 0.49              |
| 1:N:97:ILE:CG2   | 1:N:104:VAL:HG11 | 2.42                     | 0.49              |
| 1:R:27:ILE:HG23  | 1:R:28:LEU:N     | 2.27                     | 0.49              |
| 1:H:124:ALA:CA   | 1:H:169:LEU:HD21 | 2.42                     | 0.49              |
| 1:R:66:ARG:HH11  | 1:R:70:LYS:HA    | 1.77                     | 0.49              |
| 1:C:206:VAL:HG22 | 1:C:210:GLN:HB2  | 1.93                     | 0.49              |
| 1:E:178:GLN:O    | 1:E:182:GLU:N    | 2.41                     | 0.49              |
| 1:G:13:VAL:HG23  | 1:G:14:ARG:HG3   | 1.94                     | 0.49              |
| 1:A:160:LYS:CE   | 1:A:165:SER:HB2  | 2.42                     | 0.48              |
| 1:E:64:SER:OG    | 1:E:109:LYS:NZ   | 2.31                     | 0.48              |
| 1:Q:29:GLU:HB2   | 1:U:35:LEU:HD11  | 1.95                     | 0.48              |
| 1:W:76:LEU:HD13  | 1:W:195:THR:HG23 | 1.95                     | 0.48              |
| 1:G:10:GLU:CA    | 1:G:13:VAL:HG22  | 2.43                     | 0.48              |
| 1:Y:74:LEU:CD2   | 1:Y:76:LEU:HD12  | 2.43                     | 0.48              |
| 1:G:84[B]:CYS:SG | 1:G:87[B]:CYS:N  | 2.81                     | 0.48              |
| 1:Q:94:LEU:HD13  | 1:Q:211:LEU:HB3  | 1.96                     | 0.48              |
| 1:X:83:ASN:OD1   | 1:X:117:SER:OG   | 2.18                     | 0.48              |
| 1:Y:202:LEU:HD21 | 1:Y:206:VAL:CG2  | 2.44                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:67:ILE:HB    | 1:E:106:VAL:HG23 | 1.95                     | 0.48              |
| 1:N:87:CYS:SG    | 1:N:192:THR:HB   | 2.53                     | 0.48              |
| 1:B:96:LYS:O     | 1:B:100:GLN:N    | 2.43                     | 0.48              |
| 1:F:151:ASP:OD1  | 1:F:154:SER:N    | 2.39                     | 0.48              |
| 1:G:139:LEU:HB2  | 1:G:162:THR:HG21 | 1.96                     | 0.48              |
| 1:I:113:PHE:CE1  | 1:I:181:LEU:HD11 | 2.49                     | 0.48              |
| 1:J:159:MSE:O    | 1:J:163:ASN:N    | 2.47                     | 0.48              |
| 1:R:90:PHE:HE1   | 1:R:206:VAL:HG22 | 1.78                     | 0.48              |
| 1:H:55:HIS:O     | 1:H:55:HIS:ND1   | 2.40                     | 0.48              |
| 1:M:35:LEU:HD11  | 1:N:29:GLU:HB2   | 1.96                     | 0.48              |
| 1:M:101:TYR:C    | 1:M:103:ASP:H    | 2.17                     | 0.48              |
| 1:M:170:THR:O    | 1:M:173:SER:OG   | 2.28                     | 0.48              |
| 1:M:94:LEU:O     | 1:M:98:THR:N     | 2.44                     | 0.48              |
| 1:O:98:THR:HG21  | 1:O:106:VAL:HG22 | 1.96                     | 0.48              |
| 1:P:159:MSE:O    | 1:P:164:THR:OG1  | 2.25                     | 0.48              |
| 1:V:46:GLN:HB2   | 1:V:49:GLN:HE22  | 1.79                     | 0.48              |
| 1:X:92:PRO:HD3   | 1:X:144:MSE:HE2  | 1.95                     | 0.48              |
| 1:N:74:LEU:O     | 1:N:104:VAL:HA   | 2.13                     | 0.48              |
| 1:R:223:LYS:HG3  | 1:R:224:LYS:H    | 1.79                     | 0.48              |
| 1:I:11:LYS:HA    | 1:I:14:ARG:HB2   | 1.96                     | 0.47              |
| 1:L:74:LEU:HD23  | 1:L:215:VAL:CG2  | 2.44                     | 0.47              |
| 1:M:160:LYS:HG3  | 1:M:165:SER:OG   | 2.14                     | 0.47              |
| 1:Q:28:LEU:HD21  | 1:U:32:ILE:HD13  | 1.96                     | 0.47              |
| 1:X:167:ILE:HG13 | 1:X:167:ILE:O    | 2.12                     | 0.47              |
| 1:B:66:ARG:HH11  | 1:B:70:LYS:HA    | 1.80                     | 0.47              |
| 1:F:99:GLU:HA    | 1:F:102:PRO:HA   | 1.95                     | 0.47              |
| 1:L:83:ASN:ND2   | 1:L:150:LEU:HD13 | 2.29                     | 0.47              |
| 1:Q:210:GLN:NE2  | 1:X:199:ASP:OD1  | 2.46                     | 0.47              |
| 1:V:77:VAL:HB    | 1:V:196:VAL:HB   | 1.96                     | 0.47              |
| 1:M:20:THR:HG22  | 1:M:27:ILE:HD12  | 1.97                     | 0.47              |
| 1:P:46:GLN:HB2   | 1:P:49:GLN:CB    | 2.44                     | 0.47              |
| 1:Q:197:ILE:HD13 | 1:Q:202:LEU:HB2  | 1.97                     | 0.47              |
| 1:R:219:LEU:HD12 | 1:R:220:ALA:N    | 2.29                     | 0.47              |
| 1:J:144:MSE:HE2  | 1:J:146:LYS:HB3  | 1.96                     | 0.47              |
| 1:N:83:ASN:OD1   | 1:N:118:SER:OG   | 2.24                     | 0.47              |
| 1:X:116:GLU:OE2  | 1:Y:37:THR:HG22  | 2.13                     | 0.47              |
| 1:E:149:MSE:HG3  | 1:E:150:LEU:H    | 1.80                     | 0.47              |
| 1:F:130:LYS:O    | 1:F:130:LYS:HD2  | 2.15                     | 0.47              |
| 1:G:166:LYS:H    | 1:G:166:LYS:HD2  | 1.80                     | 0.47              |
| 1:H:125:VAL:HG13 | 1:H:136:PHE:CE1  | 2.49                     | 0.47              |
| 1:V:79:PHE:HB2   | 1:V:194:ALA:HB3  | 1.97                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:48:ARG:NH1   | 1:W:200:THR:HA   | 2.30                     | 0.47              |
| 1:Y:34:ALA:O     | 1:Y:37:THR:OG1   | 2.33                     | 0.47              |
| 1:O:39:LYS:HG2   | 1:O:185:ARG:CZ   | 2.44                     | 0.47              |
| 1:W:66:ARG:HH12  | 1:W:70:LYS:HD3   | 1.79                     | 0.47              |
| 1:Y:142:ARG:CZ   | 1:Y:162:THR:HG23 | 2.45                     | 0.47              |
| 1:G:112:PRO:HA   | 1:G:118:SER:HB3  | 1.96                     | 0.47              |
| 1:G:150:LEU:HD13 | 1:G:155:ILE:HD13 | 1.97                     | 0.47              |
| 1:K:87[A]:CYS:SG | 1:K:192:THR:HB   | 2.54                     | 0.47              |
| 1:R:206:VAL:HG21 | 1:R:211:LEU:HB2  | 1.97                     | 0.47              |
| 1:D:223:LYS:HE3  | 1:L:134:LYS:HB3  | 1.96                     | 0.47              |
| 1:F:139:LEU:HA   | 1:F:162:THR:HG21 | 1.97                     | 0.47              |
| 1:Y:74:LEU:CD2   | 1:Y:76:LEU:CD1   | 2.93                     | 0.47              |
| 1:M:83:ASN:ND2   | 1:M:117:SER:OG   | 2.47                     | 0.47              |
| 1:E:20:THR:HG21  | 1:J:14:ARG:HG2   | 1.97                     | 0.47              |
| 1:Y:48:ARG:NH2   | 1:Y:187:LEU:HG   | 2.29                     | 0.47              |
| 1:A:200:THR:HG22 | 1:A:201:ILE:N    | 2.30                     | 0.46              |
| 1:D:58:LEU:HD21  | 1:D:187:LEU:HD11 | 1.96                     | 0.46              |
| 1:T:147:LYS:O    | 1:T:148:THR:OG1  | 2.19                     | 0.46              |
| 1:W:179:ASN:O    | 1:W:183:LEU:N    | 2.45                     | 0.46              |
| 1:C:222:VAL:HG23 | 1:C:224:LYS:HZ1  | 1.79                     | 0.46              |
| 1:L:119:ALA:O    | 1:L:123:GLN:HG3  | 2.15                     | 0.46              |
| 1:N:159:MSE:O    | 1:N:164:THR:OG1  | 2.30                     | 0.46              |
| 1:M:221:LYS:HB3  | 1:Q:138:ALA:HB2  | 1.97                     | 0.46              |
| 1:V:206:VAL:HG13 | 1:V:211:LEU:HD11 | 1.96                     | 0.46              |
| 1:W:79:PHE:CE2   | 1:W:183:LEU:HD22 | 2.50                     | 0.46              |
| 1:T:29:GLU:OE1   | 1:Y:185:ARG:NH1  | 2.48                     | 0.46              |
| 1:A:142:ARG:NH1  | 1:A:161:SER:OG   | 2.49                     | 0.46              |
| 1:E:147:LYS:O    | 1:E:148:THR:HB   | 2.15                     | 0.46              |
| 1:E:27:ILE:HG12  | 1:J:18:ARG:HA    | 1.97                     | 0.46              |
| 1:J:77:VAL:HB    | 1:J:196:VAL:HG22 | 1.97                     | 0.46              |
| 1:M:79:PHE:HZ    | 1:M:183:LEU:HD22 | 1.79                     | 0.46              |
| 1:G:58:LEU:HD21  | 1:G:77:VAL:HG21  | 1.98                     | 0.46              |
| 1:Q:215:VAL:O    | 1:Q:215:VAL:HG13 | 2.16                     | 0.46              |
| 1:Y:48:ARG:HG3   | 1:Y:50:ALA:HB3   | 1.97                     | 0.46              |
| 1:T:25:PRO:O     | 1:Y:35:LEU:HD12  | 2.16                     | 0.46              |
| 1:A:159:MSE:HB2  | 1:A:165:SER:OG   | 2.15                     | 0.46              |
| 1:B:47:PHE:CZ    | 1:B:201:ILE:HG12 | 2.51                     | 0.46              |
| 1:F:66:ARG:NH1   | 1:F:66:ARG:HB3   | 2.30                     | 0.46              |
| 1:G:156:GLU:O    | 1:G:160:LYS:HG2  | 2.15                     | 0.46              |
| 1:O:91:ASP:HB3   | 1:O:92:PRO:HD3   | 1.97                     | 0.46              |
| 1:P:152:ASN:HA   | 1:P:155:ILE:HG12 | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:121:ALA:HB2  | 1:G:155:ILE:HD12 | 1.97                     | 0.46              |
| 1:X:87:CYS:SG    | 1:X:193:PRO:HB3  | 2.56                     | 0.46              |
| 1:B:47:PHE:HE1   | 1:B:201:ILE:HG12 | 1.81                     | 0.46              |
| 1:E:67:ILE:HB    | 1:E:106:VAL:CG2  | 2.46                     | 0.46              |
| 1:E:76:LEU:HB2   | 1:E:106:VAL:HG12 | 1.97                     | 0.46              |
| 1:I:170:THR:HG23 | 1:I:173:SER:H    | 1.80                     | 0.46              |
| 1:K:6:ASN:OD1    | 1:K:9:GLN:N      | 2.44                     | 0.46              |
| 1:E:190:GLN:OE1  | 1:E:190:GLN:N    | 2.48                     | 0.46              |
| 1:F:134:LYS:HE2  | 1:J:222:VAL:HG12 | 1.98                     | 0.46              |
| 1:G:224:LYS:NZ   | 1:K:99:GLU:OE1   | 2.45                     | 0.46              |
| 1:N:101:TYR:HB2  | 1:N:104:VAL:HG12 | 1.96                     | 0.46              |
| 1:B:92:PRO:O     | 1:B:95:GLU:HG2   | 2.15                     | 0.46              |
| 1:E:76:LEU:N     | 1:E:76:LEU:HD12  | 2.31                     | 0.46              |
| 1:P:168:LYS:CD   | 1:P:168:LYS:H    | 2.28                     | 0.46              |
| 1:R:151:ASP:H    | 1:R:154:SER:HB2  | 1.80                     | 0.46              |
| 1:I:75:VAL:HG12  | 1:I:105:ALA:HB3  | 1.98                     | 0.45              |
| 1:O:96:LYS:O     | 1:O:99:GLU:HG2   | 2.16                     | 0.45              |
| 1:X:90:PHE:O     | 1:X:94:LEU:HD12  | 2.16                     | 0.45              |
| 1:I:195:THR:HG23 | 1:I:202:LEU:HB2  | 1.98                     | 0.45              |
| 1:J:182:GLU:HG2  | 1:J:185:ARG:NH2  | 2.32                     | 0.45              |
| 1:N:73:LYS:HG2   | 1:N:103:ASP:HB3  | 1.99                     | 0.45              |
| 1:U:65:PRO:HA    | 1:U:129:TRP:CE2  | 2.52                     | 0.45              |
| 1:Q:82:TYR:HD1   | 1:Q:144:MSE:HG2  | 1.81                     | 0.45              |
| 1:Q:214:ILE:HG12 | 1:X:214:ILE:HG12 | 1.98                     | 0.45              |
| 1:F:50:ALA:O     | 1:F:54:GLU:N     | 2.50                     | 0.45              |
| 1:H:86:TYR:HB2   | 1:H:193:PRO:HD3  | 1.98                     | 0.45              |
| 1:J:144:MSE:HE3  | 1:J:150:LEU:CD1  | 2.46                     | 0.45              |
| 1:W:76:LEU:HD11  | 1:W:106:VAL:HG22 | 1.97                     | 0.45              |
| 1:B:92:PRO:O     | 1:B:96:LYS:HD3   | 2.17                     | 0.45              |
| 1:E:74:LEU:HD22  | 1:E:104:VAL:HG22 | 1.98                     | 0.45              |
| 1:L:74:LEU:HD23  | 1:L:215:VAL:HG22 | 1.98                     | 0.45              |
| 1:N:112:PRO:HD3  | 1:N:177:LEU:HD11 | 1.98                     | 0.45              |
| 1:P:168:LYS:CD   | 1:P:168:LYS:N    | 2.80                     | 0.45              |
| 1:Q:211:LEU:O    | 1:Q:215:VAL:HG12 | 2.17                     | 0.45              |
| 1:T:197:ILE:HG22 | 1:T:218:GLN:HG3  | 1.98                     | 0.45              |
| 1:U:204:GLY:HA3  | 1:Y:203:PRO:HG2  | 1.98                     | 0.45              |
| 1:E:77:VAL:HB    | 1:E:196:VAL:HB   | 1.99                     | 0.45              |
| 1:P:168:LYS:N    | 1:P:168:LYS:HD2  | 2.32                     | 0.45              |
| 1:Q:97:ILE:HG23  | 1:Q:101:TYR:HD2  | 1.82                     | 0.45              |
| 1:R:47:PHE:CZ    | 1:R:201:ILE:HG12 | 2.52                     | 0.45              |
| 1:D:197:ILE:HD13 | 1:D:202:LEU:HD13 | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:148:THR:HG22 | 1:X:149:MSE:N    | 2.30                     | 0.45              |
| 1:B:193:PRO:HD2  | 1:B:204:GLY:HA2  | 1.98                     | 0.45              |
| 1:H:142:ARG:HA   | 1:H:145:GLN:HG2  | 1.98                     | 0.45              |
| 1:O:14:ARG:HA    | 1:O:17:VAL:HG12  | 1.99                     | 0.45              |
| 1:W:179:ASN:O    | 1:W:183:LEU:HB2  | 2.16                     | 0.45              |
| 1:X:13:VAL:O     | 1:X:17:VAL:HG23  | 2.17                     | 0.45              |
| 1:X:65:PRO:HA    | 1:X:129:TRP:CE2  | 2.52                     | 0.45              |
| 1:Y:148:THR:OG1  | 1:Y:149:MSE:N    | 2.49                     | 0.45              |
| 1:A:206:VAL:HG12 | 1:A:210:GLN:HB2  | 1.98                     | 0.45              |
| 1:O:18:ARG:NH2   | 1:P:30:GLU:CD    | 2.70                     | 0.45              |
| 1:Q:97:ILE:HA    | 1:Q:100:GLN:HB2  | 1.99                     | 0.45              |
| 1:Y:48:ARG:CD    | 1:Y:186:LYS:HB3  | 2.47                     | 0.45              |
| 1:A:40:ALA:HA    | 1:A:43:GLN:HB3   | 1.98                     | 0.44              |
| 1:A:80:THR:O     | 1:A:111:LEU:N    | 2.48                     | 0.44              |
| 1:C:128:VAL:O    | 1:C:132:ASP:N    | 2.44                     | 0.44              |
| 1:G:146:LYS:CD   | 1:G:150:LEU:HD21 | 2.47                     | 0.44              |
| 1:J:43:GLN:HG3   | 1:J:44:GLN:HG3   | 2.00                     | 0.44              |
| 1:T:210:GLN:HE22 | 1:V:197:ILE:HD12 | 1.82                     | 0.44              |
| 1:T:17:VAL:HG21  | 1:Y:17:VAL:HA    | 1.99                     | 0.44              |
| 1:C:222:VAL:HG23 | 1:C:224:LYS:NZ   | 2.32                     | 0.44              |
| 1:E:82:TYR:CD1   | 1:E:144:MSE:HE3  | 2.52                     | 0.44              |
| 1:E:193:PRO:O    | 1:E:204:GLY:N    | 2.50                     | 0.44              |
| 1:F:59:TYR:CD1   | 1:F:75:VAL:HG23  | 2.52                     | 0.44              |
| 1:I:58:LEU:CD2   | 1:I:77:VAL:HG21  | 2.47                     | 0.44              |
| 1:N:28:LEU:O     | 1:N:32:ILE:HG12  | 2.17                     | 0.44              |
| 1:Q:79:PHE:HB2   | 1:Q:194:ALA:HB3  | 1.98                     | 0.44              |
| 1:U:151:ASP:H    | 1:U:154:SER:HB2  | 1.82                     | 0.44              |
| 1:X:140:HIS:O    | 1:X:144:MSE:HB3  | 2.18                     | 0.44              |
| 1:I:33:MSE:HA    | 1:I:36:GLN:HB2   | 1.99                     | 0.44              |
| 1:M:194:ALA:HA   | 1:M:203:PRO:HA   | 1.99                     | 0.44              |
| 1:M:39:LYS:HD3   | 1:M:185:ARG:CZ   | 2.47                     | 0.44              |
| 1:O:76:LEU:HD22  | 1:O:197:ILE:HD13 | 1.99                     | 0.44              |
| 1:R:73:LYS:HE2   | 1:R:224:LYS:HD2  | 1.99                     | 0.44              |
| 1:A:91:ASP:HB3   | 1:A:92:PRO:HD3   | 2.00                     | 0.44              |
| 1:B:35:LEU:HD21  | 1:F:29:GLU:HB3   | 1.99                     | 0.44              |
| 1:E:137:LEU:HD21 | 1:E:141:GLN:NE2  | 2.33                     | 0.44              |
| 1:E:74:LEU:HD21  | 1:E:76:LEU:CD1   | 2.48                     | 0.44              |
| 1:G:104:VAL:HG22 | 1:G:219:LEU:HD21 | 1.99                     | 0.44              |
| 1:G:212:GLU:O    | 1:G:216:LYS:N    | 2.44                     | 0.44              |
| 1:I:77:VAL:HG22  | 1:I:107:ILE:HB   | 2.00                     | 0.44              |
| 1:L:207:ASP:OD1  | 1:L:208:TYR:N    | 2.50                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:66:ARG:HB2   | 1:E:107:ILE:HD13  | 2.00                     | 0.44              |
| 1:I:190:GLN:O    | 1:I:190:GLN:HG2   | 2.17                     | 0.44              |
| 1:N:147:LYS:O    | 1:N:148:THR:OG1   | 2.26                     | 0.44              |
| 1:O:80:THR:HG1   | 1:O:87[B]:CYS:HB3 | 1.83                     | 0.44              |
| 1:B:142:ARG:HE   | 1:B:158:ALA:HA    | 1.83                     | 0.44              |
| 1:F:98:THR:C     | 1:F:99:GLU:HG2    | 2.37                     | 0.44              |
| 1:I:125:VAL:HG12 | 1:I:139:LEU:HD22  | 1.97                     | 0.44              |
| 1:M:120:LYS:HD3  | 1:N:37:THR:CG2    | 2.47                     | 0.44              |
| 1:N:83:ASN:HB2   | 1:N:114:LYS:HB3   | 1.99                     | 0.44              |
| 1:N:6:ASN:OD1    | 1:N:9:GLN:N       | 2.43                     | 0.44              |
| 1:P:97:ILE:HD13  | 1:P:215:VAL:HG21  | 1.99                     | 0.44              |
| 1:T:21:LEU:HD21  | 1:X:21:LEU:CD1    | 2.47                     | 0.44              |
| 1:X:139:LEU:HD12 | 1:X:164:THR:OG1   | 2.17                     | 0.44              |
| 1:C:29:GLU:HB3   | 1:D:35:LEU:HD21   | 2.00                     | 0.44              |
| 1:F:66:ARG:HB3   | 1:F:66:ARG:CZ     | 2.48                     | 0.44              |
| 1:V:207:ASP:OD1  | 1:V:208:TYR:N     | 2.50                     | 0.44              |
| 1:E:222:VAL:HG22 | 1:E:222:VAL:O     | 2.18                     | 0.44              |
| 1:F:73:LYS:HG2   | 1:F:103:ASP:CG    | 2.37                     | 0.44              |
| 1:I:13:VAL:CG2   | 1:J:16:LEU:HD13   | 2.47                     | 0.44              |
| 1:I:83:ASN:HD21  | 1:I:150:LEU:HG    | 1.83                     | 0.44              |
| 1:K:217:GLU:HB3  | 1:K:218:GLN:OE1   | 2.18                     | 0.44              |
| 1:N:172:ASP:O    | 1:N:175:LYS:HB3   | 2.18                     | 0.44              |
| 1:P:146:LYS:NZ   | 1:P:147:LYS:O     | 2.51                     | 0.44              |
| 1:P:181:LEU:O    | 1:P:184:SER:OG    | 2.27                     | 0.44              |
| 1:W:139:LEU:HA   | 1:W:162:THR:HG21  | 1.99                     | 0.44              |
| 1:E:16:LEU:O     | 1:E:20:THR:HG23   | 2.18                     | 0.43              |
| 1:E:206:VAL:HG23 | 1:E:211:LEU:HB2   | 1.99                     | 0.43              |
| 1:F:141:GLN:OE1  | 1:J:221:LYS:HD3   | 2.18                     | 0.43              |
| 1:G:223:LYS:HE2  | 1:G:224:LYS:HD3   | 1.99                     | 0.43              |
| 1:J:87:CYS:HA    | 1:J:193:PRO:HG3   | 2.00                     | 0.43              |
| 1:K:73:LYS:HD3   | 1:K:103:ASP:HB3   | 1.99                     | 0.43              |
| 1:M:48:ARG:NH2   | 1:O:89:ARG:HD3    | 2.33                     | 0.43              |
| 1:N:218:GLN:HA   | 1:N:221:LYS:HG3   | 1.99                     | 0.43              |
| 1:N:49:GLN:HG3   | 1:N:52:ALA:HB3    | 2.00                     | 0.43              |
| 1:N:89:ARG:HD2   | 1:N:89:ARG:O      | 2.19                     | 0.43              |
| 1:R:14:ARG:CZ    | 1:R:14:ARG:HB3    | 2.47                     | 0.43              |
| 1:X:3:ALA:O      | 1:X:5:LEU:N       | 2.46                     | 0.43              |
| 1:X:81:ASP:OD1   | 1:X:118:SER:OG    | 2.29                     | 0.43              |
| 1:A:3:ALA:CA     | 1:A:4:ALA:HB3     | 2.47                     | 0.43              |
| 1:E:61:ASP:OD2   | 1:E:64:SER:OG     | 2.37                     | 0.43              |
| 1:M:19:ASP:O     | 1:M:23:SER:OG     | 2.33                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:97:ILE:HD12  | 1:O:211:LEU:HG   | 2.00                     | 0.43              |
| 1:U:79:PHE:N     | 1:U:194:ALA:O    | 2.43                     | 0.43              |
| 1:Y:187:LEU:HD23 | 1:Y:189:ILE:HD13 | 2.00                     | 0.43              |
| 1:I:147:LYS:O    | 1:I:148:THR:HG22 | 2.18                     | 0.43              |
| 1:O:94:LEU:HD23  | 1:O:211:LEU:HD21 | 2.00                     | 0.43              |
| 1:M:199:ASP:OD1  | 1:Q:160:LYS:NZ   | 2.51                     | 0.43              |
| 1:T:35:LEU:HD21  | 1:X:29:GLU:HB3   | 2.00                     | 0.43              |
| 1:V:151:ASP:O    | 1:V:155:ILE:HG12 | 2.18                     | 0.43              |
| 1:X:128:VAL:HG21 | 1:X:139:LEU:HD13 | 2.00                     | 0.43              |
| 1:E:89:ARG:O     | 1:E:89:ARG:HG3   | 2.17                     | 0.43              |
| 1:G:125:VAL:O    | 1:G:128:VAL:HG22 | 2.18                     | 0.43              |
| 1:G:13:VAL:CG2   | 1:G:14:ARG:N     | 2.82                     | 0.43              |
| 1:P:219:LEU:O    | 1:P:223:LYS:N    | 2.47                     | 0.43              |
| 1:O:5:LEU:HD11   | 1:P:9:GLN:HG2    | 2.00                     | 0.43              |
| 1:Q:146:LYS:HD2  | 1:Q:150:LEU:HD11 | 2.00                     | 0.43              |
| 1:B:87[A]:CYS:HA | 1:B:193:PRO:HG3  | 2.01                     | 0.43              |
| 1:C:164:THR:HA   | 1:C:167:ILE:CD1  | 2.49                     | 0.43              |
| 1:Q:6:ASN:OD1    | 1:Q:9:GLN:N      | 2.47                     | 0.43              |
| 1:R:25:PRO:HA    | 1:R:27:ILE:HG22  | 2.01                     | 0.43              |
| 1:B:27:ILE:HG23  | 1:F:18:ARG:HG3   | 2.00                     | 0.43              |
| 1:E:207:ASP:OD1  | 1:E:208:TYR:N    | 2.51                     | 0.43              |
