



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:09 PM GMT

PDB ID : 1IS8  
Title : Crystal structure of rat GTPCHI/GFRP stimulatory complex plus Zn  
Authors : Maita, N.; Okada, K.; Hatakeyama, K.; Hakoshima, T.  
Deposited on : 2001-11-18  
Resolution : 2.70 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

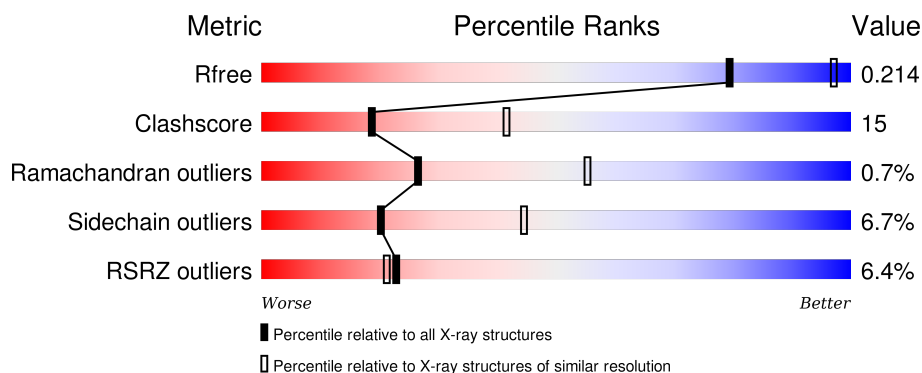
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 91344                       | 2103 (2.70-2.70)                                      |
| Clashscore            | 102246                      | 2422 (2.70-2.70)                                      |
| Ramachandran outliers | 100387                      | 2382 (2.70-2.70)                                      |
| Sidechain outliers    | 100360                      | 2382 (2.70-2.70)                                      |
| RSRZ outliers         | 91569                       | 2107 (2.70-2.70)                                      |

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     | 230    | <div> <div>11%</div> <div> <div>54%</div> <div>26%</div> <div>•</div> <div>17%</div> </div> </div> |
| 1   | B     | 230    | <div> <div>6%</div> <div> <div>58%</div> <div>22%</div> <div>•</div> <div>17%</div> </div> </div>  |
| 1   | C     | 230    | <div> <div>7%</div> <div> <div>57%</div> <div>24%</div> <div>•</div> <div>17%</div> </div> </div>  |
| 1   | D     | 230    | <div> <div>7%</div> <div> <div>56%</div> <div>26%</div> <div>•</div> <div>17%</div> </div> </div>  |
| 1   | E     | 230    | <div> <div>5%</div> <div> <div>57%</div> <div>23%</div> <div>•</div> <div>17%</div> </div> </div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | F     | 230    |                  |
| 1   | G     | 230    |                  |
| 1   | H     | 230    |                  |
| 1   | I     | 230    |                  |
| 1   | J     | 230    |                  |
| 2   | K     | 84     |                  |
| 2   | L     | 84     |                  |
| 2   | M     | 84     |                  |
| 2   | N     | 84     |                  |
| 2   | O     | 84     |                  |
| 2   | P     | 84     |                  |
| 2   | Q     | 84     |                  |
| 2   | R     | 84     |                  |
| 2   | S     | 84     |                  |
| 2   | T     | 84     |                  |

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 22511 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 GTP Cyclohydrolase I.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 1   | A     | 192      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1524  | 959 | 269 | 285 | 11 |         |         |       |
| 1   | B     | 192      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1524  | 959 | 269 | 285 | 11 |         |         |       |
| 1   | C     | 192      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1524  | 959 | 269 | 285 | 11 |         |         |       |
| 1   | D     | 192      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1524  | 959 | 269 | 285 | 11 |         |         |       |
| 1   | E     | 192      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1524  | 959 | 269 | 285 | 11 |         |         |       |
| 1   | F     | 192      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1524  | 959 | 269 | 285 | 11 |         |         |       |
| 1   | G     | 192      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1524  | 959 | 269 | 285 | 11 |         |         |       |
| 1   | H     | 192      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1524  | 959 | 269 | 285 | 11 |         |         |       |
| 1   | I     | 192      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1524  | 959 | 269 | 285 | 11 |         |         |       |
| 1   | J     | 192      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1524  | 959 | 269 | 285 | 11 |         |         |       |

