



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:35 AM GMT

PDB ID : 2R6C  
Title : Crystal Form BH2  
Authors : Bailey, S.; Eliason, W.K.; Steitz, T.A.  
Deposited on : 2007-09-05  
Resolution : 4.00 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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

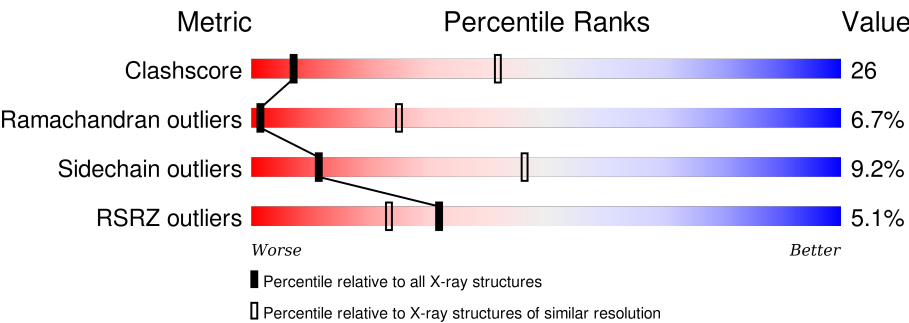
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore            | 102246                      | 1052 (4.40-3.60)                                      |
| Ramachandran outliers | 100387                      | 1005 (4.40-3.60)                                      |
| Sidechain outliers    | 100360                      | 1013 (4.42-3.58)                                      |
| RSRZ outliers         | 91569                       | 1013 (4.42-3.56)                                      |

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     | 454    | <div><div>3%</div><div><div></div><div>46%</div><div>25%</div><div>7%</div><div>•</div><div>21%</div></div></div> |
| 1   | B     | 454    | <div><div>4%</div><div><div></div><div>44%</div><div>27%</div><div>7%</div><div>•</div><div>21%</div></div></div> |
| 1   | C     | 454    | <div><div>3%</div><div><div></div><div>45%</div><div>25%</div><div>8%</div><div>•</div><div>21%</div></div></div> |
| 1   | D     | 454    | <div><div>3%</div><div><div></div><div>42%</div><div>28%</div><div>8%</div><div>•</div><div>21%</div></div></div> |
| 1   | E     | 454    | <div><div>4%</div><div><div></div><div>46%</div><div>25%</div><div>8%</div><div>•</div><div>21%</div></div></div> |
| 1   | F     | 454    | <div><div>9%</div><div><div></div><div>48%</div><div>24%</div><div>6%</div><div>•</div><div>21%</div></div></div> |
| 2   | G     | 143    | <div><div>%</div><div><div></div><div>59%</div><div>29%</div><div>8%</div><div>• •</div></div></div>              |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 2   | H     | 143    | <div><div><div>3%</div><div>54%</div><div>34%</div><div>8%</div><div></div></div></div> |
| 2   | I     | 143    | <div><div><div>3%</div><div>52%</div><div>36%</div><div>8%</div><div></div></div></div> |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19920 atoms, of which 0 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 Replicative helicase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 358      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2759  | 1737 | 473 | 536 | 13 |         |         |       |
| 1   | B     | 358      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2759  | 1737 | 473 | 536 | 13 |         |         |       |
| 1   | C     | 358      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2759  | 1737 | 473 | 536 | 13 |         |         |       |
| 1   | D     | 358      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2759  | 1737 | 473 | 536 | 13 |         |         |       |
| 1   | E     | 358      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2759  | 1737 | 473 | 536 | 13 |         |         |       |
| 1   | F     | 358      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2759  | 1737 | 473 | 536 | 13 |         |         |       |

- Molecule 2 is a protein called DnaG Primase, Helicase Binding Domain.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 2   | G     | 138      | Total | C   | N   | O   | Se | 0       | 0       | 0     |
|     |       |          | 1122  | 712 | 199 | 205 | 6  |         |         |       |
| 2   | H     | 138      | Total | C   | N   | O   | Se | 0       | 0       | 0     |
|     |       |          | 1122  | 712 | 199 | 205 | 6  |         |         |       |
| 2   | I     | 138      | Total | C   | N   | O   | Se | 0       | 0       | 0     |
|     |       |          | 1122  | 712 | 199 | 205 | 6  |         |         |       |

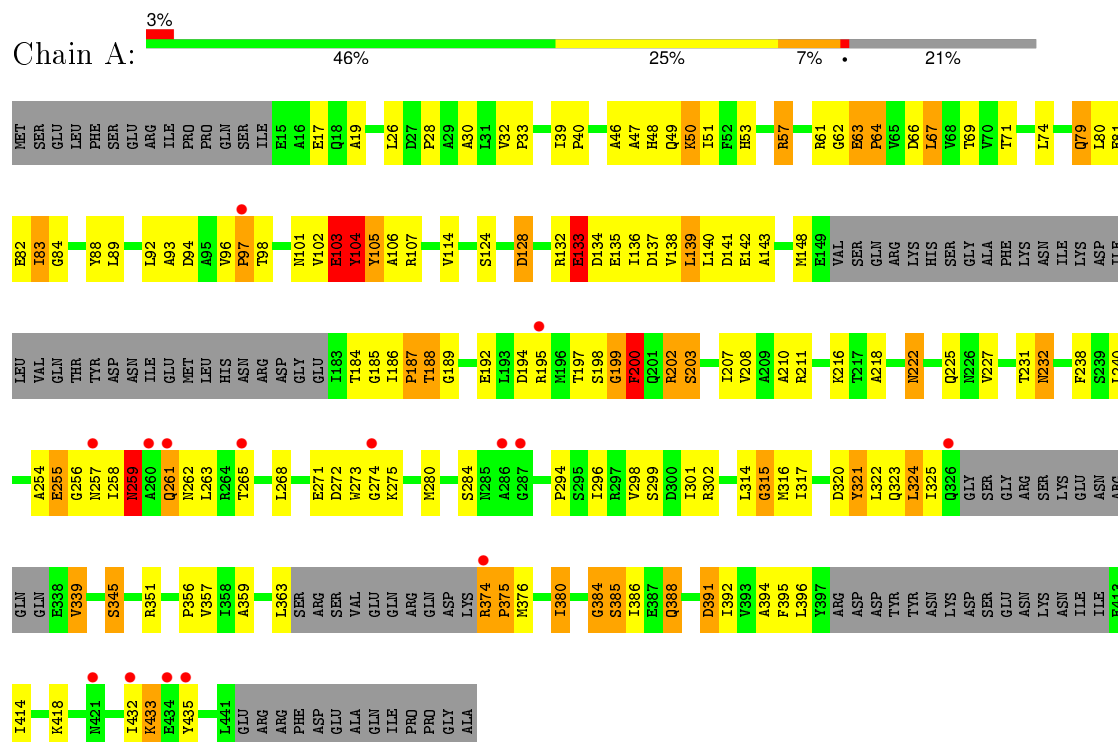
There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| G     | 530     | GLU      | ASP    | CONFLICT | UNP Q9X4D0 |
| G     | 531     | LEU      | VAL    | CONFLICT | UNP Q9X4D0 |
| H     | 530     | GLU      | ASP    | CONFLICT | UNP Q9X4D0 |
| H     | 531     | LEU      | VAL    | CONFLICT | UNP Q9X4D0 |
| I     | 530     | GLU      | ASP    | CONFLICT | UNP Q9X4D0 |
| I     | 531     | LEU      | VAL    | CONFLICT | UNP Q9X4D0 |

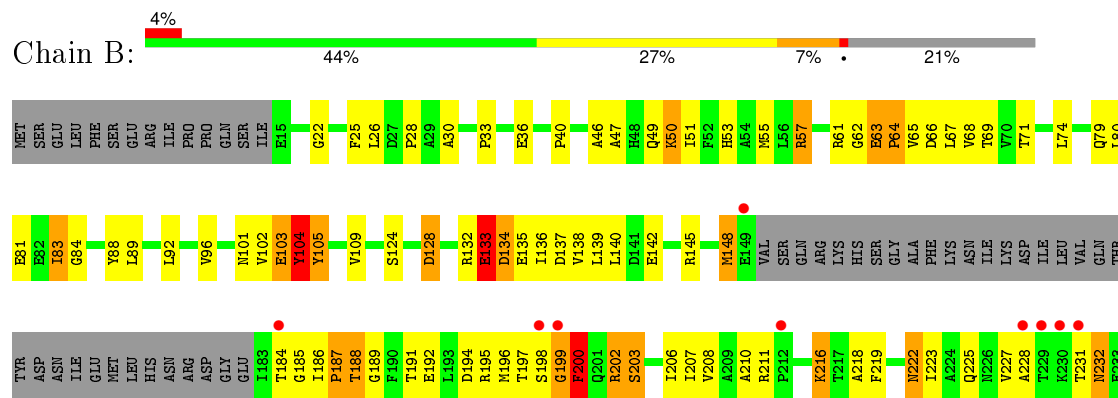
### 3 Residue-property plots

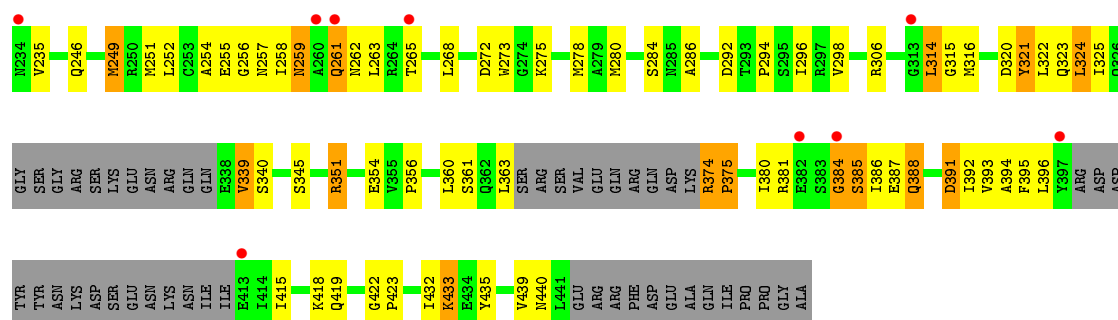
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Replicative helicase

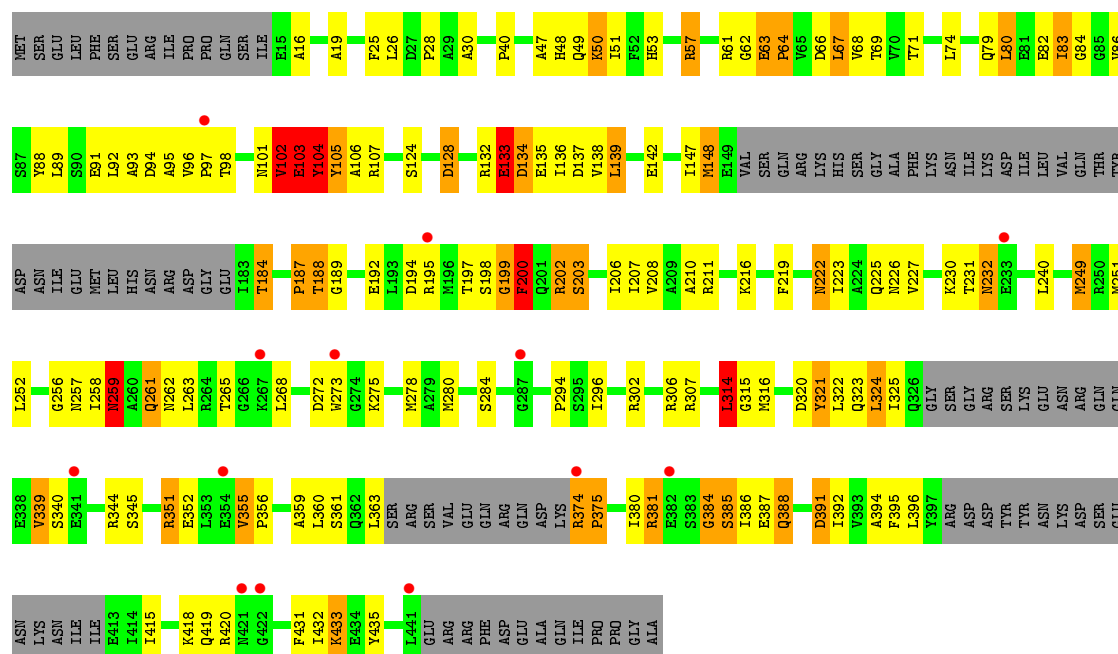
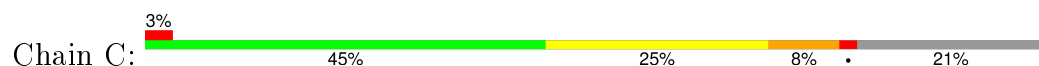


#### • Molecule 1: Replicative helicase

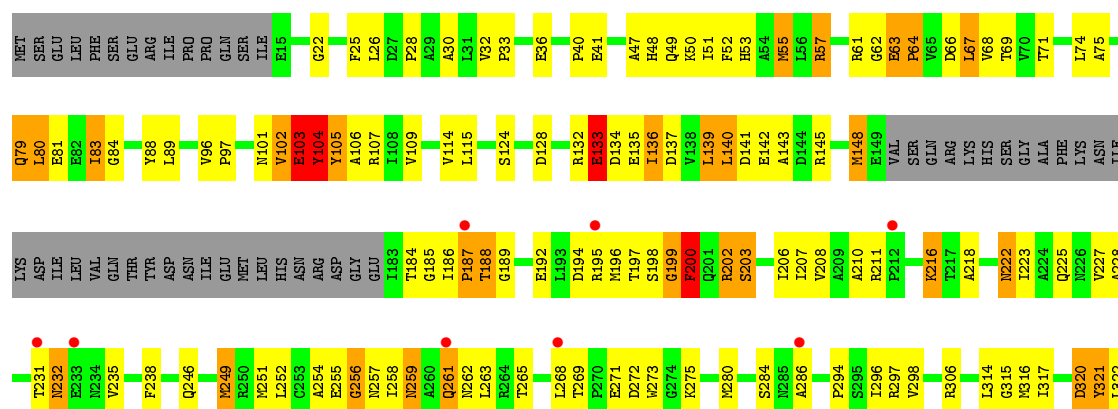
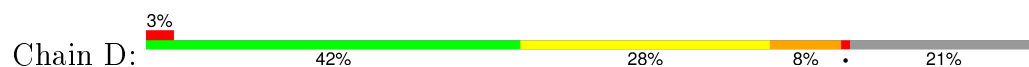


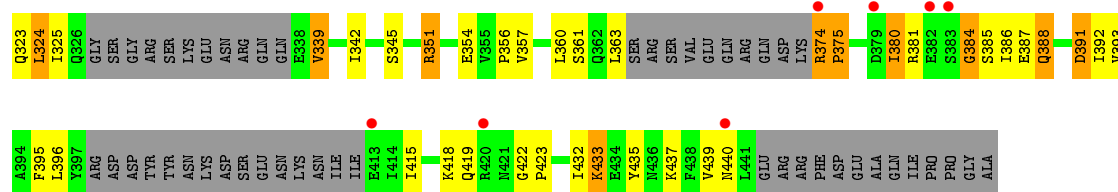


• Molecule 1: Replicative helicase

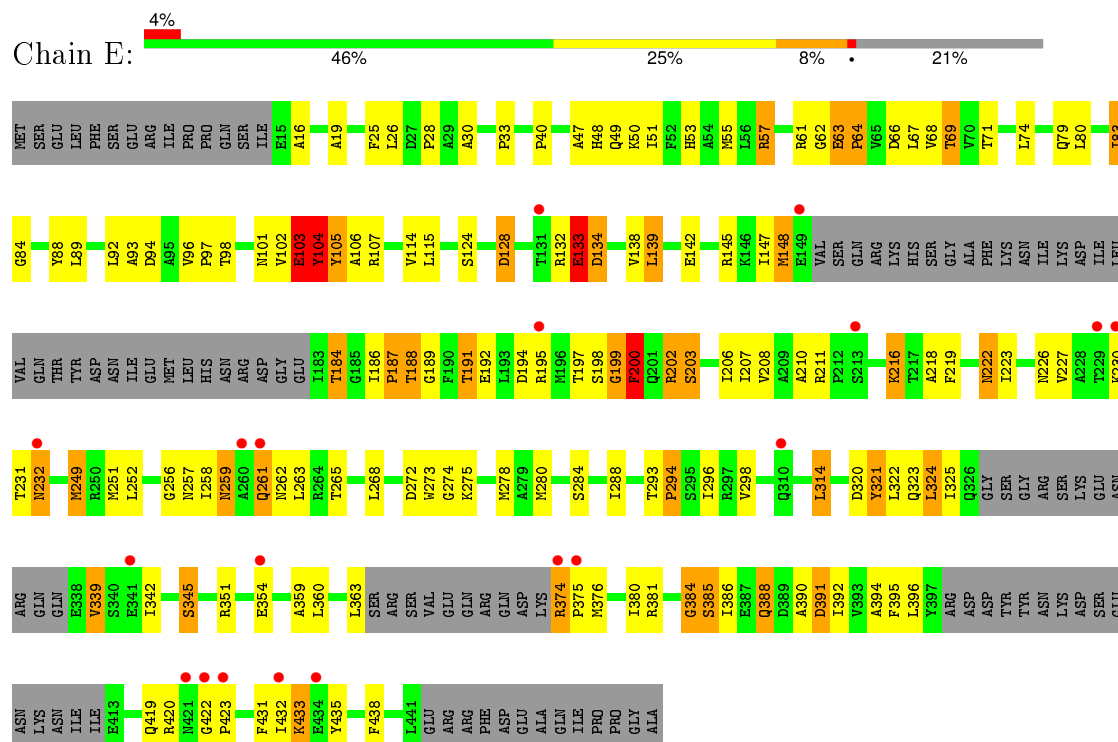


• Molecule 1: Replicative helicase

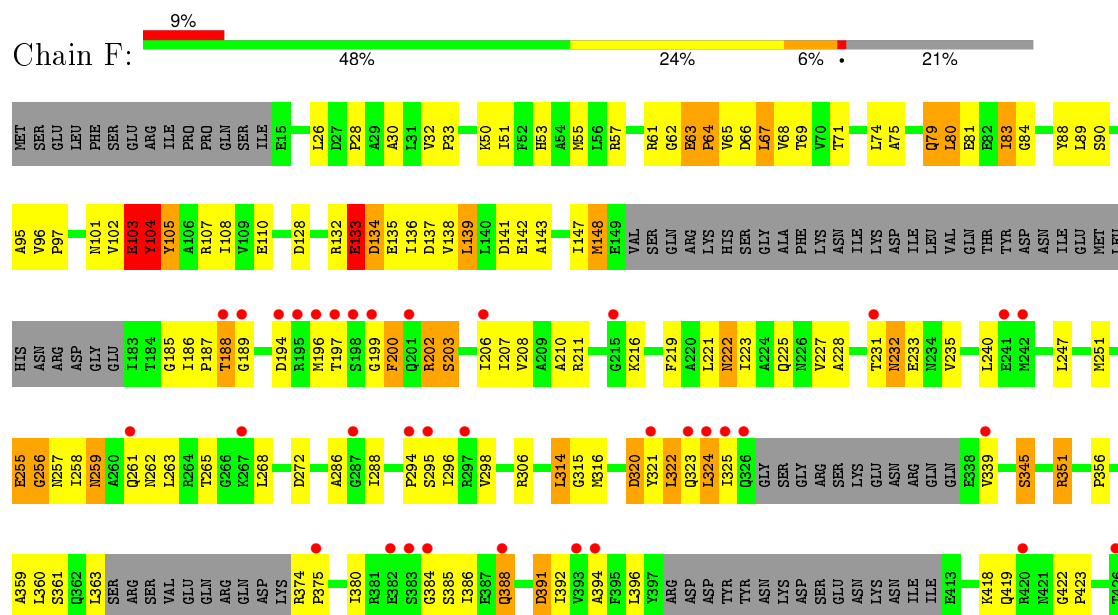


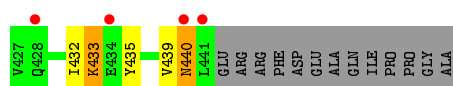


### • Molecule 1: Replicative helicase

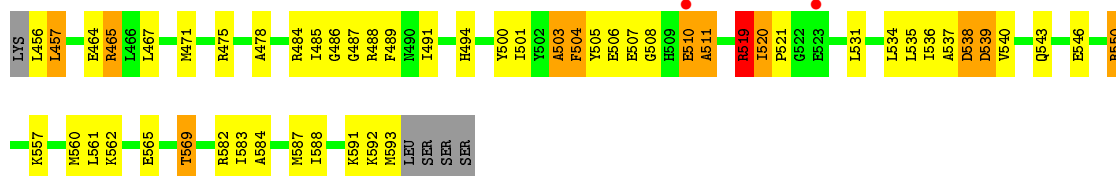


### • Molecule 1: Replicative helicase

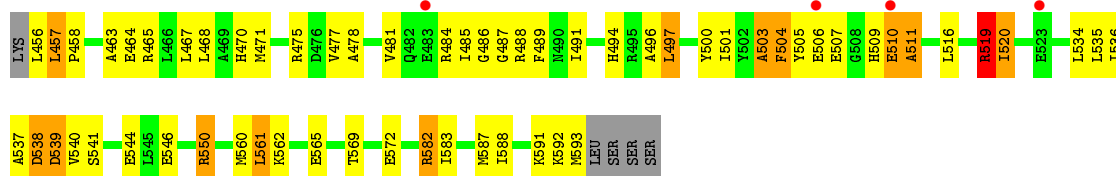




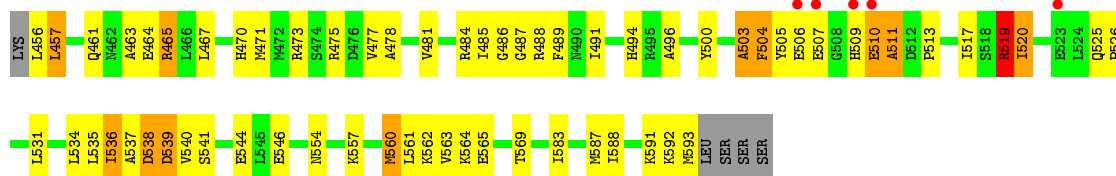
• Molecule 2: DnaG Primase, Helicase Binding Domain



• Molecule 2: DnaG Primase, Helicase Binding Domain



• Molecule 2: DnaG Primase, Helicase Binding Domain





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 31 2 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 228.78Å 228.78Å 192.98Å<br>90.00° 90.00° 120.00°            | Depositor        |
| Resolution (Å)  | 20.00 – 4.00<br>19.98 – 4.00                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 90.8 (20.00-4.00)<br>90.8 (19.98-4.00)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | 0.10  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 4.60 (at 4.07Å)   | Xtriage          |
| Refinement program  | REFMAC 5.2  | Depositor        |
| R, $R_{free}$   | 0.320 , 0.344<br>0.310 , (Not available)                    | Depositor<br>DCC |
| $R_{free}$ test set   | No test flags present.                                      | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 127.3   | Xtriage          |
| Anisotropy  | 0.073   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.26 , 176.0  | EDS              |
| Estimated twinning fraction   | 0.037 for -h,-k,l   | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$ | Xtriage          |
| Outliers  | 1 of 44598 reflections (0.002%)                             | Xtriage          |
| $F_o, F_c$ correlation  | 0.86  | EDS              |
| Total number of atoms   | 19920   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 166.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<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     | 0.51         | 0/2789      | 0.79        | 7/3770 (0.2%)   |
| 1   | B     | 0.47         | 0/2789      | 0.78        | 4/3770 (0.1%)   |
| 1   | C     | 0.51         | 0/2789      | 0.81        | 7/3770 (0.2%)   |
| 1   | D     | 0.51         | 0/2789      | 0.79        | 6/3770 (0.2%)   |
| 1   | E     | 0.50         | 0/2789      | 0.80        | 8/3770 (0.2%)   |
| 1   | F     | 0.47         | 0/2789      | 0.76        | 3/3770 (0.1%)   |
| 2   | G     | 0.42         | 0/1134      | 0.70        | 1/1514 (0.1%)   |
| 2   | H     | 0.47         | 0/1134      | 0.71        | 1/1514 (0.1%)   |
| 2   | I     | 0.42         | 0/1134      | 0.69        | 1/1514 (0.1%)   |
| All | All   | 0.49         | 0/20136     | 0.77        | 38/27162 (0.1%) |

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   | A     | 1                   | 5                   |
| 1   | B     | 1                   | 3                   |
| 1   | C     | 1                   | 5                   |
| 1   | D     | 2                   | 4                   |
| 1   | E     | 2                   | 4                   |
| 1   | F     | 1                   | 2                   |
| 2   | G     | 0                   | 1                   |
| 2   | H     | 0                   | 1                   |
| 2   | I     | 0                   | 1                   |
| All | All   | 8                   | 26                  |

There are no bond length outliers.