| 1:E:89:ARG:NH1   | 1:E:93:LEU:CD1   | 2.81                     | 0.43              |
| 1:L:95:GLU:O     | 1:L:98:THR:OG1   | 2.29                     | 0.43              |
| 1:N:128:VAL:HA   | 1:N:167:ILE:HG21 | 2.01                     | 0.43              |
| 1:M:214:ILE:HG12 | 1:O:210:GLN:HB3  | 2.00                     | 0.43              |
| 1:U:188:GLY:O    | 1:Y:86:TYR:OH    | 2.23                     | 0.43              |
| 1:X:112:PRO:HD2  | 1:X:181:LEU:HD13 | 2.01                     | 0.43              |
| 1:Y:35:LEU:HD21  | 1:Y:39:LYS:HE3   | 1.99                     | 0.43              |
| 1:E:91:ASP:N     | 1:E:92:PRO:HD2   | 2.33                     | 0.43              |
| 1:H:3:ALA:HA     | 1:H:5:LEU:N      | 2.34                     | 0.43              |
| 1:N:101:TYR:HB2  | 1:N:104:VAL:CG1  | 2.48                     | 0.43              |
| 1:Q:38:LYS:HZ1   | 1:V:26:GLU:N     | 2.17                     | 0.43              |
| 1:T:29:GLU:HB3   | 1:Y:35:LEU:HD11  | 2.00                     | 0.43              |
| 1:X:141:GLN:HA   | 1:X:144:MSE:HB3  | 2.00                     | 0.43              |
| 1:X:218:GLN:C    | 1:X:220:ALA:N    | 2.72                     | 0.43              |
| 1:D:83:ASN:OD1   | 1:D:118:SER:OG   | 2.28                     | 0.43              |
| 1:G:185:ARG:NH1  | 2:G:304:HOH:O    | 2.50                     | 0.43              |
| 1:H:89:ARG:O     | 1:H:89:ARG:HG2   | 2.19                     | 0.43              |
| 1:P:222:VAL:HG13 | 1:P:223:LYS:N    | 2.34                     | 0.43              |
| 1:R:131:GLU:OE2  | 1:R:167:ILE:HD12 | 2.19                     | 0.43              |
| 1:G:113:PHE:HE1  | 1:G:181:LEU:HD21 | 1.84                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:97:ILE:HD13  | 1:N:208:TYR:OH   | 2.19                     | 0.43              |
| 1:P:151:ASP:H    | 1:P:154:SER:HB2  | 1.84                     | 0.43              |
| 1:R:170:THR:O    | 1:R:173:SER:OG   | 2.36                     | 0.43              |
| 1:T:97:ILE:HG23  | 1:T:208:TYR:HE1  | 1.84                     | 0.43              |
| 1:W:109:LYS:O    | 1:W:111:LEU:HD13 | 2.18                     | 0.43              |
| 1:X:88:LYS:HA    | 1:X:144:MSE:HE1  | 2.00                     | 0.43              |
| 1:C:148:THR:HG22 | 1:C:149:MSE:H    | 1.84                     | 0.42              |
| 1:G:132:ASP:OD1  | 1:G:134:LYS:HE2  | 2.19                     | 0.42              |
| 1:G:80:THR:CG2   | 1:G:144:MSE:SE   | 3.17                     | 0.42              |
| 1:K:97:ILE:HA    | 1:K:100:GLN:HB2  | 2.01                     | 0.42              |
| 1:N:208:TYR:O    | 1:N:212:GLU:N    | 2.42                     | 0.42              |
| 1:P:202:LEU:HD21 | 1:P:206:VAL:HG21 | 2.01                     | 0.42              |
| 1:P:26:GLU:O     | 1:W:178:GLN:NE2  | 2.34                     | 0.42              |
| 1:P:28:LEU:O     | 1:P:32:ILE:HG13  | 2.18                     | 0.42              |
| 1:V:83:ASN:OD1   | 1:V:150:LEU:N    | 2.47                     | 0.42              |
| 1:B:77:VAL:HB    | 1:B:196:VAL:HB   | 2.01                     | 0.42              |
| 1:G:35:LEU:O     | 1:G:39:LYS:N     | 2.44                     | 0.42              |
| 1:J:65:PRO:HA    | 1:J:129:TRP:CE2  | 2.54                     | 0.42              |
| 1:J:202:LEU:CD2  | 1:J:206:VAL:HG11 | 2.49                     | 0.42              |
| 1:J:74:LEU:CD2   | 1:J:215:VAL:HG13 | 2.49                     | 0.42              |
| 1:W:49:GLN:O     | 1:W:53:SER:N     | 2.52                     | 0.42              |
| 1:E:89:ARG:NH1   | 1:E:92:PRO:HG2   | 2.34                     | 0.42              |
| 1:G:193:PRO:O    | 1:G:204:GLY:N    | 2.53                     | 0.42              |
| 1:L:111:LEU:HD23 | 1:L:113:PHE:CZ   | 2.55                     | 0.42              |
| 1:L:74:LEU:CD2   | 1:L:218:GLN:HB3  | 2.49                     | 0.42              |
| 1:O:171:ASP:HB2  | 1:P:22:VAL:HG12  | 2.00                     | 0.42              |
| 1:R:25:PRO:C     | 1:R:27:ILE:N     | 2.73                     | 0.42              |
| 1:B:87[B]:CYS:HA | 1:B:193:PRO:HG3  | 2.01                     | 0.42              |
| 1:D:175:LYS:O    | 1:D:179:ASN:ND2  | 2.43                     | 0.42              |
| 1:D:77:VAL:HB    | 1:D:196:VAL:HB   | 2.02                     | 0.42              |
| 1:E:58:LEU:HD21  | 1:E:79:PHE:HZ    | 1.84                     | 0.42              |
| 1:H:97:ILE:HG23  | 1:H:101:TYR:CD2  | 2.55                     | 0.42              |
| 1:I:90:PHE:CE2   | 1:I:94:LEU:HD11  | 2.54                     | 0.42              |
| 1:M:97:ILE:HD13  | 1:M:211:LEU:HD21 | 2.01                     | 0.42              |
| 1:M:47:PHE:CE1   | 1:M:188:GLY:HA3  | 2.54                     | 0.42              |
| 1:O:66:ARG:HG2   | 1:O:107:ILE:HG12 | 2.02                     | 0.42              |
| 1:R:210:GLN:HA   | 1:W:217:GLU:OE1  | 2.19                     | 0.42              |
| 1:X:112:PRO:HB3  | 1:X:119:ALA:HB2  | 2.01                     | 0.42              |
| 1:Y:74:LEU:HD11  | 1:Y:218:GLN:HB3  | 2.01                     | 0.42              |
| 1:C:148:THR:HG22 | 1:C:149:MSE:N    | 2.34                     | 0.42              |
| 1:G:47:PHE:CD1   | 1:G:201:ILE:HD11 | 2.55                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:35:LEU:HD23  | 1:H:39:LYS:HE2   | 2.01                     | 0.42              |
| 1:I:137:LEU:O    | 1:I:141:GLN:HG3  | 2.19                     | 0.42              |
| 1:N:132:ASP:O    | 1:N:135:ALA:HB3  | 2.20                     | 0.42              |
| 1:G:222:VAL:HG13 | 1:G:223:LYS:N    | 2.35                     | 0.42              |
| 1:G:80:THR:HG22  | 1:G:81:ASP:N     | 2.34                     | 0.42              |
| 1:H:6:ASN:OD1    | 1:H:9:GLN:N      | 2.43                     | 0.42              |
| 1:H:77:VAL:HB    | 1:H:196:VAL:HB   | 2.00                     | 0.42              |
| 1:I:145:GLN:O    | 1:I:145:GLN:HG2  | 2.19                     | 0.42              |
| 1:M:98:THR:C     | 1:M:99:GLU:HG3   | 2.39                     | 0.42              |
| 1:N:160:LYS:HB2  | 1:N:165:SER:OG   | 2.18                     | 0.42              |
| 1:O:58:LEU:CD2   | 1:O:183:LEU:HD21 | 2.49                     | 0.42              |
| 1:P:159:MSE:O    | 1:P:164:THR:N    | 2.49                     | 0.42              |
| 1:P:26:GLU:HB3   | 1:W:38:LYS:NZ    | 2.35                     | 0.42              |
| 1:R:120:LYS:O    | 1:R:124:ALA:N    | 2.49                     | 0.42              |
| 1:T:96:LYS:HE3   | 1:T:208:TYR:CZ   | 2.55                     | 0.42              |
| 1:G:140:HIS:CE1  | 1:G:144:MSE:HE1  | 2.55                     | 0.42              |
| 1:L:194:ALA:HA   | 1:L:203:PRO:HA   | 2.01                     | 0.42              |
| 1:M:164:THR:HB   | 1:M:167:ILE:HD12 | 2.01                     | 0.42              |
| 1:X:142:ARG:HH22 | 1:X:161:SER:HB3  | 1.84                     | 0.42              |
| 1:A:52:ALA:HB2   | 1:E:160:LYS:HB3  | 2.01                     | 0.42              |
| 1:L:189:ILE:C    | 1:L:191:GLY:HA2  | 2.40                     | 0.42              |
| 1:Q:160:LYS:C    | 1:Q:162:THR:H    | 2.22                     | 0.42              |
| 1:V:185:ARG:C    | 1:V:188:GLY:H    | 2.23                     | 0.42              |
| 1:V:101:TYR:OH   | 1:V:212:GLU:OE2  | 2.38                     | 0.42              |
| 1:X:77:VAL:HA    | 1:X:107:ILE:O    | 2.19                     | 0.42              |
| 1:X:91:ASP:N     | 1:X:92:PRO:CD    | 2.83                     | 0.42              |
| 1:G:124:ALA:HA   | 1:G:169:LEU:HG   | 2.02                     | 0.42              |
| 1:G:146:LYS:HD2  | 1:G:150:LEU:HD21 | 2.01                     | 0.42              |
| 1:G:159:MSE:HE1  | 1:G:169:LEU:CD1  | 2.50                     | 0.42              |
| 1:I:101:TYR:O    | 1:I:104:VAL:HG12 | 2.20                     | 0.42              |
| 1:M:47:PHE:CE2   | 1:O:86:TYR:CZ    | 3.07                     | 0.42              |
| 1:O:216:LYS:HA   | 1:O:219:LEU:HG   | 2.02                     | 0.42              |
| 1:P:95:GLU:OE1   | 1:P:141:GLN:NE2  | 2.53                     | 0.42              |
| 1:Y:45:ALA:O     | 1:Y:47:PHE:N     | 2.53                     | 0.42              |
| 1:C:77:VAL:HB    | 1:C:196:VAL:HB   | 2.02                     | 0.42              |
| 1:C:148:THR:OG1  | 1:F:151:ASP:OD2  | 2.37                     | 0.42              |
| 1:G:146:LYS:HZ3  | 1:G:158:ALA:HB2  | 1.83                     | 0.42              |
| 1:I:111:LEU:HD22 | 1:I:181:LEU:HD12 | 2.01                     | 0.42              |
| 1:J:144:MSE:HE3  | 1:J:150:LEU:HD12 | 2.02                     | 0.42              |
| 1:U:96:LYS:HD2   | 1:U:208:TYR:CZ   | 2.55                     | 0.42              |
| 1:W:76:LEU:HD11  | 1:W:106:VAL:HG13 | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:142:ARG:O    | 1:G:146:LYS:N    | 2.53                     | 0.41              |
| 1:J:174:LEU:HA   | 1:J:177:LEU:HB3  | 2.02                     | 0.41              |
| 1:L:221:LYS:HG2  | 1:L:221:LYS:O    | 2.20                     | 0.41              |
| 1:H:174:LEU:HD11 | 1:L:33:MSE:HG2   | 2.02                     | 0.41              |
| 1:W:208:TYR:O    | 1:W:212:GLU:N    | 2.53                     | 0.41              |
| 1:X:170:THR:O    | 1:X:173:SER:OG   | 2.37                     | 0.41              |
| 1:E:32:ILE:HA    | 1:J:28:LEU:CD2   | 2.49                     | 0.41              |
| 1:E:49:GLN:CG    | 1:E:52:ALA:HB3   | 2.51                     | 0.41              |
| 1:G:172:ASP:O    | 1:G:175:LYS:HG2  | 2.20                     | 0.41              |
| 1:I:139:LEU:HB2  | 1:I:162:THR:HG21 | 2.02                     | 0.41              |
| 1:M:208:TYR:O    | 1:M:212:GLU:HG2  | 2.20                     | 0.41              |
| 1:N:29:GLU:HG2   | 1:N:33:MSE:HE3   | 2.02                     | 0.41              |
| 1:P:55:HIS:O     | 1:P:59:TYR:N     | 2.42                     | 0.41              |
| 1:Q:150:LEU:HG   | 1:Q:154:SER:HB2  | 2.01                     | 0.41              |
| 1:N:32:ILE:CD1   | 1:R:28:LEU:HD21  | 2.50                     | 0.41              |
| 1:V:76:LEU:HD21  | 1:V:195:THR:HG23 | 2.02                     | 0.41              |
| 1:Y:202:LEU:HD21 | 1:Y:206:VAL:HG21 | 2.02                     | 0.41              |
| 1:B:51:LEU:HD12  | 1:B:187:LEU:HD22 | 2.01                     | 0.41              |
| 1:B:85:PRO:HG2   | 1:D:47:PHE:CE2   | 2.55                     | 0.41              |
| 1:D:6:ASN:OD1    | 1:D:9:GLN:N      | 2.47                     | 0.41              |
| 1:G:121:ALA:HB2  | 1:G:155:ILE:CD1  | 2.50                     | 0.41              |
| 1:G:12:GLU:HB3   | 1:H:5:LEU:HD12   | 2.03                     | 0.41              |
| 1:I:79:PHE:HB3   | 1:I:111:LEU:HD11 | 2.02                     | 0.41              |
| 1:J:139:LEU:HD13 | 1:J:159:MSE:HA   | 2.02                     | 0.41              |
| 1:O:89:ARG:O     | 1:O:89:ARG:HG2   | 2.20                     | 0.41              |
| 1:Q:56:ASP:OD1   | 1:Q:57:ALA:N     | 2.53                     | 0.41              |
| 1:U:206:VAL:HG22 | 1:U:210:GLN:HB2  | 2.02                     | 0.41              |
| 1:V:121:ALA:HB1  | 1:V:143:LEU:HD13 | 2.02                     | 0.41              |
| 1:V:89:ARG:O     | 1:V:89:ARG:HG2   | 2.21                     | 0.41              |
| 1:W:48:ARG:HD2   | 1:W:199:ASP:O    | 2.19                     | 0.41              |
| 1:Y:202:LEU:CD1  | 1:Y:214:ILE:HD13 | 2.50                     | 0.41              |
| 1:Y:48:ARG:HD3   | 1:Y:186:LYS:HB3  | 2.02                     | 0.41              |
| 1:I:81:ASP:OD1   | 1:I:118:SER:OG   | 2.30                     | 0.41              |
| 1:M:96:LYS:HD2   | 1:M:96:LYS:C     | 2.41                     | 0.41              |
| 1:Q:74:LEU:CD2   | 1:Q:104:VAL:HG23 | 2.50                     | 0.41              |
| 1:R:208:TYR:CE2  | 1:R:212:GLU:HB2  | 2.54                     | 0.41              |
| 1:Y:202:LEU:HD12 | 1:Y:214:ILE:HD13 | 2.02                     | 0.41              |
| 1:E:112:PRO:HG3  | 1:J:33:MSE:HE1   | 2.02                     | 0.41              |
| 1:F:192:THR:HG23 | 1:F:193:PRO:HA   | 2.03                     | 0.41              |
| 1:F:90:PHE:CE2   | 1:F:94:LEU:HD21  | 2.55                     | 0.41              |
| 1:G:156:GLU:HG3  | 1:G:159:MSE:HG2  | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:124:ALA:CA   | 1:H:169:LEU:CD2  | 2.99                     | 0.41              |
| 1:K:178:GLN:HE21 | 1:K:182:GLU:CG   | 2.34                     | 0.41              |
| 1:M:96:LYS:HE3   | 1:M:208:TYR:HE1  | 1.81                     | 0.41              |
| 1:O:124:ALA:CA   | 1:O:169:LEU:HD21 | 2.40                     | 0.41              |
| 1:P:10:GLU:HA    | 1:P:13:VAL:HG22  | 2.03                     | 0.41              |
| 1:U:97:ILE:HG13  | 1:U:208:TYR:HE1  | 1.85                     | 0.41              |
| 1:A:155:ILE:O    | 1:A:159:MSE:HG3  | 2.21                     | 0.41              |
| 1:K:80:THR:O     | 1:K:111:LEU:N    | 2.53                     | 0.41              |
| 1:P:120:LYS:HD3  | 1:P:152:ASN:OD1  | 2.20                     | 0.41              |
| 1:P:101:TYR:OH   | 1:P:212:GLU:OE2  | 2.35                     | 0.41              |
| 1:V:61:ASP:C     | 1:V:63:ALA:H     | 2.23                     | 0.41              |
| 1:W:212:GLU:O    | 1:W:216:LYS:NZ   | 2.41                     | 0.41              |
| 1:X:76:LEU:N     | 1:X:76:LEU:CD1   | 2.84                     | 0.41              |
| 1:X:97:ILE:HB    | 1:X:101:TYR:CE1  | 2.56                     | 0.41              |
| 1:A:29:GLU:HA    | 1:A:32:ILE:HD12  | 2.02                     | 0.41              |
| 1:E:40:ALA:O     | 1:E:44:GLN:HG2   | 2.20                     | 0.41              |
| 1:E:58:LEU:HD23  | 1:E:109:LYS:HE3  | 2.03                     | 0.41              |
| 1:I:65:PRO:HA    | 1:I:129:TRP:CE2  | 2.55                     | 0.41              |
| 1:N:221:LYS:NZ   | 2:N:303:HOH:O    | 2.50                     | 0.41              |
| 1:W:97:ILE:HD11  | 1:W:211:LEU:HG   | 2.02                     | 0.41              |
| 1:X:124:ALA:HB1  | 1:X:159:MSE:HE1  | 2.02                     | 0.41              |
| 1:B:17:VAL:HA    | 1:F:17:VAL:HG21  | 2.02                     | 0.41              |
| 1:I:83:ASN:OD1   | 1:I:117:SER:OG   | 2.15                     | 0.41              |
| 1:J:77:VAL:H     | 1:J:196:VAL:HG22 | 1.85                     | 0.41              |
| 1:P:90:PHE:HZ    | 1:P:195:THR:HG1  | 1.68                     | 0.41              |
| 1:R:146:LYS:CE   | 1:R:154:SER:HB3  | 2.51                     | 0.41              |
| 1:M:13:VAL:HG21  | 1:R:16:LEU:HD13  | 2.03                     | 0.41              |
| 1:V:147:LYS:O    | 1:V:148:THR:OG1  | 2.20                     | 0.41              |
| 1:E:28:LEU:O     | 1:E:32:ILE:HG13  | 2.20                     | 0.41              |
| 1:E:38:LYS:HE3   | 1:J:23:SER:O     | 2.21                     | 0.41              |
| 1:L:190:GLN:N    | 1:L:191:GLY:HA2  | 2.36                     | 0.41              |
| 1:O:190:GLN:O    | 1:O:190:GLN:HG2  | 2.20                     | 0.41              |
| 1:P:206:VAL:HG12 | 1:P:210:GLN:HB2  | 2.02                     | 0.41              |
| 1:R:159:MSE:HE2  | 1:R:164:THR:O    | 2.21                     | 0.41              |
| 1:W:51:LEU:HD11  | 1:W:201:ILE:HD11 | 2.03                     | 0.41              |
| 1:W:91:ASP:N     | 1:W:92:PRO:CD    | 2.84                     | 0.41              |
| 1:X:211:LEU:HD12 | 1:X:211:LEU:H    | 1.86                     | 0.41              |
| 1:K:73:LYS:HD2   | 1:K:73:LYS:N     | 2.36                     | 0.41              |
| 1:N:32:ILE:HD13  | 1:R:28:LEU:CD2   | 2.50                     | 0.41              |
| 1:N:42:GLU:OE1   | 1:N:185:ARG:NE   | 2.48                     | 0.41              |
| 1:O:17:VAL:HG11  | 1:P:20:THR:HG21  | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:88:LYS:HE2   | 1:P:88:LYS:HB3   | 1.93                     | 0.41              |
| 1:Q:96:LYS:NZ    | 1:Q:100:GLN:N    | 2.69                     | 0.41              |
| 1:Q:125:VAL:HG13 | 1:Q:136:PHE:HE1  | 1.86                     | 0.41              |
| 1:N:35:LEU:HD22  | 1:R:28:LEU:HD23  | 2.03                     | 0.41              |
| 1:T:86:TYR:OH    | 1:V:188:GLY:O    | 2.38                     | 0.41              |
| 1:W:125:VAL:HG13 | 1:W:136:PHE:CD1  | 2.55                     | 0.41              |
| 1:X:77:VAL:HG22  | 1:X:196:VAL:HB   | 2.02                     | 0.41              |
| 1:H:217:GLU:O    | 1:H:221:LYS:HG3  | 2.21                     | 0.41              |
| 1:L:91:ASP:N     | 1:L:92:PRO:HD2   | 2.35                     | 0.41              |
| 1:O:6:ASN:ND2    | 2:O:307:HOH:O    | 2.52                     | 0.41              |
| 1:Q:219:LEU:O    | 1:Q:223:LYS:N    | 2.53                     | 0.41              |
| 1:Q:3:ALA:O      | 1:Q:5:LEU:N      | 2.48                     | 0.41              |
| 1:R:150:LEU:HD23 | 1:R:155:ILE:HG12 | 2.03                     | 0.41              |
| 1:U:137:LEU:HG   | 1:U:141:GLN:HE21 | 1.86                     | 0.41              |
| 1:A:97:ILE:HG23  | 1:A:101:TYR:HD2  | 1.85                     | 0.40              |
| 1:K:121:ALA:HB1  | 1:K:143:LEU:HD13 | 2.03                     | 0.40              |
| 1:K:3:ALA:HA     | 1:K:4:ALA:HA     | 1.86                     | 0.40              |
| 1:L:150:LEU:HD23 | 1:L:155:ILE:HG12 | 2.04                     | 0.40              |
| 1:P:47:PHE:HD2   | 1:P:47:PHE:H     | 1.69                     | 0.40              |
| 1:V:189:ILE:HD13 | 1:V:194:ALA:CB   | 2.50                     | 0.40              |
| 1:V:90:PHE:CZ    | 1:V:211:LEU:HD21 | 2.55                     | 0.40              |
| 1:W:151:ASP:OD1  | 1:W:152:ASN:N    | 2.55                     | 0.40              |
| 1:X:74:LEU:HD22  | 1:X:222:VAL:CG1  | 2.51                     | 0.40              |
| 1:X:39:LYS:O     | 1:X:43:GLN:HG3   | 2.21                     | 0.40              |
| 1:F:66:ARG:NH1   | 1:F:70:LYS:HE2   | 2.37                     | 0.40              |
| 1:J:135:ALA:HB1  | 1:J:164:THR:CG2  | 2.52                     | 0.40              |
| 1:N:101:TYR:CB   | 1:N:104:VAL:HG12 | 2.52                     | 0.40              |
| 1:O:35:LEU:HD21  | 1:W:29:GLU:HB2   | 2.02                     | 0.40              |
| 1:R:91:ASP:N     | 1:R:92:PRO:CD    | 2.83                     | 0.40              |
| 1:T:151:ASP:H    | 1:T:154:SER:HB2  | 1.85                     | 0.40              |
| 1:T:213:ILE:HD13 | 1:V:213:ILE:HG12 | 2.02                     | 0.40              |
| 1:X:119:ALA:O    | 1:X:123:GLN:N    | 2.45                     | 0.40              |
| 1:X:33:MSE:HA    | 1:X:36:GLN:HG2   | 2.02                     | 0.40              |
| 1:Y:206:VAL:HG12 | 1:Y:210:GLN:HB2  | 2.02                     | 0.40              |
| 1:M:98:THR:O     | 1:M:104:VAL:O    | 2.39                     | 0.40              |
| 1:N:145:GLN:OE1  | 1:N:147:LYS:NZ   | 2.49                     | 0.40              |
| 1:P:156:GLU:HA   | 1:P:159:MSE:HB2  | 2.03                     | 0.40              |
| 1:R:86:TYR:OH    | 1:W:47:PHE:HB3   | 2.22                     | 0.40              |
| 1:V:77:VAL:HG13  | 1:V:109:LYS:HD3  | 2.04                     | 0.40              |
| 1:T:204:GLY:HA3  | 1:V:203:PRO:HD2  | 2.02                     | 0.40              |
| 1:W:163:ASN:ND2  | 1:W:163:ASN:O    | 2.49                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:91:ASP:N     | 1:W:92:PRO:HD2   | 2.37                     | 0.40              |
| 1:A:47:PHE:CZ    | 1:A:201:ILE:HG12 | 2.57                     | 0.40              |
| 1:H:125:VAL:HG13 | 1:H:136:PHE:HE1  | 1.86                     | 0.40              |
| 1:L:87:CYS:SG    | 1:L:193:PRO:HB3  | 2.62                     | 0.40              |
| 1:N:97:ILE:HG22  | 1:N:104:VAL:CG1  | 2.50                     | 0.40              |
| 1:O:160:LYS:CE   | 1:O:165:SER:HB3  | 2.51                     | 0.40              |
| 1:P:61:ASP:CG    | 1:P:64:SER:HG    | 2.18                     | 0.40              |
| 1:Q:98:THR:HA    | 1:Q:104:VAL:CG1  | 2.52                     | 0.40              |
| 1:B:6:ASN:OD1    | 1:B:9:GLN:N      | 2.48                     | 0.40              |
| 1:E:66:ARG:NH1   | 1:E:68:GLY:O     | 2.55                     | 0.40              |
| 1:F:153:ALA:O    | 1:F:156:GLU:HG2  | 2.21                     | 0.40              |
| 1:G:142:ARG:NH2  | 1:G:161:SER:CB   | 2.85                     | 0.40              |
| 1:H:123:GLN:HG2  | 1:H:169:LEU:HD22 | 2.04                     | 0.40              |
| 1:I:83:ASN:ND2   | 1:I:148:THR:O    | 2.54                     | 0.40              |
| 1:N:147:LYS:O    | 1:N:148:THR:HG23 | 2.21                     | 0.40              |
| 1:Q:77:VAL:CG2   | 1:Q:196:VAL:HB   | 2.52                     | 0.40              |
| 1:X:164:THR:O    | 1:X:167:ILE:HG12 | 2.22                     | 0.40              |
| 1:X:87:CYS:HA    | 1:X:90:PHE:HB3   | 2.04                     | 0.40              |