- Molecule 2 is a protein called GTP Cyclohydrolase I Feedback Regulatory Protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | K     | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 676   | 428 | 117 | 124 | 7 |         |         |       |
| 2   | L     | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 676   | 428 | 117 | 124 | 7 |         |         |       |
| 2   | M     | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 676   | 428 | 117 | 124 | 7 |         |         |       |
| 2   | N     | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 676   | 428 | 117 | 124 | 7 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | O     | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 676   | 428 | 117 | 124 | 7 |         |         |       |
| 2   | P     | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 676   | 428 | 117 | 124 | 7 |         |         |       |
| 2   | Q     | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 676   | 428 | 117 | 124 | 7 |         |         |       |
| 2   | R     | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 676   | 428 | 117 | 124 | 7 |         |         |       |
| 2   | S     | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 676   | 428 | 117 | 124 | 7 |         |         |       |
| 2   | T     | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 676   | 428 | 117 | 124 | 7 |         |         |       |

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 3   | P     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 3   | Q     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 3   | K     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 3   | T     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 3   | N     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 3   | O     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 3   | R     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 3   | L     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 3   | S     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 3   | M     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

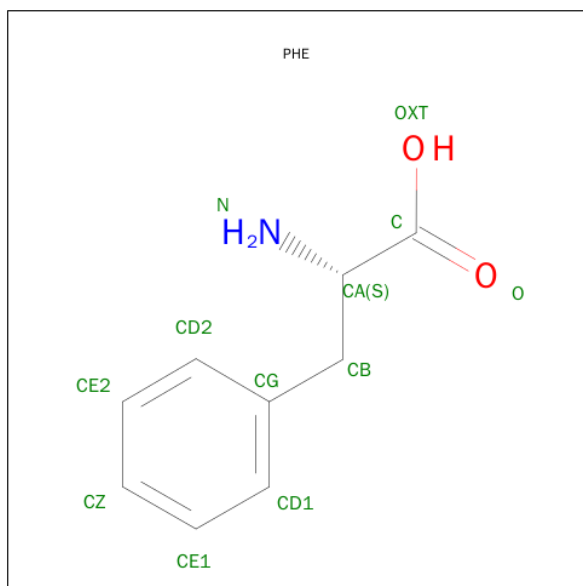
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | G     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | J     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | D     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | E     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | H     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | B     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | I     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | C     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | A     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | F     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 5 is PHENYLALANINE (three-letter code: PHE) (formula: C<sub>9</sub>H<sub>11</sub>NO<sub>2</sub>).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 5   | Q     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 12    | 9 | 1 | 2 |         |         |
| 5   | R     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 12    | 9 | 1 | 2 |         |         |

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| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 5   | P     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 12    | 9 | 1 | 2 |         |         |
| 5   | S     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 12    | 9 | 1 | 2 |         |         |
| 5   | T     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 12    | 9 | 1 | 2 |         |         |
| 5   | N     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 12    | 9 | 1 | 2 |         |         |
| 5   | N     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 12    | 9 | 1 | 2 |         |         |
| 5   | O     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 12    | 9 | 1 | 2 |         |         |
| 5   | K     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 12    | 9 | 1 | 2 |         |         |
| 5   | M     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 12    | 9 | 1 | 2 |         |         |

- Molecule 6 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 6   | A     | 17       | Total | O  | 0       | 0       |
|     |       |          | 17    | 17 |         |         |
| 6   | B     | 18       | Total | O  | 0       | 0       |
|     |       |          | 18    | 18 |         |         |
| 6   | C     | 13       | Total | O  | 0       | 0       |
|     |       |          | 13    | 13 |         |         |
| 6   | D     | 10       | Total | O  | 0       | 0       |
|     |       |          | 10    | 10 |         |         |
| 6   | E     | 13       | Total | O  | 0       | 0       |
|     |       |          | 13    | 13 |         |         |
| 6   | F     | 15       | Total | O  | 0       | 0       |
|     |       |          | 15    | 15 |         |         |
| 6   | G     | 16       | Total | O  | 0       | 0       |
|     |       |          | 16    | 16 |         |         |
| 6   | H     | 21       | Total | O  | 0       | 0       |
|     |       |          | 21    | 21 |         |         |
| 6   | I     | 20       | Total | O  | 0       | 0       |
|     |       |          | 20    | 20 |         |         |
| 6   | J     | 20       | Total | O  | 0       | 0       |
|     |       |          | 20    | 20 |         |         |
| 6   | K     | 17       | Total | O  | 0       | 0       |
|     |       |          | 17    | 17 |         |         |