All (38) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2   | H     | 519 | ARG  | N-CA-C | 7.51 | 131.28      | 111.00   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | I     | 519 | ARG  | N-CA-C   | 7.41  | 131.01      | 111.00   |
| 2   | G     | 519 | ARG  | N-CA-C   | 7.37  | 130.89      | 111.00   |
| 1   | D     | 261 | GLN  | N-CA-C   | 6.80  | 129.35      | 111.00   |
| 1   | A     | 261 | GLN  | N-CA-C   | 6.45  | 128.43      | 111.00   |
| 1   | E     | 133 | GLU  | N-CA-C   | 6.38  | 128.21      | 111.00   |
| 1   | C     | 261 | GLN  | N-CA-C   | 6.20  | 127.75      | 111.00   |
| 1   | A     | 133 | GLU  | N-CA-C   | 6.18  | 127.69      | 111.00   |
| 1   | B     | 133 | GLU  | N-CA-C   | 6.06  | 127.37      | 111.00   |
| 1   | E     | 261 | GLN  | N-CA-C   | 6.03  | 127.29      | 111.00   |
| 1   | F     | 133 | GLU  | N-CA-C   | 6.00  | 127.21      | 111.00   |
| 1   | B     | 261 | GLN  | N-CA-C   | 5.99  | 127.17      | 111.00   |
| 1   | C     | 104 | TYR  | CA-CB-CG | -5.96 | 102.08      | 113.40   |
| 1   | D     | 133 | GLU  | N-CA-C   | 5.93  | 127.02      | 111.00   |
| 1   | A     | 199 | GLY  | N-CA-C   | -5.93 | 98.28       | 113.10   |
| 1   | C     | 199 | GLY  | N-CA-C   | -5.93 | 98.28       | 113.10   |
| 1   | C     | 133 | GLU  | N-CA-C   | 5.87  | 126.83      | 111.00   |
| 1   | C     | 103 | GLU  | N-CA-C   | 5.85  | 126.80      | 111.00   |
| 1   | E     | 199 | GLY  | N-CA-C   | -5.82 | 98.55       | 113.10   |
| 1   | A     | 321 | TYR  | N-CA-C   | 5.79  | 126.64      | 111.00   |
| 1   | F     | 104 | TYR  | CA-CB-CG | -5.74 | 102.49      | 113.40   |
| 1   | E     | 184 | THR  | N-CA-C   | 5.72  | 126.45      | 111.00   |
| 1   | A     | 103 | GLU  | N-CA-C   | 5.65  | 126.26      | 111.00   |
| 1   | A     | 184 | THR  | N-CA-C   | 5.63  | 126.19      | 111.00   |
| 1   | E     | 104 | TYR  | CA-CB-CG | -5.54 | 102.87      | 113.40   |
| 1   | D     | 199 | GLY  | N-CA-C   | -5.54 | 99.26       | 113.10   |
| 1   | C     | 321 | TYR  | N-CA-C   | 5.45  | 125.72      | 111.00   |
| 1   | A     | 104 | TYR  | CA-CB-CG | -5.38 | 103.19      | 113.40   |
| 1   | E     | 321 | TYR  | N-CA-C   | 5.36  | 125.48      | 111.00   |
| 1   | D     | 321 | TYR  | N-CA-C   | 5.35  | 125.43      | 111.00   |
| 1   | B     | 199 | GLY  | N-CA-C   | -5.32 | 99.81       | 113.10   |
| 1   | D     | 104 | TYR  | CA-CB-CG | -5.32 | 103.30      | 113.40   |
| 1   | E     | 104 | TYR  | N-CA-CB  | 5.31  | 120.16      | 110.60   |
| 1   | D     | 103 | GLU  | N-CA-C   | 5.30  | 125.30      | 111.00   |
| 1   | C     | 184 | THR  | N-CA-C   | 5.21  | 125.08      | 111.00   |
| 1   | F     | 103 | GLU  | N-CA-C   | 5.19  | 125.01      | 111.00   |
| 1   | E     | 103 | GLU  | N-CA-C   | 5.16  | 124.92      | 111.00   |
| 1   | B     | 321 | TYR  | N-CA-C   | 5.04  | 124.62      | 111.00   |

All (8) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1   | A     | 104 | TYR  | CA   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1   | B     | 104 | TYR  | CA   |
| 1   | C     | 104 | TYR  | CA   |
| 1   | D     | 104 | TYR  | CA   |
| 1   | D     | 184 | THR  | CA   |
| 1   | E     | 104 | TYR  | CA   |
| 1   | E     | 184 | THR  | CA   |
| 1   | F     | 104 | TYR  | CA   |