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:C:161:SER:OG  | 1:H:99:GLU:OE2[1_655]  | 1.95                     | 0.25              |
| 1:H:86:TYR:OH   | 1:J:187:LEU:O[1_455]   | 2.12                     | 0.08              |
| 1:G:134:LYS:NZ  | 1:M:134:LYS:O[2_456]   | 2.13                     | 0.07              |
| 1:G:148:THR:OG1 | 1:J:148:THR:OG1[1_455] | 2.17                     | 0.03              |
| 1:C:7:ALA:H     | 1:U:3:ALA:O[1_554]     | 1.59                     | 0.01              |

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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   | A     | 223/224 (100%)  | 212 (95%)  | 8 (4%)   | 3 (1%)   | 15          | 30  |
| 1   | B     | 223/224 (100%)  | 216 (97%)  | 6 (3%)   | 1 (0%)   | 39          | 65  |
| 1   | C     | 223/224 (100%)  | 214 (96%)  | 8 (4%)   | 1 (0%)   | 39          | 65  |
| 1   | D     | 223/224 (100%)  | 216 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 1   | E     | 216/224 (96%)   | 203 (94%)  | 12 (6%)  | 1 (0%)   | 34          | 60  |
| 1   | F     | 223/224 (100%)  | 214 (96%)  | 7 (3%)   | 2 (1%)   | 21          | 42  |
| 1   | G     | 220/224 (98%)   | 208 (94%)  | 10 (4%)  | 2 (1%)   | 21          | 42  |
| 1   | H     | 223/224 (100%)  | 212 (95%)  | 9 (4%)   | 2 (1%)   | 21          | 42  |
| 1   | I     | 196/224 (88%)   | 188 (96%)  | 6 (3%)   | 2 (1%)   | 19          | 39  |
| 1   | J     | 217/224 (97%)   | 210 (97%)  | 5 (2%)   | 2 (1%)   | 21          | 42  |
| 1   | K     | 223/224 (100%)  | 215 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 1   | L     | 172/224 (77%)   | 162 (94%)  | 6 (4%)   | 4 (2%)   | 8           | 14  |
| 1   | M     | 221/224 (99%)   | 210 (95%)  | 10 (4%)  | 1 (0%)   | 34          | 60  |
| 1   | N     | 218/224 (97%)   | 210 (96%)  | 7 (3%)   | 1 (0%)   | 34          | 60  |
| 1   | O     | 221/224 (99%)   | 213 (96%)  | 7 (3%)   | 1 (0%)   | 34          | 60  |
| 1   | P     | 220/224 (98%)   | 210 (96%)  | 8 (4%)   | 2 (1%)   | 21          | 42  |
| 1   | Q     | 222/224 (99%)   | 198 (89%)  | 20 (9%)  | 4 (2%)   | 11          | 21  |
| 1   | R     | 219/224 (98%)   | 208 (95%)  | 7 (3%)   | 4 (2%)   | 11          | 21  |
| 1   | T     | 222/224 (99%)   | 216 (97%)  | 5 (2%)   | 1 (0%)   | 34          | 60  |
| 1   | U     | 223/224 (100%)  | 214 (96%)  | 8 (4%)   | 1 (0%)   | 39          | 65  |
| 1   | V     | 222/224 (99%)   | 211 (95%)  | 9 (4%)   | 2 (1%)   | 21          | 42  |
| 1   | W     | 222/224 (99%)   | 211 (95%)  | 10 (4%)  | 1 (0%)   | 34          | 60  |
| 1   | X     | 220/224 (98%)   | 196 (89%)  | 20 (9%)  | 4 (2%)   | 11          | 21  |
| 1   | Y     | 223/224 (100%)  | 206 (92%)  | 10 (4%)  | 7 (3%)   | 5           | 8   |
| All | All   | 5235/5376 (97%) | 4973 (95%) | 213 (4%) | 49 (1%)  | 21          | 42  |