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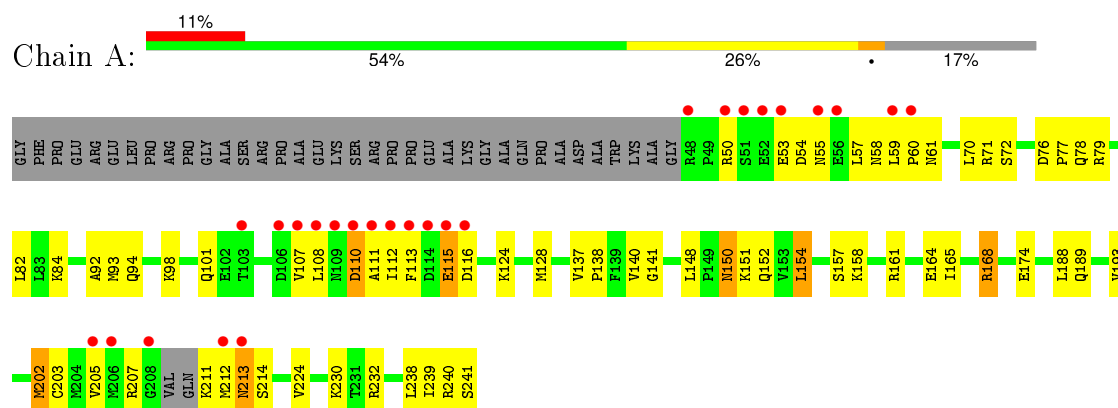
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 6   | L     | 19       | Total | O  | 0       | 0       |
|     |       |          | 19    | 19 |         |         |
| 6   | M     | 16       | Total | O  | 0       | 0       |
|     |       |          | 16    | 16 |         |         |
| 6   | N     | 16       | Total | O  | 0       | 0       |
|     |       |          | 16    | 16 |         |         |
| 6   | O     | 16       | Total | O  | 0       | 0       |
|     |       |          | 16    | 16 |         |         |
| 6   | P     | 27       | Total | O  | 0       | 0       |
|     |       |          | 27    | 27 |         |         |
| 6   | Q     | 31       | Total | O  | 0       | 0       |
|     |       |          | 31    | 31 |         |         |
| 6   | R     | 28       | Total | O  | 0       | 0       |
|     |       |          | 28    | 28 |         |         |
| 6   | S     | 22       | Total | O  | 0       | 0       |
|     |       |          | 22    | 22 |         |         |
| 6   | T     | 16       | Total | O  | 0       | 0       |
|     |       |          | 16    | 16 |         |         |



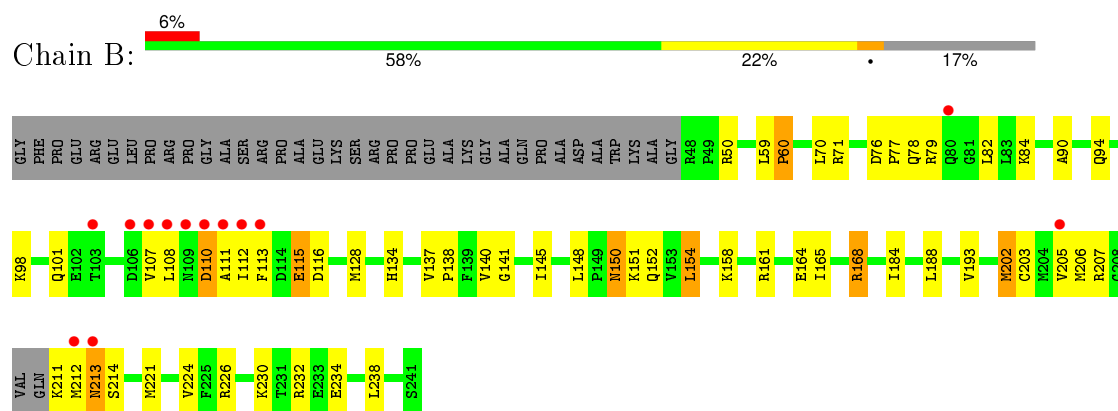
### 3 Residue-property plots

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.