All (26) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 103 | GLU  | Peptide |
| 1   | A     | 187 | PRO  | Peptide |
| 1   | A     | 259 | ASN  | Peptide |
| 1   | A     | 320 | ASP  | Peptide |
| 1   | A     | 374 | ARG  | Peptide |
| 1   | B     | 187 | PRO  | Peptide |
| 1   | B     | 320 | ASP  | Peptide |
| 1   | B     | 374 | ARG  | Peptide |
| 1   | C     | 103 | GLU  | Peptide |
| 1   | C     | 187 | PRO  | Peptide |
| 1   | C     | 259 | ASN  | Peptide |
| 1   | C     | 320 | ASP  | Peptide |
| 1   | C     | 374 | ARG  | Peptide |
| 1   | D     | 103 | GLU  | Peptide |
| 1   | D     | 187 | PRO  | Peptide |
| 1   | D     | 320 | ASP  | Peptide |
| 1   | D     | 374 | ARG  | Peptide |
| 1   | E     | 103 | GLU  | Peptide |
| 1   | E     | 187 | PRO  | Peptide |
| 1   | E     | 320 | ASP  | Peptide |
| 1   | E     | 374 | ARG  | Peptide |
| 1   | F     | 103 | GLU  | Peptide |
| 1   | F     | 320 | ASP  | Peptide |
| 2   | G     | 519 | ARG  | Peptide |
| 2   | H     | 519 | ARG  | Peptide |
| 2   | I     | 519 | ARG  | 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     | 2759  | 0        | 2806     | 160     | 0            |
| 1   | B     | 2759  | 0        | 2806     | 151     | 0            |
| 1   | C     | 2759  | 0        | 2805     | 163     | 0            |
| 1   | D     | 2759  | 0        | 2807     | 187     | 0            |
| 1   | E     | 2759  | 0        | 2806     | 162     | 0            |
| 1   | F     | 2759  | 0        | 2807     | 124     | 0            |
| 2   | G     | 1122  | 0        | 1144     | 62      | 0            |
| 2   | H     | 1122  | 0        | 1144     | 61      | 0            |
| 2   | I     | 1122  | 0        | 1144     | 56      | 0            |
| All | All   | 19920 | 0        | 20269    | 1051    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (1051) 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:A:255:GLU:O   | 1:A:257:ASN:N    | 1.60                     | 1.34              |
| 1:C:188:THR:OG1 | 1:C:194:ASP:OD1  | 1.52                     | 1.27              |
| 1:C:306:ARG:CZ  | 1:D:32:VAL:HG21  | 1.64                     | 1.26              |
| 1:D:255:GLU:O   | 1:D:257:ASN:N    | 1.70                     | 1.23              |
| 1:A:132:ARG:O   | 1:A:133:GLU:HB2  | 1.40                     | 1.20              |
| 1:E:188:THR:OG1 | 1:E:194:ASP:OD1  | 1.60                     | 1.16              |
| 1:D:188:THR:OG1 | 1:D:194:ASP:OD1  | 1.63                     | 1.14              |
| 1:B:132:ARG:O   | 1:B:133:GLU:HB2  | 1.46                     | 1.14              |
| 1:F:255:GLU:O   | 1:F:257:ASN:N    | 1.79                     | 1.14              |
| 1:C:227:VAL:O   | 1:C:231:THR:HG22 | 1.49                     | 1.13              |
| 2:H:475:ARG:NH1 | 2:H:505:TYR:HB2  | 1.64                     | 1.12              |
| 1:B:63:GLU:H    | 1:B:64:PRO:HA    | 0.99                     | 1.11              |
| 1:E:104:TYR:HE2 | 1:F:63:GLU:HB2   | 1.16                     | 1.10              |
| 1:D:63:GLU:H    | 1:D:64:PRO:HA    | 1.12                     | 1.08              |
| 1:C:132:ARG:O   | 1:C:133:GLU:HB2  | 1.43                     | 1.08              |
| 1:E:132:ARG:O   | 1:E:133:GLU:HB2  | 1.47                     | 1.07              |
| 1:F:132:ARG:O   | 1:F:133:GLU:HB2  | 1.50                     | 1.07              |
| 1:F:227:VAL:O   | 1:F:231:THR:HG22 | 1.56                     | 1.06              |
| 1:C:94:ASP:HB3  | 2:H:591:LYS:NZ   | 1.69                     | 1.06              |
| 1:E:63:GLU:H    | 1:E:64:PRO:HA    | 1.13                     | 1.06              |
| 1:D:132:ARG:HD2 | 1:D:139:LEU:HG   | 1.35                     | 1.05              |
| 1:F:188:THR:OG1 | 1:F:194:ASP:OD1  | 1.74                     | 1.05              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:63:GLU:N     | 1:D:64:PRO:HA    | 1.71                     | 1.05              |
| 1:B:227:VAL:O    | 1:B:231:THR:HG22 | 1.56                     | 1.05              |
| 1:A:227:VAL:O    | 1:A:231:THR:HG22 | 1.52                     | 1.05              |
| 1:D:132:ARG:O    | 1:D:133:GLU:HB2  | 1.50                     | 1.04              |
| 1:A:63:GLU:H     | 1:A:64:PRO:HA    | 1.18                     | 1.04              |
| 1:F:63:GLU:H     | 1:F:64:PRO:HA    | 1.17                     | 1.03              |
| 1:A:104:TYR:HE2  | 1:B:63:GLU:HB2   | 1.17                     | 1.03              |
| 1:C:104:TYR:CE2  | 1:D:63:GLU:HB2   | 1.93                     | 1.02              |
| 1:B:132:ARG:HD2  | 1:B:139:LEU:HG   | 1.41                     | 1.02              |
| 1:C:133:GLU:N    | 1:C:134:ASP:HB2  | 1.74                     | 1.02              |
| 2:H:475:ARG:HH12 | 2:H:505:TYR:HB2  | 1.23                     | 1.02              |
| 1:B:63:GLU:N     | 1:B:64:PRO:HA    | 1.71                     | 1.01              |
| 1:D:101:ASN:O    | 1:D:103:GLU:N    | 1.93                     | 1.01              |
| 1:C:63:GLU:H     | 1:C:64:PRO:HA    | 1.23                     | 1.01              |
| 1:D:61:ARG:HB2   | 1:D:62:GLY:HA3   | 1.43                     | 1.00              |
| 1:C:94:ASP:HB3   | 2:H:591:LYS:HZ3  | 1.15                     | 1.00              |
| 1:B:188:THR:OG1  | 1:B:194:ASP:OD1  | 1.80                     | 0.99              |
| 1:E:104:TYR:CE2  | 1:F:63:GLU:HB2   | 1.96                     | 0.99              |
| 1:C:104:TYR:HE2  | 1:D:63:GLU:HB2   | 1.23                     | 0.99              |
| 1:E:257:ASN:C    | 1:E:435:TYR:CE2  | 2.35                     | 0.99              |
| 1:B:63:GLU:H     | 1:B:64:PRO:CA    | 1.77                     | 0.98              |
| 1:A:104:TYR:CE2  | 1:B:63:GLU:HB2   | 1.99                     | 0.98              |
| 1:A:188:THR:OG1  | 1:A:194:ASP:OD1  | 1.83                     | 0.96              |
| 1:D:227:VAL:O    | 1:D:231:THR:HG22 | 1.62                     | 0.96              |
| 1:E:133:GLU:N    | 1:E:134:ASP:HB2  | 1.80                     | 0.96              |
| 1:C:257:ASN:C    | 1:C:435:TYR:CE2  | 2.39                     | 0.96              |
| 1:B:133:GLU:N    | 1:B:134:ASP:HB2  | 1.80                     | 0.95              |
| 1:C:61:ARG:HB2   | 1:C:62:GLY:HA3   | 1.45                     | 0.95              |
| 1:D:257:ASN:C    | 1:D:435:TYR:CE2  | 2.40                     | 0.95              |
| 1:B:104:TYR:OH   | 2:G:537:ALA:HB2  | 1.67                     | 0.94              |
| 1:D:63:GLU:H     | 1:D:64:PRO:CA    | 1.82                     | 0.93              |
| 1:B:62:GLY:HA2   | 1:B:63:GLU:HB3   | 1.50                     | 0.93              |
| 1:F:63:GLU:N     | 1:F:64:PRO:HA    | 1.82                     | 0.93              |
| 1:A:61:ARG:HB2   | 1:A:62:GLY:HA3   | 1.49                     | 0.93              |
| 1:A:257:ASN:C    | 1:A:435:TYR:CE2  | 2.43                     | 0.93              |
| 1:E:227:VAL:O    | 1:E:231:THR:HG22 | 1.68                     | 0.92              |
| 1:B:257:ASN:C    | 1:B:435:TYR:CE2  | 2.43                     | 0.92              |
| 1:C:231:THR:HG23 | 1:C:232:ASN:H    | 1.33                     | 0.92              |
| 1:E:63:GLU:N     | 1:E:64:PRO:HA    | 1.83                     | 0.92              |
| 1:C:132:ARG:HD2  | 1:C:139:LEU:HG   | 1.52                     | 0.92              |
| 1:E:322:LEU:O    | 1:E:325:ILE:HG22 | 1.70                     | 0.92              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:101:ASN:O    | 1:B:103:GLU:N    | 2.02                     | 0.91              |
| 1:F:61:ARG:HB2   | 1:F:62:GLY:HA3   | 1.53                     | 0.90              |
| 1:B:66:ASP:H     | 1:B:69:THR:HG22  | 1.35                     | 0.90              |
| 1:C:322:LEU:O    | 1:C:325:ILE:HG22 | 1.70                     | 0.90              |
| 2:H:475:ARG:HH12 | 2:H:505:TYR:CB   | 1.84                     | 0.89              |
| 1:F:363:LEU:HD23 | 1:F:380:ILE:HG23 | 1.51                     | 0.89              |
| 1:A:104:TYR:HH   | 1:B:69:THR:HG1   | 1.17                     | 0.89              |
| 1:E:61:ARG:HB2   | 1:E:62:GLY:HA3   | 1.54                     | 0.89              |
| 1:D:322:LEU:O    | 1:D:325:ILE:HG22 | 1.73                     | 0.89              |
| 1:E:63:GLU:H     | 1:E:64:PRO:CA    | 1.86                     | 0.89              |
| 1:A:322:LEU:O    | 1:A:325:ILE:HG22 | 1.73                     | 0.89              |
| 1:F:132:ARG:HD2  | 1:F:139:LEU:HG   | 1.54                     | 0.88              |
| 1:E:257:ASN:C    | 1:E:435:TYR:HE2  | 1.77                     | 0.88              |
| 1:E:94:ASP:HB3   | 2:I:591:LYS:NZ   | 1.88                     | 0.88              |
| 1:F:322:LEU:O    | 1:F:325:ILE:HG22 | 1.72                     | 0.88              |
| 1:B:322:LEU:O    | 1:B:325:ILE:HG22 | 1.72                     | 0.87              |
| 1:F:63:GLU:H     | 1:F:64:PRO:CA    | 1.87                     | 0.87              |
| 2:G:475:ARG:NH1  | 2:G:505:TYR:HB2  | 1.89                     | 0.87              |
| 1:E:93:ALA:HB1   | 2:I:588:ILE:HD11 | 1.56                     | 0.87              |
| 1:C:302:ARG:HG2  | 1:C:306:ARG:HH12 | 1.40                     | 0.87              |
| 1:D:66:ASP:H     | 1:D:69:THR:CG2   | 1.88                     | 0.87              |
| 1:A:63:GLU:H     | 1:A:64:PRO:CA    | 1.88                     | 0.86              |
| 1:F:101:ASN:O    | 1:F:103:GLU:N    | 2.08                     | 0.86              |
| 1:F:67:LEU:O     | 1:F:71:THR:HG23  | 1.75                     | 0.86              |
| 1:B:363:LEU:HD23 | 1:B:380:ILE:HG23 | 1.56                     | 0.86              |
| 2:H:484:ARG:HH22 | 2:H:546:GLU:HG2  | 1.39                     | 0.86              |
| 1:A:101:ASN:O    | 1:A:103:GLU:N    | 2.10                     | 0.85              |
| 1:E:231:THR:HG23 | 1:E:232:ASN:H    | 1.40                     | 0.84              |
| 1:F:133:GLU:N    | 1:F:134:ASP:HB2  | 1.91                     | 0.84              |
| 1:A:63:GLU:N     | 1:A:64:PRO:HA    | 1.89                     | 0.84              |
| 2:H:475:ARG:HH11 | 2:H:475:ARG:HG3  | 1.41                     | 0.84              |
| 1:D:133:GLU:N    | 1:D:134:ASP:HB2  | 1.93                     | 0.83              |
| 2:G:456:LEU:O    | 2:G:457:LEU:HB2  | 1.78                     | 0.83              |
| 1:C:93:ALA:HB1   | 2:H:588:ILE:HD11 | 1.61                     | 0.83              |
| 2:I:475:ARG:NH1  | 2:I:505:TYR:HB2  | 1.94                     | 0.83              |
| 1:E:83:ILE:HG22  | 1:E:84:GLY:H     | 1.42                     | 0.83              |
| 1:D:231:THR:HG23 | 1:D:232:ASN:H    | 1.43                     | 0.83              |
| 1:E:101:ASN:O    | 1:E:103:GLU:N    | 2.11                     | 0.82              |
| 1:D:255:GLU:C    | 1:D:257:ASN:H    | 1.81                     | 0.82              |
| 1:E:132:ARG:HD2  | 1:E:139:LEU:HG   | 1.62                     | 0.82              |
| 1:D:66:ASP:H     | 1:D:69:THR:HG22  | 1.44                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:66:ASP:H     | 1:F:69:THR:HG22  | 1.44                     | 0.81              |
| 1:C:63:GLU:N     | 1:C:64:PRO:HA    | 1.96                     | 0.81              |
| 1:A:67:LEU:O     | 1:A:71:THR:HG23  | 1.81                     | 0.81              |
| 1:B:66:ASP:H     | 1:B:69:THR:CG2   | 1.93                     | 0.80              |
| 1:B:62:GLY:HA2   | 1:B:63:GLU:CB    | 2.07                     | 0.80              |
| 1:C:187:PRO:O    | 1:C:189:GLY:N    | 2.14                     | 0.80              |
| 1:A:61:ARG:CB    | 1:A:62:GLY:HA3   | 2.12                     | 0.80              |
| 1:B:227:VAL:O    | 1:B:231:THR:CG2  | 2.31                     | 0.79              |
| 1:F:66:ASP:H     | 1:F:69:THR:CG2   | 1.95                     | 0.79              |
| 1:B:257:ASN:C    | 1:B:435:TYR:HE2  | 1.86                     | 0.79              |
| 1:B:231:THR:O    | 1:B:232:ASN:HB2  | 1.81                     | 0.79              |
| 1:E:258:ILE:O    | 1:E:259:ASN:HB3  | 1.81                     | 0.79              |
| 1:B:135:GLU:O    | 1:B:137:ASP:N    | 2.13                     | 0.79              |
| 2:G:475:ARG:HG3  | 2:G:475:ARG:HH11 | 1.47                     | 0.79              |
| 1:A:133:GLU:N    | 1:A:134:ASP:HB2  | 1.97                     | 0.79              |
| 1:C:63:GLU:H     | 1:C:64:PRO:CA    | 1.95                     | 0.79              |
| 1:A:197:THR:HB   | 1:A:199:GLY:O    | 1.81                     | 0.79              |
| 1:A:94:ASP:HB3   | 2:G:591:LYS:NZ   | 1.98                     | 0.78              |
| 1:A:231:THR:HG23 | 1:A:232:ASN:H    | 1.49                     | 0.78              |
| 1:C:67:LEU:O     | 1:C:71:THR:HG23  | 1.83                     | 0.78              |
| 1:C:74:LEU:HD22  | 1:C:83:ILE:HD11  | 1.65                     | 0.78              |
| 1:F:148:MET:HA   | 1:F:148:MET:CE   | 2.13                     | 0.78              |
| 1:A:66:ASP:H     | 1:A:69:THR:HG22  | 1.48                     | 0.78              |
| 1:D:61:ARG:CB    | 1:D:62:GLY:HA3   | 2.07                     | 0.77              |
| 1:B:61:ARG:HB2   | 1:B:62:GLY:HA3   | 1.66                     | 0.77              |
| 1:F:62:GLY:HA2   | 1:F:63:GLU:HB3   | 1.65                     | 0.77              |
| 1:C:51:ILE:HD11  | 1:C:83:ILE:HG21  | 1.66                     | 0.77              |
| 1:B:132:ARG:O    | 1:B:133:GLU:CB   | 2.30                     | 0.77              |
| 1:E:74:LEU:HD22  | 1:E:83:ILE:HD11  | 1.66                     | 0.77              |
| 1:A:363:LEU:HD23 | 1:A:380:ILE:HG23 | 1.67                     | 0.76              |
| 1:A:62:GLY:HA2   | 1:A:63:GLU:HB3   | 1.67                     | 0.76              |
| 1:C:315:GLY:O    | 1:C:356:PRO:HD2  | 1.85                     | 0.76              |
| 1:C:61:ARG:CB    | 1:C:62:GLY:HA3   | 2.15                     | 0.76              |
| 1:F:71:THR:HG22  | 1:F:89:LEU:HD12  | 1.68                     | 0.76              |
| 1:E:62:GLY:HA2   | 1:E:63:GLU:HB3   | 1.66                     | 0.75              |
| 1:A:222:ASN:N    | 1:A:222:ASN:HD22 | 1.85                     | 0.75              |
| 1:D:363:LEU:HD23 | 1:D:380:ILE:HG23 | 1.65                     | 0.75              |
| 1:C:306:ARG:NH2  | 1:D:32:VAL:HG21  | 2.00                     | 0.75              |
| 1:E:257:ASN:O    | 1:E:435:TYR:HE2  | 1.69                     | 0.75              |
| 1:C:101:ASN:O    | 1:C:103:GLU:N    | 2.19                     | 0.75              |
| 1:A:93:ALA:HB1   | 2:G:588:ILE:HD11 | 1.67                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:104:TYR:HH   | 1:D:69:THR:HG1   | 0.97                     | 0.75              |
| 1:C:66:ASP:H     | 1:C:69:THR:HG22  | 1.50                     | 0.75              |
| 1:B:187:PRO:O    | 1:B:189:GLY:N    | 2.19                     | 0.74              |
| 1:B:30:ALA:O     | 1:B:33:PRO:HD2   | 1.87                     | 0.74              |
| 1:F:132:ARG:O    | 1:F:133:GLU:CB   | 2.35                     | 0.74              |
| 1:E:363:LEU:HD23 | 1:E:380:ILE:HG23 | 1.70                     | 0.74              |
| 2:G:475:ARG:HH12 | 2:G:505:TYR:CB   | 2.00                     | 0.73              |
| 1:F:135:GLU:O    | 1:F:137:ASP:N    | 2.21                     | 0.73              |
| 1:D:218:ALA:O    | 1:D:222:ASN:ND2  | 2.21                     | 0.73              |
| 1:A:218:ALA:O    | 1:A:222:ASN:ND2  | 2.21                     | 0.73              |
| 1:C:104:TYR:H    | 1:C:107:ARG:H    | 1.36                     | 0.73              |
| 1:E:104:TYR:HH   | 1:F:69:THR:HG1   | 0.83                     | 0.73              |
| 1:B:74:LEU:HD22  | 1:B:83:ILE:HD11  | 1.71                     | 0.73              |
| 1:C:307:ARG:CZ   | 1:D:36:GLU:OE2   | 2.36                     | 0.73              |
| 1:E:66:ASP:H     | 1:E:69:THR:HG22  | 1.53                     | 0.73              |
| 1:E:67:LEU:O     | 1:E:71:THR:HG23  | 1.88                     | 0.73              |
| 1:E:132:ARG:O    | 1:E:133:GLU:CB   | 2.31                     | 0.72              |
| 1:C:363:LEU:HD23 | 1:C:380:ILE:HG23 | 1.71                     | 0.72              |
| 1:A:132:ARG:HD2  | 1:A:139:LEU:HG   | 1.70                     | 0.72              |
| 1:A:104:TYR:H    | 1:A:107:ARG:H    | 1.38                     | 0.72              |
| 1:C:258:ILE:O    | 1:C:259:ASN:HB3  | 1.90                     | 0.72              |
| 1:E:388:GLN:H    | 1:E:388:GLN:HE21 | 1.36                     | 0.72              |
| 1:D:135:GLU:O    | 1:D:137:ASP:N    | 2.15                     | 0.72              |
| 1:A:132:ARG:O    | 1:A:133:GLU:CB   | 2.27                     | 0.72              |
| 1:E:94:ASP:HB3   | 2:I:591:LYS:HZ3  | 1.54                     | 0.72              |
| 1:A:26:LEU:HD22  | 2:G:592:LYS:HE3  | 1.72                     | 0.72              |
| 1:D:257:ASN:O    | 1:D:435:TYR:CE2  | 2.42                     | 0.71              |
| 1:F:62:GLY:HA2   | 1:F:63:GLU:CB    | 2.19                     | 0.71              |
| 1:A:94:ASP:HB3   | 2:G:591:LYS:HZ3  | 1.54                     | 0.71              |
| 1:F:231:THR:HG23 | 1:F:232:ASN:H    | 1.55                     | 0.71              |
| 1:D:104:TYR:OH   | 2:H:537:ALA:HB2  | 1.90                     | 0.71              |
| 1:F:74:LEU:HD22  | 1:F:83:ILE:HD11  | 1.73                     | 0.71              |
| 1:A:268:LEU:HB3  | 1:A:272:ASP:HB2  | 1.73                     | 0.71              |
| 1:A:74:LEU:HD22  | 1:A:83:ILE:HD11  | 1.72                     | 0.71              |
| 1:C:132:ARG:O    | 1:C:133:GLU:CB   | 2.30                     | 0.70              |
| 1:B:218:ALA:O    | 1:B:222:ASN:ND2  | 2.24                     | 0.70              |
| 1:D:187:PRO:O    | 1:D:189:GLY:N    | 2.24                     | 0.70              |
| 1:A:255:GLU:C    | 1:A:257:ASN:N    | 2.44                     | 0.70              |
| 1:D:62:GLY:HA2   | 1:D:63:GLU:HB3   | 1.71                     | 0.70              |
| 1:E:197:THR:HB   | 1:E:199:GLY:O    | 1.91                     | 0.70              |
| 1:A:114:VAL:HG11 | 1:D:140:LEU:HD11 | 1.72                     | 0.70              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:H:484:ARG:NH2  | 2:H:546:GLU:HG2 | 2.06                     | 0.70              |
| 1:C:187:PRO:C    | 1:C:189:GLY:H   | 1.95                     | 0.70              |
| 1:B:257:ASN:O    | 1:B:435:TYR:HE2 | 1.74                     | 0.70              |
| 1:B:339:VAL:HG13 | 1:B:384:GLY:HA3 | 1.73                     | 0.70              |
| 1:A:231:THR:O    | 1:A:232:ASN:HB2 | 1.90                     | 0.70              |
| 2:H:475:ARG:NH1  | 2:H:505:TYR:CB  | 2.47                     | 0.70              |
| 1:C:257:ASN:C    | 1:C:435:TYR:HE2 | 1.90                     | 0.70              |
| 2:G:475:ARG:NH1  | 2:G:505:TYR:CB  | 2.54                     | 0.70              |
| 1:F:227:VAL:O    | 1:F:231:THR:CG2 | 2.39                     | 0.69              |
| 1:C:257:ASN:O    | 1:C:435:TYR:CE2 | 2.44                     | 0.69              |
| 2:I:475:ARG:HG2  | 2:I:511:ALA:CB  | 2.22                     | 0.69              |
| 1:B:47:ALA:HB1   | 1:B:83:ILE:HG23 | 1.74                     | 0.69              |
| 1:A:187:PRO:O    | 1:A:189:GLY:N   | 2.24                     | 0.69              |
| 1:A:192:GLU:HA   | 1:A:195:ARG:HG3 | 1.73                     | 0.69              |
| 2:G:487:GLY:HA3  | 2:G:489:PHE:H   | 1.57                     | 0.69              |
| 1:B:258:ILE:O    | 1:B:259:ASN:HB3 | 1.92                     | 0.69              |
| 1:C:306:ARG:NH1  | 1:D:32:VAL:HG21 | 2.08                     | 0.69              |
| 1:A:258:ILE:O    | 1:A:259:ASN:HB3 | 1.93                     | 0.69              |
| 2:H:510:GLU:O    | 2:H:511:ALA:HB2 | 1.92                     | 0.68              |
| 1:A:62:GLY:CA    | 1:A:63:GLU:HB3  | 2.23                     | 0.68              |
| 1:B:148:MET:CE   | 1:B:148:MET:HA  | 2.24                     | 0.68              |
| 1:F:104:TYR:OH   | 2:I:537:ALA:HB2 | 1.93                     | 0.68              |
| 1:E:227:VAL:O    | 1:E:231:THR:CG2 | 2.41                     | 0.68              |
| 1:D:51:ILE:HD11  | 1:D:83:ILE:HG21 | 1.76                     | 0.68              |
| 1:D:388:GLN:HE21 | 1:D:388:GLN:H   | 1.40                     | 0.68              |
| 1:F:132:ARG:C    | 1:F:134:ASP:HB2 | 2.14                     | 0.68              |
| 1:C:83:ILE:HG22  | 1:C:84:GLY:H    | 1.58                     | 0.68              |
| 1:A:210:ALA:HB2  | 1:A:396:LEU:HB2 | 1.76                     | 0.68              |
| 1:E:218:ALA:O    | 1:E:222:ASN:ND2 | 2.27                     | 0.68              |
| 1:E:268:LEU:HB3  | 1:E:272:ASP:HB2 | 1.76                     | 0.68              |
| 1:E:257:ASN:O    | 1:E:435:TYR:CE2 | 2.44                     | 0.67              |
| 1:E:94:ASP:HB3   | 2:I:591:LYS:HZ2 | 1.57                     | 0.67              |
| 1:A:257:ASN:C    | 1:A:435:TYR:HE2 | 1.94                     | 0.67              |
| 1:A:299:SER:HB3  | 1:B:36:GLU:HB3  | 1.75                     | 0.67              |
| 1:A:432:ILE:O    | 1:A:433:LYS:HB2 | 1.94                     | 0.67              |
| 2:G:491:ILE:HB   | 2:G:494:HIS:HD2 | 1.59                     | 0.67              |
| 1:F:233:GLU:HG2  | 1:F:315:GLY:HA3 | 1.76                     | 0.67              |
| 2:H:491:ILE:HB   | 2:H:494:HIS:HD2 | 1.60                     | 0.67              |
| 1:E:105:TYR:HE2  | 1:F:68:VAL:HG12 | 1.59                     | 0.67              |
| 1:A:197:THR:CB   | 1:A:199:GLY:O   | 2.41                     | 0.67              |
| 1:F:148:MET:HA   | 1:F:148:MET:HE3 | 1.75                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:583:ILE:O    | 2:H:587:MSE:HG3  | 1.94                     | 0.67              |
| 1:E:257:ASN:HA   | 1:E:435:TYR:CD2  | 2.29                     | 0.67              |
| 1:A:388:GLN:HE21 | 1:A:388:GLN:H    | 1.43                     | 0.67              |
| 1:E:192:GLU:HA   | 1:E:195:ARG:HG3  | 1.77                     | 0.67              |
| 1:D:258:ILE:O    | 1:D:259:ASN:HB3  | 1.95                     | 0.66              |
| 1:D:231:THR:O    | 1:D:232:ASN:HB2  | 1.95                     | 0.66              |
| 1:C:257:ASN:O    | 1:C:435:TYR:HE2  | 1.76                     | 0.66              |
| 1:E:231:THR:O    | 1:E:232:ASN:HB2  | 1.94                     | 0.66              |
| 2:H:487:GLY:HA3  | 2:H:489:PHE:H    | 1.61                     | 0.66              |
| 1:E:105:TYR:OH   | 1:F:68:VAL:HB    | 1.95                     | 0.66              |
| 1:C:62:GLY:HA2   | 1:C:63:GLU:HB3   | 1.75                     | 0.66              |
| 1:B:262:ASN:OD1  | 1:B:263:LEU:N    | 2.29                     | 0.66              |
| 1:D:62:GLY:HA2   | 1:D:63:GLU:CB    | 2.24                     | 0.66              |
| 1:E:432:ILE:O    | 1:E:433:LYS:HB2  | 1.96                     | 0.66              |
| 1:E:83:ILE:HG22  | 1:E:84:GLY:N     | 2.10                     | 0.66              |
| 1:A:47:ALA:HB1   | 1:A:83:ILE:HG23  | 1.76                     | 0.66              |
| 1:B:222:ASN:N    | 1:B:222:ASN:HD22 | 1.93                     | 0.66              |
| 1:D:262:ASN:HB3  | 1:D:265:THR:HG22 | 1.78                     | 0.66              |
| 1:A:257:ASN:O    | 1:A:435:TYR:CE2  | 2.49                     | 0.66              |
| 1:C:194:ASP:O    | 1:C:198:SER:N    | 2.29                     | 0.66              |
| 1:B:231:THR:HG23 | 1:B:232:ASN:H    | 1.61                     | 0.66              |
| 1:C:222:ASN:HD22 | 1:C:222:ASN:N    | 1.93                     | 0.66              |
| 1:B:257:ASN:O    | 1:B:435:TYR:CE2  | 2.48                     | 0.65              |
| 1:B:197:THR:HB   | 1:B:199:GLY:O    | 1.95                     | 0.65              |
| 1:A:114:VAL:CG1  | 1:D:140:LEU:HD11 | 2.26                     | 0.65              |
| 1:D:74:LEU:HD22  | 1:D:83:ILE:HD11  | 1.78                     | 0.65              |
| 2:H:491:ILE:HB   | 2:H:494:HIS:CD2  | 2.32                     | 0.65              |
| 1:C:388:GLN:H    | 1:C:388:GLN:HE21 | 1.44                     | 0.65              |
| 1:D:141:ASP:OD2  | 1:D:297:ARG:HD3  | 1.95                     | 0.65              |
| 2:I:484:ARG:HH22 | 2:I:546:GLU:HG2  | 1.60                     | 0.65              |
| 1:E:187:PRO:O    | 1:E:189:GLY:N    | 2.28                     | 0.65              |
| 1:F:374:ARG:HB3  | 1:F:375:PRO:HA   | 1.77                     | 0.65              |
| 1:C:432:ILE:O    | 1:C:433:LYS:HB2  | 1.97                     | 0.65              |
| 2:G:475:ARG:HG2  | 2:G:511:ALA:CB   | 2.26                     | 0.65              |
| 1:C:19:ALA:HA    | 1:C:96:VAL:HG21  | 1.79                     | 0.64              |
| 1:F:339:VAL:HG13 | 1:F:384:GLY:HA3  | 1.79                     | 0.64              |
| 1:A:227:VAL:O    | 1:A:231:THR:CG2  | 2.38                     | 0.64              |
| 1:B:432:ILE:O    | 1:B:433:LYS:HB2  | 1.97                     | 0.64              |
| 1:D:257:ASN:O    | 1:D:435:TYR:HE2  | 1.79                     | 0.64              |
| 1:D:71:THR:HG22  | 1:D:89:LEU:HD12  | 1.79                     | 0.64              |
| 1:A:138:VAL:O    | 1:A:142:GLU:HG2  | 1.98                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:510:GLU:O    | 2:H:511:ALA:CB   | 2.44                     | 0.64              |
| 1:F:262:ASN:HB3  | 1:F:265:THR:HG22 | 1.80                     | 0.64              |
| 1:F:66:ASP:O     | 1:F:69:THR:HG22  | 1.98                     | 0.64              |
| 1:A:66:ASP:H     | 1:A:69:THR:CG2   | 2.11                     | 0.64              |
| 2:I:538:ASP:O    | 2:I:539:ASP:HB2  | 1.98                     | 0.64              |
| 1:B:388:GLN:HE21 | 1:B:388:GLN:H    | 1.46                     | 0.64              |
| 1:D:197:THR:HB   | 1:D:199:GLY:O    | 1.97                     | 0.63              |
| 1:D:30:ALA:O     | 1:D:33:PRO:HD2   | 1.99                     | 0.63              |
| 2:G:486:GLY:H    | 2:G:488:ARG:HB2  | 1.64                     | 0.63              |
| 1:F:28:PRO:C     | 1:F:30:ALA:H     | 2.01                     | 0.63              |
| 1:C:94:ASP:HB3   | 2:H:591:LYS:HZ2  | 1.63                     | 0.63              |
| 2:I:456:LEU:O    | 2:I:457:LEU:HB2  | 1.98                     | 0.63              |
| 1:A:97:PRO:HG2   | 1:A:98:THR:HG22  | 1.80                     | 0.63              |
| 1:F:388:GLN:H    | 1:F:388:GLN:HE21 | 1.45                     | 0.63              |
| 1:E:273:TRP:C    | 1:E:275:LYS:H    | 2.03                     | 0.63              |
| 1:D:222:ASN:N    | 1:D:222:ASN:HD22 | 1.96                     | 0.63              |
| 1:F:63:GLU:N     | 1:F:64:PRO:CA    | 2.55                     | 0.62              |
| 1:C:431:PHE:CE2  | 1:C:433:LYS:HG3  | 2.33                     | 0.62              |
| 1:F:262:ASN:OD1  | 1:F:263:LEU:N    | 2.31                     | 0.62              |
| 1:C:26:LEU:HD22  | 2:H:592:LYS:HE3  | 1.81                     | 0.62              |
| 1:E:222:ASN:N    | 1:E:222:ASN:HD22 | 1.97                     | 0.62              |
| 2:G:491:ILE:HB   | 2:G:494:HIS:CD2  | 2.34                     | 0.62              |
| 1:E:280:MET:O    | 1:E:284:SER:HB2  | 1.99                     | 0.62              |
| 2:H:562:LYS:HA   | 2:H:565:GLU:HB3  | 1.81                     | 0.62              |
| 1:C:66:ASP:H     | 1:C:69:THR:CG2   | 2.12                     | 0.62              |
| 1:A:296:ILE:O    | 1:A:325:ILE:HG13 | 1.98                     | 0.62              |
| 1:C:197:THR:HB   | 1:C:199:GLY:O    | 1.98                     | 0.62              |
| 2:H:456:LEU:O    | 2:H:457:LEU:HB2  | 2.00                     | 0.62              |
| 1:F:228:ALA:HB1  | 1:F:286:ALA:HB1  | 1.82                     | 0.62              |
| 1:D:432:ILE:O    | 1:D:433:LYS:HB2  | 1.99                     | 0.62              |
| 2:I:475:ARG:HG2  | 2:I:511:ALA:HB1  | 1.80                     | 0.62              |
| 1:D:104:TYR:HA   | 1:D:106:ALA:H    | 1.65                     | 0.62              |
| 1:F:210:ALA:HB2  | 1:F:396:LEU:HB2  | 1.81                     | 0.62              |
| 1:F:231:THR:O    | 1:F:232:ASN:HB2  | 1.99                     | 0.62              |
| 1:C:257:ASN:C    | 1:C:435:TYR:CD2  | 2.73                     | 0.62              |
| 2:G:464:GLU:HG3  | 2:G:489:PHE:CD1  | 2.35                     | 0.62              |
| 1:C:148:MET:HA   | 1:C:148:MET:CE   | 2.30                     | 0.62              |
| 1:C:105:TYR:OH   | 1:D:68:VAL:HB    | 2.00                     | 0.62              |
| 2:G:464:GLU:HG3  | 2:G:489:PHE:HD1  | 1.64                     | 0.62              |
| 1:C:268:LEU:HB3  | 1:C:272:ASP:HB2  | 1.81                     | 0.62              |
| 1:A:257:ASN:O    | 1:A:435:TYR:HE2  | 1.82                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:104:TYR:HA   | 1:A:106:ALA:N    | 2.14                     | 0.61              |
| 2:I:560:MSE:O    | 2:I:562:LYS:N    | 2.32                     | 0.61              |
| 2:I:464:GLU:HG3  | 2:I:489:PHE:HD1  | 1.65                     | 0.61              |
| 1:B:132:ARG:C    | 1:B:134:ASP:HB2  | 2.20                     | 0.61              |
| 1:A:208:VAL:HG22 | 1:A:394:ALA:HB3  | 1.81                     | 0.61              |
| 1:F:258:ILE:O    | 1:F:259:ASN:CB   | 2.48                     | 0.61              |
| 1:E:61:ARG:CB    | 1:E:62:GLY:HA3   | 2.26                     | 0.61              |
| 1:D:187:PRO:C    | 1:D:189:GLY:H    | 2.04                     | 0.61              |
| 1:A:187:PRO:C    | 1:A:189:GLY:H    | 2.04                     | 0.61              |
| 1:D:208:VAL:HB   | 1:D:360:LEU:HD23 | 1.81                     | 0.61              |
| 2:G:510:GLU:O    | 2:G:511:ALA:CB   | 2.49                     | 0.61              |
| 2:I:519:ARG:H    | 2:I:520:ILE:HB   | 1.65                     | 0.61              |
| 1:C:105:TYR:HE2  | 1:D:68:VAL:HG12  | 1.65                     | 0.61              |
| 1:B:63:GLU:N     | 1:B:64:PRO:CA    | 2.48                     | 0.61              |
| 1:D:63:GLU:N     | 1:D:64:PRO:CA    | 2.45                     | 0.61              |
| 1:C:231:THR:O    | 1:C:232:ASN:HB2  | 2.01                     | 0.60              |
| 1:E:197:THR:CB   | 1:E:199:GLY:O    | 2.49                     | 0.60              |
| 1:C:105:TYR:CE2  | 1:D:68:VAL:HG12  | 2.36                     | 0.60              |
| 1:A:188:THR:HG22 | 1:A:200:PHE:CE2  | 2.37                     | 0.60              |
| 1:A:93:ALA:HB1   | 2:G:588:ILE:CD1  | 2.30                     | 0.60              |
| 1:C:431:PHE:HE2  | 1:C:433:LYS:HG3  | 1.65                     | 0.60              |
| 1:A:53:HIS:CE1   | 1:A:57:ARG:NH1   | 2.69                     | 0.60              |
| 2:H:475:ARG:NH1  | 2:H:475:ARG:HG3  | 2.15                     | 0.60              |
| 1:D:391:ASP:OD1  | 1:D:391:ASP:N    | 2.33                     | 0.60              |
| 1:D:339:VAL:HG13 | 1:D:384:GLY:HA3  | 1.82                     | 0.60              |
| 1:D:257:ASN:C    | 1:D:435:TYR:HE2  | 1.98                     | 0.60              |
| 1:D:75:ALA:HB2   | 1:D:80:LEU:HD12  | 1.82                     | 0.60              |
| 1:D:132:ARG:O    | 1:D:133:GLU:CB   | 2.34                     | 0.60              |
| 1:A:104:TYR:HA   | 1:A:106:ALA:H    | 1.67                     | 0.60              |
| 2:I:463:ALA:O    | 2:I:467:LEU:HB2  | 2.01                     | 0.60              |