All (49) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 223 | LYS  |
| 1   | F     | 148 | THR  |
| 1   | I     | 148 | THR  |
| 1   | L     | 145 | GLN  |
| 1   | N     | 148 | THR  |
| 1   | O     | 148 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | P     | 148 | THR  |
| 1   | Q     | 97  | ILE  |
| 1   | Q     | 218 | GLN  |
| 1   | T     | 148 | THR  |
| 1   | V     | 148 | THR  |
| 1   | Y     | 46  | GLN  |
| 1   | Y     | 223 | LYS  |
| 1   | A     | 148 | THR  |
| 1   | B     | 148 | THR  |
| 1   | E     | 148 | THR  |
| 1   | H     | 48  | ARG  |
| 1   | J     | 148 | THR  |
| 1   | L     | 148 | THR  |
| 1   | L     | 191 | GLY  |
| 1   | P     | 223 | LYS  |
| 1   | U     | 148 | THR  |
| 1   | X     | 148 | THR  |
| 1   | X     | 155 | ILE  |
| 1   | Y     | 47  | PHE  |
| 1   | Y     | 145 | GLN  |
| 1   | A     | 223 | LYS  |
| 1   | F     | 223 | LYS  |
| 1   | G     | 11  | LYS  |
| 1   | Q     | 159 | MSE  |
| 1   | W     | 148 | THR  |
| 1   | X     | 149 | MSE  |
| 1   | M     | 102 | PRO  |
| 1   | R     | 148 | THR  |
| 1   | R     | 223 | LYS  |
| 1   | X     | 223 | LYS  |
| 1   | Y     | 48  | ARG  |
| 1   | G     | 223 | LYS  |
| 1   | R     | 23  | SER  |
| 1   | R     | 26  | GLU  |
| 1   | Y     | 72  | ALA  |
| 1   | Y     | 144 | MSE  |
| 1   | H     | 4   | ALA  |
| 1   | L     | 144 | MSE  |
| 1   | Q     | 85  | PRO  |
| 1   | I     | 206 | VAL  |
| 1   | V     | 112 | PRO  |
| 1   | A     | 112 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 112 | 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 X-ray entries followed by that with respect to entries of similar resolution.

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   | A     | 192/187 (103%) | 191 (100%) | 1 (0%)   | 92          | 98  |
| 1   | B     | 192/187 (103%) | 191 (100%) | 1 (0%)   | 92          | 98  |
| 1   | C     | 192/187 (103%) | 188 (98%)  | 4 (2%)   | 61          | 85  |
| 1   | D     | 192/187 (103%) | 191 (100%) | 1 (0%)   | 92          | 98  |
| 1   | E     | 189/187 (101%) | 186 (98%)  | 3 (2%)   | 70          | 89  |
| 1   | F     | 192/187 (103%) | 190 (99%)  | 2 (1%)   | 82          | 94  |
| 1   | G     | 191/187 (102%) | 190 (100%) | 1 (0%)   | 92          | 98  |
| 1   | H     | 192/187 (103%) | 189 (98%)  | 3 (2%)   | 70          | 89  |
| 1   | I     | 170/187 (91%)  | 168 (99%)  | 2 (1%)   | 78          | 92  |
| 1   | J     | 187/187 (100%) | 182 (97%)  | 5 (3%)   | 52          | 79  |
| 1   | K     | 192/187 (103%) | 189 (98%)  | 3 (2%)   | 70          | 89  |
| 1   | L     | 156/187 (83%)  | 153 (98%)  | 3 (2%)   | 65          | 86  |
| 1   | M     | 190/187 (102%) | 184 (97%)  | 6 (3%)   | 46          | 74  |
| 1   | N     | 188/187 (100%) | 185 (98%)  | 3 (2%)   | 70          | 89  |
| 1   | O     | 190/187 (102%) | 189 (100%) | 1 (0%)   | 92          | 98  |
| 1   | P     | 189/187 (101%) | 187 (99%)  | 2 (1%)   | 80          | 93  |
| 1   | Q     | 191/187 (102%) | 188 (98%)  | 3 (2%)   | 70          | 89  |
| 1   | R     | 190/187 (102%) | 187 (98%)  | 3 (2%)   | 70          | 89  |
| 1   | T     | 191/187 (102%) | 191 (100%) | 0        | 100         | 100 |
| 1   | U     | 192/187 (103%) | 191 (100%) | 1 (0%)   | 92          | 98  |
| 1   | V     | 191/187 (102%) | 189 (99%)  | 2 (1%)   | 82          | 94  |
| 1   | W     | 191/187 (102%) | 184 (96%)  | 7 (4%)   | 41          | 69  |
| 1   | X     | 189/187 (101%) | 185 (98%)  | 4 (2%)   | 61          | 85  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|-------------|----|
| 1   | Y     | 192/187 (103%)   | 189 (98%)  | 3 (2%)   | 70          | 89 |
| All | All   | 4521/4488 (101%) | 4457 (99%) | 64 (1%)  | 74          | 90 |

All (64) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 99     | GLU  |
| 1   | B     | 71     | ASP  |
| 1   | C     | 89     | ARG  |
| 1   | C     | 160    | LYS  |
| 1   | C     | 190    | GLN  |
| 1   | C     | 222    | VAL  |
| 1   | D     | 190    | GLN  |
| 1   | E     | 26     | GLU  |
| 1   | E     | 33     | MSE  |
| 1   | E     | 178    | GLN  |
| 1   | F     | 99     | GLU  |
| 1   | F     | 160    | LYS  |
| 1   | G     | 12     | GLU  |
| 1   | H     | 55     | HIS  |
| 1   | H     | 73     | LYS  |
| 1   | H     | 200    | THR  |
| 1   | I     | 12     | GLU  |
| 1   | I     | 202    | LEU  |
| 1   | J     | 39     | LYS  |
| 1   | J     | 48     | ARG  |
| 1   | J     | 49     | GLN  |
| 1   | J     | 148    | THR  |
| 1   | J     | 222    | VAL  |
| 1   | K     | 144[A] | MSE  |
| 1   | K     | 144[B] | MSE  |
| 1   | K     | 209    | ASP  |
| 1   | L     | 120    | LYS  |
| 1   | L     | 123    | GLN  |
| 1   | L     | 152    | ASN  |
| 1   | M     | 51     | LEU  |
| 1   | M     | 73     | LYS  |
| 1   | M     | 96     | LYS  |
| 1   | M     | 134    | LYS  |
| 1   | M     | 185    | ARG  |
| 1   | M     | 218    | GLN  |
| 1   | N     | 43     | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | N     | 77  | VAL  |
| 1   | N     | 190 | GLN  |
| 1   | O     | 46  | GLN  |
| 1   | P     | 54  | GLU  |
| 1   | P     | 160 | LYS  |
| 1   | Q     | 130 | LYS  |
| 1   | Q     | 159 | MSE  |
| 1   | Q     | 160 | LYS  |
| 1   | R     | 14  | ARG  |
| 1   | R     | 73  | LYS  |
| 1   | R     | 142 | ARG  |
| 1   | U     | 141 | GLN  |
| 1   | V     | 55  | HIS  |
| 1   | V     | 192 | THR  |
| 1   | W     | 99  | GLU  |
| 1   | W     | 125 | VAL  |
| 1   | W     | 136 | PHE  |
| 1   | W     | 137 | LEU  |
| 1   | W     | 147 | LYS  |
| 1   | W     | 163 | ASN  |
| 1   | W     | 206 | VAL  |
| 1   | X     | 76  | LEU  |
| 1   | X     | 97  | ILE  |
| 1   | X     | 146 | LYS  |
| 1   | X     | 200 | THR  |
| 1   | Y     | 49  | GLN  |
| 1   | Y     | 192 | THR  |
| 1   | Y     | 218 | GLN  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 83  | ASN  |
| 1   | G     | 43  | GLN  |
| 1   | G     | 190 | GLN  |
| 1   | R     | 210 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|---------------|-----------------------|-------|
| 1   | A     | 218/224 (97%) | 0.73   | 14 (6%) 23 17 | 19, 39, 60, 83        | 0     |
| 1   | B     | 216/224 (96%) | 0.85   | 18 (8%) 14 9  | 24, 42, 62, 90        | 0     |
| 1   | C     | 218/224 (97%) | 0.86   | 19 (8%) 13 8  | 29, 47, 64, 82        | 0     |
| 1   | D     | 218/224 (97%) | 0.88   | 16 (7%) 18 12 | 26, 44, 62, 68        | 0     |
| 1   | E     | 211/224 (94%) | 1.80   | 74 (35%) 0 0  | 38, 66, 86, 99        | 0     |
| 1   | F     | 218/224 (97%) | 0.88   | 25 (11%) 6 4  | 26, 45, 70, 90        | 0     |
| 1   | G     | 215/224 (95%) | 2.02   | 80 (37%) 0 0  | 43, 67, 87, 104       | 0     |
| 1   | H     | 218/224 (97%) | 1.80   | 66 (30%) 1 0  | 40, 61, 90, 103       | 0     |
| 1   | I     | 194/224 (86%) | 1.94   | 67 (34%) 0 0  | 39, 66, 85, 100       | 0     |
| 1   | J     | 215/224 (95%) | 2.08   | 88 (40%) 0 0  | 45, 66, 93, 112       | 0     |
| 1   | K     | 216/224 (96%) | 0.85   | 18 (8%) 14 9  | 25, 42, 68, 81        | 0     |
| 1   | L     | 172/224 (76%) | 1.75   | 55 (31%) 1 0  | 41, 62, 78, 88        | 0     |
| 1   | M     | 216/224 (96%) | 2.49   | 102 (47%) 0 0 | 45, 69, 91, 124       | 0     |
| 1   | N     | 216/224 (96%) | 2.24   | 95 (43%) 0 0  | 33, 71, 95, 122       | 0     |
| 1   | O     | 216/224 (96%) | 2.46   | 92 (42%) 0 0  | 42, 66, 94, 109       | 0     |
| 1   | P     | 218/224 (97%) | 2.58   | 97 (44%) 0 0  | 39, 70, 89, 102       | 0     |
| 1   | Q     | 217/224 (96%) | 1.55   | 58 (26%) 1 0  | 28, 66, 95, 107       | 0     |
| 1   | R     | 214/224 (95%) | 2.20   | 102 (47%) 0 0 | 45, 68, 91, 104       | 0     |
| 1   | T     | 217/224 (96%) | 0.78   | 17 (7%) 16 11 | 25, 47, 66, 81        | 0     |
| 1   | U     | 218/224 (97%) | 0.87   | 12 (5%) 29 21 | 29, 48, 70, 96        | 0     |
| 1   | V     | 217/224 (96%) | 1.18   | 32 (14%) 3 2  | 31, 58, 84, 97        | 0     |
| 1   | W     | 217/224 (96%) | 2.23   | 92 (42%) 0 0  | 40, 66, 91, 124       | 0     |
| 1   | X     | 218/224 (97%) | 1.68   | 72 (33%) 0 0  | 29, 67, 90, 108       | 0     |
| 1   | Y     | 218/224 (97%) | 0.97   | 19 (8%) 13 8  | 25, 48, 70, 85        | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2                      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|------------------------------|-----------------------|-------|
| All | All   | 5131/5376 (95%) | 1.56   | 1330 (25%) <b>1</b> <b>0</b> | 19, 59, 86, 124       | 0     |

All (1330) RSRZ outliers are listed below:

| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 1   | P     | 105   | ALA  | 19.9 |
| 1   | P     | 21    | LEU  | 16.6 |
| 1   | P     | 17    | VAL  | 15.9 |
| 1   | M     | 69    | ALA  | 15.7 |
| 1   | O     | 105   | ALA  | 15.5 |
| 1   | L     | 170   | THR  | 15.5 |
| 1   | O     | 40    | ALA  | 14.9 |
| 1   | O     | 103   | ASP  | 14.0 |
| 1   | W     | 88[A] | LYS  | 13.4 |
| 1   | O     | 104   | VAL  | 13.1 |
| 1   | O     | 106   | VAL  | 12.9 |
| 1   | P     | 15    | ALA  | 12.2 |
| 1   | W     | 170   | THR  | 11.8 |
| 1   | X     | 197   | ILE  | 11.7 |
| 1   | M     | 211   | LEU  | 11.6 |
| 1   | L     | 126   | LEU  | 11.4 |
| 1   | L     | 171   | ASP  | 10.8 |
| 1   | H     | 56    | ASP  | 10.7 |
| 1   | I     | 148   | THR  | 10.4 |
| 1   | N     | 100   | GLN  | 10.4 |
| 1   | G     | 17    | VAL  | 10.4 |
| 1   | M     | 203   | PRO  | 10.2 |
| 1   | J     | 210   | GLN  | 9.8  |
| 1   | M     | 97    | ILE  | 9.5  |
| 1   | W     | 63    | ALA  | 9.4  |
| 1   | E     | 169   | LEU  | 9.3  |
| 1   | P     | 104   | VAL  | 9.2  |
| 1   | O     | 56    | ASP  | 9.0  |
| 1   | L     | 75    | VAL  | 9.0  |
| 1   | L     | 132   | ASP  | 8.9  |
| 1   | W     | 198   | GLY  | 8.9  |
| 1   | J     | 5     | LEU  | 8.8  |
| 1   | J     | 23    | SER  | 8.8  |
| 1   | P     | 171   | ASP  | 8.7  |
| 1   | O     | 199   | ASP  | 8.7  |
| 1   | O     | 171   | ASP  | 8.7  |
| 1   | P     | 167   | ILE  | 8.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | O     | 220 | ALA  | 8.6  |
| 1   | Q     | 105 | ALA  | 8.6  |
| 1   | W     | 199 | ASP  | 8.5  |
| 1   | Q     | 86  | TYR  | 8.4  |
| 1   | O     | 45  | ALA  | 8.4  |
| 1   | O     | 17  | VAL  | 8.3  |
| 1   | H     | 7   | ALA  | 8.2  |
| 1   | G     | 45  | ALA  | 8.1  |
| 1   | W     | 169 | LEU  | 8.1  |
| 1   | R     | 106 | VAL  | 8.0  |
| 1   | M     | 143 | LEU  | 8.0  |
| 1   | G     | 26  | GLU  | 8.0  |
| 1   | O     | 5   | LEU  | 7.9  |
| 1   | J     | 138 | ALA  | 7.9  |
| 1   | R     | 219 | LEU  | 7.8  |
| 1   | W     | 13  | VAL  | 7.8  |
| 1   | P     | 168 | LYS  | 7.6  |
| 1   | I     | 114 | LYS  | 7.6  |
| 1   | M     | 126 | LEU  | 7.6  |
| 1   | M     | 75  | VAL  | 7.6  |
| 1   | P     | 195 | THR  | 7.6  |
| 1   | M     | 127 | SER  | 7.6  |
| 1   | O     | 55  | HIS  | 7.6  |
| 1   | L     | 168 | LYS  | 7.6  |
| 1   | Q     | 82  | TYR  | 7.6  |
| 1   | V     | 213 | ILE  | 7.6  |
| 1   | I     | 188 | GLY  | 7.5  |
| 1   | O     | 59  | TYR  | 7.5  |
| 1   | R     | 135 | ALA  | 7.5  |
| 1   | R     | 21  | LEU  | 7.5  |
| 1   | H     | 55  | HIS  | 7.4  |
| 1   | R     | 28  | LEU  | 7.4  |
| 1   | O     | 4   | ALA  | 7.3  |
| 1   | J     | 206 | VAL  | 7.3  |
| 1   | W     | 206 | VAL  | 7.2  |
| 1   | H     | 72  | ALA  | 7.2  |
| 1   | G     | 169 | LEU  | 7.1  |
| 1   | N     | 90  | PHE  | 7.1  |
| 1   | N     | 222 | VAL  | 7.0  |
| 1   | X     | 143 | LEU  | 7.0  |
| 1   | M     | 112 | PRO  | 6.9  |
| 1   | M     | 200 | THR  | 6.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | V     | 55  | HIS  | 6.9  |
| 1   | J     | 169 | LEU  | 6.9  |
| 1   | M     | 5   | LEU  | 6.9  |
| 1   | O     | 124 | ALA  | 6.8  |
| 1   | R     | 137 | LEU  | 6.8  |
| 1   | R     | 206 | VAL  | 6.8  |
| 1   | P     | 169 | LEU  | 6.8  |
| 1   | O     | 44  | GLN  | 6.8  |
| 1   | N     | 189 | ILE  | 6.8  |
| 1   | H     | 105 | ALA  | 6.8  |
| 1   | N     | 87  | CYS  | 6.7  |
| 1   | H     | 104 | VAL  | 6.7  |
| 1   | P     | 213 | ILE  | 6.6  |
| 1   | I     | 130 | LYS  | 6.6  |
| 1   | P     | 7   | ALA  | 6.6  |
| 1   | P     | 106 | VAL  | 6.6  |
| 1   | M     | 201 | ILE  | 6.5  |
| 1   | N     | 81  | ASP  | 6.5  |
| 1   | G     | 220 | ALA  | 6.5  |
| 1   | I     | 52  | ALA  | 6.5  |
| 1   | M     | 9   | GLN  | 6.5  |
| 1   | N     | 148 | THR  | 6.5  |
| 1   | Q     | 46  | GLN  | 6.5  |
| 1   | O     | 74  | LEU  | 6.5  |
| 1   | L     | 209 | ASP  | 6.4  |
| 1   | E     | 208 | TYR  | 6.4  |
| 1   | P     | 199 | ASP  | 6.4  |
| 1   | P     | 141 | GLN  | 6.3  |
| 1   | W     | 200 | THR  | 6.3  |
| 1   | P     | 75  | VAL  | 6.3  |
| 1   | H     | 124 | ALA  | 6.3  |
| 1   | W     | 135 | ALA  | 6.3  |
| 1   | G     | 13  | VAL  | 6.3  |
| 1   | O     | 10  | GLU  | 6.3  |
| 1   | G     | 164 | THR  | 6.3  |
| 1   | J     | 163 | ASN  | 6.2  |
| 1   | G     | 153 | ALA  | 6.2  |
| 1   | P     | 158 | ALA  | 6.2  |
| 1   | Q     | 221 | LYS  | 6.2  |
| 1   | N     | 117 | SER  | 6.2  |
| 1   | O     | 47  | PHE  | 6.2  |
| 1   | G     | 168 | LYS  | 6.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | R     | 32  | ILE  | 6.2  |
| 1   | X     | 145 | GLN  | 6.1  |
| 1   | J     | 87  | CYS  | 6.1  |
| 1   | G     | 167 | ILE  | 6.1  |
| 1   | N     | 223 | LYS  | 6.1  |
| 1   | W     | 5   | LEU  | 6.1  |
| 1   | V     | 113 | PHE  | 6.1  |
| 1   | H     | 178 | GLN  | 6.0  |
| 1   | N     | 194 | ALA  | 6.0  |
| 1   | W     | 86  | TYR  | 6.0  |
| 1   | M     | 37  | THR  | 6.0  |
| 1   | W     | 17  | VAL  | 6.0  |
| 1   | N     | 28  | LEU  | 6.0  |
| 1   | J     | 139 | LEU  | 5.9  |
| 1   | G     | 76  | LEU  | 5.9  |
| 1   | G     | 105 | ALA  | 5.9  |
| 1   | M     | 101 | TYR  | 5.9  |
| 1   | E     | 215 | VAL  | 5.9  |
| 1   | M     | 4   | ALA  | 5.8  |
| 1   | R     | 215 | VAL  | 5.8  |
| 1   | Q     | 220 | ALA  | 5.8  |
| 1   | G     | 118 | SER  | 5.8  |
| 1   | R     | 193 | PRO  | 5.8  |
| 1   | M     | 98  | THR  | 5.8  |
| 1   | N     | 101 | TYR  | 5.8  |
| 1   | W     | 85  | PRO  | 5.8  |
| 1   | P     | 173 | SER  | 5.8  |
| 1   | G     | 15  | ALA  | 5.7  |
| 1   | N     | 72  | ALA  | 5.7  |
| 1   | I     | 90  | PHE  | 5.7  |
| 1   | R     | 208 | TYR  | 5.7  |
| 1   | W     | 56  | ASP  | 5.7  |
| 1   | W     | 15  | ALA  | 5.7  |
| 1   | R     | 136 | PHE  | 5.7  |
| 1   | E     | 52  | ALA  | 5.7  |
| 1   | H     | 19  | ASP  | 5.7  |
| 1   | H     | 76  | LEU  | 5.7  |
| 1   | R     | 211 | LEU  | 5.7  |
| 1   | O     | 50  | ALA  | 5.6  |
| 1   | X     | 208 | TYR  | 5.6  |
| 1   | H     | 131 | GLU  | 5.6  |
| 1   | R     | 158 | ALA  | 5.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | M     | 102 | PRO  | 5.5  |
| 1   | L     | 128 | VAL  | 5.5  |
| 1   | F     | 105 | ALA  | 5.5  |
| 1   | P     | 13  | VAL  | 5.5  |
| 1   | R     | 76  | LEU  | 5.5  |
| 1   | G     | 23  | SER  | 5.5  |
| 1   | G     | 148 | THR  | 5.4  |
| 1   | G     | 104 | VAL  | 5.4  |
| 1   | H     | 169 | LEU  | 5.4  |
| 1   | J     | 68  | GLY  | 5.4  |
| 1   | X     | 74  | LEU  | 5.4  |
| 1   | G     | 20  | THR  | 5.3  |
| 1   | R     | 167 | ILE  | 5.3  |
| 1   | I     | 45  | ALA  | 5.3  |
| 1   | X     | 72  | ALA  | 5.3  |
| 1   | Q     | 191 | GLY  | 5.3  |
| 1   | G     | 112 | PRO  | 5.3  |
| 1   | P     | 42  | GLU  | 5.3  |
| 1   | I     | 16  | LEU  | 5.3  |
| 1   | P     | 16  | LEU  | 5.3  |
| 1   | P     | 19  | ASP  | 5.3  |
| 1   | O     | 108 | ILE  | 5.3  |
| 1   | R     | 191 | GLY  | 5.3  |
| 1   | N     | 20  | THR  | 5.2  |
| 1   | M     | 190 | GLN  | 5.2  |
| 1   | G     | 83  | ASN  | 5.2  |
| 1   | I     | 20  | THR  | 5.2  |
| 1   | X     | 138 | ALA  | 5.2  |
| 1   | P     | 162 | THR  | 5.2  |
| 1   | O     | 3   | ALA  | 5.2  |
| 1   | J     | 199 | ASP  | 5.1  |
| 1   | P     | 115 | GLY  | 5.1  |
| 1   | O     | 170 | THR  | 5.1  |
| 1   | I     | 76  | LEU  | 5.1  |
| 1   | G     | 54  | GLU  | 5.1  |
| 1   | O     | 169 | LEU  | 5.1  |
| 1   | E     | 72  | ALA  | 5.1  |
| 1   | H     | 30  | GLU  | 5.1  |
| 1   | W     | 152 | ASN  | 5.1  |
| 1   | H     | 74  | LEU  | 5.1  |
| 1   | P     | 86  | TYR  | 5.1  |
| 1   | X     | 76  | LEU  | 5.1  |