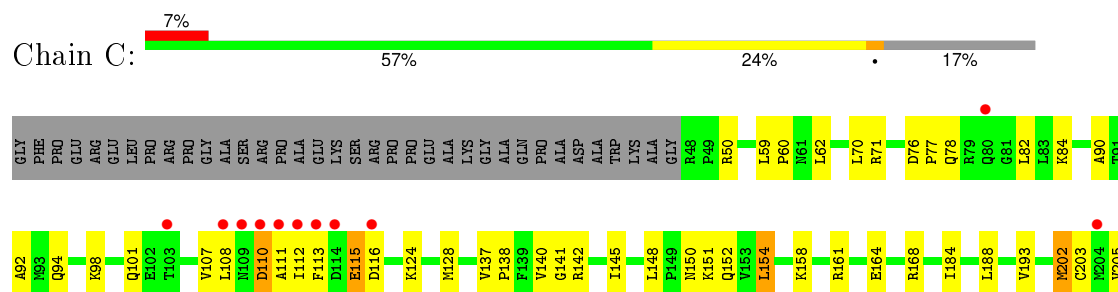
#### • Molecule 1: GTP Cyclohydrolase I



#### • Molecule 1: GTP Cyclohydrolase I

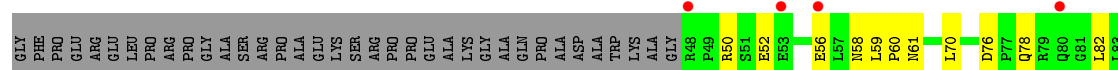


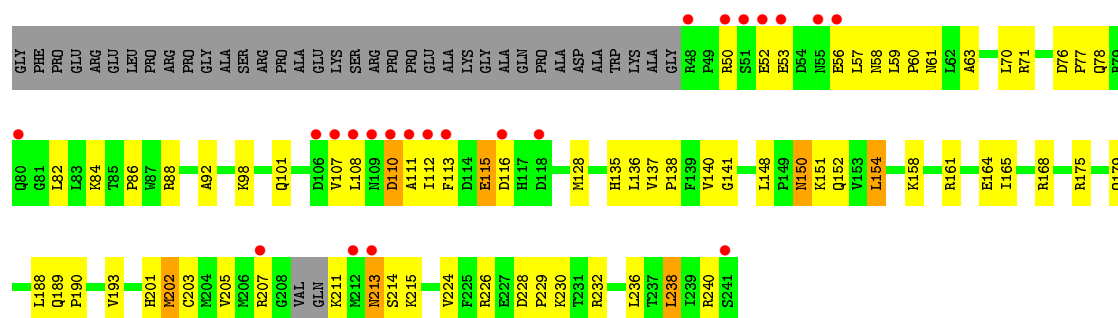
#### • Molecule 1: GTP Cyclohydrolase I



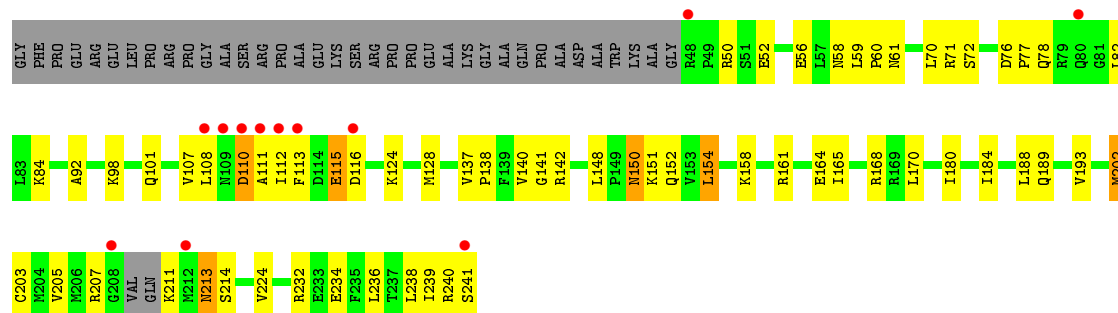


• Molecule 1: GTP Cyclohydrolase I

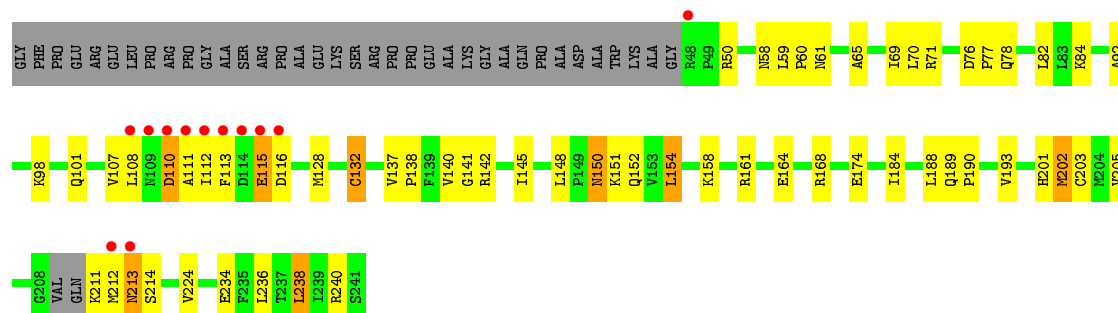




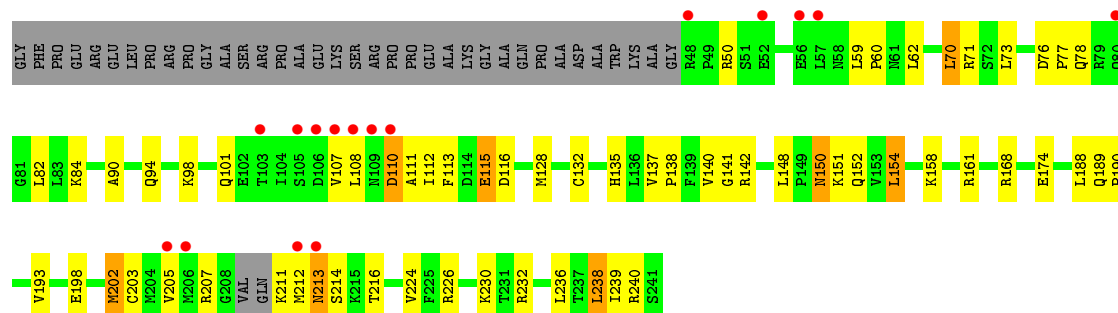
• Molecule 1: GTP Cyclohydrolase I



• Molecule 1: GTP Cyclohydrolase I

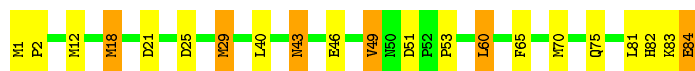


• Molecule 1: GTP Cyclohydrolase I




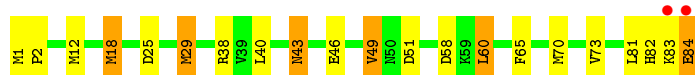
- Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