| 2:G:562:LYS:HA   | 2:G:565:GLU:HB3  | 1.83                     | 0.60              |
| 1:E:187:PRO:C    | 1:E:189:GLY:H    | 2.05                     | 0.60              |
| 1:C:64:PRO:O     | 1:C:69:THR:HG21  | 2.01                     | 0.59              |
| 2:I:562:LYS:HA   | 2:I:565:GLU:HB3  | 1.83                     | 0.59              |
| 1:C:28:PRO:C     | 1:C:30:ALA:H     | 2.05                     | 0.59              |
| 1:D:257:ASN:C    | 1:D:435:TYR:CD2  | 2.75                     | 0.59              |
| 1:E:93:ALA:HB1   | 2:I:588:ILE:CD1  | 2.29                     | 0.59              |
| 1:B:392:ILE:HA   | 1:B:418:LYS:O    | 2.01                     | 0.59              |
| 1:E:257:ASN:C    | 1:E:435:TYR:CD2  | 2.75                     | 0.59              |
| 1:A:273:TRP:C    | 1:A:275:LYS:H    | 2.04                     | 0.59              |
| 1:B:374:ARG:HB3  | 1:B:375:PRO:HA   | 1.83                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:47:ALA:HB1   | 1:E:83:ILE:HG23  | 1.84                     | 0.59              |
| 1:A:93:ALA:CB    | 2:G:588:ILE:HD11 | 2.31                     | 0.59              |
| 1:C:296:ILE:O    | 1:C:325:ILE:HG13 | 2.02                     | 0.59              |
| 2:G:583:ILE:O    | 2:G:587:MSE:HG3  | 2.02                     | 0.59              |
| 2:H:486:GLY:H    | 2:H:488:ARG:HB2  | 1.67                     | 0.59              |
| 1:C:50:LYS:NZ    | 1:C:82:GLU:OE2   | 2.35                     | 0.59              |
| 1:A:262:ASN:HB3  | 1:A:265:THR:HG22 | 1.85                     | 0.59              |
| 1:A:83:ILE:HG22  | 1:A:84:GLY:H     | 1.68                     | 0.59              |
| 2:I:464:GLU:HG3  | 2:I:489:PHE:CD1  | 2.38                     | 0.59              |
| 1:B:67:LEU:O     | 1:B:71:THR:HG23  | 2.02                     | 0.59              |
| 2:G:475:ARG:HG2  | 2:G:511:ALA:HB2  | 1.84                     | 0.59              |
| 2:I:510:GLU:O    | 2:I:511:ALA:CB   | 2.49                     | 0.59              |
| 2:I:487:GLY:HA3  | 2:I:489:PHE:H    | 1.67                     | 0.59              |
| 1:D:32:VAL:O     | 1:D:36:GLU:HG3   | 2.03                     | 0.59              |
| 1:B:133:GLU:HG2  | 1:E:115:LEU:CD1  | 2.33                     | 0.59              |
| 1:E:93:ALA:CB    | 2:I:588:ILE:HD11 | 2.30                     | 0.59              |
| 1:A:257:ASN:HA   | 1:A:435:TYR:CD2  | 2.38                     | 0.58              |
| 1:A:105:TYR:CE2  | 1:B:68:VAL:HG12  | 2.38                     | 0.58              |
| 1:E:64:PRO:O     | 1:E:69:THR:HG21  | 2.02                     | 0.58              |
| 1:A:199:GLY:HA3  | 1:A:200:PHE:O    | 2.03                     | 0.58              |
| 1:D:227:VAL:O    | 1:D:231:THR:CG2  | 2.44                     | 0.58              |
| 1:E:138:VAL:O    | 1:E:142:GLU:HG2  | 2.03                     | 0.58              |
| 1:C:93:ALA:CB    | 2:H:588:ILE:HD11 | 2.31                     | 0.58              |
| 2:G:471:MSE:HB2  | 2:G:478:ALA:HB2  | 1.85                     | 0.58              |
| 2:H:485:ILE:HG22 | 2:H:487:GLY:HA2  | 1.86                     | 0.58              |
| 1:E:104:TYR:HB3  | 1:E:105:TYR:HB2  | 1.84                     | 0.58              |
| 1:B:194:ASP:O    | 1:B:198:SER:N    | 2.31                     | 0.58              |
| 1:D:249:MET:HA   | 1:D:252:LEU:HB2  | 1.86                     | 0.58              |
| 1:B:66:ASP:O     | 1:B:69:THR:HG22  | 2.04                     | 0.58              |
| 1:F:187:PRO:O    | 1:F:189:GLY:N    | 2.37                     | 0.58              |
| 2:G:465:ARG:HG3  | 2:G:531:LEU:HD21 | 1.85                     | 0.58              |
| 1:E:26:LEU:HD22  | 2:I:592:LYS:HE3  | 1.85                     | 0.58              |
| 1:B:104:TYR:HA   | 1:B:105:TYR:HB2  | 1.86                     | 0.58              |
| 1:F:74:LEU:HD13  | 1:F:83:ILE:CD1   | 2.34                     | 0.58              |
| 1:C:207:ILE:HD13 | 1:C:386:ILE:HG21 | 1.85                     | 0.58              |
| 1:C:188:THR:HG22 | 1:C:200:PHE:CE2  | 2.39                     | 0.57              |
| 1:B:187:PRO:C    | 1:B:189:GLY:H    | 2.06                     | 0.57              |
| 1:B:273:TRP:C    | 1:B:275:LYS:H    | 2.07                     | 0.57              |
| 2:G:504:PHE:O    | 2:G:507:GLU:HB3  | 2.05                     | 0.57              |
| 1:D:67:LEU:O     | 1:D:71:THR:HG23  | 2.04                     | 0.57              |
| 1:F:61:ARG:CB    | 1:F:62:GLY:HA3   | 2.23                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:88:TYR:O     | 1:B:92:LEU:HG    | 2.04                     | 0.57              |
| 1:A:202:ARG:O    | 1:A:203:SER:HB2  | 2.03                     | 0.57              |
| 1:C:208:VAL:HG22 | 1:C:394:ALA:HB3  | 1.87                     | 0.57              |
| 1:A:322:LEU:HB3  | 1:A:323:GLN:NE2  | 2.19                     | 0.57              |
| 1:C:47:ALA:HB1   | 1:C:83:ILE:HG23  | 1.86                     | 0.57              |
| 1:E:105:TYR:CE2  | 1:F:68:VAL:HG12  | 2.39                     | 0.57              |
| 1:B:225:GLN:NE2  | 1:B:251:MET:HB2  | 2.19                     | 0.57              |
| 1:F:391:ASP:N    | 1:F:391:ASP:OD1  | 2.38                     | 0.57              |
| 2:I:510:GLU:O    | 2:I:511:ALA:HB2  | 2.03                     | 0.57              |
| 1:F:268:LEU:HB3  | 1:F:272:ASP:HB2  | 1.85                     | 0.57              |
| 1:B:207:ILE:HD13 | 1:B:386:ILE:HG21 | 1.87                     | 0.57              |
| 1:E:257:ASN:CA   | 1:E:435:TYR:CD2  | 2.87                     | 0.57              |
| 2:G:538:ASP:O    | 2:G:539:ASP:HB2  | 2.05                     | 0.57              |
| 1:C:104:TYR:HA   | 1:C:106:ALA:N    | 2.20                     | 0.57              |
| 1:E:148:MET:HA   | 1:E:148:MET:CE   | 2.34                     | 0.57              |
| 1:E:28:PRO:C     | 1:E:30:ALA:H     | 2.07                     | 0.56              |
| 1:B:51:ILE:HD11  | 1:B:83:ILE:HG21  | 1.86                     | 0.56              |
| 1:B:262:ASN:HB3  | 1:B:265:THR:HG22 | 1.88                     | 0.56              |
| 1:A:374:ARG:HB3  | 1:A:375:PRO:HA   | 1.86                     | 0.56              |
| 1:D:273:TRP:C    | 1:D:275:LYS:H    | 2.08                     | 0.56              |
| 1:C:138:VAL:O    | 1:C:142:GLU:HG2  | 2.05                     | 0.56              |
| 2:I:475:ARG:HH12 | 2:I:505:TYR:CB   | 2.19                     | 0.56              |
| 1:F:196:MET:O    | 1:F:419:GLN:NE2  | 2.34                     | 0.56              |
| 1:D:148:MET:CE   | 1:D:148:MET:HA   | 2.35                     | 0.56              |
| 1:A:135:GLU:O    | 1:A:137:ASP:N    | 2.33                     | 0.56              |
| 2:H:504:PHE:O    | 2:H:507:GLU:HB3  | 2.06                     | 0.56              |
| 1:C:132:ARG:C    | 1:C:134:ASP:HB2  | 2.25                     | 0.56              |
| 2:I:475:ARG:NH1  | 2:I:505:TYR:CB   | 2.67                     | 0.56              |
| 1:C:71:THR:HG22  | 1:C:89:LEU:CD1   | 2.36                     | 0.56              |
| 1:B:148:MET:HE2  | 1:B:148:MET:HA   | 1.86                     | 0.56              |
| 1:B:71:THR:HG22  | 1:B:89:LEU:HD12  | 1.88                     | 0.56              |
| 1:E:296:ILE:O    | 1:E:325:ILE:HG13 | 2.05                     | 0.56              |
| 1:D:296:ILE:O    | 1:D:325:ILE:HG13 | 2.05                     | 0.56              |
| 1:F:258:ILE:O    | 1:F:259:ASN:HB3  | 2.06                     | 0.56              |
| 1:D:53:HIS:CE1   | 1:D:57:ARG:HD2   | 2.40                     | 0.56              |
| 1:B:71:THR:HG22  | 1:B:89:LEU:CD1   | 2.36                     | 0.56              |
| 1:D:381:ARG:HD3  | 1:D:387:GLU:HB2  | 1.85                     | 0.56              |
| 1:B:257:ASN:C    | 1:B:435:TYR:CD2  | 2.79                     | 0.56              |
| 1:E:66:ASP:H     | 1:E:69:THR:CG2   | 2.16                     | 0.56              |
| 1:C:62:GLY:CA    | 1:C:63:GLU:HB3   | 2.35                     | 0.56              |
| 1:F:83:ILE:HG22  | 1:F:84:GLY:H     | 1.71                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:302:ARG:HD2  | 1:B:36:GLU:OE2   | 2.05                     | 0.55              |
| 1:C:262:ASN:OD1  | 1:C:263:LEU:N    | 2.39                     | 0.55              |
| 1:E:202:ARG:O    | 1:E:203:SER:HB2  | 2.06                     | 0.55              |
| 2:H:475:ARG:HG2  | 2:H:511:ALA:CB   | 2.35                     | 0.55              |
| 1:E:105:TYR:CE2  | 1:F:68:VAL:CG1   | 2.90                     | 0.55              |
| 1:C:227:VAL:O    | 1:C:231:THR:CG2  | 2.39                     | 0.55              |
| 1:F:79:GLN:O     | 1:F:83:ILE:HG13  | 2.07                     | 0.55              |
| 1:A:257:ASN:C    | 1:A:435:TYR:CD2  | 2.80                     | 0.55              |
| 1:E:194:ASP:O    | 1:E:198:SER:N    | 2.29                     | 0.55              |
| 1:A:64:PRO:O     | 1:A:69:THR:HG21  | 2.06                     | 0.55              |
| 1:A:53:HIS:CE1   | 1:A:57:ARG:HH11  | 2.25                     | 0.55              |
| 1:C:262:ASN:HB3  | 1:C:265:THR:HG22 | 1.89                     | 0.55              |
| 1:F:207:ILE:HD11 | 1:F:361:SER:HB2  | 1.89                     | 0.55              |
| 1:D:40:PRO:O     | 1:D:49:GLN:HG3   | 2.05                     | 0.55              |
| 2:G:510:GLU:O    | 2:G:511:ALA:HB2  | 2.07                     | 0.55              |
| 1:A:67:LEU:CD1   | 2:G:584:ALA:HB3  | 2.36                     | 0.55              |
| 1:D:262:ASN:OD1  | 1:D:263:LEU:N    | 2.38                     | 0.55              |
| 2:H:519:ARG:H    | 2:H:520:ILE:HB   | 1.71                     | 0.55              |
| 1:E:53:HIS:CE1   | 1:E:57:ARG:HD2   | 2.42                     | 0.55              |
| 1:A:207:ILE:HD13 | 1:A:386:ILE:HG21 | 1.89                     | 0.55              |
| 2:I:583:ILE:O    | 2:I:587:MSE:HG3  | 2.06                     | 0.55              |
| 1:D:52:PHE:CD1   | 1:D:55:MET:HE2   | 2.42                     | 0.55              |
| 1:C:93:ALA:HB1   | 2:H:588:ILE:CD1  | 2.35                     | 0.54              |
| 1:F:148:MET:HE2  | 1:F:148:MET:HA   | 1.89                     | 0.54              |
| 2:H:538:ASP:O    | 2:H:539:ASP:HB2  | 2.07                     | 0.54              |
| 1:E:262:ASN:OD1  | 1:E:263:LEU:N    | 2.40                     | 0.54              |
| 1:B:257:ASN:HA   | 1:B:435:TYR:CD2  | 2.41                     | 0.54              |
| 1:C:83:ILE:HG22  | 1:C:84:GLY:N     | 2.22                     | 0.54              |
| 1:D:200:PHE:CD1  | 1:D:206:ILE:HD13 | 2.42                     | 0.54              |
| 1:A:315:GLY:O    | 1:A:356:PRO:HD2  | 2.07                     | 0.54              |
| 1:B:62:GLY:CA    | 1:B:63:GLU:CB    | 2.83                     | 0.54              |
| 1:D:61:ARG:CB    | 1:D:62:GLY:CA    | 2.82                     | 0.54              |
| 1:C:210:ALA:HB2  | 1:C:396:LEU:HB2  | 1.87                     | 0.54              |
| 1:B:210:ALA:HB2  | 1:B:396:LEU:HB2  | 1.90                     | 0.54              |
| 1:B:197:THR:CB   | 1:B:199:GLY:O    | 2.55                     | 0.54              |
| 1:A:262:ASN:OD1  | 1:A:263:LEU:N    | 2.40                     | 0.54              |
| 1:E:262:ASN:HB3  | 1:E:265:THR:HG22 | 1.88                     | 0.54              |
| 1:E:374:ARG:HB3  | 1:E:375:PRO:HA   | 1.89                     | 0.54              |
| 1:F:202:ARG:O    | 1:F:203:SER:HB2  | 2.08                     | 0.54              |
| 1:C:103:GLU:N    | 1:C:104:TYR:CB   | 2.71                     | 0.54              |
| 1:E:258:ILE:O    | 1:E:259:ASN:CB   | 2.54                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:477:VAL:O    | 2:H:481:VAL:HG23 | 2.07                     | 0.54              |
| 1:E:19:ALA:HA    | 1:E:96:VAL:HG21  | 1.90                     | 0.54              |
| 1:C:257:ASN:HA   | 1:C:435:TYR:CD2  | 2.42                     | 0.54              |
| 1:D:315:GLY:O    | 1:D:356:PRO:HD2  | 2.08                     | 0.54              |
| 1:C:202:ARG:O    | 1:C:203:SER:HB2  | 2.07                     | 0.54              |
| 1:D:194:ASP:O    | 1:D:198:SER:N    | 2.38                     | 0.54              |
| 1:A:71:THR:HG22  | 1:A:89:LEU:HD12  | 1.90                     | 0.54              |
| 2:I:538:ASP:O    | 2:I:539:ASP:CB   | 2.56                     | 0.54              |
| 1:B:391:ASP:N    | 1:B:391:ASP:OD1  | 2.37                     | 0.54              |
| 1:D:392:ILE:HA   | 1:D:418:LYS:O    | 2.08                     | 0.54              |
| 1:D:64:PRO:O     | 1:D:69:THR:HG21  | 2.08                     | 0.54              |
| 1:C:225:GLN:NE2  | 1:C:251:MET:HB2  | 2.23                     | 0.54              |
| 2:H:471:MSE:HB2  | 2:H:478:ALA:HB2  | 1.90                     | 0.53              |
| 1:A:222:ASN:HD22 | 1:A:222:ASN:H    | 1.56                     | 0.53              |
| 1:C:306:ARG:NH2  | 1:C:352:GLU:OE1  | 2.41                     | 0.53              |
| 1:D:32:VAL:HB    | 1:D:33:PRO:HD3   | 1.89                     | 0.53              |
| 1:C:231:THR:HG23 | 1:C:232:ASN:N    | 2.13                     | 0.53              |
| 1:D:132:ARG:C    | 1:D:134:ASP:HB2  | 2.28                     | 0.53              |
| 1:E:51:ILE:HD11  | 1:E:83:ILE:HG21  | 1.89                     | 0.53              |
| 1:A:105:TYR:HE2  | 1:B:68:VAL:HG12  | 1.71                     | 0.53              |
| 1:F:185:GLY:O    | 1:F:186:ILE:HG13 | 2.09                     | 0.53              |
| 1:D:141:ASP:C    | 1:D:143:ALA:H    | 2.12                     | 0.53              |
| 2:I:560:MSE:O    | 2:I:563:VAL:N    | 2.36                     | 0.53              |
| 2:H:475:ARG:HG2  | 2:H:511:ALA:HB1  | 1.90                     | 0.53              |
| 1:D:231:THR:HG23 | 1:D:232:ASN:N    | 2.21                     | 0.53              |
| 1:B:246:GLN:HE22 | 1:E:376:MET:CE   | 2.21                     | 0.53              |
| 1:E:257:ASN:CA   | 1:E:435:TYR:CE2  | 2.92                     | 0.53              |
| 1:F:322:LEU:HD12 | 1:F:359:ALA:HB1  | 1.91                     | 0.53              |
| 2:I:475:ARG:HG2  | 2:I:511:ALA:HB2  | 1.90                     | 0.53              |
| 2:G:560:MSE:O    | 2:G:562:LYS:N    | 2.42                     | 0.53              |
| 1:E:40:PRO:O     | 1:E:49:GLN:HG3   | 2.08                     | 0.53              |
| 1:E:62:GLY:CA    | 1:E:63:GLU:HB3   | 2.35                     | 0.53              |
| 1:C:374:ARG:HB3  | 1:C:375:PRO:HA   | 1.91                     | 0.53              |
| 1:E:210:ALA:HB2  | 1:E:396:LEU:HB2  | 1.91                     | 0.53              |
| 1:F:208:VAL:HG22 | 1:F:394:ALA:HB3  | 1.90                     | 0.53              |
| 1:B:268:LEU:HB3  | 1:B:272:ASP:HB2  | 1.91                     | 0.53              |
| 1:B:83:ILE:HG22  | 1:B:84:GLY:H     | 1.74                     | 0.52              |
| 1:E:207:ILE:HA   | 1:E:359:ALA:O    | 2.09                     | 0.52              |
| 1:D:257:ASN:HA   | 1:D:435:TYR:CD2  | 2.45                     | 0.52              |
| 1:A:105:TYR:OH   | 1:B:68:VAL:HB    | 2.09                     | 0.52              |
| 1:F:71:THR:HG22  | 1:F:89:LEU:CD1   | 2.38                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:51:ILE:HD11  | 1:A:83:ILE:HG21  | 1.90                     | 0.52              |
| 1:E:431:PHE:CE2  | 1:E:433:LYS:HG3  | 2.44                     | 0.52              |
| 2:H:560:MSE:O    | 2:H:562:LYS:N    | 2.43                     | 0.52              |
| 1:F:221:LEU:HD21 | 1:F:247:LEU:HD11 | 1.91                     | 0.52              |
| 1:B:53:HIS:CE1   | 1:B:57:ARG:HD2   | 2.45                     | 0.52              |
| 1:E:200:PHE:CD1  | 1:E:206:ILE:HD13 | 2.44                     | 0.52              |
| 1:F:62:GLY:CA    | 1:F:63:GLU:CB    | 2.87                     | 0.52              |
| 1:A:79:GLN:O     | 1:A:83:ILE:HG13  | 2.09                     | 0.52              |
| 1:F:235:VAL:HG12 | 1:F:316:MET:HB2  | 1.91                     | 0.52              |
| 1:E:88:TYR:O     | 1:E:92:LEU:HG    | 2.09                     | 0.52              |
| 1:B:104:TYR:HH   | 2:G:537:ALA:HB2  | 1.70                     | 0.52              |
| 1:C:84:GLY:HA3   | 1:C:88:TYR:HB2   | 1.92                     | 0.52              |
| 1:A:202:ARG:O    | 1:A:203:SER:CB   | 2.58                     | 0.52              |
| 1:B:185:GLY:O    | 1:B:186:ILE:HG13 | 2.09                     | 0.52              |
| 1:A:19:ALA:HA    | 1:A:96:VAL:HG21  | 1.92                     | 0.52              |
| 1:B:296:ILE:O    | 1:B:325:ILE:HG13 | 2.10                     | 0.52              |
| 1:F:28:PRO:C     | 1:F:30:ALA:N     | 2.62                     | 0.52              |
| 1:D:223:ILE:HG22 | 1:D:316:MET:HE1  | 1.91                     | 0.52              |
| 1:C:97:PRO:HG2   | 1:C:98:THR:HG22  | 1.92                     | 0.52              |
| 1:D:66:ASP:N     | 1:D:69:THR:HG22  | 2.21                     | 0.52              |
| 2:I:475:ARG:HG3  | 2:I:475:ARG:HH11 | 1.75                     | 0.52              |
| 1:D:432:ILE:HD12 | 1:D:437:LYS:HE3  | 1.92                     | 0.52              |
| 1:E:231:THR:HG23 | 1:E:232:ASN:N    | 2.19                     | 0.51              |
| 1:E:25:PHE:CZ    | 1:E:89:LEU:HD22  | 2.44                     | 0.51              |
| 1:A:83:ILE:CG2   | 1:A:84:GLY:H     | 2.22                     | 0.51              |
| 1:E:101:ASN:C    | 1:E:103:GLU:H    | 2.10                     | 0.51              |
| 1:A:32:VAL:HB    | 1:A:33:PRO:HD3   | 1.91                     | 0.51              |
| 1:A:141:ASP:C    | 1:A:143:ALA:H    | 2.14                     | 0.51              |
| 1:B:105:TYR:O    | 1:B:109:VAL:HG23 | 2.09                     | 0.51              |
| 1:A:339:VAL:HG13 | 1:A:384:GLY:HA3  | 1.92                     | 0.51              |
| 1:E:206:ILE:HG23 | 1:E:392:ILE:HG12 | 1.92                     | 0.51              |
| 1:F:432:ILE:O    | 1:F:433:LYS:HB2  | 2.10                     | 0.51              |
| 1:A:103:GLU:N    | 1:A:104:TYR:CB   | 2.74                     | 0.51              |
| 1:A:375:PRO:HG2  | 1:A:395:PHE:HB3  | 1.93                     | 0.51              |
| 1:D:210:ALA:HB2  | 1:D:396:LEU:HB2  | 1.91                     | 0.51              |
| 2:H:501:ILE:O    | 2:H:504:PHE:HB3  | 2.11                     | 0.51              |
| 2:H:507:GLU:O    | 2:H:507:GLU:HG3  | 2.10                     | 0.51              |
| 1:F:139:LEU:O    | 1:F:143:ALA:HB2  | 2.10                     | 0.51              |
| 1:C:197:THR:CB   | 1:C:199:GLY:O    | 2.58                     | 0.51              |
| 1:A:17:GLU:HB3   | 1:A:48:HIS:HD1   | 1.74                     | 0.51              |
| 2:I:477:VAL:O    | 2:I:481:VAL:HG23 | 2.11                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:395:PHE:HB2  | 1:C:415:ILE:HB   | 1.93                     | 0.51              |
| 1:C:105:TYR:CE2  | 1:D:68:VAL:CG1   | 2.94                     | 0.51              |
| 1:C:187:PRO:C    | 1:C:189:GLY:N    | 2.62                     | 0.51              |
| 1:A:268:LEU:HB3  | 1:A:272:ASP:CB   | 2.38                     | 0.51              |
| 1:A:30:ALA:O     | 1:A:33:PRO:HD2   | 2.10                     | 0.51              |
| 1:D:280:MET:O    | 1:D:284:SER:HB2  | 2.11                     | 0.51              |
| 1:A:194:ASP:O    | 1:A:198:SER:N    | 2.39                     | 0.51              |
| 2:G:475:ARG:HH12 | 2:G:505:TYR:HB3  | 1.74                     | 0.51              |
| 1:D:197:THR:CB   | 1:D:199:GLY:O    | 2.58                     | 0.51              |
| 2:G:519:ARG:H    | 2:G:520:ILE:HB   | 1.75                     | 0.51              |
| 1:C:257:ASN:CA   | 1:C:435:TYR:CD2  | 2.94                     | 0.51              |
| 2:G:538:ASP:O    | 2:G:539:ASP:CB   | 2.59                     | 0.51              |
| 1:A:104:TYR:OH   | 1:B:69:THR:OG1   | 2.05                     | 0.51              |
| 1:B:28:PRO:C     | 1:B:30:ALA:H     | 2.13                     | 0.51              |
| 1:C:307:ARG:NH2  | 1:D:36:GLU:OE2   | 2.43                     | 0.50              |
| 2:I:486:GLY:H    | 2:I:488:ARG:HB2  | 1.76                     | 0.50              |
| 1:C:202:ARG:O    | 1:C:203:SER:CB   | 2.59                     | 0.50              |
| 1:D:207:ILE:HD13 | 1:D:386:ILE:HG21 | 1.93                     | 0.50              |
| 1:C:135:GLU:O    | 1:C:137:ASP:N    | 2.38                     | 0.50              |
| 1:E:25:PHE:HZ    | 1:E:89:LEU:HD22  | 1.75                     | 0.50              |
| 1:E:202:ARG:O    | 1:E:203:SER:CB   | 2.58                     | 0.50              |
| 1:E:385:SER:OG   | 1:E:386:ILE:N    | 2.44                     | 0.50              |
| 1:D:202:ARG:O    | 1:D:203:SER:CB   | 2.60                     | 0.50              |
| 1:E:391:ASP:HB3  | 1:E:420:ARG:HD2  | 1.93                     | 0.50              |
| 1:B:133:GLU:CA   | 1:B:134:ASP:HB2  | 2.41                     | 0.50              |
| 1:A:28:PRO:C     | 1:A:30:ALA:H     | 2.14                     | 0.50              |
| 1:F:197:THR:HB   | 1:F:199:GLY:O    | 2.10                     | 0.50              |
| 1:A:258:ILE:O    | 1:A:259:ASN:CB   | 2.59                     | 0.50              |
| 1:B:340:SER:CB   | 1:B:385:SER:HB3  | 2.41                     | 0.50              |
| 1:F:75:ALA:HB2   | 1:F:80:LEU:HD12  | 1.93                     | 0.50              |
| 1:D:66:ASP:O     | 1:D:69:THR:HG22  | 2.12                     | 0.50              |
| 1:D:101:ASN:C    | 1:D:103:GLU:N    | 2.64                     | 0.50              |
| 1:D:104:TYR:HA   | 1:D:106:ALA:N    | 2.25                     | 0.50              |
| 2:H:487:GLY:CA   | 2:H:489:PHE:H    | 2.23                     | 0.50              |
| 1:C:273:TRP:C    | 1:C:275:LYS:H    | 2.14                     | 0.50              |
| 1:E:104:TYR:H    | 1:E:107:ARG:H    | 1.59                     | 0.50              |
| 1:C:71:THR:HG22  | 1:C:89:LEU:HD12  | 1.92                     | 0.50              |
| 1:C:192:GLU:HA   | 1:C:195:ARG:HG3  | 1.92                     | 0.50              |
| 1:E:219:PHE:HB2  | 1:E:438:PHE:CE1  | 2.47                     | 0.50              |
| 1:C:96:VAL:HG13  | 1:C:97:PRO:HD2   | 1.94                     | 0.50              |
| 1:A:66:ASP:O     | 1:A:69:THR:HG22  | 2.12                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:222:ASN:ND2  | 1:A:222:ASN:N    | 2.57                     | 0.50              |
| 2:H:470:HIS:HE1  | 2:H:537:ALA:O    | 1.95                     | 0.50              |
| 2:G:485:ILE:HG22 | 2:G:487:GLY:HA2  | 1.94                     | 0.50              |
| 2:G:467:LEU:O    | 2:G:471:MSE:HG2  | 2.11                     | 0.50              |
| 1:B:25:PHE:HZ    | 1:B:89:LEU:HD22  | 1.77                     | 0.49              |
| 1:D:139:LEU:O    | 1:D:143:ALA:HB2  | 2.12                     | 0.49              |
| 1:B:315:GLY:O    | 1:B:356:PRO:HD2  | 2.10                     | 0.49              |
| 1:A:257:ASN:CA   | 1:A:435:TYR:CD2  | 2.95                     | 0.49              |
| 1:B:101:ASN:C    | 1:B:103:GLU:H    | 2.06                     | 0.49              |
| 1:F:207:ILE:HD13 | 1:F:386:ILE:HG21 | 1.93                     | 0.49              |
| 1:A:385:SER:OG   | 1:A:386:ILE:N    | 2.46                     | 0.49              |
| 1:E:103:GLU:N    | 1:E:104:TYR:CB   | 2.76                     | 0.49              |
| 2:H:464:GLU:HG3  | 2:H:489:PHE:HD1  | 1.77                     | 0.49              |
| 1:B:208:VAL:HB   | 1:B:360:LEU:HD23 | 1.94                     | 0.49              |
| 1:A:140:LEU:HD11 | 1:D:114:VAL:HG11 | 1.94                     | 0.49              |
| 1:F:200:PHE:CD1  | 1:F:206:ILE:HD13 | 2.47                     | 0.49              |
| 1:B:257:ASN:CA   | 1:B:435:TYR:CD2  | 2.96                     | 0.49              |
| 1:F:84:GLY:HA3   | 1:F:88:TYR:HB2   | 1.95                     | 0.49              |
| 1:D:25:PHE:HZ    | 1:D:89:LEU:HD22  | 1.77                     | 0.49              |
| 1:F:138:VAL:O    | 1:F:142:GLU:HG2  | 2.12                     | 0.49              |
| 2:I:471:MSE:HB2  | 2:I:478:ALA:HB2  | 1.95                     | 0.49              |
| 1:D:268:LEU:HB3  | 1:D:272:ASP:HB2  | 1.93                     | 0.49              |
| 2:G:475:ARG:HH21 | 2:G:501:ILE:HG22 | 1.77                     | 0.49              |
| 1:D:71:THR:HG22  | 1:D:89:LEU:CD1   | 2.42                     | 0.49              |
| 1:B:83:ILE:CG2   | 1:B:84:GLY:H     | 2.25                     | 0.49              |
| 1:B:140:LEU:HD11 | 1:E:114:VAL:HG11 | 1.95                     | 0.49              |
| 1:F:222:ASN:N    | 1:F:222:ASN:HD22 | 2.11                     | 0.49              |
| 1:B:25:PHE:CZ    | 1:B:89:LEU:HD22  | 2.48                     | 0.49              |
| 1:F:53:HIS:CE1   | 1:F:57:ARG:NH1   | 2.81                     | 0.49              |
| 1:D:142:GLU:HA   | 1:D:145:ARG:HB3  | 1.95                     | 0.49              |
| 1:B:192:GLU:HA   | 1:B:195:ARG:HG3  | 1.94                     | 0.49              |
| 1:D:192:GLU:HA   | 1:D:195:ARG:HG3  | 1.94                     | 0.49              |
| 1:E:71:THR:HG22  | 1:E:89:LEU:HD13  | 1.93                     | 0.49              |
| 1:D:104:TYR:O    | 1:D:104:TYR:CD2  | 2.66                     | 0.49              |
| 1:F:392:ILE:HA   | 1:F:418:LYS:O    | 2.12                     | 0.49              |
| 1:D:228:ALA:HB1  | 1:D:286:ALA:HB1  | 1.95                     | 0.49              |
| 1:E:97:PRO:HG2   | 1:E:98:THR:HG22  | 1.95                     | 0.49              |
| 1:D:62:GLY:CA    | 1:D:63:GLU:CB    | 2.89                     | 0.49              |
| 1:A:63:GLU:N     | 1:A:64:PRO:CA    | 2.59                     | 0.49              |
| 1:C:259:ASN:OD1  | 1:C:259:ASN:C    | 2.51                     | 0.49              |
| 1:D:104:TYR:HD1  | 1:D:105:TYR:CG   | 2.31                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:238:PHE:CE2  | 1:A:301:ILE:HG23 | 2.48                     | 0.49              |
| 1:C:53:HIS:CE1   | 1:C:57:ARG:NH1   | 2.81                     | 0.49              |
| 1:F:255:GLU:C    | 1:F:257:ASN:H    | 2.05                     | 0.49              |
| 1:C:84:GLY:HA3   | 1:C:88:TYR:CB    | 2.43                     | 0.49              |
| 2:H:464:GLU:HG3  | 2:H:489:PHE:CD1  | 2.47                     | 0.49              |
| 1:D:317:ILE:HB   | 1:D:357:VAL:HG22 | 1.95                     | 0.49              |
| 1:D:262:ASN:HB3  | 1:D:265:THR:CG2  | 2.43                     | 0.48              |
| 1:A:53:HIS:CE1   | 1:A:57:ARG:HD2   | 2.48                     | 0.48              |
| 1:E:28:PRO:C     | 1:E:30:ALA:N     | 2.67                     | 0.48              |
| 1:D:202:ARG:HB3  | 1:D:354:GLU:C    | 2.32                     | 0.48              |
| 1:B:228:ALA:HB1  | 1:B:286:ALA:HB1  | 1.95                     | 0.48              |
| 1:E:249:MET:HA   | 1:E:252:LEU:HB2  | 1.95                     | 0.48              |
| 1:A:83:ILE:HG22  | 1:A:84:GLY:N     | 2.29                     | 0.48              |
| 2:G:487:GLY:CA   | 2:G:489:PHE:H    | 2.24                     | 0.48              |
| 1:F:132:ARG:NH1  | 1:F:135:GLU:OE1  | 2.46                     | 0.48              |
| 2:G:503:ALA:O    | 2:G:506:GLU:N    | 2.46                     | 0.48              |
| 1:B:133:GLU:N    | 1:B:134:ASP:CB   | 2.67                     | 0.48              |
| 1:D:141:ASP:OD2  | 1:D:297:ARG:CD   | 2.59                     | 0.48              |
| 1:E:104:TYR:OH   | 1:F:69:THR:OG1   | 1.87                     | 0.48              |
| 1:E:259:ASN:OD1  | 1:E:259:ASN:C    | 2.51                     | 0.48              |
| 1:D:25:PHE:CZ    | 1:D:89:LEU:HD22  | 2.49                     | 0.48              |
| 1:C:226:ASN:O    | 1:C:230:LYS:HB2  | 2.14                     | 0.48              |
| 1:A:105:TYR:CE2  | 1:B:68:VAL:CG1   | 2.96                     | 0.48              |
| 1:B:219:PHE:CZ   | 1:B:223:ILE:HD11 | 2.48                     | 0.48              |
| 1:F:219:PHE:CZ   | 1:F:223:ILE:HD11 | 2.48                     | 0.48              |
| 1:B:381:ARG:HD3  | 1:B:387:GLU:HB2  | 1.96                     | 0.48              |
| 1:E:322:LEU:HB3  | 1:E:323:GLN:NE2  | 2.28                     | 0.48              |
| 1:B:83:ILE:HG22  | 1:B:84:GLY:N     | 2.28                     | 0.48              |
| 1:A:46:ALA:O     | 1:A:50:LYS:HD2   | 2.14                     | 0.48              |
| 1:C:258:ILE:N    | 1:C:435:TYR:CD2  | 2.82                     | 0.48              |
| 2:G:475:ARG:HG2  | 2:G:511:ALA:HB1  | 1.94                     | 0.48              |
| 1:D:222:ASN:HD22 | 1:D:222:ASN:H    | 1.60                     | 0.48              |
| 2:H:541:SER:HB3  | 2:H:544:GLU:HG3  | 1.96                     | 0.48              |
| 2:H:475:ARG:CG   | 2:H:475:ARG:NH1  | 2.77                     | 0.48              |
| 1:C:66:ASP:O     | 1:C:69:THR:HG22  | 2.14                     | 0.48              |
| 1:B:391:ASP:O    | 1:B:419:GLN:HA   | 2.14                     | 0.48              |
| 2:I:504:PHE:O    | 2:I:507:GLU:HB3  | 2.14                     | 0.48              |
| 1:D:225:GLN:HE22 | 1:D:254:ALA:HB3  | 1.78                     | 0.48              |
| 1:D:255:GLU:C    | 1:D:257:ASN:N    | 2.45                     | 0.47              |
| 2:H:503:ALA:O    | 2:H:506:GLU:N    | 2.45                     | 0.47              |
| 1:C:104:TYR:HD1  | 1:C:105:TYR:CG   | 2.31                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:325:ILE:HG23 | 1:D:342:ILE:HD13 | 1.95                     | 0.47              |
| 2:G:487:GLY:HA3  | 2:G:489:PHE:N    | 2.27                     | 0.47              |
| 2:G:464:GLU:CG   | 2:G:489:PHE:HD1  | 2.27                     | 0.47              |
| 1:B:395:PHE:HB2  | 1:B:415:ILE:HB   | 1.95                     | 0.47              |
| 2:I:465:ARG:HG3  | 2:I:531:LEU:HD21 | 1.95                     | 0.47              |
| 1:D:132:ARG:NH1  | 1:D:135:GLU:OE1  | 2.48                     | 0.47              |
| 1:A:271:GLU:O    | 1:A:275:LYS:HB2  | 2.14                     | 0.47              |
| 1:E:216:LYS:HA   | 1:E:396:LEU:HD12 | 1.96                     | 0.47              |
| 1:D:225:GLN:NE2  | 1:D:251:MET:HB2  | 2.29                     | 0.47              |
| 1:C:280:MET:O    | 1:C:284:SER:HB2  | 2.14                     | 0.47              |
| 1:C:392:ILE:HA   | 1:C:418:LYS:O    | 2.14                     | 0.47              |
| 1:E:63:GLU:N     | 1:E:64:PRO:CA    | 2.56                     | 0.47              |
| 1:B:222:ASN:H    | 1:B:222:ASN:HD22 | 1.61                     | 0.47              |
| 1:D:235:VAL:HG12 | 1:D:316:MET:HB2  | 1.96                     | 0.47              |
| 1:D:257:ASN:CA   | 1:D:435:TYR:CD2  | 2.98                     | 0.47              |
| 2:H:538:ASP:O    | 2:H:539:ASP:CB   | 2.61                     | 0.47              |
| 1:F:32:VAL:HB    | 1:F:33:PRO:HD3   | 1.96                     | 0.47              |
| 1:A:392:ILE:HA   | 1:A:418:LYS:O    | 2.14                     | 0.47              |
| 1:B:66:ASP:N     | 1:B:69:THR:HG22  | 2.16                     | 0.47              |
| 1:B:104:TYR:HB3  | 1:B:105:TYR:HB2  | 1.95                     | 0.47              |
| 1:F:83:ILE:CG2   | 1:F:84:GLY:H     | 2.26                     | 0.47              |
| 1:A:50:LYS:NZ    | 1:A:82:GLU:OE2   | 2.48                     | 0.47              |