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| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 1   | M     | 115   | GLY  | 5.1  |
| 1   | E     | 224   | LYS  | 5.0  |
| 1   | N     | 141   | GLN  | 5.0  |
| 1   | N     | 191   | GLY  | 5.0  |
| 1   | W     | 182   | GLU  | 5.0  |
| 1   | M     | 41    | ASP  | 5.0  |
| 1   | P     | 198   | GLY  | 5.0  |
| 1   | E     | 88[A] | LYS  | 5.0  |
| 1   | I     | 75    | VAL  | 5.0  |
| 1   | P     | 58    | LEU  | 5.0  |
| 1   | H     | 8     | ALA  | 5.0  |
| 1   | X     | 77    | VAL  | 5.0  |
| 1   | H     | 111   | LEU  | 5.0  |
| 1   | H     | 220   | ALA  | 4.9  |
| 1   | J     | 9     | GLN  | 4.9  |
| 1   | J     | 162   | THR  | 4.9  |
| 1   | P     | 219   | LEU  | 4.9  |
| 1   | R     | 155   | ILE  | 4.9  |
| 1   | W     | 167   | ILE  | 4.9  |
| 1   | X     | 89    | ARG  | 4.9  |
| 1   | W     | 122   | SER  | 4.9  |
| 1   | E     | 219   | LEU  | 4.9  |
| 1   | Q     | 93    | LEU  | 4.9  |
| 1   | F     | 54    | GLU  | 4.9  |
| 1   | E     | 21    | LEU  | 4.9  |
| 1   | N     | 152   | ASN  | 4.9  |
| 1   | J     | 209   | ASP  | 4.9  |
| 1   | O     | 132   | ASP  | 4.9  |
| 1   | X     | 102   | PRO  | 4.9  |
| 1   | W     | 129   | TRP  | 4.8  |
| 1   | W     | 127   | SER  | 4.8  |
| 1   | R     | 17    | VAL  | 4.8  |
| 1   | M     | 12    | GLU  | 4.8  |
| 1   | O     | 42    | GLU  | 4.8  |
| 1   | L     | 129   | TRP  | 4.8  |
| 1   | H     | 103   | ASP  | 4.8  |
| 1   | J     | 201   | ILE  | 4.8  |
| 1   | I     | 84    | CYS  | 4.8  |
| 1   | M     | 26    | GLU  | 4.8  |
| 1   | J     | 164   | THR  | 4.7  |
| 1   | W     | 98    | THR  | 4.7  |
| 1   | J     | 19    | ASP  | 4.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 128 | VAL  | 4.7  |
| 1   | M     | 214 | ILE  | 4.7  |
| 1   | J     | 157 | ASP  | 4.7  |
| 1   | N     | 76  | LEU  | 4.7  |
| 1   | M     | 32  | ILE  | 4.7  |
| 1   | E     | 171 | ASP  | 4.7  |
| 1   | I     | 28  | LEU  | 4.7  |
| 1   | J     | 143 | LEU  | 4.7  |
| 1   | P     | 108 | ILE  | 4.7  |
| 1   | W     | 208 | TYR  | 4.7  |
| 1   | X     | 46  | GLN  | 4.7  |
| 1   | I     | 150 | LEU  | 4.7  |
| 1   | O     | 198 | GLY  | 4.7  |
| 1   | K     | 3   | ALA  | 4.7  |
| 1   | M     | 15  | ALA  | 4.7  |
| 1   | H     | 17  | VAL  | 4.7  |
| 1   | N     | 70  | LYS  | 4.6  |
| 1   | G     | 171 | ASP  | 4.6  |
| 1   | W     | 197 | ILE  | 4.6  |
| 1   | W     | 89  | ARG  | 4.6  |
| 1   | G     | 162 | THR  | 4.6  |
| 1   | E     | 71  | ASP  | 4.6  |
| 1   | P     | 156 | GLU  | 4.6  |
| 1   | G     | 106 | VAL  | 4.6  |
| 1   | X     | 205 | ALA  | 4.6  |
| 1   | J     | 22  | VAL  | 4.6  |
| 1   | M     | 164 | THR  | 4.6  |
| 1   | P     | 174 | LEU  | 4.6  |
| 1   | K     | 68  | GLY  | 4.5  |
| 1   | P     | 191 | GLY  | 4.5  |
| 1   | P     | 103 | ASP  | 4.5  |
| 1   | I     | 40  | ALA  | 4.5  |
| 1   | W     | 51  | LEU  | 4.5  |
| 1   | I     | 32  | ILE  | 4.5  |
| 1   | M     | 170 | THR  | 4.5  |
| 1   | P     | 164 | THR  | 4.5  |
| 1   | N     | 82  | TYR  | 4.5  |
| 1   | G     | 65  | PRO  | 4.5  |
| 1   | J     | 200 | THR  | 4.5  |
| 1   | J     | 174 | LEU  | 4.5  |
| 1   | P     | 41  | ASP  | 4.5  |
| 1   | M     | 206 | VAL  | 4.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | O     | 69  | ALA  | 4.5  |
| 1   | M     | 10  | GLU  | 4.5  |
| 1   | O     | 197 | ILE  | 4.5  |
| 1   | R     | 51  | LEU  | 4.4  |
| 1   | W     | 128 | VAL  | 4.4  |
| 1   | L     | 93  | LEU  | 4.4  |
| 1   | I     | 115 | GLY  | 4.4  |
| 1   | G     | 161 | SER  | 4.4  |
| 1   | N     | 147 | LYS  | 4.4  |
| 1   | H     | 109 | LYS  | 4.4  |
| 1   | C     | 213 | ILE  | 4.4  |
| 1   | Q     | 192 | THR  | 4.4  |
| 1   | N     | 206 | VAL  | 4.4  |
| 1   | J     | 156 | GLU  | 4.4  |
| 1   | W     | 213 | ILE  | 4.4  |
| 1   | L     | 74  | LEU  | 4.4  |
| 1   | X     | 139 | LEU  | 4.4  |
| 1   | J     | 161 | SER  | 4.3  |
| 1   | O     | 101 | TYR  | 4.3  |
| 1   | J     | 69  | ALA  | 4.3  |
| 1   | M     | 11  | LYS  | 4.3  |
| 1   | P     | 54  | GLU  | 4.3  |
| 1   | W     | 20  | THR  | 4.3  |
| 1   | H     | 129 | TRP  | 4.3  |
| 1   | G     | 221 | LYS  | 4.3  |
| 1   | W     | 126 | LEU  | 4.3  |
| 1   | N     | 207 | ASP  | 4.3  |
| 1   | M     | 47  | PHE  | 4.3  |
| 1   | M     | 113 | PHE  | 4.3  |
| 1   | R     | 124 | ALA  | 4.3  |
| 1   | O     | 214 | ILE  | 4.3  |
| 1   | J     | 165 | SER  | 4.3  |
| 1   | L     | 154 | SER  | 4.3  |
| 1   | R     | 183 | LEU  | 4.3  |
| 1   | H     | 3   | ALA  | 4.3  |
| 1   | M     | 209 | ASP  | 4.3  |
| 1   | E     | 217 | GLU  | 4.3  |
| 1   | W     | 76  | LEU  | 4.3  |
| 1   | M     | 155 | ILE  | 4.3  |
| 1   | N     | 6   | ASN  | 4.3  |
| 1   | M     | 166 | LYS  | 4.2  |
| 1   | N     | 56  | ASP  | 4.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | P     | 50  | ALA  | 4.2  |
| 1   | F     | 47  | PHE  | 4.2  |
| 1   | O     | 60  | ASN  | 4.2  |
| 1   | L     | 125 | VAL  | 4.2  |
| 1   | E     | 23  | SER  | 4.2  |
| 1   | J     | 134 | LYS  | 4.2  |
| 1   | X     | 91  | ASP  | 4.2  |
| 1   | M     | 3   | ALA  | 4.2  |
| 1   | U     | 52  | ALA  | 4.2  |
| 1   | O     | 15  | ALA  | 4.2  |
| 1   | N     | 188 | GLY  | 4.2  |
| 1   | I     | 92  | PRO  | 4.2  |
| 1   | W     | 47  | PHE  | 4.1  |
| 1   | X     | 105 | ALA  | 4.1  |
| 1   | V     | 74  | LEU  | 4.1  |
| 1   | W     | 74  | LEU  | 4.1  |
| 1   | F     | 50  | ALA  | 4.1  |
| 1   | W     | 31  | ALA  | 4.1  |
| 1   | O     | 19  | ASP  | 4.1  |
| 1   | N     | 139 | LEU  | 4.1  |
| 1   | W     | 111 | LEU  | 4.1  |
| 1   | W     | 203 | PRO  | 4.1  |
| 1   | F     | 208 | TYR  | 4.1  |
| 1   | G     | 9   | GLN  | 4.1  |
| 1   | E     | 79  | PHE  | 4.1  |
| 1   | I     | 55  | HIS  | 4.1  |
| 1   | L     | 35  | LEU  | 4.1  |
| 1   | N     | 104 | VAL  | 4.1  |
| 1   | E     | 220 | ALA  | 4.1  |
| 1   | X     | 55  | HIS  | 4.0  |
| 1   | G     | 16  | LEU  | 4.0  |
| 1   | P     | 136 | PHE  | 4.0  |
| 1   | E     | 143 | LEU  | 4.0  |
| 1   | E     | 115 | GLY  | 4.0  |
| 1   | L     | 102 | PRO  | 4.0  |
| 1   | P     | 32  | ILE  | 4.0  |
| 1   | N     | 209 | ASP  | 4.0  |
| 1   | R     | 56  | ASP  | 4.0  |
| 1   | N     | 26  | GLU  | 4.0  |
| 1   | I     | 27  | ILE  | 4.0  |
| 1   | Y     | 213 | ILE  | 4.0  |
| 1   | Q     | 206 | VAL  | 4.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | J     | 15  | ALA  | 4.0  |
| 1   | N     | 187 | LEU  | 4.0  |
| 1   | G     | 8   | ALA  | 4.0  |
| 1   | H     | 45  | ALA  | 4.0  |
| 1   | M     | 162 | THR  | 4.0  |
| 1   | L     | 199 | ASP  | 4.0  |
| 1   | I     | 50  | ALA  | 4.0  |
| 1   | P     | 101 | TYR  | 4.0  |
| 1   | R     | 143 | LEU  | 4.0  |
| 1   | T     | 186 | LYS  | 4.0  |
| 1   | M     | 221 | LYS  | 4.0  |
| 1   | E     | 170 | THR  | 3.9  |
| 1   | G     | 19  | ASP  | 3.9  |
| 1   | L     | 76  | LEU  | 3.9  |
| 1   | V     | 155 | ILE  | 3.9  |
| 1   | E     | 69  | ALA  | 3.9  |
| 1   | P     | 8   | ALA  | 3.9  |
| 1   | W     | 75  | VAL  | 3.9  |
| 1   | H     | 5   | LEU  | 3.9  |
| 1   | N     | 211 | LEU  | 3.9  |
| 1   | P     | 155 | ILE  | 3.9  |
| 1   | P     | 90  | PHE  | 3.9  |
| 1   | P     | 3   | ALA  | 3.9  |
| 1   | E     | 211 | LEU  | 3.9  |
| 1   | M     | 131 | GLU  | 3.9  |
| 1   | G     | 46  | GLN  | 3.9  |
| 1   | J     | 131 | GLU  | 3.9  |
| 1   | N     | 4   | ALA  | 3.9  |
| 1   | Q     | 57  | ALA  | 3.9  |
| 1   | Q     | 202 | LEU  | 3.9  |
| 1   | W     | 176 | THR  | 3.9  |
| 1   | N     | 95  | GLU  | 3.9  |
| 1   | X     | 54  | GLU  | 3.9  |
| 1   | Q     | 77  | VAL  | 3.9  |
| 1   | R     | 45  | ALA  | 3.9  |
| 1   | N     | 110 | PRO  | 3.9  |
| 1   | I     | 113 | PHE  | 3.9  |
| 1   | N     | 7   | ALA  | 3.9  |
| 1   | N     | 215 | VAL  | 3.9  |
| 1   | E     | 28  | LEU  | 3.9  |
| 1   | W     | 52  | ALA  | 3.8  |
| 1   | M     | 70  | LYS  | 3.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 101 | TYR  | 3.8  |
| 1   | J     | 41  | ASP  | 3.8  |
| 1   | W     | 132 | ASP  | 3.8  |
| 1   | W     | 27  | ILE  | 3.8  |
| 1   | A     | 22  | VAL  | 3.8  |
| 1   | G     | 202 | LEU  | 3.8  |
| 1   | L     | 174 | LEU  | 3.8  |
| 1   | W     | 187 | LEU  | 3.8  |
| 1   | R     | 148 | THR  | 3.8  |
| 1   | J     | 92  | PRO  | 3.8  |
| 1   | H     | 128 | VAL  | 3.8  |
| 1   | J     | 154 | SER  | 3.8  |
| 1   | P     | 184 | SER  | 3.8  |
| 1   | M     | 191 | GLY  | 3.8  |
| 1   | W     | 92  | PRO  | 3.8  |
| 1   | I     | 23  | SER  | 3.8  |
| 1   | N     | 8   | ALA  | 3.8  |
| 1   | R     | 168 | LYS  | 3.8  |
| 1   | W     | 83  | ASN  | 3.8  |
| 1   | I     | 208 | TYR  | 3.8  |
| 1   | O     | 79  | PHE  | 3.8  |
| 1   | I     | 81  | ASP  | 3.8  |
| 1   | O     | 209 | ASP  | 3.8  |
| 1   | K     | 46  | GLN  | 3.8  |
| 1   | N     | 143 | LEU  | 3.8  |
| 1   | Q     | 211 | LEU  | 3.8  |
| 1   | R     | 74  | LEU  | 3.8  |
| 1   | W     | 62  | ALA  | 3.8  |
| 1   | X     | 211 | LEU  | 3.8  |
| 1   | Y     | 211 | LEU  | 3.8  |
| 1   | R     | 222 | VAL  | 3.8  |
| 1   | M     | 207 | ASP  | 3.8  |
| 1   | W     | 193 | PRO  | 3.8  |
| 1   | P     | 44  | GLN  | 3.8  |
| 1   | J     | 218 | GLN  | 3.7  |
| 1   | R     | 99  | GLU  | 3.7  |
| 1   | O     | 72  | ALA  | 3.7  |
| 1   | Q     | 97  | ILE  | 3.7  |
| 1   | X     | 47  | PHE  | 3.7  |
| 1   | R     | 57  | ALA  | 3.7  |
| 1   | P     | 148 | THR  | 3.7  |
| 1   | G     | 150 | LEU  | 3.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | O     | 7   | ALA  | 3.7  |
| 1   | I     | 67  | ILE  | 3.7  |
| 1   | Q     | 90  | PHE  | 3.7  |
| 1   | W     | 190 | GLN  | 3.7  |
| 1   | I     | 66  | ARG  | 3.7  |
| 1   | E     | 162 | THR  | 3.7  |
| 1   | P     | 102 | PRO  | 3.7  |
| 1   | O     | 58  | LEU  | 3.7  |
| 1   | C     | 45  | ALA  | 3.7  |
| 1   | H     | 214 | ILE  | 3.7  |
| 1   | Q     | 222 | VAL  | 3.7  |
| 1   | O     | 221 | LYS  | 3.7  |
| 1   | K     | 218 | GLN  | 3.7  |
| 1   | O     | 61  | ASP  | 3.7  |
| 1   | R     | 108 | ILE  | 3.6  |
| 1   | X     | 213 | ILE  | 3.6  |
| 1   | X     | 160 | LYS  | 3.6  |
| 1   | O     | 112 | PRO  | 3.6  |
| 1   | M     | 7   | ALA  | 3.6  |
| 1   | R     | 72  | ALA  | 3.6  |
| 1   | I     | 197 | ILE  | 3.6  |
| 1   | Q     | 196 | VAL  | 3.6  |
| 1   | R     | 189 | ILE  | 3.6  |
| 1   | W     | 103 | ASP  | 3.6  |
| 1   | G     | 173 | SER  | 3.6  |
| 1   | J     | 148 | THR  | 3.6  |
| 1   | P     | 217 | GLU  | 3.6  |
| 1   | R     | 210 | GLN  | 3.6  |
| 1   | O     | 216 | LYS  | 3.6  |
| 1   | X     | 167 | ILE  | 3.6  |
| 1   | D     | 31  | ALA  | 3.6  |
| 1   | N     | 62  | ALA  | 3.6  |
| 1   | E     | 132 | ASP  | 3.6  |
| 1   | G     | 92  | PRO  | 3.6  |
| 1   | N     | 49  | GLN  | 3.6  |
| 1   | J     | 160 | LYS  | 3.6  |
| 1   | Q     | 205 | ALA  | 3.6  |
| 1   | N     | 174 | LEU  | 3.6  |
| 1   | J     | 140 | HIS  | 3.5  |
| 1   | L     | 192 | THR  | 3.5  |
| 1   | I     | 87  | CYS  | 3.5  |
| 1   | P     | 209 | ASP  | 3.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | W     | 207 | ASP  | 3.5  |
| 1   | I     | 68  | GLY  | 3.5  |
| 1   | N     | 102 | PRO  | 3.5  |
| 1   | P     | 202 | LEU  | 3.5  |
| 1   | Q     | 169 | LEU  | 3.5  |
| 1   | R     | 95  | GLU  | 3.5  |
| 1   | R     | 139 | LEU  | 3.5  |
| 1   | M     | 90  | PHE  | 3.5  |
| 1   | P     | 11  | LYS  | 3.5  |
| 1   | L     | 178 | GLN  | 3.5  |
| 1   | P     | 40  | ALA  | 3.5  |
| 1   | M     | 20  | THR  | 3.5  |
| 1   | I     | 72  | ALA  | 3.5  |
| 1   | O     | 194 | ALA  | 3.5  |
| 1   | L     | 191 | GLY  | 3.5  |
| 1   | M     | 110 | PRO  | 3.5  |
| 1   | N     | 171 | ASP  | 3.5  |
| 1   | P     | 47  | PHE  | 3.5  |
| 1   | K     | 53  | SER  | 3.5  |
| 1   | X     | 53  | SER  | 3.5  |
| 1   | I     | 196 | VAL  | 3.5  |
| 1   | N     | 75  | VAL  | 3.5  |
| 1   | X     | 17  | VAL  | 3.5  |
| 1   | H     | 139 | LEU  | 3.5  |
| 1   | R     | 111 | LEU  | 3.5  |
| 1   | M     | 123 | GLN  | 3.5  |
| 1   | W     | 73  | LYS  | 3.5  |
| 1   | P     | 56  | ASP  | 3.5  |
| 1   | R     | 13  | VAL  | 3.5  |
| 1   | M     | 21  | LEU  | 3.5  |
| 1   | E     | 194 | ALA  | 3.4  |
| 1   | H     | 15  | ALA  | 3.4  |
| 1   | E     | 32  | ILE  | 3.4  |
| 1   | N     | 12  | GLU  | 3.4  |
| 1   | J     | 4   | ALA  | 3.4  |
| 1   | R     | 62  | ALA  | 3.4  |
| 1   | E     | 65  | PRO  | 3.4  |
| 1   | H     | 183 | LEU  | 3.4  |
| 1   | J     | 187 | LEU  | 3.4  |
| 1   | M     | 150 | LEU  | 3.4  |
| 1   | M     | 156 | GLU  | 3.4  |
| 1   | P     | 196 | VAL  | 3.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | R     | 122 | SER  | 3.4  |
| 1   | H     | 194 | ALA  | 3.4  |
| 1   | P     | 197 | ILE  | 3.4  |
| 1   | N     | 160 | LYS  | 3.4  |
| 1   | C     | 220 | ALA  | 3.4  |
| 1   | P     | 138 | ALA  | 3.4  |
| 1   | J     | 147 | LYS  | 3.4  |
| 1   | V     | 115 | GLY  | 3.4  |
| 1   | M     | 163 | ASN  | 3.4  |
| 1   | N     | 71  | ASP  | 3.4  |
| 1   | G     | 133 | PRO  | 3.4  |
| 1   | H     | 108 | ILE  | 3.4  |
| 1   | O     | 189 | ILE  | 3.4  |
| 1   | N     | 129 | TRP  | 3.4  |
| 1   | L     | 172 | ASP  | 3.4  |
| 1   | M     | 172 | ASP  | 3.4  |
| 1   | P     | 61  | ASP  | 3.4  |
| 1   | G     | 126 | LEU  | 3.4  |
| 1   | M     | 111 | LEU  | 3.4  |
| 1   | I     | 62  | ALA  | 3.4  |
| 1   | T     | 220 | ALA  | 3.4  |
| 1   | P     | 46  | GLN  | 3.4  |
| 1   | Q     | 162 | THR  | 3.3  |
| 1   | U     | 224 | LYS  | 3.3  |
| 1   | G     | 158 | ALA  | 3.3  |
| 1   | H     | 10  | GLU  | 3.3  |
| 1   | J     | 102 | PRO  | 3.3  |
| 1   | M     | 95  | GLU  | 3.3  |
| 1   | G     | 183 | LEU  | 3.3  |
| 1   | Q     | 148 | THR  | 3.3  |
| 1   | R     | 175 | LYS  | 3.3  |
| 1   | X     | 201 | ILE  | 3.3  |
| 1   | Y     | 47  | PHE  | 3.3  |
| 1   | M     | 6   | ASN  | 3.3  |
| 1   | F     | 74  | LEU  | 3.3  |
| 1   | Y     | 148 | THR  | 3.3  |
| 1   | Q     | 136 | PHE  | 3.3  |
| 1   | R     | 188 | GLY  | 3.3  |
| 1   | H     | 65  | PRO  | 3.3  |
| 1   | L     | 176 | THR  | 3.3  |
| 1   | R     | 154 | SER  | 3.3  |
| 1   | V     | 158 | ALA  | 3.3  |

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| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 1   | I     | 184   | SER  | 3.3  |
| 1   | R     | 165   | SER  | 3.3  |
| 1   | R     | 90    | PHE  | 3.3  |
| 1   | E     | 50    | ALA  | 3.3  |
| 1   | Q     | 94    | LEU  | 3.3  |
| 1   | N     | 128   | VAL  | 3.3  |
| 1   | P     | 145   | GLN  | 3.3  |
| 1   | E     | 87[A] | CYS  | 3.3  |
| 1   | H     | 110   | PRO  | 3.3  |
| 1   | H     | 156   | GLU  | 3.3  |
| 1   | H     | 66    | ARG  | 3.3  |
| 1   | I     | 206   | VAL  | 3.3  |
| 1   | R     | 31    | ALA  | 3.3  |
| 1   | X     | 150   | LEU  | 3.3  |
| 1   | E     | 48    | ARG  | 3.3  |
| 1   | P     | 78    | SER  | 3.2  |
| 1   | R     | 152   | ASN  | 3.2  |
| 1   | X     | 59    | TYR  | 3.2  |
| 1   | X     | 148   | THR  | 3.2  |
| 1   | L     | 131   | GLU  | 3.2  |
| 1   | H     | 51    | LEU  | 3.2  |
| 1   | M     | 74    | LEU  | 3.2  |
| 1   | M     | 157   | ASP  | 3.2  |
| 1   | R     | 187   | LEU  | 3.2  |
| 1   | H     | 60    | ASN  | 3.2  |
| 1   | M     | 93    | LEU  | 3.2  |
| 1   | P     | 183   | LEU  | 3.2  |
| 1   | R     | 23    | SER  | 3.2  |
| 1   | M     | 80    | THR  | 3.2  |
| 1   | X     | 84    | CYS  | 3.2  |
| 1   | E     | 45    | ALA  | 3.2  |
| 1   | I     | 190   | GLN  | 3.2  |
| 1   | R     | 110   | PRO  | 3.2  |
| 1   | R     | 20    | THR  | 3.2  |
| 1   | E     | 51    | LEU  | 3.2  |
| 1   | W     | 217   | GLU  | 3.2  |
| 1   | W     | 163   | ASN  | 3.2  |
| 1   | G     | 198   | GLY  | 3.2  |
| 1   | W     | 115   | GLY  | 3.2  |
| 1   | N     | 21    | LEU  | 3.2  |
| 1   | V     | 202   | LEU  | 3.2  |
| 1   | N     | 67    | ILE  | 3.2  |

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| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 1   | H     | 57    | ALA  | 3.2  |
| 1   | E     | 24    | ASN  | 3.2  |
| 1   | Q     | 79    | PHE  | 3.2  |
| 1   | W     | 148   | THR  | 3.2  |
| 1   | E     | 131   | GLU  | 3.2  |
| 1   | E     | 199   | ASP  | 3.2  |
| 1   | N     | 24    | ASN  | 3.2  |
| 1   | N     | 60    | ASN  | 3.2  |
| 1   | W     | 87[A] | CYS  | 3.2  |
| 1   | M     | 215   | VAL  | 3.1  |
| 1   | R     | 47    | PHE  | 3.1  |
| 1   | L     | 134   | LYS  | 3.1  |
| 1   | L     | 190   | GLN  | 3.1  |
| 1   | R     | 174   | LEU  | 3.1  |
| 1   | K     | 20    | THR  | 3.1  |
| 1   | H     | 49    | GLN  | 3.1  |
| 1   | J     | 124   | ALA  | 3.1  |
| 1   | M     | 29    | GLU  | 3.1  |
| 1   | P     | 189   | ILE  | 3.1  |
| 1   | J     | 110   | PRO  | 3.1  |
| 1   | P     | 25    | PRO  | 3.1  |
| 1   | N     | 98    | THR  | 3.1  |
| 1   | X     | 192   | THR  | 3.1  |
| 1   | I     | 94    | LEU  | 3.1  |
| 1   | V     | 69    | ALA  | 3.1  |
| 1   | N     | 114   | LYS  | 3.1  |
| 1   | P     | 133   | PRO  | 3.1  |
| 1   | G     | 178   | GLN  | 3.1  |
| 1   | J     | 6     | ASN  | 3.1  |
| 1   | J     | 135   | ALA  | 3.1  |
| 1   | O     | 217   | GLU  | 3.1  |
| 1   | E     | 164   | THR  | 3.1  |
| 1   | W     | 158   | ALA  | 3.1  |
| 1   | E     | 203   | PRO  | 3.1  |
| 1   | G     | 108   | ILE  | 3.1  |
| 1   | V     | 142   | ARG  | 3.1  |
| 1   | H     | 170   | THR  | 3.1  |
| 1   | J     | 105   | ALA  | 3.1  |
| 1   | O     | 161   | SER  | 3.1  |
| 1   | P     | 79    | PHE  | 3.0  |
| 1   | O     | 125   | VAL  | 3.0  |
| 1   | Q     | 104   | VAL  | 3.0  |

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| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 1   | L     | 26    | GLU  | 3.0  |
| 1   | M     | 31    | ALA  | 3.0  |
| 1   | Q     | 187   | LEU  | 3.0  |
| 1   | O     | 164   | THR  | 3.0  |
| 1   | Q     | 96    | LYS  | 3.0  |
| 1   | O     | 46    | GLN  | 3.0  |
| 1   | R     | 153   | ALA  | 3.0  |
| 1   | Q     | 87[A] | CYS  | 3.0  |
| 1   | M     | 99    | GLU  | 3.0  |
| 1   | N     | 137   | LEU  | 3.0  |
| 1   | R     | 107   | ILE  | 3.0  |
| 1   | V     | 67    | ILE  | 3.0  |
| 1   | J     | 170   | THR  | 3.0  |
| 1   | R     | 177   | LEU  | 3.0  |
| 1   | R     | 220   | ALA  | 3.0  |
| 1   | J     | 80    | THR  | 3.0  |
| 1   | Q     | 74    | LEU  | 3.0  |
| 1   | C     | 62    | ALA  | 3.0  |
| 1   | O     | 57    | ALA  | 3.0  |
| 1   | W     | 69    | ALA  | 3.0  |
| 1   | X     | 119   | ALA  | 3.0  |
| 1   | J     | 167   | ILE  | 3.0  |
| 1   | L     | 214   | ILE  | 3.0  |
| 1   | E     | 47    | PHE  | 3.0  |
| 1   | J     | 90    | PHE  | 3.0  |
| 1   | M     | 84[A] | CYS  | 3.0  |
| 1   | H     | 44    | GLN  | 3.0  |
| 1   | I     | 83    | ASN  | 3.0  |
| 1   | X     | 209   | ASP  | 3.0  |
| 1   | M     | 94    | LEU  | 3.0  |
| 1   | P     | 116   | GLU  | 3.0  |
| 1   | B     | 67    | ILE  | 2.9  |
| 1   | R     | 60    | ASN  | 2.9  |
| 1   | O     | 41    | ASP  | 2.9  |
| 1   | G     | 37    | THR  | 2.9  |
| 1   | E     | 22    | VAL  | 2.9  |
| 1   | R     | 66    | ARG  | 2.9  |
| 1   | W     | 45    | ALA  | 2.9  |
| 1   | L     | 167   | ILE  | 2.9  |
| 1   | N     | 201   | ILE  | 2.9  |
| 1   | O     | 18    | ARG  | 2.9  |
| 1   | O     | 126   | LEU  | 2.9  |