Chain K:  75% 18% 7%




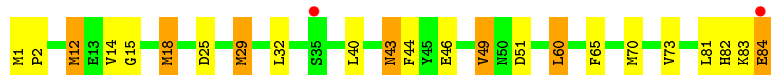
- Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

Chain L:  2% 75% 18% 7%



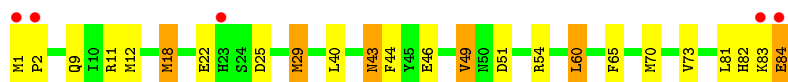
- Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

Chain M:  2% 73% 19% 8%



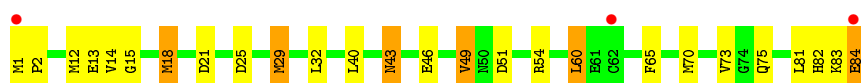
- Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

Chain N:  6% 71% 21% 7%



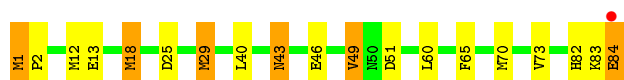
- Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

Chain O:  4% 69% 24% 7%




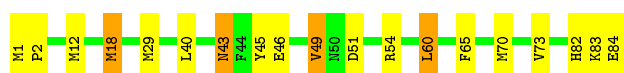
- Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