| 1:C:391:ASP:O    | 1:C:419:GLN:HA   | 2.15                     | 0.47              |
| 1:A:185:GLY:O    | 1:A:186:ILE:HG13 | 2.13                     | 0.47              |
| 1:D:66:ASP:OD1   | 1:D:69:THR:HG22  | 2.15                     | 0.47              |
| 1:D:105:TYR:O    | 1:D:109:VAL:HG23 | 2.15                     | 0.47              |
| 2:I:503:ALA:O    | 2:I:506:GLU:N    | 2.46                     | 0.47              |
| 1:A:104:TYR:HD1  | 1:A:105:TYR:CG   | 2.33                     | 0.47              |
| 1:A:231:THR:HG23 | 1:A:232:ASN:N    | 2.25                     | 0.47              |
| 1:D:323:GLN:HE21 | 1:D:361:SER:HA   | 1.79                     | 0.47              |
| 1:A:322:LEU:C    | 1:A:324:LEU:H    | 2.18                     | 0.47              |
| 2:G:507:GLU:O    | 2:G:507:GLU:HG3  | 2.15                     | 0.47              |
| 2:H:463:ALA:O    | 2:H:467:LEU:HB2  | 2.14                     | 0.47              |
| 1:C:258:ILE:O    | 1:C:259:ASN:CB   | 2.61                     | 0.47              |
| 1:C:148:MET:HE3  | 1:C:148:MET:HA   | 1.97                     | 0.47              |
| 1:F:202:ARG:O    | 1:F:203:SER:CB   | 2.63                     | 0.47              |
| 1:D:298:VAL:HG11 | 1:D:345:SER:HB3  | 1.96                     | 0.47              |
| 2:I:513:PRO:O    | 2:I:517:ILE:HG12 | 2.15                     | 0.47              |
| 1:E:104:TYR:HD1  | 1:E:105:TYR:CG   | 2.32                     | 0.47              |
| 1:B:223:ILE:O    | 1:B:227:VAL:HG23 | 2.15                     | 0.47              |
| 1:E:83:ILE:CG2   | 1:E:84:GLY:H     | 2.09                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:207:ILE:CD1  | 1:D:386:ILE:HG21 | 2.45                     | 0.47              |
| 1:C:216:LYS:HB2  | 1:C:360:LEU:HD22 | 1.97                     | 0.47              |
| 1:E:208:VAL:HG22 | 1:E:394:ALA:HB3  | 1.96                     | 0.47              |
| 1:A:391:ASP:N    | 1:A:391:ASP:OD1  | 2.43                     | 0.47              |
| 1:F:251:MET:CE   | 1:F:288:ILE:HD13 | 2.45                     | 0.47              |
| 1:B:196:MET:O    | 1:B:419:GLN:NE2  | 2.40                     | 0.46              |
| 1:F:208:VAL:HA   | 1:F:394:ALA:O    | 2.15                     | 0.46              |
| 1:D:374:ARG:HB3  | 1:D:375:PRO:HA   | 1.96                     | 0.46              |
| 2:G:475:ARG:NH1  | 2:G:475:ARG:HG3  | 2.20                     | 0.46              |
| 1:B:258:ILE:O    | 1:B:259:ASN:CB   | 2.62                     | 0.46              |
| 1:C:28:PRO:C     | 1:C:30:ALA:N     | 2.68                     | 0.46              |
| 1:C:86:VAL:HG22  | 2:H:572:GLU:HG3  | 1.98                     | 0.46              |
| 1:C:104:TYR:N    | 1:C:107:ARG:H    | 2.09                     | 0.46              |
| 1:D:202:ARG:O    | 1:D:203:SER:HB2  | 2.15                     | 0.46              |
| 1:A:132:ARG:NH1  | 1:A:135:GLU:OE1  | 2.48                     | 0.46              |
| 1:E:132:ARG:C    | 1:E:134:ASP:HB2  | 2.36                     | 0.46              |
| 1:E:62:GLY:HA2   | 1:E:63:GLU:CB    | 2.33                     | 0.46              |
| 1:F:315:GLY:O    | 1:F:356:PRO:HD2  | 2.16                     | 0.46              |
| 1:B:235:VAL:HG12 | 1:B:316:MET:HB2  | 1.98                     | 0.46              |
| 1:C:104:TYR:HA   | 1:C:106:ALA:H    | 1.79                     | 0.46              |
| 1:F:188:THR:HG22 | 1:F:200:PHE:CE2  | 2.51                     | 0.46              |
| 1:C:25:PHE:CZ    | 1:C:89:LEU:HD22  | 2.51                     | 0.46              |
| 1:E:339:VAL:HG13 | 1:E:384:GLY:HA3  | 1.98                     | 0.46              |
| 2:G:550:ARG:CB   | 2:G:550:ARG:HH11 | 2.28                     | 0.46              |
| 1:F:187:PRO:C    | 1:F:189:GLY:H    | 2.18                     | 0.46              |
| 2:H:467:LEU:HA   | 2:H:467:LEU:HD12 | 1.85                     | 0.46              |
| 1:F:240:LEU:HD22 | 1:F:295:SER:HA   | 1.97                     | 0.46              |
| 1:A:280:MET:O    | 1:A:284:SER:HB2  | 2.15                     | 0.46              |
| 1:E:191:THR:O    | 1:E:194:ASP:HB2  | 2.16                     | 0.45              |
| 2:H:471:MSE:O    | 2:H:475:ARG:HD2  | 2.16                     | 0.45              |
| 1:F:64:PRO:HB2   | 1:F:65:VAL:H     | 1.64                     | 0.45              |
| 1:C:101:ASN:HB2  | 1:C:105:TYR:CD1  | 2.51                     | 0.45              |
| 1:D:128:ASP:HB3  | 1:D:139:LEU:HD21 | 1.96                     | 0.45              |
| 1:C:62:GLY:CA    | 1:C:63:GLU:CB    | 2.93                     | 0.45              |
| 1:B:222:ASN:ND2  | 1:B:222:ASN:N    | 2.63                     | 0.45              |
| 2:I:519:ARG:O    | 2:I:519:ARG:HD3  | 2.16                     | 0.45              |
| 1:D:200:PHE:CD1  | 1:D:200:PHE:N    | 2.83                     | 0.45              |
| 2:I:541:SER:HB3  | 2:I:544:GLU:HG3  | 1.98                     | 0.45              |
| 1:A:88:TYR:O     | 1:A:92:LEU:HG    | 2.16                     | 0.45              |
| 2:I:491:ILE:HB   | 2:I:494:HIS:CD2  | 2.51                     | 0.45              |
| 1:D:28:PRO:C     | 1:D:30:ALA:H     | 2.19                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:104:TYR:HD1  | 1:B:105:TYR:CG   | 2.34                     | 0.45              |
| 1:D:322:LEU:HB3  | 1:D:323:GLN:NE2  | 2.31                     | 0.45              |
| 1:B:148:MET:HE3  | 1:B:148:MET:HA   | 1.97                     | 0.45              |
| 2:I:487:GLY:HA2  | 2:I:488:ARG:HB2  | 1.97                     | 0.45              |
| 2:G:565:GLU:O    | 2:G:569:THR:HG22 | 2.15                     | 0.45              |
| 1:C:351:ARG:HH11 | 1:C:351:ARG:HB2  | 1.80                     | 0.45              |
| 1:A:61:ARG:CB    | 1:A:62:GLY:CA    | 2.90                     | 0.45              |
| 1:E:202:ARG:HB3  | 1:E:354:GLU:C    | 2.36                     | 0.45              |
| 2:G:519:ARG:O    | 2:G:519:ARG:HD3  | 2.17                     | 0.45              |
| 1:C:258:ILE:N    | 1:C:435:TYR:CE2  | 2.85                     | 0.45              |
| 1:E:84:GLY:HA3   | 1:E:88:TYR:CB    | 2.46                     | 0.45              |
| 1:D:185:GLY:O    | 1:D:186:ILE:HG13 | 2.17                     | 0.45              |
| 1:E:187:PRO:C    | 1:E:189:GLY:N    | 2.69                     | 0.45              |
| 1:D:246:GLN:HG2  | 1:D:246:GLN:O    | 2.17                     | 0.45              |
| 1:B:249:MET:HA   | 1:B:252:LEU:HB2  | 1.98                     | 0.45              |
| 1:F:298:VAL:HG11 | 1:F:345:SER:HB3  | 1.98                     | 0.45              |
| 1:B:280:MET:O    | 1:B:284:SER:HB2  | 2.17                     | 0.45              |
| 1:A:67:LEU:HD12  | 2:G:584:ALA:HB3  | 1.98                     | 0.45              |
| 1:D:148:MET:HE3  | 1:D:148:MET:HA   | 1.98                     | 0.45              |
| 1:C:219:PHE:CZ   | 1:C:223:ILE:HD11 | 2.51                     | 0.45              |
| 1:E:251:MET:HE3  | 1:E:288:ILE:HD13 | 1.99                     | 0.45              |
| 1:A:104:TYR:CD2  | 1:A:104:TYR:O    | 2.69                     | 0.45              |
| 1:B:200:PHE:CD1  | 1:B:206:ILE:HD13 | 2.52                     | 0.45              |
| 2:G:475:ARG:CG   | 2:G:475:ARG:HH11 | 2.23                     | 0.45              |
| 1:E:48:HIS:NE2   | 1:E:88:TYR:OH    | 2.37                     | 0.45              |
| 1:F:51:ILE:HD11  | 1:F:83:ILE:HG21  | 1.99                     | 0.45              |
| 1:F:233:GLU:CG   | 1:F:315:GLY:HA3  | 2.43                     | 0.45              |
| 2:H:487:GLY:HA3  | 2:H:489:PHE:N    | 2.27                     | 0.45              |
| 1:E:273:TRP:O    | 1:E:275:LYS:N    | 2.47                     | 0.45              |
| 1:E:208:VAL:HB   | 1:E:360:LEU:HD23 | 1.99                     | 0.45              |
| 2:I:470:HIS:HE1  | 2:I:537:ALA:O    | 2.00                     | 0.45              |
| 1:C:222:ASN:ND2  | 1:C:222:ASN:N    | 2.62                     | 0.45              |
| 1:C:148:MET:HA   | 1:C:148:MET:HE2  | 1.99                     | 0.45              |
| 1:C:135:GLU:C    | 1:C:137:ASP:H    | 2.19                     | 0.45              |
| 1:C:101:ASN:C    | 1:C:103:GLU:H    | 2.17                     | 0.45              |
| 1:D:74:LEU:HD13  | 1:D:83:ILE:CD1   | 2.47                     | 0.45              |
| 1:C:385:SER:OG   | 1:C:386:ILE:N    | 2.49                     | 0.45              |
| 1:E:251:MET:CE   | 1:E:288:ILE:HD13 | 2.47                     | 0.45              |
| 1:B:439:VAL:HG12 | 1:B:440:ASN:N    | 2.32                     | 0.45              |
| 1:B:202:ARG:O    | 1:B:203:SER:CB   | 2.64                     | 0.45              |
| 1:E:298:VAL:HG11 | 1:E:345:SER:HB3  | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:439:VAL:HG12 | 1:F:440:ASN:H    | 1.82                     | 0.45              |
| 1:D:259:ASN:OD1  | 1:D:259:ASN:C    | 2.56                     | 0.45              |
| 1:A:200:PHE:N    | 1:A:200:PHE:CD1  | 2.85                     | 0.45              |
| 1:F:296:ILE:O    | 1:F:325:ILE:HG13 | 2.17                     | 0.45              |
| 1:C:200:PHE:CD1  | 1:C:206:ILE:HD13 | 2.52                     | 0.44              |
| 1:C:133:GLU:CA   | 1:C:134:ASP:HB2  | 2.46                     | 0.44              |
| 1:C:322:LEU:C    | 1:C:324:LEU:H    | 2.21                     | 0.44              |
| 1:C:322:LEU:HB3  | 1:C:323:GLN:NE2  | 2.31                     | 0.44              |
| 1:A:187:PRO:C    | 1:A:189:GLY:N    | 2.69                     | 0.44              |
| 2:I:473:ARG:HD2  | 2:I:536:ILE:HD11 | 1.99                     | 0.44              |
| 1:C:231:THR:CG2  | 1:C:232:ASN:H    | 2.15                     | 0.44              |
| 1:C:316:MET:HG2  | 1:C:356:PRO:HG2  | 1.99                     | 0.44              |
| 1:B:259:ASN:C    | 1:B:259:ASN:OD1  | 2.55                     | 0.44              |
| 1:B:202:ARG:HB3  | 1:B:354:GLU:C    | 2.37                     | 0.44              |
| 1:B:28:PRO:C     | 1:B:30:ALA:N     | 2.68                     | 0.44              |
| 1:F:104:TYR:H    | 1:F:107:ARG:HB2  | 1.82                     | 0.44              |
| 1:E:142:GLU:HA   | 1:E:145:ARG:HB3  | 1.99                     | 0.44              |
| 1:E:219:PHE:CZ   | 1:E:223:ILE:HD11 | 2.52                     | 0.44              |
| 1:A:298:VAL:HG11 | 1:A:345:SER:HB3  | 2.00                     | 0.44              |
| 1:D:196:MET:O    | 1:D:419:GLN:NE2  | 2.43                     | 0.44              |
| 1:A:257:ASN:CA   | 1:A:435:TYR:CE2  | 3.00                     | 0.44              |
| 1:E:104:TYR:HA   | 1:E:106:ALA:N    | 2.33                     | 0.44              |
| 1:D:104:TYR:H    | 1:D:107:ARG:H    | 1.65                     | 0.44              |
| 1:F:197:THR:CB   | 1:F:199:GLY:O    | 2.65                     | 0.44              |
| 1:C:104:TYR:HB3  | 1:C:105:TYR:HB2  | 2.00                     | 0.44              |
| 1:F:83:ILE:HG22  | 1:F:84:GLY:N     | 2.32                     | 0.44              |
| 1:A:273:TRP:C    | 1:A:275:LYS:N    | 2.70                     | 0.44              |
| 2:I:503:ALA:O    | 2:I:504:PHE:C    | 2.56                     | 0.44              |
| 1:C:391:ASP:OD1  | 1:C:391:ASP:N    | 2.46                     | 0.44              |
| 2:H:496:ALA:O    | 2:H:500:TYR:HD2  | 2.00                     | 0.44              |
| 1:A:104:TYR:OH   | 1:B:63:GLU:HG3   | 2.17                     | 0.44              |
| 1:E:16:ALA:HA    | 1:F:68:VAL:HG11  | 2.00                     | 0.44              |
| 1:D:133:GLU:N    | 1:D:134:ASP:CB   | 2.74                     | 0.44              |
| 1:C:88:TYR:O     | 1:C:92:LEU:HG    | 2.18                     | 0.44              |
| 2:G:582:ARG:HB3  | 2:G:582:ARG:HE   | 1.56                     | 0.44              |
| 1:C:83:ILE:CG2   | 1:C:84:GLY:H     | 2.17                     | 0.44              |
| 1:C:48:HIS:NE2   | 1:C:88:TYR:OH    | 2.42                     | 0.44              |
| 1:A:207:ILE:HA   | 1:A:359:ALA:O    | 2.17                     | 0.44              |
| 2:H:503:ALA:O    | 2:H:504:PHE:C    | 2.56                     | 0.44              |
| 1:E:98:THR:HG23  | 1:E:101:ASN:HD21 | 1.83                     | 0.44              |
| 1:E:133:GLU:CA   | 1:E:134:ASP:HB2  | 2.48                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:66:ASP:O     | 1:E:69:THR:HG22  | 2.18                     | 0.44              |
| 1:D:322:LEU:C    | 1:D:324:LEU:H    | 2.21                     | 0.44              |
| 1:C:207:ILE:HA   | 1:C:359:ALA:O    | 2.17                     | 0.44              |
| 1:A:132:ARG:C    | 1:A:134:ASP:HB2  | 2.38                     | 0.44              |
| 2:H:509:HIS:O    | 2:H:510:GLU:C    | 2.57                     | 0.44              |
| 1:F:141:ASP:C    | 1:F:143:ALA:H    | 2.21                     | 0.44              |
| 1:E:322:LEU:O    | 1:E:324:LEU:N    | 2.51                     | 0.44              |
| 1:E:84:GLY:HA3   | 1:E:88:TYR:HB3   | 2.00                     | 0.44              |
| 1:C:40:PRO:O     | 1:C:49:GLN:HG3   | 2.17                     | 0.44              |
| 1:E:200:PHE:CD1  | 1:E:200:PHE:N    | 2.85                     | 0.43              |
| 1:E:322:LEU:C    | 1:E:324:LEU:H    | 2.20                     | 0.43              |
| 1:A:396:LEU:CD2  | 1:A:414:ILE:HG12 | 2.48                     | 0.43              |
| 1:B:225:GLN:HE22 | 1:B:254:ALA:HB3  | 1.82                     | 0.43              |
| 1:D:28:PRO:C     | 1:D:30:ALA:N     | 2.71                     | 0.43              |
| 1:C:104:TYR:OH   | 1:D:63:GLU:HG3   | 2.18                     | 0.43              |
| 1:D:67:LEU:HD23  | 1:D:67:LEU:HA    | 1.83                     | 0.43              |
| 2:I:565:GLU:O    | 2:I:569:THR:HG22 | 2.18                     | 0.43              |
| 1:C:340:SER:HB3  | 1:C:385:SER:HB3  | 2.00                     | 0.43              |
| 1:E:422:GLY:HA3  | 1:E:423:PRO:HD3  | 1.82                     | 0.43              |
| 1:A:101:ASN:HB2  | 1:A:105:TYR:CD1  | 2.53                     | 0.43              |
| 1:E:226:ASN:O    | 1:E:230:LYS:HB2  | 2.19                     | 0.43              |
| 1:F:351:ARG:HH11 | 1:F:351:ARG:HB2  | 1.82                     | 0.43              |
| 1:F:422:GLY:HA3  | 1:F:423:PRO:HD3  | 1.83                     | 0.43              |
| 1:A:104:TYR:N    | 1:A:107:ARG:H    | 2.12                     | 0.43              |
| 1:B:61:ARG:HB2   | 1:B:62:GLY:CA    | 2.44                     | 0.43              |
| 1:E:62:GLY:CA    | 1:E:63:GLU:CB    | 2.95                     | 0.43              |
| 1:D:47:ALA:HB1   | 1:D:83:ILE:HG23  | 2.00                     | 0.43              |
| 2:G:465:ARG:CG   | 2:G:531:LEU:HD21 | 2.46                     | 0.43              |
| 1:B:216:LYS:HA   | 1:B:396:LEU:HD12 | 2.00                     | 0.43              |
| 1:B:53:HIS:CE1   | 1:B:57:ARG:NH1   | 2.86                     | 0.43              |
| 1:C:381:ARG:HD3  | 1:C:387:GLU:HB2  | 2.00                     | 0.43              |
| 1:E:101:ASN:HB2  | 1:E:105:TYR:CD1  | 2.54                     | 0.43              |
| 1:C:61:ARG:CB    | 1:C:62:GLY:CA    | 2.93                     | 0.43              |
| 1:C:323:GLN:HE21 | 1:C:361:SER:HA   | 1.83                     | 0.43              |
| 1:F:323:GLN:HE21 | 1:F:361:SER:HA   | 1.83                     | 0.43              |
| 1:D:84:GLY:HA3   | 1:D:88:TYR:CB    | 2.49                     | 0.43              |
| 1:D:273:TRP:C    | 1:D:275:LYS:N    | 2.72                     | 0.43              |
| 1:B:202:ARG:O    | 1:B:203:SER:HB2  | 2.19                     | 0.43              |
| 1:B:138:VAL:O    | 1:B:142:GLU:HG2  | 2.19                     | 0.43              |
| 1:A:124:SER:O    | 1:A:128:ASP:HB2  | 2.19                     | 0.43              |
| 1:A:101:ASN:HB3  | 1:A:104:TYR:CD1  | 2.53                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:124:SER:O    | 1:D:128:ASP:HB2  | 2.18                     | 0.43              |
| 2:G:501:ILE:O    | 2:G:504:PHE:HB3  | 2.18                     | 0.43              |
| 1:D:102:VAL:O    | 1:D:104:TYR:HA   | 2.19                     | 0.43              |
| 1:A:316:MET:HG2  | 1:A:356:PRO:HG2  | 2.01                     | 0.43              |
| 1:B:22:GLY:HA3   | 1:B:96:VAL:HG21  | 2.00                     | 0.43              |
| 1:D:133:GLU:CA   | 1:D:134:ASP:HB2  | 2.48                     | 0.43              |
| 1:A:67:LEU:HD21  | 1:A:89:LEU:HB3   | 2.00                     | 0.43              |
| 1:E:273:TRP:C    | 1:E:275:LYS:N    | 2.69                     | 0.43              |
| 1:A:28:PRO:C     | 1:A:30:ALA:N     | 2.72                     | 0.43              |
| 1:D:255:GLU:HB3  | 1:D:256:GLY:H    | 1.61                     | 0.43              |
| 1:B:322:LEU:C    | 1:B:324:LEU:H    | 2.22                     | 0.43              |
| 1:D:79:GLN:O     | 1:D:83:ILE:HG13  | 2.18                     | 0.43              |
| 1:E:148:MET:HA   | 1:E:148:MET:HE2  | 2.00                     | 0.43              |
| 1:A:374:ARG:HG2  | 1:A:376:MET:HE3  | 2.01                     | 0.43              |
| 2:G:484:ARG:HH22 | 2:G:546:GLU:HG2  | 1.84                     | 0.43              |
| 1:B:187:PRO:C    | 1:B:189:GLY:N    | 2.69                     | 0.43              |
| 2:I:461:GLN:HG3  | 2:I:491:ILE:HD11 | 2.00                     | 0.43              |
| 1:D:439:VAL:HG12 | 1:D:440:ASN:H    | 1.84                     | 0.43              |
| 1:B:61:ARG:CB    | 1:B:62:GLY:HA3   | 2.34                     | 0.42              |
| 1:E:101:ASN:HB3  | 1:E:104:TYR:CD1  | 2.53                     | 0.42              |
| 1:A:376:MET:CE   | 1:D:246:GLN:HE22 | 2.32                     | 0.42              |
| 1:D:258:ILE:N    | 1:D:435:TYR:CD2  | 2.87                     | 0.42              |
| 1:E:104:TYR:CD2  | 1:E:104:TYR:C    | 2.90                     | 0.42              |
| 2:H:546:GLU:O    | 2:H:550:ARG:HB2  | 2.19                     | 0.42              |
| 1:A:210:ALA:CB   | 1:A:396:LEU:HB2  | 2.48                     | 0.42              |
| 1:C:340:SER:CB   | 1:C:385:SER:HB3  | 2.49                     | 0.42              |
| 1:E:391:ASP:O    | 1:E:419:GLN:HA   | 2.19                     | 0.42              |
| 1:B:40:PRO:O     | 1:B:49:GLN:HG3   | 2.19                     | 0.42              |
| 1:C:101:ASN:HB2  | 1:C:102:VAL:H    | 1.69                     | 0.42              |
| 1:F:101:ASN:C    | 1:F:103:GLU:N    | 2.72                     | 0.42              |
| 2:H:565:GLU:O    | 2:H:569:THR:HG22 | 2.19                     | 0.42              |
| 1:D:207:ILE:HG23 | 1:D:393:VAL:HG13 | 2.00                     | 0.42              |
| 1:B:298:VAL:HG11 | 1:B:345:SER:HB3  | 2.00                     | 0.42              |
| 1:C:306:ARG:NH2  | 1:D:32:VAL:CG2   | 2.79                     | 0.42              |
| 1:A:101:ASN:C    | 1:A:103:GLU:N    | 2.73                     | 0.42              |
| 1:C:98:THR:HG23  | 1:C:101:ASN:HD21 | 1.85                     | 0.42              |
| 2:G:487:GLY:HA2  | 2:G:488:ARG:HB2  | 2.01                     | 0.42              |
| 1:B:207:ILE:HG23 | 1:B:393:VAL:HG13 | 2.01                     | 0.42              |
| 1:A:140:LEU:HD11 | 1:D:114:VAL:CG1  | 2.50                     | 0.42              |
| 1:F:251:MET:HE3  | 1:F:288:ILE:HD13 | 2.02                     | 0.42              |
| 1:A:40:PRO:O     | 1:A:49:GLN:HG3   | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:96:VAL:HA    | 1:F:97:PRO:HD3   | 1.92                     | 0.42              |
| 1:E:104:TYR:O    | 1:E:104:TYR:CD2  | 2.72                     | 0.42              |
| 1:A:322:LEU:O    | 1:A:324:LEU:N    | 2.52                     | 0.42              |
| 1:D:186:ILE:HA   | 1:D:187:PRO:HD3  | 1.92                     | 0.42              |
| 2:G:486:GLY:N    | 2:G:488:ARG:HB2  | 2.33                     | 0.42              |
| 1:C:339:VAL:HG13 | 1:C:384:GLY:HA3  | 2.00                     | 0.42              |
| 2:G:487:GLY:HA3  | 2:G:489:PHE:HD2  | 1.85                     | 0.42              |
| 1:D:83:ILE:CG2   | 1:D:84:GLY:H     | 2.30                     | 0.42              |
| 1:E:268:LEU:HB3  | 1:E:272:ASP:CB   | 2.46                     | 0.42              |
| 1:D:395:PHE:HB2  | 1:D:415:ILE:HB   | 2.01                     | 0.42              |
| 1:F:84:GLY:HA3   | 1:F:88:TYR:CB    | 2.49                     | 0.42              |
| 1:D:48:HIS:HE2   | 1:D:88:TYR:HH    | 1.68                     | 0.42              |
| 1:D:84:GLY:HA3   | 1:D:88:TYR:HB2   | 2.02                     | 0.42              |
| 2:H:486:GLY:N    | 2:H:488:ARG:HB2  | 2.33                     | 0.42              |
| 1:E:26:LEU:HA    | 1:E:26:LEU:HD23  | 1.76                     | 0.42              |
| 1:C:249:MET:HA   | 1:C:252:LEU:HB2  | 2.01                     | 0.42              |
| 1:D:41:GLU:N     | 1:D:41:GLU:OE1   | 2.51                     | 0.42              |
| 2:H:516:LEU:HD23 | 2:H:516:LEU:HA   | 1.93                     | 0.42              |
| 2:H:468:LEU:HD23 | 2:H:497:LEU:HD13 | 2.01                     | 0.42              |
| 1:E:105:TYR:CZ   | 1:F:68:VAL:HB    | 2.55                     | 0.42              |
| 1:C:25:PHE:HZ    | 1:C:89:LEU:HD22  | 1.84                     | 0.42              |
| 1:A:225:GLN:HE22 | 1:A:254:ALA:HB3  | 1.85                     | 0.42              |
| 1:C:391:ASP:HB3  | 1:C:420:ARG:NH1  | 2.34                     | 0.42              |
| 1:C:314:LEU:HD13 | 1:C:355:VAL:HG21 | 2.02                     | 0.42              |
| 2:H:582:ARG:HE   | 2:H:582:ARG:HB3  | 1.45                     | 0.42              |
| 1:B:351:ARG:HH11 | 1:B:351:ARG:HB2  | 1.85                     | 0.42              |
| 1:A:62:GLY:CA    | 1:A:63:GLU:CB    | 2.89                     | 0.42              |
| 1:C:66:ASP:C     | 1:C:66:ASP:OD1   | 2.58                     | 0.42              |
| 1:F:105:TYR:H    | 1:F:108:ILE:HD12 | 1.85                     | 0.42              |
| 2:I:487:GLY:HA3  | 2:I:489:PHE:N    | 2.33                     | 0.42              |
| 2:G:467:LEU:HA   | 2:G:467:LEU:HD12 | 1.91                     | 0.42              |
| 1:B:142:GLU:HA   | 1:B:145:ARG:HB3  | 2.01                     | 0.42              |
| 1:C:124:SER:O    | 1:C:128:ASP:HB2  | 2.19                     | 0.42              |
| 1:F:320:ASP:HA   | 1:F:360:LEU:HD12 | 2.01                     | 0.42              |
| 1:C:91:GLU:O     | 1:C:95:ALA:HB2   | 2.20                     | 0.42              |
| 1:D:238:PHE:O    | 1:D:320:ASP:N    | 2.46                     | 0.42              |
| 1:B:292:ASP:OD1  | 1:B:292:ASP:N    | 2.50                     | 0.42              |
| 1:F:61:ARG:HB2   | 1:F:62:GLY:CA    | 2.39                     | 0.41              |
| 1:B:84:GLY:HA3   | 1:B:88:TYR:CB    | 2.50                     | 0.41              |
| 2:H:457:LEU:HA   | 2:H:458:PRO:HD3  | 1.83                     | 0.41              |
| 1:B:375:PRO:HG2  | 1:B:395:PHE:HB3  | 2.01                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:22:GLY:HA3   | 1:D:96:VAL:HG21  | 2.02                     | 0.41              |
| 2:G:505:TYR:O    | 2:G:508:GLY:N    | 2.52                     | 0.41              |
| 1:F:74:LEU:HD13  | 1:F:83:ILE:HD11  | 2.02                     | 0.41              |
| 1:D:187:PRO:C    | 1:D:189:GLY:N    | 2.69                     | 0.41              |
| 1:F:104:TYR:HD1  | 1:F:105:TYR:CG   | 2.37                     | 0.41              |
| 1:E:222:ASN:H    | 1:E:222:ASN:HD22 | 1.67                     | 0.41              |
| 1:E:30:ALA:O     | 1:E:33:PRO:HD2   | 2.20                     | 0.41              |
| 1:D:375:PRO:HG2  | 1:D:395:PHE:HB3  | 2.02                     | 0.41              |
| 1:E:293:THR:HA   | 1:E:294:PRO:HD2  | 1.76                     | 0.41              |
| 1:D:115:LEU:HA   | 1:D:115:LEU:HD23 | 1.93                     | 0.41              |
| 1:D:256:GLY:O    | 1:D:257:ASN:C    | 2.57                     | 0.41              |
| 2:I:509:HIS:O    | 2:I:510:GLU:C    | 2.58                     | 0.41              |
| 2:I:564:LYS:HE3  | 2:I:587:MSE:HG2  | 2.01                     | 0.41              |
| 1:A:141:ASP:C    | 1:A:143:ALA:N    | 2.73                     | 0.41              |
| 1:D:216:LYS:HA   | 1:D:396:LEU:HD12 | 2.01                     | 0.41              |
| 2:I:525:GLN:N    | 2:I:526:PRO:HD2  | 2.34                     | 0.41              |
| 2:G:500:TYR:CZ   | 2:G:521:PRO:HD3  | 2.55                     | 0.41              |
| 1:F:257:ASN:C    | 1:F:435:TYR:CE2  | 2.93                     | 0.41              |
| 1:C:344:ARG:HH11 | 1:D:61:ARG:CG    | 2.33                     | 0.41              |
| 1:D:141:ASP:C    | 1:D:143:ALA:N    | 2.74                     | 0.41              |
| 1:D:104:TYR:CD1  | 1:D:105:TYR:N    | 2.88                     | 0.41              |
| 1:A:259:ASN:C    | 1:A:259:ASN:OD1  | 2.58                     | 0.41              |
| 2:G:557:LYS:O    | 2:G:560:MSE:HB3  | 2.19                     | 0.41              |
| 1:B:64:PRO:HB2   | 1:B:65:VAL:H     | 1.63                     | 0.41              |
| 1:B:200:PHE:CD1  | 1:B:200:PHE:N    | 2.87                     | 0.41              |
| 2:G:503:ALA:O    | 2:G:504:PHE:C    | 2.57                     | 0.41              |
| 2:I:496:ALA:O    | 2:I:500:TYR:HD2  | 2.03                     | 0.41              |
| 1:B:66:ASP:O     | 1:B:67:LEU:C     | 2.59                     | 0.41              |
| 1:B:64:PRO:O     | 1:B:69:THR:HG21  | 2.20                     | 0.41              |
| 1:E:186:ILE:HA   | 1:E:187:PRO:HD3  | 1.89                     | 0.41              |
| 1:D:271:GLU:O    | 1:D:275:LYS:HB2  | 2.21                     | 0.41              |
| 1:E:375:PRO:HG2  | 1:E:395:PHE:HB3  | 2.03                     | 0.41              |
| 1:D:96:VAL:HA    | 1:D:97:PRO:HD3   | 1.90                     | 0.41              |
| 1:E:104:TYR:HA   | 1:E:106:ALA:H    | 1.85                     | 0.41              |
| 2:I:554:ASN:HB2  | 2:I:557:LYS:HD2  | 2.02                     | 0.41              |
| 1:C:80:LEU:HD23  | 1:C:80:LEU:HA    | 1.93                     | 0.41              |
| 1:E:103:GLU:N    | 1:E:104:TYR:HB2  | 2.36                     | 0.41              |
| 1:E:216:LYS:HA   | 1:E:396:LEU:CD1  | 2.51                     | 0.41              |
| 1:F:225:GLN:NE2  | 1:F:251:MET:HB2  | 2.36                     | 0.41              |
| 1:B:422:GLY:HA3  | 1:B:423:PRO:HD3  | 1.84                     | 0.41              |
| 1:D:257:ASN:CA   | 1:D:435:TYR:CE2  | 3.04                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:103:GLU:N    | 1:A:104:TYR:HB2  | 2.36                     | 0.41              |
| 1:A:188:THR:CG2  | 1:A:200:PHE:CE2  | 3.04                     | 0.41              |
| 1:D:322:LEU:C    | 1:D:324:LEU:N    | 2.73                     | 0.41              |
| 2:G:475:ARG:CG   | 2:G:475:ARG:NH1  | 2.83                     | 0.41              |
| 1:E:222:ASN:N    | 1:E:222:ASN:ND2  | 2.66                     | 0.41              |
| 1:B:208:VAL:HG22 | 1:B:394:ALA:HB3  | 2.02                     | 0.41              |
| 1:D:351:ARG:HB2  | 1:D:351:ARG:HH11 | 1.86                     | 0.41              |
| 1:A:317:ILE:HB   | 1:A:357:VAL:HG22 | 2.02                     | 0.41              |
| 1:B:323:GLN:HE21 | 1:B:361:SER:HA   | 1.85                     | 0.41              |
| 1:F:255:GLU:CG   | 1:F:256:GLY:H    | 2.33                     | 0.41              |
| 1:E:104:TYR:OH   | 1:F:63:GLU:HG3   | 2.21                     | 0.41              |
| 1:C:94:ASP:CB    | 2:H:591:LYS:NZ   | 2.61                     | 0.41              |
| 1:D:135:GLU:C    | 1:D:137:ASP:N    | 2.74                     | 0.41              |
| 1:B:188:THR:HG22 | 1:B:200:PHE:CE2  | 2.56                     | 0.41              |
| 1:E:325:ILE:HG23 | 1:E:342:ILE:HD13 | 2.03                     | 0.41              |
| 2:I:484:ARG:NH2  | 2:I:546:GLU:HG2  | 2.32                     | 0.41              |
| 1:F:95:ALA:HA    | 2:I:457:LEU:O    | 2.20                     | 0.41              |
| 1:A:273:TRP:O    | 1:A:275:LYS:N    | 2.53                     | 0.41              |
| 1:B:340:SER:HB3  | 1:B:385:SER:HB3  | 2.03                     | 0.41              |
| 1:E:124:SER:O    | 1:E:128:ASP:HB2  | 2.20                     | 0.41              |
| 1:E:188:THR:HG22 | 1:E:200:PHE:CE2  | 2.57                     | 0.40              |
| 1:F:432:ILE:HG22 | 1:F:435:TYR:H    | 1.85                     | 0.40              |
| 1:E:258:ILE:N    | 1:E:435:TYR:CE2  | 2.85                     | 0.40              |
| 1:E:322:LEU:C    | 1:E:324:LEU:N    | 2.74                     | 0.40              |
| 2:I:464:GLU:CG   | 2:I:489:PHE:HD1  | 2.33                     | 0.40              |
| 1:B:273:TRP:C    | 1:B:275:LYS:N    | 2.72                     | 0.40              |
| 1:E:391:ASP:HB3  | 1:E:420:ARG:NH1  | 2.36                     | 0.40              |
| 1:B:124:SER:O    | 1:B:128:ASP:HB2  | 2.21                     | 0.40              |
| 1:C:16:ALA:HA    | 1:D:68:VAL:HG11  | 2.03                     | 0.40              |
| 1:F:322:LEU:C    | 1:F:324:LEU:H    | 2.24                     | 0.40              |
| 1:F:104:TYR:CD1  | 1:F:104:TYR:C    | 2.91                     | 0.40              |
| 2:I:485:ILE:HG22 | 2:I:487:GLY:HA2  | 2.04                     | 0.40              |
| 1:A:39:ILE:HB    | 1:A:40:PRO:HD2   | 2.03                     | 0.40              |
| 1:A:396:LEU:HD23 | 1:A:414:ILE:HG12 | 2.03                     | 0.40              |
| 1:D:422:GLY:HA3  | 1:D:423:PRO:HD3  | 1.80                     | 0.40              |
| 1:B:67:LEU:HA    | 1:B:67:LEU:HD23  | 1.94                     | 0.40              |
| 1:C:67:LEU:HA    | 1:C:67:LEU:HD23  | 1.88                     | 0.40              |
| 1:D:222:ASN:N    | 1:D:222:ASN:ND2  | 2.66                     | 0.40              |
| 1:D:439:VAL:HG12 | 1:D:440:ASN:N    | 2.36                     | 0.40              |
| 2:H:475:ARG:NH1  | 2:H:504:PHE:HD2  | 2.20                     | 0.40              |
| 1:D:104:TYR:C    | 1:D:104:TYR:CD1  | 2.81                     | 0.40              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:D:381:ARG:HD2  | 1:D:381:ARG:HA  | 1.91                     | 0.40              |
| 1:E:207:ILE:HG22 | 1:E:390:ALA:HB1 | 2.04                     | 0.40              |
| 1:D:202:ARG:HB3  | 1:D:354:GLU:O   | 2.21                     | 0.40              |
| 1:B:46:ALA:HB1   | 1:B:50:LYS:HE3  | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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     | 348/454 (77%)   | 284 (82%)  | 41 (12%)  | 23 (7%)  | 1           | 25 |
| 1   | B     | 348/454 (77%)   | 285 (82%)  | 40 (12%)  | 23 (7%)  | 1           | 25 |
| 1   | C     | 348/454 (77%)   | 283 (81%)  | 40 (12%)  | 25 (7%)  | 1           | 23 |
| 1   | D     | 348/454 (77%)   | 285 (82%)  | 42 (12%)  | 21 (6%)  | 2           | 27 |
| 1   | E     | 348/454 (77%)   | 283 (81%)  | 42 (12%)  | 23 (7%)  | 1           | 25 |
| 1   | F     | 348/454 (77%)   | 289 (83%)  | 38 (11%)  | 21 (6%)  | 2           | 27 |
| 2   | G     | 136/143 (95%)   | 113 (83%)  | 13 (10%)  | 10 (7%)  | 1           | 21 |
| 2   | H     | 136/143 (95%)   | 109 (80%)  | 17 (12%)  | 10 (7%)  | 1           | 21 |
| 2   | I     | 136/143 (95%)   | 111 (82%)  | 14 (10%)  | 11 (8%)  | 1           | 19 |
| All | All   | 2496/3153 (79%) | 2042 (82%) | 287 (12%) | 167 (7%) | 1           | 25 |