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| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 1   | M     | 25    | PRO  | 2.9  |
| 1   | R     | 7     | ALA  | 2.9  |
| 1   | R     | 205   | ALA  | 2.9  |
| 1   | L     | 103   | ASP  | 2.9  |
| 1   | M     | 71    | ASP  | 2.9  |
| 1   | N     | 103   | ASP  | 2.9  |
| 1   | O     | 80    | THR  | 2.9  |
| 1   | R     | 46    | GLN  | 2.9  |
| 1   | Q     | 106   | VAL  | 2.9  |
| 1   | B     | 8     | ALA  | 2.9  |
| 1   | G     | 40    | ALA  | 2.9  |
| 1   | L     | 124   | ALA  | 2.9  |
| 1   | Q     | 85    | PRO  | 2.9  |
| 1   | W     | 7     | ALA  | 2.9  |
| 1   | R     | 151   | ASP  | 2.9  |
| 1   | M     | 108   | ILE  | 2.9  |
| 1   | E     | 223   | LYS  | 2.9  |
| 1   | G     | 84[A] | CYS  | 2.9  |
| 1   | D     | 198   | GLY  | 2.9  |
| 1   | I     | 86    | TYR  | 2.9  |
| 1   | K     | 86    | TYR  | 2.9  |
| 1   | M     | 212   | GLU  | 2.9  |
| 1   | N     | 142   | ARG  | 2.9  |
| 1   | R     | 55    | HIS  | 2.9  |
| 1   | X     | 165   | SER  | 2.9  |
| 1   | I     | 169   | LEU  | 2.9  |
| 1   | Q     | 137   | LEU  | 2.9  |
| 1   | V     | 5     | LEU  | 2.9  |
| 1   | W     | 150   | LEU  | 2.9  |
| 1   | M     | 196   | VAL  | 2.9  |
| 1   | O     | 12    | GLU  | 2.9  |
| 1   | P     | 212   | GLU  | 2.9  |
| 1   | Q     | 208   | TYR  | 2.9  |
| 1   | G     | 11    | LYS  | 2.9  |
| 1   | O     | 190   | GLN  | 2.9  |
| 1   | G     | 174   | LEU  | 2.9  |
| 1   | J     | 26    | GLU  | 2.9  |
| 1   | O     | 192   | THR  | 2.9  |
| 1   | N     | 216   | LYS  | 2.9  |
| 1   | I     | 13    | VAL  | 2.9  |
| 1   | G     | 34    | ALA  | 2.9  |
| 1   | P     | 6     | ASN  | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | X     | 112 | PRO  | 2.9  |
| 1   | Y     | 49  | GLN  | 2.9  |
| 1   | C     | 67  | ILE  | 2.9  |
| 1   | C     | 73  | LYS  | 2.9  |
| 1   | J     | 11  | LYS  | 2.9  |
| 1   | T     | 73  | LYS  | 2.9  |
| 1   | M     | 194 | ALA  | 2.9  |
| 1   | O     | 24  | ASN  | 2.9  |
| 1   | V     | 44  | GLN  | 2.8  |
| 1   | R     | 38  | LYS  | 2.8  |
| 1   | X     | 107 | ILE  | 2.8  |
| 1   | P     | 126 | LEU  | 2.8  |
| 1   | K     | 56  | ASP  | 2.8  |
| 1   | P     | 172 | ASP  | 2.8  |
| 1   | J     | 145 | GLN  | 2.8  |
| 1   | W     | 44  | GLN  | 2.8  |
| 1   | I     | 73  | LYS  | 2.8  |
| 1   | M     | 160 | LYS  | 2.8  |
| 1   | R     | 73  | LYS  | 2.8  |
| 1   | M     | 154 | SER  | 2.8  |
| 1   | I     | 69  | ALA  | 2.8  |
| 1   | R     | 196 | VAL  | 2.8  |
| 1   | P     | 113 | PHE  | 2.8  |
| 1   | N     | 16  | LEU  | 2.8  |
| 1   | R     | 199 | ASP  | 2.8  |
| 1   | V     | 145 | GLN  | 2.8  |
| 1   | J     | 99  | GLU  | 2.8  |
| 1   | U     | 148 | THR  | 2.8  |
| 1   | X     | 60  | ASN  | 2.8  |
| 1   | R     | 67  | ILE  | 2.8  |
| 1   | J     | 171 | ASP  | 2.8  |
| 1   | W     | 172 | ASP  | 2.8  |
| 1   | Q     | 125 | VAL  | 2.8  |
| 1   | R     | 105 | ALA  | 2.8  |
| 1   | X     | 45  | ALA  | 2.8  |
| 1   | A     | 160 | LYS  | 2.8  |
| 1   | M     | 218 | GLN  | 2.8  |
| 1   | D     | 136 | PHE  | 2.8  |
| 1   | L     | 179 | ASN  | 2.8  |
| 1   | L     | 193 | PRO  | 2.8  |
| 1   | N     | 25  | PRO  | 2.8  |
| 1   | N     | 40  | ALA  | 2.8  |

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| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 1   | X     | 104   | VAL  | 2.8  |
| 1   | E     | 64    | SER  | 2.8  |
| 1   | G     | 88[A] | LYS  | 2.8  |
| 1   | G     | 142   | ARG  | 2.8  |
| 1   | J     | 18    | ARG  | 2.8  |
| 1   | B     | 97    | ILE  | 2.8  |
| 1   | Q     | 47    | PHE  | 2.8  |
| 1   | Q     | 197   | ILE  | 2.8  |
| 1   | N     | 57    | ALA  | 2.8  |
| 1   | G     | 117   | SER  | 2.8  |
| 1   | R     | 101   | TYR  | 2.8  |
| 1   | F     | 76    | LEU  | 2.8  |
| 1   | H     | 35    | LEU  | 2.8  |
| 1   | R     | 27    | ILE  | 2.8  |
| 1   | W     | 90    | PHE  | 2.8  |
| 1   | W     | 97    | ILE  | 2.8  |
| 1   | E     | 37    | THR  | 2.8  |
| 1   | O     | 63    | ALA  | 2.7  |
| 1   | P     | 161   | SER  | 2.7  |
| 1   | L     | 183   | LEU  | 2.7  |
| 1   | M     | 179   | ASN  | 2.7  |
| 1   | N     | 32    | ILE  | 2.7  |
| 1   | O     | 68    | GLY  | 2.7  |
| 1   | B     | 84[A] | CYS  | 2.7  |
| 1   | E     | 49    | GLN  | 2.7  |
| 1   | R     | 218   | GLN  | 2.7  |
| 1   | C     | 102   | PRO  | 2.7  |
| 1   | H     | 106   | VAL  | 2.7  |
| 1   | E     | 221   | LYS  | 2.7  |
| 1   | G     | 61    | ASP  | 2.7  |
| 1   | A     | 113   | PHE  | 2.7  |
| 1   | X     | 58    | LEU  | 2.7  |
| 1   | X     | 82    | TYR  | 2.7  |
| 1   | Q     | 89    | ARG  | 2.7  |
| 1   | B     | 32    | ILE  | 2.7  |
| 1   | W     | 107   | ILE  | 2.7  |
| 1   | P     | 43    | GLN  | 2.7  |
| 1   | E     | 193   | PRO  | 2.7  |
| 1   | J     | 7     | ALA  | 2.7  |
| 1   | N     | 135   | ALA  | 2.7  |
| 1   | H     | 221   | LYS  | 2.7  |
| 1   | F     | 93    | LEU  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | I     | 74  | LEU  | 2.7  |
| 1   | N     | 48  | ARG  | 2.7  |
| 1   | P     | 107 | ILE  | 2.7  |
| 1   | Q     | 214 | ILE  | 2.7  |
| 1   | L     | 20  | THR  | 2.7  |
| 1   | M     | 130 | LYS  | 2.7  |
| 1   | E     | 17  | VAL  | 2.7  |
| 1   | H     | 54  | GLU  | 2.7  |
| 1   | I     | 204 | GLY  | 2.7  |
| 1   | E     | 150 | LEU  | 2.7  |
| 1   | I     | 177 | LEU  | 2.7  |
| 1   | R     | 70  | LYS  | 2.7  |
| 1   | E     | 55  | HIS  | 2.7  |
| 1   | E     | 140 | HIS  | 2.7  |
| 1   | D     | 82  | TYR  | 2.7  |
| 1   | W     | 189 | ILE  | 2.7  |
| 1   | H     | 20  | THR  | 2.7  |
| 1   | P     | 176 | THR  | 2.7  |
| 1   | G     | 63  | ALA  | 2.7  |
| 1   | N     | 77  | VAL  | 2.7  |
| 1   | M     | 68  | GLY  | 2.7  |
| 1   | O     | 174 | LEU  | 2.7  |
| 1   | D     | 108 | ILE  | 2.7  |
| 1   | C     | 80  | THR  | 2.7  |
| 1   | I     | 56  | ASP  | 2.7  |
| 1   | J     | 132 | ASP  | 2.7  |
| 1   | O     | 157 | ASP  | 2.7  |
| 1   | Q     | 91  | ASP  | 2.7  |
| 1   | B     | 167 | ILE  | 2.7  |
| 1   | G     | 59  | TYR  | 2.7  |
| 1   | J     | 45  | ALA  | 2.6  |
| 1   | P     | 85  | PRO  | 2.6  |
| 1   | W     | 55  | HIS  | 2.6  |
| 1   | J     | 28  | LEU  | 2.6  |
| 1   | Y     | 51  | LEU  | 2.6  |
| 1   | J     | 47  | PHE  | 2.6  |
| 1   | R     | 59  | TYR  | 2.6  |
| 1   | B     | 119 | ALA  | 2.6  |
| 1   | C     | 191 | GLY  | 2.6  |
| 1   | W     | 72  | ALA  | 2.6  |
| 1   | I     | 140 | HIS  | 2.6  |
| 1   | M     | 222 | VAL  | 2.6  |

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| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 1   | F     | 73    | LYS  | 2.6  |
| 1   | H     | 224   | LYS  | 2.6  |
| 1   | T     | 66    | ARG  | 2.6  |
| 1   | J     | 35    | LEU  | 2.6  |
| 1   | I     | 71    | ASP  | 2.6  |
| 1   | O     | 43    | GLN  | 2.6  |
| 1   | L     | 173   | SER  | 2.6  |
| 1   | O     | 127   | SER  | 2.6  |
| 1   | J     | 32    | ILE  | 2.6  |
| 1   | G     | 146   | LYS  | 2.6  |
| 1   | H     | 73    | LYS  | 2.6  |
| 1   | I     | 26    | GLU  | 2.6  |
| 1   | L     | 203   | PRO  | 2.6  |
| 1   | R     | 8     | ALA  | 2.6  |
| 1   | X     | 52    | ALA  | 2.6  |
| 1   | K     | 87[A] | CYS  | 2.6  |
| 1   | X     | 87    | CYS  | 2.6  |
| 1   | F     | 106   | VAL  | 2.6  |
| 1   | G     | 21    | LEU  | 2.6  |
| 1   | X     | 113   | PHE  | 2.6  |
| 1   | F     | 53    | SER  | 2.6  |
| 1   | J     | 221   | LYS  | 2.6  |
| 1   | O     | 188   | GLY  | 2.6  |
| 1   | F     | 59    | TYR  | 2.6  |
| 1   | V     | 102   | PRO  | 2.6  |
| 1   | K     | 75    | VAL  | 2.6  |
| 1   | X     | 13    | VAL  | 2.6  |
| 1   | N     | 43    | GLN  | 2.6  |
| 1   | I     | 175   | LYS  | 2.6  |
| 1   | E     | 184   | SER  | 2.6  |
| 1   | Q     | 204   | GLY  | 2.6  |
| 1   | C     | 85    | PRO  | 2.6  |
| 1   | M     | 192   | THR  | 2.6  |
| 1   | C     | 86    | TYR  | 2.6  |
| 1   | Y     | 44    | GLN  | 2.6  |
| 1   | I     | 111   | LEU  | 2.6  |
| 1   | J     | 212   | GLU  | 2.6  |
| 1   | O     | 23    | SER  | 2.6  |
| 1   | Q     | 66    | ARG  | 2.6  |
| 1   | P     | 92    | PRO  | 2.6  |
| 1   | M     | 46    | GLN  | 2.6  |
| 1   | Q     | 72    | ALA  | 2.6  |

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| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 1   | P     | 39    | LYS  | 2.6  |
| 1   | T     | 46    | GLN  | 2.6  |
| 1   | L     | 104   | VAL  | 2.6  |
| 1   | Y     | 196   | VAL  | 2.6  |
| 1   | H     | 174   | LEU  | 2.6  |
| 1   | G     | 203   | PRO  | 2.5  |
| 1   | V     | 170   | THR  | 2.5  |
| 1   | Y     | 83    | ASN  | 2.5  |
| 1   | B     | 57    | ALA  | 2.5  |
| 1   | J     | 30    | GLU  | 2.5  |
| 1   | P     | 59    | TYR  | 2.5  |
| 1   | Q     | 75    | VAL  | 2.5  |
| 1   | G     | 223   | LYS  | 2.5  |
| 1   | J     | 216   | LYS  | 2.5  |
| 1   | R     | 39    | LYS  | 2.5  |
| 1   | X     | 123   | GLN  | 2.5  |
| 1   | C     | 214   | ILE  | 2.5  |
| 1   | G     | 29    | GLU  | 2.5  |
| 1   | J     | 20    | THR  | 2.5  |
| 1   | W     | 50    | ALA  | 2.5  |
| 1   | N     | 185   | ARG  | 2.5  |
| 1   | X     | 70    | LYS  | 2.5  |
| 1   | J     | 220   | ALA  | 2.5  |
| 1   | W     | 19    | ASP  | 2.5  |
| 1   | X     | 80    | THR  | 2.5  |
| 1   | G     | 77    | VAL  | 2.5  |
| 1   | Q     | 88[A] | LYS  | 2.5  |
| 1   | I     | 100   | GLN  | 2.5  |
| 1   | I     | 145   | GLN  | 2.5  |
| 1   | E     | 102   | PRO  | 2.5  |
| 1   | G     | 214   | ILE  | 2.5  |
| 1   | I     | 195   | THR  | 2.5  |
| 1   | J     | 120   | LYS  | 2.5  |
| 1   | J     | 153   | ALA  | 2.5  |
| 1   | O     | 8     | ALA  | 2.5  |
| 1   | G     | 82    | TYR  | 2.5  |
| 1   | H     | 58    | LEU  | 2.5  |
| 1   | Y     | 111   | LEU  | 2.5  |
| 1   | I     | 79    | PHE  | 2.5  |
| 1   | U     | 154   | SER  | 2.5  |
| 1   | N     | 146   | LYS  | 2.5  |
| 1   | W     | 186   | LYS  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 135 | ALA  | 2.5  |
| 1   | G     | 14  | ARG  | 2.5  |
| 1   | G     | 107 | ILE  | 2.5  |
| 1   | M     | 124 | ALA  | 2.5  |
| 1   | O     | 66  | ARG  | 2.5  |
| 1   | O     | 93  | LEU  | 2.5  |
| 1   | E     | 75  | VAL  | 2.5  |
| 1   | E     | 82  | TYR  | 2.5  |
| 1   | G     | 10  | GLU  | 2.5  |
| 1   | R     | 26  | GLU  | 2.5  |
| 1   | X     | 83  | ASN  | 2.5  |
| 1   | X     | 71  | ASP  | 2.5  |
| 1   | E     | 15  | ALA  | 2.5  |
| 1   | X     | 135 | ALA  | 2.5  |
| 1   | L     | 187 | LEU  | 2.5  |
| 1   | P     | 9   | GLN  | 2.5  |
| 1   | U     | 219 | LEU  | 2.5  |
| 1   | W     | 12  | GLU  | 2.5  |
| 1   | Q     | 114 | LYS  | 2.5  |
| 1   | H     | 71  | ASP  | 2.5  |
| 1   | W     | 112 | PRO  | 2.5  |
| 1   | E     | 124 | ALA  | 2.5  |
| 1   | R     | 80  | THR  | 2.5  |
| 1   | L     | 137 | LEU  | 2.5  |
| 1   | X     | 96  | LYS  | 2.5  |
| 1   | T     | 215 | VAL  | 2.5  |
| 1   | P     | 142 | ARG  | 2.5  |
| 1   | F     | 224 | LYS  | 2.4  |
| 1   | P     | 20  | THR  | 2.4  |
| 1   | Q     | 219 | LEU  | 2.4  |
| 1   | R     | 197 | ILE  | 2.4  |
| 1   | U     | 16  | LEU  | 2.4  |
| 1   | V     | 51  | LEU  | 2.4  |
| 1   | B     | 125 | VAL  | 2.4  |
| 1   | M     | 13  | VAL  | 2.4  |
| 1   | O     | 152 | ASN  | 2.4  |
| 1   | X     | 156 | GLU  | 2.4  |
| 1   | Q     | 223 | LYS  | 2.4  |
| 1   | Y     | 73  | LYS  | 2.4  |
| 1   | N     | 200 | THR  | 2.4  |
| 1   | B     | 107 | ILE  | 2.4  |
| 1   | L     | 169 | LEU  | 2.4  |