Chain P:  0% 77% 15% 7%

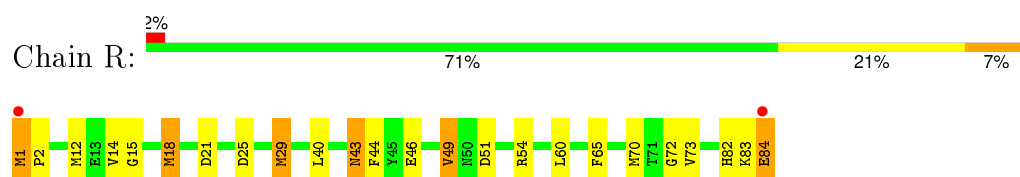


- Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

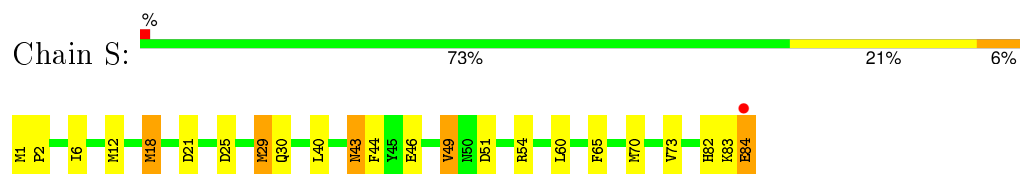
Chain Q:  77% 18% 5%



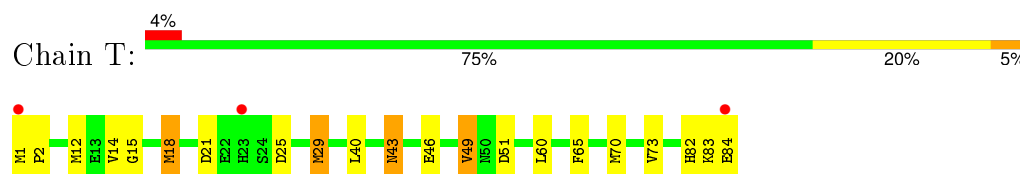
- Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein



- Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein



- Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 123.90Å 111.43Å 125.91Å<br>90.00° 97.32° 90.00°             | Depositor        |
| Resolution (Å)  | 15.00 – 2.70<br>29.65 – 2.70                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.9 (15.00-2.70)<br>95.5 (29.65-2.70)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | 0.10  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 4.30 (at 2.68Å)   | Xtriage          |
| Refinement program  | CNS 0.9   | Depositor        |
| R, $R_{free}$   | 0.219 , 0.245<br>0.215 , 0.214                              | Depositor<br>DCC |
| $R_{free}$ test set   | 4648 reflections (5.27%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 16.8  | Xtriage          |
| Anisotropy  | 0.171   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.24 , 21.1   | EDS              |
| Estimated twinning fraction   | 0.199 for l,-k,h  | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.29$ , $\langle L^2 \rangle = 0.12$ | Xtriage          |
| Outliers  | 0 of 93283 reflections                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.84  | EDS              |
| Total number of atoms   | 22511   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 43.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.07% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, K

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     | 0.43         | 0/1548  | 0.65        | 0/2087          |
| 1   | B     | 0.40         | 0/1548  | 0.64        | 0/2087          |
| 1   | C     | 0.41         | 0/1548  | 0.63        | 0/2087          |
| 1   | D     | 0.41         | 0/1548  | 0.63        | 0/2087          |
| 1   | E     | 0.41         | 0/1548  | 0.69        | 2/2087 (0.1%)   |
| 1   | F     | 0.39         | 0/1548  | 0.63        | 0/2087          |
| 1   | G     | 0.41         | 0/1548  | 0.64        | 0/2087          |
| 1   | H     | 0.42         | 0/1548  | 0.63        | 1/2087 (0.0%)   |
| 1   | I     | 0.40         | 0/1548  | 0.66        | 1/2087 (0.0%)   |
| 1   | J     | 0.40         | 0/1548  | 0.64        | 0/2087          |
| 2   | K     | 0.39         | 0/690   | 0.75        | 5/931 (0.5%)    |
| 2   | L     | 0.38         | 0/690   | 0.75        | 5/931 (0.5%)    |
| 2   | M     | 0.38         | 0/690   | 0.76        | 5/931 (0.5%)    |
| 2   | N     | 0.38         | 0/690   | 0.76        | 5/931 (0.5%)    |
| 2   | O     | 0.38         | 0/690   | 0.76        | 5/931 (0.5%)    |
| 2   | P     | 0.38         | 0/690   | 0.76        | 5/931 (0.5%)    |
| 2   | Q     | 0.40         | 0/690   | 0.76        | 5/931 (0.5%)    |
| 2   | R     | 0.40         | 0/690   | 0.77        | 5/931 (0.5%)    |
| 2   | S     | 0.41         | 0/690   | 0.76        | 5/931 (0.5%)    |
| 2   | T     | 0.39         | 0/690   | 0.76        | 5/931 (0.5%)    |
| All | All   | 0.40         | 0/22380 | 0.68        | 54/30180 (0.2%) |

There are no bond length outliers.