All (167) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 63  | GLU  |
| 1   | A     | 188 | THR  |
| 1   | A     | 200 | PHE  |
| 1   | A     | 203 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 232 | ASN  |
| 1   | A     | 256 | GLY  |
| 1   | A     | 259 | ASN  |
| 1   | A     | 385 | SER  |
| 1   | B     | 63  | GLU  |
| 1   | B     | 102 | VAL  |
| 1   | B     | 104 | TYR  |
| 1   | B     | 188 | THR  |
| 1   | B     | 200 | PHE  |
| 1   | B     | 203 | SER  |
| 1   | B     | 232 | ASN  |
| 1   | B     | 256 | GLY  |
| 1   | B     | 259 | ASN  |
| 1   | B     | 385 | SER  |
| 1   | C     | 63  | GLU  |
| 1   | C     | 104 | TYR  |
| 1   | C     | 188 | THR  |
| 1   | C     | 200 | PHE  |
| 1   | C     | 203 | SER  |
| 1   | C     | 232 | ASN  |
| 1   | C     | 256 | GLY  |
| 1   | C     | 259 | ASN  |
| 1   | C     | 385 | SER  |
| 1   | D     | 102 | VAL  |
| 1   | D     | 136 | ILE  |
| 1   | D     | 188 | THR  |
| 1   | D     | 200 | PHE  |
| 1   | D     | 203 | SER  |
| 1   | D     | 232 | ASN  |
| 1   | D     | 256 | GLY  |
| 1   | D     | 385 | SER  |
| 1   | E     | 63  | GLU  |
| 1   | E     | 104 | TYR  |
| 1   | E     | 188 | THR  |
| 1   | E     | 200 | PHE  |
| 1   | E     | 203 | SER  |
| 1   | E     | 232 | ASN  |
| 1   | E     | 256 | GLY  |
| 1   | E     | 259 | ASN  |
| 1   | E     | 385 | SER  |
| 1   | F     | 63  | GLU  |
| 1   | F     | 102 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 104 | TYR  |
| 1   | F     | 188 | THR  |
| 1   | F     | 203 | SER  |
| 1   | F     | 232 | ASN  |
| 1   | F     | 256 | GLY  |
| 1   | F     | 259 | ASN  |
| 1   | F     | 385 | SER  |
| 2   | G     | 504 | PHE  |
| 2   | G     | 510 | GLU  |
| 2   | G     | 511 | ALA  |
| 2   | G     | 534 | LEU  |
| 2   | G     | 535 | LEU  |
| 2   | G     | 539 | ASP  |
| 2   | H     | 504 | PHE  |
| 2   | H     | 510 | GLU  |
| 2   | H     | 511 | ALA  |
| 2   | H     | 535 | LEU  |
| 2   | H     | 539 | ASP  |
| 2   | I     | 504 | PHE  |
| 2   | I     | 510 | GLU  |
| 2   | I     | 511 | ALA  |
| 2   | I     | 534 | LEU  |
| 2   | I     | 539 | ASP  |
| 1   | A     | 83  | ILE  |
| 1   | A     | 102 | VAL  |
| 1   | A     | 104 | TYR  |
| 1   | A     | 133 | GLU  |
| 1   | A     | 433 | LYS  |
| 1   | B     | 83  | ILE  |
| 1   | B     | 133 | GLU  |
| 1   | B     | 136 | ILE  |
| 1   | B     | 433 | LYS  |
| 1   | C     | 83  | ILE  |
| 1   | C     | 102 | VAL  |
| 1   | C     | 133 | GLU  |
| 1   | C     | 384 | GLY  |
| 1   | D     | 63  | GLU  |
| 1   | D     | 83  | ILE  |
| 1   | D     | 133 | GLU  |
| 1   | D     | 184 | THR  |
| 1   | D     | 259 | ASN  |
| 1   | D     | 433 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 83  | ILE  |
| 1   | E     | 102 | VAL  |
| 1   | E     | 133 | GLU  |
| 1   | E     | 433 | LYS  |
| 1   | F     | 83  | ILE  |
| 1   | F     | 133 | GLU  |
| 1   | F     | 136 | ILE  |
| 2   | G     | 503 | ALA  |
| 2   | H     | 503 | ALA  |
| 2   | H     | 534 | LEU  |
| 2   | I     | 561 | LEU  |
| 1   | A     | 294 | PRO  |
| 1   | B     | 184 | THR  |
| 1   | C     | 134 | ASP  |
| 1   | D     | 104 | TYR  |
| 1   | D     | 105 | TYR  |
| 1   | D     | 294 | PRO  |
| 1   | D     | 321 | TYR  |
| 1   | E     | 184 | THR  |
| 1   | E     | 294 | PRO  |
| 1   | F     | 294 | PRO  |
| 1   | F     | 440 | ASN  |
| 2   | I     | 503 | ALA  |
| 2   | I     | 535 | LEU  |
| 1   | A     | 105 | TYR  |
| 1   | A     | 384 | GLY  |
| 1   | B     | 64  | PRO  |
| 1   | B     | 105 | TYR  |
| 1   | B     | 294 | PRO  |
| 1   | B     | 384 | GLY  |
| 1   | C     | 240 | LEU  |
| 1   | C     | 294 | PRO  |
| 1   | C     | 321 | TYR  |
| 1   | C     | 433 | LYS  |
| 1   | D     | 384 | GLY  |
| 1   | E     | 105 | TYR  |
| 1   | E     | 134 | ASP  |
| 1   | E     | 384 | GLY  |
| 1   | F     | 64  | PRO  |
| 1   | F     | 105 | TYR  |
| 1   | F     | 200 | PHE  |
| 1   | F     | 321 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | G     | 457 | LEU  |
| 2   | G     | 561 | LEU  |
| 2   | H     | 561 | LEU  |
| 1   | A     | 136 | ILE  |
| 1   | A     | 240 | LEU  |
| 1   | B     | 134 | ASP  |
| 1   | B     | 314 | LEU  |
| 1   | C     | 105 | TYR  |
| 1   | C     | 184 | THR  |
| 1   | C     | 314 | LEU  |
| 1   | C     | 375 | PRO  |
| 1   | E     | 191 | THR  |
| 1   | E     | 314 | LEU  |
| 1   | F     | 134 | ASP  |
| 1   | F     | 314 | LEU  |
| 1   | F     | 433 | LYS  |
| 2   | H     | 457 | LEU  |
| 2   | I     | 457 | LEU  |
| 2   | I     | 560 | MSE  |
| 1   | B     | 321 | TYR  |
| 1   | D     | 375 | PRO  |
| 1   | E     | 274 | GLY  |
| 1   | A     | 274 | GLY  |
| 1   | A     | 315 | GLY  |
| 1   | B     | 375 | PRO  |
| 2   | G     | 520 | ILE  |
| 2   | H     | 520 | ILE  |
| 1   | A     | 97  | PRO  |
| 1   | C     | 68  | VAL  |
| 1   | C     | 136 | ILE  |
| 1   | E     | 68  | VAL  |
| 2   | I     | 520 | ILE  |
| 1   | A     | 375 | PRO  |
| 1   | A     | 64  | PRO  |
| 1   | C     | 64  | PRO  |
| 1   | E     | 64  | PRO  |
| 1   | D     | 64  | 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     | 297/386 (77%)   | 269 (91%)  | 28 (9%)  | 11          | 45 |
| 1   | B     | 297/386 (77%)   | 269 (91%)  | 28 (9%)  | 11          | 45 |
| 1   | C     | 297/386 (77%)   | 269 (91%)  | 28 (9%)  | 11          | 45 |
| 1   | D     | 297/386 (77%)   | 267 (90%)  | 30 (10%) | 9           | 41 |
| 1   | E     | 297/386 (77%)   | 268 (90%)  | 29 (10%) | 10          | 43 |
| 1   | F     | 297/386 (77%)   | 269 (91%)  | 28 (9%)  | 11          | 45 |
| 2   | G     | 117/116 (101%)  | 108 (92%)  | 9 (8%)   | 16          | 55 |
| 2   | H     | 117/116 (101%)  | 107 (92%)  | 10 (8%)  | 13          | 51 |
| 2   | I     | 117/116 (101%)  | 111 (95%)  | 6 (5%)   | 29          | 68 |
| All | All   | 2133/2664 (80%) | 1937 (91%) | 196 (9%) | 11          | 46 |