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| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 1   | X     | 94    | LEU  | 2.4  |
| 1   | K     | 206   | VAL  | 2.4  |
| 1   | W     | 66    | ARG  | 2.4  |
| 1   | E     | 56    | ASP  | 2.4  |
| 1   | F     | 61    | ASP  | 2.4  |
| 1   | B     | 49    | GLN  | 2.4  |
| 1   | D     | 86    | TYR  | 2.4  |
| 1   | M     | 152   | ASN  | 2.4  |
| 1   | T     | 182   | GLU  | 2.4  |
| 1   | R     | 186   | LYS  | 2.4  |
| 1   | X     | 216   | LYS  | 2.4  |
| 1   | N     | 55    | HIS  | 2.4  |
| 1   | R     | 102   | PRO  | 2.4  |
| 1   | J     | 211   | LEU  | 2.4  |
| 1   | D     | 30    | GLU  | 2.4  |
| 1   | N     | 131   | GLU  | 2.4  |
| 1   | B     | 71    | ASP  | 2.4  |
| 1   | I     | 19    | ASP  | 2.4  |
| 1   | W     | 82    | TYR  | 2.4  |
| 1   | J     | 109   | LYS  | 2.4  |
| 1   | P     | 214   | ILE  | 2.4  |
| 1   | B     | 222   | VAL  | 2.4  |
| 1   | N     | 163   | ASN  | 2.4  |
| 1   | U     | 222   | VAL  | 2.4  |
| 1   | X     | 48    | ARG  | 2.4  |
| 1   | O     | 39    | LYS  | 2.4  |
| 1   | N     | 37    | THR  | 2.4  |
| 1   | L     | 208   | TYR  | 2.4  |
| 1   | M     | 217   | GLU  | 2.4  |
| 1   | M     | 138   | ALA  | 2.4  |
| 1   | Q     | 135   | ALA  | 2.4  |
| 1   | P     | 151   | ASP  | 2.4  |
| 1   | C     | 205   | ALA  | 2.4  |
| 1   | J     | 93    | LEU  | 2.4  |
| 1   | W     | 138   | ALA  | 2.4  |
| 1   | X     | 31    | ALA  | 2.4  |
| 1   | J     | 207   | ASP  | 2.4  |
| 1   | D     | 87[A] | CYS  | 2.4  |
| 1   | G     | 189   | ILE  | 2.4  |
| 1   | M     | 168   | LYS  | 2.4  |
| 1   | A     | 48    | ARG  | 2.4  |
| 1   | N     | 106   | VAL  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | R     | 129 | TRP  | 2.4  |
| 1   | N     | 203 | PRO  | 2.3  |
| 1   | E     | 35  | LEU  | 2.3  |
| 1   | G     | 103 | ASP  | 2.3  |
| 1   | I     | 127 | SER  | 2.3  |
| 1   | L     | 111 | LEU  | 2.3  |
| 1   | P     | 118 | SER  | 2.3  |
| 1   | Q     | 174 | LEU  | 2.3  |
| 1   | R     | 41  | ASP  | 2.3  |
| 1   | W     | 71  | ASP  | 2.3  |
| 1   | O     | 11  | LYS  | 2.3  |
| 1   | E     | 99  | GLU  | 2.3  |
| 1   | J     | 189 | ILE  | 2.3  |
| 1   | J     | 84  | CYS  | 2.3  |
| 1   | D     | 202 | LEU  | 2.3  |
| 1   | E     | 207 | ASP  | 2.3  |
| 1   | Q     | 151 | ASP  | 2.3  |
| 1   | L     | 122 | SER  | 2.3  |
| 1   | G     | 217 | GLU  | 2.3  |
| 1   | Q     | 68  | GLY  | 2.3  |
| 1   | R     | 104 | VAL  | 2.3  |
| 1   | F     | 55  | HIS  | 2.3  |
| 1   | J     | 133 | PRO  | 2.3  |
| 1   | I     | 53  | SER  | 2.3  |
| 1   | M     | 188 | GLY  | 2.3  |
| 1   | N     | 51  | LEU  | 2.3  |
| 1   | O     | 208 | TYR  | 2.3  |
| 1   | X     | 191 | GLY  | 2.3  |
| 1   | A     | 162 | THR  | 2.3  |
| 1   | O     | 83  | ASN  | 2.3  |
| 1   | F     | 100 | GLN  | 2.3  |
| 1   | W     | 123 | GLN  | 2.3  |
| 1   | E     | 12  | GLU  | 2.3  |
| 1   | O     | 191 | GLY  | 2.3  |
| 1   | V     | 203 | PRO  | 2.3  |
| 1   | B     | 16  | LEU  | 2.3  |
| 1   | F     | 21  | LEU  | 2.3  |
| 1   | F     | 51  | LEU  | 2.3  |
| 1   | B     | 52  | ALA  | 2.3  |
| 1   | N     | 44  | GLN  | 2.3  |
| 1   | Y     | 155 | ILE  | 2.3  |
| 1   | G     | 48  | ARG  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | N     | 19  | ASP  | 2.3  |
| 1   | N     | 91  | ASP  | 2.3  |
| 1   | N     | 74  | LEU  | 2.3  |
| 1   | R     | 150 | LEU  | 2.3  |
| 1   | V     | 184 | SER  | 2.3  |
| 1   | N     | 83  | ASN  | 2.3  |
| 1   | K     | 213 | ILE  | 2.3  |
| 1   | D     | 13  | VAL  | 2.3  |
| 1   | E     | 116 | GLU  | 2.3  |
| 1   | V     | 114 | LYS  | 2.3  |
| 1   | V     | 60  | ASN  | 2.3  |
| 1   | J     | 31  | ALA  | 2.3  |
| 1   | L     | 200 | THR  | 2.3  |
| 1   | D     | 156 | GLU  | 2.3  |
| 1   | H     | 125 | VAL  | 2.3  |
| 1   | J     | 13  | VAL  | 2.3  |
| 1   | E     | 109 | LYS  | 2.3  |
| 1   | V     | 221 | LYS  | 2.3  |
| 1   | X     | 103 | ASP  | 2.3  |
| 1   | X     | 186 | LYS  | 2.3  |
| 1   | A     | 55  | HIS  | 2.3  |
| 1   | E     | 165 | SER  | 2.3  |
| 1   | F     | 174 | LEU  | 2.3  |
| 1   | J     | 111 | LEU  | 2.3  |
| 1   | L     | 152 | ASN  | 2.3  |
| 1   | M     | 165 | SER  | 2.3  |
| 1   | T     | 49  | GLN  | 2.3  |
| 1   | F     | 63  | ALA  | 2.3  |
| 1   | E     | 136 | PHE  | 2.3  |
| 1   | L     | 107 | ILE  | 2.3  |
| 1   | E     | 196 | VAL  | 2.3  |
| 1   | K     | 17  | VAL  | 2.3  |
| 1   | R     | 49  | GLN  | 2.2  |
| 1   | D     | 76  | LEU  | 2.2  |
| 1   | K     | 133 | PRO  | 2.2  |
| 1   | O     | 85  | PRO  | 2.2  |
| 1   | Y     | 112 | PRO  | 2.2  |
| 1   | X     | 212 | GLU  | 2.2  |
| 1   | N     | 192 | THR  | 2.2  |
| 1   | A     | 214 | ILE  | 2.2  |
| 1   | O     | 13  | VAL  | 2.2  |
| 1   | N     | 36  | GLN  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | H     | 24  | ASN  | 2.2  |
| 1   | O     | 129 | TRP  | 2.2  |
| 1   | W     | 95  | GLU  | 2.2  |
| 1   | T     | 31  | ALA  | 2.2  |
| 1   | F     | 148 | THR  | 2.2  |
| 1   | O     | 145 | GLN  | 2.2  |
| 1   | J     | 150 | LEU  | 2.2  |
| 1   | E     | 98  | THR  | 2.2  |
| 1   | H     | 192 | THR  | 2.2  |
| 1   | D     | 47  | PHE  | 2.2  |
| 1   | E     | 191 | GLY  | 2.2  |
| 1   | J     | 113 | PHE  | 2.2  |
| 1   | F     | 214 | ILE  | 2.2  |
| 1   | N     | 213 | ILE  | 2.2  |
| 1   | N     | 184 | SER  | 2.2  |
| 1   | C     | 74  | LEU  | 2.2  |
| 1   | G     | 18  | ARG  | 2.2  |
| 1   | P     | 76  | LEU  | 2.2  |
| 1   | T     | 150 | LEU  | 2.2  |
| 1   | V     | 72  | ALA  | 2.2  |
| 1   | P     | 37  | THR  | 2.2  |
| 1   | L     | 30  | GLU  | 2.2  |
| 1   | O     | 204 | GLY  | 2.2  |
| 1   | I     | 134 | LYS  | 2.2  |
| 1   | N     | 113 | PHE  | 2.2  |
| 1   | C     | 125 | VAL  | 2.2  |
| 1   | X     | 22  | VAL  | 2.2  |
| 1   | F     | 66  | ARG  | 2.2  |
| 1   | D     | 94  | LEU  | 2.2  |
| 1   | P     | 146 | LYS  | 2.2  |
| 1   | R     | 44  | GLN  | 2.2  |
| 1   | Y     | 194 | ALA  | 2.2  |
| 1   | A     | 73  | LYS  | 2.2  |
| 1   | M     | 42  | GLU  | 2.2  |
| 1   | W     | 192 | THR  | 2.2  |
| 1   | L     | 161 | SER  | 2.2  |
| 1   | N     | 64  | SER  | 2.2  |
| 1   | W     | 125 | VAL  | 2.2  |
| 1   | I     | 143 | LEU  | 2.2  |
| 1   | M     | 58  | LEU  | 2.2  |
| 1   | R     | 207 | ASP  | 2.2  |
| 1   | W     | 205 | ALA  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | V     | 80  | THR  | 2.2  |
| 1   | V     | 148 | THR  | 2.2  |
| 1   | A     | 14  | ARG  | 2.2  |
| 1   | X     | 14  | ARG  | 2.2  |
| 1   | R     | 82  | TYR  | 2.2  |
| 1   | G     | 155 | ILE  | 2.2  |
| 1   | V     | 201 | ILE  | 2.2  |
| 1   | A     | 187 | LEU  | 2.2  |
| 1   | C     | 76  | LEU  | 2.2  |
| 1   | E     | 93  | LEU  | 2.2  |
| 1   | N     | 166 | LYS  | 2.2  |
| 1   | R     | 146 | LYS  | 2.2  |
| 1   | H     | 193 | PRO  | 2.2  |
| 1   | R     | 169 | LEU  | 2.2  |
| 1   | G     | 172 | ASP  | 2.2  |
| 1   | K     | 71  | ASP  | 2.2  |
| 1   | A     | 45  | ALA  | 2.2  |
| 1   | X     | 158 | ALA  | 2.2  |
| 1   | R     | 89  | ARG  | 2.2  |
| 1   | G     | 47  | PHE  | 2.2  |
| 1   | E     | 222 | VAL  | 2.1  |
| 1   | O     | 213 | ILE  | 2.1  |
| 1   | T     | 97  | ILE  | 2.1  |
| 1   | X     | 196 | VAL  | 2.1  |
| 1   | O     | 51  | LEU  | 2.1  |
| 1   | O     | 111 | LEU  | 2.1  |
| 1   | O     | 137 | LEU  | 2.1  |
| 1   | P     | 190 | GLN  | 2.1  |
| 1   | Q     | 92  | PRO  | 2.1  |
| 1   | R     | 71  | ASP  | 2.1  |
| 1   | J     | 119 | ALA  | 2.1  |
| 1   | O     | 62  | ALA  | 2.1  |
| 1   | P     | 49  | GLN  | 2.1  |
| 1   | R     | 127 | SER  | 2.1  |
| 1   | F     | 128 | VAL  | 2.1  |
| 1   | R     | 128 | VAL  | 2.1  |
| 1   | V     | 210 | GLN  | 2.1  |
| 1   | J     | 203 | PRO  | 2.1  |
| 1   | M     | 139 | LEU  | 2.1  |
| 1   | T     | 126 | LEU  | 2.1  |
| 1   | A     | 209 | ASP  | 2.1  |
| 1   | M     | 171 | ASP  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 89  | ARG  | 2.1  |
| 1   | L     | 166 | LYS  | 2.1  |
| 1   | M     | 63  | ALA  | 2.1  |
| 1   | G     | 156 | GLU  | 2.1  |
| 1   | Q     | 67  | ILE  | 2.1  |
| 1   | X     | 101 | TYR  | 2.1  |
| 1   | H     | 28  | LEU  | 2.1  |
| 1   | I     | 199 | ASP  | 2.1  |
| 1   | J     | 183 | LEU  | 2.1  |
| 1   | M     | 177 | LEU  | 2.1  |
| 1   | V     | 143 | LEU  | 2.1  |
| 1   | X     | 28  | LEU  | 2.1  |
| 1   | H     | 14  | ARG  | 2.1  |
| 1   | M     | 85  | PRO  | 2.1  |
| 1   | N     | 112 | PRO  | 2.1  |
| 1   | H     | 168 | LYS  | 2.1  |
| 1   | W     | 11  | LYS  | 2.1  |
| 1   | C     | 119 | ALA  | 2.1  |
| 1   | G     | 7   | ALA  | 2.1  |
| 1   | P     | 62  | ALA  | 2.1  |
| 1   | U     | 220 | ALA  | 2.1  |
| 1   | Y     | 192 | THR  | 2.1  |
| 1   | G     | 90  | PHE  | 2.1  |
| 1   | R     | 180 | ASN  | 2.1  |
| 1   | L     | 86  | TYR  | 2.1  |
| 1   | R     | 172 | ASP  | 2.1  |
| 1   | V     | 157 | ASP  | 2.1  |
| 1   | W     | 124 | ALA  | 2.1  |
| 1   | I     | 80  | THR  | 2.1  |
| 1   | R     | 176 | THR  | 2.1  |
| 1   | I     | 38  | LYS  | 2.1  |
| 1   | W     | 168 | LYS  | 2.1  |
| 1   | M     | 35  | LEU  | 2.1  |
| 1   | O     | 143 | LEU  | 2.1  |
| 1   | X     | 75  | VAL  | 2.1  |
| 1   | L     | 85  | PRO  | 2.1  |
| 1   | Y     | 203 | PRO  | 2.1  |
| 1   | C     | 15  | ALA  | 2.1  |
| 1   | J     | 8   | ALA  | 2.1  |
| 1   | J     | 168 | LYS  | 2.1  |
| 1   | M     | 24  | ASN  | 2.1  |
| 1   | N     | 11  | LYS  | 2.1  |

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| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 1   | T     | 37    | THR  | 2.1  |
| 1   | D     | 23    | SER  | 2.1  |
| 1   | I     | 89    | ARG  | 2.1  |
| 1   | M     | 18    | ARG  | 2.1  |
| 1   | Q     | 165   | SER  | 2.1  |
| 1   | R     | 161   | SER  | 2.1  |
| 1   | Y     | 142   | ARG  | 2.1  |
| 1   | X     | 140   | HIS  | 2.1  |
| 1   | O     | 84[A] | CYS  | 2.1  |
| 1   | U     | 193   | PRO  | 2.1  |
| 1   | B     | 145   | GLN  | 2.1  |
| 1   | D     | 46    | GLN  | 2.1  |
| 1   | U     | 205   | ALA  | 2.1  |
| 1   | T     | 192   | THR  | 2.1  |
| 1   | X     | 66    | ARG  | 2.1  |
| 1   | K     | 171   | ASP  | 2.1  |
| 1   | I     | 17    | VAL  | 2.1  |
| 1   | Q     | 21    | LEU  | 2.1  |
| 1   | Q     | 108   | ILE  | 2.1  |
| 1   | W     | 222   | VAL  | 2.1  |
| 1   | H     | 96    | LYS  | 2.1  |
| 1   | H     | 186   | LYS  | 2.1  |
| 1   | T     | 88[A] | LYS  | 2.1  |
| 1   | P     | 57    | ALA  | 2.1  |
| 1   | V     | 105   | ALA  | 2.1  |
| 1   | W     | 121   | ALA  | 2.1  |
| 1   | M     | 185   | ARG  | 2.1  |
| 1   | H     | 199   | ASP  | 2.1  |
| 1   | L     | 23    | SER  | 2.1  |
| 1   | P     | 122   | SER  | 2.1  |
| 1   | V     | 192   | THR  | 2.1  |
| 1   | X     | 217   | GLU  | 2.1  |
| 1   | A     | 28    | LEU  | 2.0  |
| 1   | A     | 166   | LYS  | 2.0  |
| 1   | E     | 177   | LEU  | 2.0  |
| 1   | H     | 137   | LEU  | 2.0  |
| 1   | O     | 73    | LYS  | 2.0  |
| 1   | T     | 70    | LYS  | 2.0  |
| 1   | O     | 128   | VAL  | 2.0  |
| 1   | W     | 77    | VAL  | 2.0  |
| 1   | K     | 167   | ILE  | 2.0  |
| 1   | R     | 18    | ARG  | 2.0  |

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| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 1   | B     | 151   | ASP  | 2.0  |
| 1   | L     | 41    | ASP  | 2.0  |
| 1   | T     | 19    | ASP  | 2.0  |
| 1   | K     | 147   | LYS  | 2.0  |
| 1   | E     | 44    | GLN  | 2.0  |
| 1   | N     | 150   | LEU  | 2.0  |
| 1   | W     | 143   | LEU  | 2.0  |
| 1   | O     | 158   | ALA  | 2.0  |
| 1   | E     | 120   | LYS  | 2.0  |
| 1   | H     | 184   | SER  | 2.0  |
| 1   | E     | 43    | GLN  | 2.0  |
| 1   | M     | 100   | GLN  | 2.0  |
| 1   | B     | 5     | LEU  | 2.0  |
| 1   | W     | 137   | LEU  | 2.0  |
| 1   | E     | 112   | PRO  | 2.0  |
| 1   | W     | 142   | ARG  | 2.0  |
| 1   | Y     | 89    | ARG  | 2.0  |
| 1   | H     | 155   | ILE  | 2.0  |
| 1   | H     | 213   | ILE  | 2.0  |
| 1   | G     | 24    | ASN  | 2.0  |
| 1   | P     | 134   | LYS  | 2.0  |
| 1   | L     | 198   | GLY  | 2.0  |
| 1   | P     | 194   | ALA  | 2.0  |
| 1   | E     | 36    | GLN  | 2.0  |
| 1   | U     | 165   | SER  | 2.0  |
| 1   | X     | 173   | SER  | 2.0  |
| 1   | V     | 84[A] | CYS  | 2.0  |
| 1   | Q     | 76    | LEU  | 2.0  |
| 1   | Y     | 48    | ARG  | 2.0  |
| 1   | I     | 168   | LYS  | 2.0  |
| 1   | J     | 77    | VAL  | 2.0  |
| 1   | M     | 114   | LYS  | 2.0  |
| 1   | U     | 175   | LYS  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.