All (54) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | E     | 240 | ARG  | NE-CZ-NH1 | -8.20 | 116.20      | 120.30   |
| 1   | E     | 240 | ARG  | NE-CZ-NH2 | 7.99  | 124.29      | 120.30   |
| 2   | R     | 70  | MET  | CG-SD-CE  | 5.92  | 109.68      | 100.20   |
| 2   | K     | 1   | MET  | CG-SD-CE  | 5.91  | 109.66      | 100.20   |

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| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 2   | S     | 70  | MET  | CG-SD-CE | 5.91 | 109.66      | 100.20   |
| 2   | N     | 1   | MET  | CG-SD-CE | 5.89 | 109.62      | 100.20   |
| 2   | P     | 70  | MET  | CG-SD-CE | 5.89 | 109.62      | 100.20   |
| 2   | Q     | 70  | MET  | CG-SD-CE | 5.89 | 109.62      | 100.20   |
| 2   | O     | 1   | MET  | CG-SD-CE | 5.88 | 109.60      | 100.20   |
| 2   | S     | 1   | MET  | CG-SD-CE | 5.88 | 109.61      | 100.20   |
| 2   | M     | 1   | MET  | CG-SD-CE | 5.88 | 109.60      | 100.20   |
| 2   | K     | 70  | MET  | CG-SD-CE | 5.87 | 109.59      | 100.20   |
| 2   | L     | 70  | MET  | CG-SD-CE | 5.86 | 109.57      | 100.20   |
| 2   | L     | 1   | MET  | CG-SD-CE | 5.86 | 109.57      | 100.20   |
| 2   | N     | 70  | MET  | CG-SD-CE | 5.86 | 109.57      | 100.20   |
| 2   | T     | 1   | MET  | CG-SD-CE | 5.86 | 109.57      | 100.20   |
| 2   | T     | 70  | MET  | CG-SD-CE | 5.86 | 109.57      | 100.20   |
| 2   | R     | 1   | MET  | CG-SD-CE | 5.84 | 109.54      | 100.20   |
| 2   | M     | 70  | MET  | CG-SD-CE | 5.83 | 109.53      | 100.20   |
| 2   | Q     | 1   | MET  | CG-SD-CE | 5.83 | 109.53      | 100.20   |
| 2   | P     | 1   | MET  | CG-SD-CE | 5.82 | 109.52      | 100.20   |
| 2   | O     | 70  | MET  | CG-SD-CE | 5.80 | 109.49      | 100.20   |
| 2   | P     | 12  | MET  | CG-SD-CE | 5.79 | 109.47      | 100.20   |
| 2   | M     | 12  | MET  | CG-SD-CE | 5.79 | 109.46      | 100.20   |
| 2   | M     | 18  | MET  | CG-SD-CE | 5.79 | 109.46      | 100.20   |
| 2   | S     | 18  | MET  | CG-SD-CE | 5.76 | 109.41      | 100.20   |
| 2   | Q     | 12  | MET  | CG-SD-CE | 5.75 | 109.41      | 100.20   |
| 2   | K     | 18  | MET  | CG-SD-CE | 5.74 | 109.38      | 100.20   |
| 2   | T     | 12  | MET  | CG-SD-CE | 5.72 | 109.35      | 100.20   |
| 2   | R     | 18  | MET  | CG-SD-CE | 5.71 | 109.34      | 100.20   |
| 2   | R     | 12  | MET  | CG-SD-CE | 5.71 | 109.33      | 100.20   |
| 2   | S     | 12  | MET  | CG-SD-CE | 5.71 | 109.33      | 100.20   |
| 2   | O     | 18  | MET  | CG-SD-CE | 5.70 | 109.31      | 100.20   |
| 2   | N     | 12  | MET  | CG-SD-CE | 5.69 | 109.31      | 100.20   |
| 2   | N     | 18  | MET  | CG-SD-CE | 5.67 | 109.28      | 100.20   |
| 1   | I     | 132 | CYS  | CA-CB-SG | 5.67 | 124.20      | 114.00   |
| 2   | O     | 12  | MET  | CG-SD-CE | 5.66 | 109.26      | 100.20   |
| 2   | K     | 12  | MET  | CG-SD-CE | 5.65 | 109.24      | 100.20   |
| 2   | P     | 18  | MET  | CG-SD-CE | 5.65 | 109.24      | 100.20   |
| 2   | L     | 12  | MET  | CG-SD-CE | 5.64 | 109.23      | 100.20   |
| 2   | N     | 29  | MET  | CG-SD-CE | 5.64 | 109.22      | 100.20   |
| 2   | T     | 18  | MET  | CG-SD-CE | 5.62 | 109.19      | 100.20   |
| 2   | L     | 18  | MET  | CG-SD-CE | 5.60 | 109.16      | 100.20   |
| 2   | Q     | 18  | MET  | CG-SD-CE | 5.59 | 109.14      | 100.20   |
| 2   | O     | 29  | MET  | CG-SD-CE | 5.56 | 109.09      | 100.20   |
| 2   | S     | 29  | MET  | CG-SD-CE | 5.54 | 109.06      | 100.20   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | M     | 29  | MET  | CG-SD-CE | 5.48  | 108.97      | 100.20   |
| 2   | L     | 29  | MET  | CG-SD-CE | 5.47  | 108.96      | 100.20   |
| 2   | P     | 29  | MET  | CG-SD-CE | 5.46  | 108.94      | 100.20   |
| 2   | Q     | 29  | MET  | CG-SD-CE | 5.46  | 108.94      | 100.20   |
| 2   | T     | 29  | MET  | CG-SD-CE | 5.45  | 108.91      | 100.20   |
| 2   | K     | 29  | MET  | CG-SD-CE | 5.43  | 108.89      | 100.20   |
| 2   | R     | 29  | MET  | CG-SD-CE | 5.39  | 108.83      | 100.20   |
| 1   | H     | 170 | LEU  | N-CA-C   | -5.08 | 97.30       | 111.00   |