All (196) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 50  | LYS  |
| 1   | A     | 57  | ARG  |
| 1   | A     | 67  | LEU  |
| 1   | A     | 79  | GLN  |
| 1   | A     | 80  | LEU  |
| 1   | A     | 81  | GLU  |
| 1   | A     | 103 | GLU  |
| 1   | A     | 104 | TYR  |
| 1   | A     | 128 | ASP  |
| 1   | A     | 133 | GLU  |
| 1   | A     | 139 | LEU  |
| 1   | A     | 148 | MET  |
| 1   | A     | 200 | PHE  |
| 1   | A     | 202 | ARG  |
| 1   | A     | 211 | ARG  |
| 1   | A     | 216 | LYS  |
| 1   | A     | 222 | ASN  |
| 1   | A     | 255 | GLU  |
| 1   | A     | 261 | GLN  |
| 1   | A     | 314 | LEU  |
| 1   | A     | 321 | TYR  |
| 1   | A     | 324 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 339 | VAL  |
| 1   | A     | 345 | SER  |
| 1   | A     | 351 | ARG  |
| 1   | A     | 380 | ILE  |
| 1   | A     | 388 | GLN  |
| 1   | A     | 391 | ASP  |
| 1   | B     | 26  | LEU  |
| 1   | B     | 50  | LYS  |
| 1   | B     | 55  | MET  |
| 1   | B     | 57  | ARG  |
| 1   | B     | 79  | GLN  |
| 1   | B     | 80  | LEU  |
| 1   | B     | 81  | GLU  |
| 1   | B     | 103 | GLU  |
| 1   | B     | 104 | TYR  |
| 1   | B     | 128 | ASP  |
| 1   | B     | 148 | MET  |
| 1   | B     | 191 | THR  |
| 1   | B     | 200 | PHE  |
| 1   | B     | 202 | ARG  |
| 1   | B     | 211 | ARG  |
| 1   | B     | 216 | LYS  |
| 1   | B     | 222 | ASN  |
| 1   | B     | 249 | MET  |
| 1   | B     | 255 | GLU  |
| 1   | B     | 261 | GLN  |
| 1   | B     | 278 | MET  |
| 1   | B     | 306 | ARG  |
| 1   | B     | 314 | LEU  |
| 1   | B     | 324 | LEU  |
| 1   | B     | 339 | VAL  |
| 1   | B     | 351 | ARG  |
| 1   | B     | 388 | GLN  |
| 1   | B     | 391 | ASP  |
| 1   | C     | 50  | LYS  |
| 1   | C     | 57  | ARG  |
| 1   | C     | 67  | LEU  |
| 1   | C     | 79  | GLN  |
| 1   | C     | 80  | LEU  |
| 1   | C     | 102 | VAL  |
| 1   | C     | 104 | TYR  |
| 1   | C     | 128 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 133 | GLU  |
| 1   | C     | 139 | LEU  |
| 1   | C     | 147 | ILE  |
| 1   | C     | 148 | MET  |
| 1   | C     | 200 | PHE  |
| 1   | C     | 202 | ARG  |
| 1   | C     | 211 | ARG  |
| 1   | C     | 222 | ASN  |
| 1   | C     | 249 | MET  |
| 1   | C     | 261 | GLN  |
| 1   | C     | 278 | MET  |
| 1   | C     | 314 | LEU  |
| 1   | C     | 324 | LEU  |
| 1   | C     | 339 | VAL  |
| 1   | C     | 345 | SER  |
| 1   | C     | 351 | ARG  |
| 1   | C     | 355 | VAL  |
| 1   | C     | 381 | ARG  |
| 1   | C     | 388 | GLN  |
| 1   | C     | 391 | ASP  |
| 1   | D     | 26  | LEU  |
| 1   | D     | 50  | LYS  |
| 1   | D     | 55  | MET  |
| 1   | D     | 57  | ARG  |
| 1   | D     | 67  | LEU  |
| 1   | D     | 79  | GLN  |
| 1   | D     | 80  | LEU  |
| 1   | D     | 81  | GLU  |
| 1   | D     | 103 | GLU  |
| 1   | D     | 104 | TYR  |
| 1   | D     | 136 | ILE  |
| 1   | D     | 139 | LEU  |
| 1   | D     | 140 | LEU  |
| 1   | D     | 148 | MET  |
| 1   | D     | 200 | PHE  |
| 1   | D     | 202 | ARG  |
| 1   | D     | 211 | ARG  |
| 1   | D     | 216 | LYS  |
| 1   | D     | 222 | ASN  |
| 1   | D     | 249 | MET  |
| 1   | D     | 261 | GLN  |
| 1   | D     | 269 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 306 | ARG  |
| 1   | D     | 314 | LEU  |
| 1   | D     | 324 | LEU  |
| 1   | D     | 339 | VAL  |
| 1   | D     | 351 | ARG  |
| 1   | D     | 380 | ILE  |
| 1   | D     | 388 | GLN  |
| 1   | D     | 391 | ASP  |
| 1   | E     | 50  | LYS  |
| 1   | E     | 55  | MET  |
| 1   | E     | 57  | ARG  |
| 1   | E     | 69  | THR  |
| 1   | E     | 79  | GLN  |
| 1   | E     | 80  | LEU  |
| 1   | E     | 103 | GLU  |
| 1   | E     | 104 | TYR  |
| 1   | E     | 128 | ASP  |
| 1   | E     | 139 | LEU  |
| 1   | E     | 147 | ILE  |
| 1   | E     | 148 | MET  |
| 1   | E     | 200 | PHE  |
| 1   | E     | 202 | ARG  |
| 1   | E     | 211 | ARG  |
| 1   | E     | 216 | LYS  |
| 1   | E     | 222 | ASN  |
| 1   | E     | 249 | MET  |
| 1   | E     | 261 | GLN  |
| 1   | E     | 278 | MET  |
| 1   | E     | 314 | LEU  |
| 1   | E     | 321 | TYR  |
| 1   | E     | 324 | LEU  |
| 1   | E     | 339 | VAL  |
| 1   | E     | 345 | SER  |
| 1   | E     | 351 | ARG  |
| 1   | E     | 381 | ARG  |
| 1   | E     | 388 | GLN  |
| 1   | E     | 391 | ASP  |
| 1   | F     | 26  | LEU  |
| 1   | F     | 50  | LYS  |
| 1   | F     | 55  | MET  |
| 1   | F     | 67  | LEU  |
| 1   | F     | 79  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 80  | LEU  |
| 1   | F     | 81  | GLU  |
| 1   | F     | 90  | SER  |
| 1   | F     | 104 | TYR  |
| 1   | F     | 110 | GLU  |
| 1   | F     | 128 | ASP  |
| 1   | F     | 139 | LEU  |
| 1   | F     | 147 | ILE  |
| 1   | F     | 148 | MET  |
| 1   | F     | 202 | ARG  |
| 1   | F     | 211 | ARG  |
| 1   | F     | 216 | LYS  |
| 1   | F     | 222 | ASN  |
| 1   | F     | 255 | GLU  |
| 1   | F     | 261 | GLN  |
| 1   | F     | 306 | ARG  |
| 1   | F     | 314 | LEU  |
| 1   | F     | 322 | LEU  |
| 1   | F     | 324 | LEU  |
| 1   | F     | 345 | SER  |
| 1   | F     | 351 | ARG  |
| 1   | F     | 388 | GLN  |
| 1   | F     | 391 | ASP  |
| 2   | G     | 465 | ARG  |
| 2   | G     | 519 | ARG  |
| 2   | G     | 536 | ILE  |
| 2   | G     | 538 | ASP  |
| 2   | G     | 540 | VAL  |
| 2   | G     | 543 | GLN  |
| 2   | G     | 550 | ARG  |
| 2   | G     | 569 | THR  |
| 2   | G     | 593 | MSE  |
| 2   | H     | 465 | ARG  |
| 2   | H     | 497 | LEU  |
| 2   | H     | 519 | ARG  |
| 2   | H     | 536 | ILE  |
| 2   | H     | 538 | ASP  |
| 2   | H     | 540 | VAL  |
| 2   | H     | 550 | ARG  |
| 2   | H     | 561 | LEU  |
| 2   | H     | 582 | ARG  |
| 2   | H     | 593 | MSE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | I     | 465 | ARG  |
| 2   | I     | 519 | ARG  |
| 2   | I     | 536 | ILE  |
| 2   | I     | 538 | ASP  |
| 2   | I     | 540 | VAL  |
| 2   | I     | 593 | MSE  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 53  | HIS  |
| 1   | A     | 222 | ASN  |
| 1   | A     | 225 | GLN  |
| 1   | A     | 323 | GLN  |
| 1   | A     | 388 | GLN  |
| 1   | B     | 53  | HIS  |
| 1   | B     | 201 | GLN  |
| 1   | B     | 222 | ASN  |
| 1   | B     | 225 | GLN  |
| 1   | B     | 245 | GLN  |
| 1   | B     | 246 | GLN  |
| 1   | B     | 323 | GLN  |
| 1   | B     | 388 | GLN  |
| 1   | B     | 421 | ASN  |
| 1   | C     | 53  | HIS  |
| 1   | C     | 201 | GLN  |
| 1   | C     | 222 | ASN  |
| 1   | C     | 225 | GLN  |
| 1   | C     | 234 | ASN  |
| 1   | C     | 245 | GLN  |
| 1   | C     | 246 | GLN  |
| 1   | C     | 323 | GLN  |
| 1   | C     | 388 | GLN  |
| 1   | C     | 421 | ASN  |
| 1   | D     | 53  | HIS  |
| 1   | D     | 201 | GLN  |
| 1   | D     | 222 | ASN  |
| 1   | D     | 225 | GLN  |
| 1   | D     | 246 | GLN  |
| 1   | D     | 323 | GLN  |
| 1   | D     | 388 | GLN  |
| 1   | E     | 53  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 201 | GLN  |
| 1   | E     | 222 | ASN  |
| 1   | E     | 225 | GLN  |
| 1   | E     | 323 | GLN  |
| 1   | E     | 388 | GLN  |
| 1   | E     | 421 | ASN  |
| 1   | F     | 53  | HIS  |
| 1   | F     | 201 | GLN  |
| 1   | F     | 225 | GLN  |
| 1   | F     | 226 | ASN  |
| 1   | F     | 246 | GLN  |
| 1   | F     | 323 | GLN  |
| 1   | F     | 388 | GLN  |
| 2   | G     | 470 | HIS  |
| 2   | G     | 494 | HIS  |
| 2   | H     | 470 | HIS  |
| 2   | H     | 494 | HIS  |
| 2   | H     | 509 | HIS  |
| 2   | H     | 554 | ASN  |
| 2   | I     | 470 | HIS  |
| 2   | I     | 494 | HIS  |

### 5.3.3 RNA [i](#)

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     | 358/454 (78%)   | 0.02   | 15 (4%)  | 40 | 30 | 156, 167, 168, 170    | 0     |
| 1   | B     | 358/454 (78%)   | 0.13   | 18 (5%)  | 32 | 24 | 163, 167, 168, 175    | 0     |
| 1   | C     | 358/454 (78%)   | -0.01  | 13 (3%)  | 46 | 36 | 157, 167, 168, 170    | 0     |
| 1   | D     | 358/454 (78%)   | 0.00   | 15 (4%)  | 40 | 30 | 163, 167, 168, 182    | 0     |
| 1   | E     | 358/454 (78%)   | 0.10   | 19 (5%)  | 30 | 22 | 163, 167, 168, 170    | 0     |
| 1   | F     | 358/454 (78%)   | 0.59   | 39 (10%) | 7  | 6  | 162, 167, 168, 187    | 0     |
| 2   | G     | 132/143 (92%)   | -0.18  | 2 (1%)   | 76 | 66 | 163, 167, 168, 169    | 0     |
| 2   | H     | 132/143 (92%)   | -0.16  | 4 (3%)   | 54 | 41 | 162, 167, 168, 169    | 0     |
| 2   | I     | 132/143 (92%)   | 0.07   | 5 (3%)   | 44 | 34 | 163, 167, 168, 169    | 0     |
| All | All   | 2544/3153 (80%) | 0.10   | 130 (5%) | 32 | 23 | 156, 167, 168, 187    | 0     |

All (130) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 326 | GLN  | 7.5  |
| 2   | I     | 510 | GLU  | 7.4  |
| 1   | B     | 260 | ALA  | 6.5  |
| 1   | F     | 199 | GLY  | 6.5  |
| 1   | A     | 287 | GLY  | 5.6  |
| 1   | F     | 197 | THR  | 5.3  |
| 2   | H     | 510 | GLU  | 5.1  |
| 1   | F     | 394 | ALA  | 5.0  |
| 1   | F     | 198 | SER  | 4.9  |
| 1   | F     | 426 | THR  | 4.9  |
| 1   | F     | 383 | SER  | 4.8  |
| 1   | F     | 324 | LEU  | 4.8  |
| 1   | A     | 260 | ALA  | 4.8  |
| 1   | F     | 382 | GLU  | 4.8  |
| 1   | D     | 383 | SER  | 4.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 261 | GLN  | 4.6  |
| 1   | F     | 384 | GLY  | 4.4  |
| 1   | C     | 441 | LEU  | 4.2  |
| 2   | I     | 506 | GLU  | 4.2  |
| 1   | F     | 231 | THR  | 4.2  |
| 1   | A     | 421 | ASN  | 4.1  |
| 1   | F     | 428 | GLN  | 4.1  |
| 1   | B     | 230 | LYS  | 4.1  |
| 1   | F     | 297 | ARG  | 4.0  |
| 1   | F     | 420 | ARG  | 4.0  |
| 2   | I     | 507 | GLU  | 3.9  |
| 1   | F     | 188 | THR  | 3.8  |
| 1   | D     | 379 | ASP  | 3.8  |
| 2   | H     | 523 | GLU  | 3.8  |
| 1   | F     | 441 | LEU  | 3.7  |
| 1   | D     | 413 | GLU  | 3.7  |
| 1   | F     | 295 | SER  | 3.6  |
| 1   | E     | 310 | GLN  | 3.6  |
| 2   | I     | 523 | GLU  | 3.6  |
| 1   | F     | 261 | GLN  | 3.6  |
| 1   | E     | 229 | THR  | 3.5  |
| 1   | F     | 323 | GLN  | 3.5  |
| 1   | A     | 434 | GLU  | 3.4  |
| 2   | G     | 523 | GLU  | 3.4  |
| 1   | F     | 375 | PRO  | 3.4  |
| 1   | F     | 325 | ILE  | 3.4  |
| 1   | E     | 375 | PRO  | 3.3  |
| 1   | C     | 421 | ASN  | 3.3  |
| 1   | A     | 286 | ALA  | 3.3  |
| 1   | F     | 287 | GLY  | 3.3  |
| 1   | E     | 374 | ARG  | 3.3  |
| 1   | E     | 232 | ASN  | 3.3  |
| 1   | E     | 434 | GLU  | 3.2  |
| 1   | F     | 215 | GLY  | 3.2  |
| 1   | A     | 265 | THR  | 3.2  |
| 1   | F     | 195 | ARG  | 3.1  |
| 1   | B     | 231 | THR  | 3.0  |
| 1   | E     | 195 | ARG  | 3.0  |
| 1   | A     | 257 | ASN  | 3.0  |
| 1   | E     | 421 | ASN  | 3.0  |
| 1   | F     | 241 | GLU  | 3.0  |
| 1   | B     | 261 | GLN  | 3.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | G     | 510 | GLU  | 3.0  |
| 1   | B     | 313 | GLY  | 2.9  |
| 1   | F     | 388 | GLN  | 2.9  |
| 1   | B     | 413 | GLU  | 2.9  |
| 1   | A     | 432 | ILE  | 2.8  |
| 1   | F     | 196 | MET  | 2.8  |
| 1   | B     | 265 | THR  | 2.8  |
| 1   | F     | 321 | TYR  | 2.8  |
| 1   | F     | 242 | MET  | 2.7  |
| 1   | D     | 231 | THR  | 2.7  |
| 1   | F     | 201 | GLN  | 2.7  |
| 1   | B     | 198 | SER  | 2.7  |
| 1   | B     | 397 | TYR  | 2.7  |
| 1   | E     | 131 | THR  | 2.7  |
| 1   | D     | 212 | PRO  | 2.6  |
| 1   | D     | 261 | GLN  | 2.6  |
| 1   | B     | 229 | THR  | 2.6  |
| 1   | E     | 230 | LYS  | 2.6  |
| 1   | B     | 184 | THR  | 2.6  |
| 1   | F     | 294 | PRO  | 2.6  |
| 1   | C     | 341 | GLU  | 2.6  |
| 1   | D     | 382 | GLU  | 2.6  |
| 1   | B     | 212 | PRO  | 2.5  |
| 1   | B     | 228 | ALA  | 2.5  |
| 1   | E     | 422 | GLY  | 2.5  |
| 1   | E     | 260 | ALA  | 2.5  |
| 1   | F     | 194 | ASP  | 2.5  |
| 1   | D     | 187 | PRO  | 2.5  |
| 2   | I     | 509 | HIS  | 2.4  |
| 1   | C     | 195 | ARG  | 2.4  |
| 1   | E     | 213 | SER  | 2.4  |
| 1   | E     | 354 | GLU  | 2.4  |
| 2   | H     | 483 | GLU  | 2.4  |
| 1   | F     | 339 | VAL  | 2.4  |
| 1   | D     | 195 | ARG  | 2.4  |
| 1   | B     | 234 | ASN  | 2.4  |
| 1   | C     | 422 | GLY  | 2.4  |
| 1   | A     | 374 | ARG  | 2.3  |
| 1   | B     | 149 | GLU  | 2.3  |
| 1   | F     | 189 | GLY  | 2.3  |
| 1   | F     | 440 | ASN  | 2.3  |
| 1   | D     | 286 | ALA  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 233 | GLU  | 2.2  |
| 2   | H     | 506 | GLU  | 2.2  |
| 1   | F     | 206 | ILE  | 2.2  |
| 1   | B     | 199 | GLY  | 2.2  |
| 1   | D     | 440 | ASN  | 2.2  |
| 1   | E     | 432 | ILE  | 2.2  |
| 1   | A     | 97  | PRO  | 2.2  |
| 1   | A     | 326 | GLN  | 2.2  |
| 1   | F     | 393 | VAL  | 2.2  |
| 1   | C     | 354 | GLU  | 2.2  |
| 1   | F     | 434 | GLU  | 2.2  |
| 1   | C     | 273 | TRP  | 2.2  |
| 1   | C     | 267 | LYS  | 2.2  |
| 1   | E     | 261 | GLN  | 2.2  |
| 1   | E     | 423 | PRO  | 2.1  |
| 1   | C     | 374 | ARG  | 2.1  |
| 1   | D     | 374 | ARG  | 2.1  |
| 1   | D     | 268 | LEU  | 2.1  |
| 1   | A     | 195 | ARG  | 2.1  |
| 1   | C     | 287 | GLY  | 2.1  |
| 1   | F     | 267 | LYS  | 2.1  |
| 1   | C     | 382 | GLU  | 2.1  |
| 1   | B     | 384 | GLY  | 2.0  |
| 1   | D     | 233 | GLU  | 2.0  |
| 1   | E     | 341 | GLU  | 2.0  |
| 1   | B     | 382 | GLU  | 2.0  |
| 1   | D     | 420 | ARG  | 2.0  |
| 1   | A     | 435 | TYR  | 2.0  |
| 1   | E     | 149 | GLU  | 2.0  |
| 1   | C     | 97  | PRO  | 2.0  |
| 1   | A     | 274 | GLY  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

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.