There are no chirality outliers.

There are no planarity outliers.

## 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     | 1524  | 0        | 1543     | 62      | 0            |
| 1   | B     | 1524  | 0        | 1543     | 54      | 0            |
| 1   | C     | 1524  | 0        | 1543     | 44      | 0            |
| 1   | D     | 1524  | 0        | 1543     | 47      | 0            |
| 1   | E     | 1524  | 0        | 1543     | 57      | 0            |
| 1   | F     | 1524  | 0        | 1543     | 56      | 0            |
| 1   | G     | 1524  | 0        | 1543     | 59      | 0            |
| 1   | H     | 1524  | 0        | 1543     | 55      | 0            |
| 1   | I     | 1524  | 0        | 1545     | 53      | 0            |
| 1   | J     | 1524  | 0        | 1543     | 62      | 0            |
| 2   | K     | 676   | 0        | 677      | 16      | 0            |
| 2   | L     | 676   | 0        | 677      | 18      | 0            |
| 2   | M     | 676   | 0        | 677      | 18      | 0            |
| 2   | N     | 676   | 0        | 677      | 18      | 0            |
| 2   | O     | 676   | 0        | 677      | 23      | 0            |
| 2   | P     | 676   | 0        | 677      | 14      | 0            |
| 2   | Q     | 676   | 0        | 677      | 15      | 1            |
| 2   | R     | 676   | 0        | 677      | 20      | 0            |
| 2   | S     | 676   | 0        | 677      | 19      | 1            |
| 2   | T     | 676   | 0        | 677      | 18      | 0            |
| 3   | K     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | L     | 1     | 0        | 0        | 0       | 0            |
| 3   | M     | 1     | 0        | 0        | 0       | 0            |
| 3   | N     | 1     | 0        | 0        | 0       | 0            |
| 3   | O     | 1     | 0        | 0        | 0       | 0            |
| 3   | P     | 1     | 0        | 0        | 0       | 0            |
| 3   | Q     | 1     | 0        | 0        | 0       | 0            |
| 3   | R     | 1     | 0        | 0        | 0       | 0            |
| 3   | S     | 1     | 0        | 0        | 0       | 0            |
| 3   | T     | 1     | 0        | 0        | 0       | 0            |
| 4   | A     | 1     | 0        | 0        | 0       | 0            |
| 4   | B     | 1     | 0        | 0        | 0       | 0            |
| 4   | C     | 1     | 0        | 0        | 0       | 0            |
| 4   | D     | 1     | 0        | 0        | 0       | 0            |
| 4   | E     | 1     | 0        | 0        | 0       | 0            |
| 4   | F     | 1     | 0        | 0        | 0       | 0            |
| 4   | G     | 1     | 0        | 0        | 0       | 0            |
| 4   | H     | 1     | 0        | 0        | 0       | 0            |
| 4   | I     | 1     | 0        | 0        | 1       | 0            |
| 4   | J     | 1     | 0        | 0        | 0       | 0            |
| 5   | K     | 12    | 0        | 8        | 2       | 0            |
| 5   | M     | 12    | 0        | 8        | 1       | 0            |
| 5   | N     | 24    | 0        | 16       | 1       | 0            |
| 5   | O     | 12    | 0        | 8        | 1       | 0            |
| 5   | P     | 12    | 0        | 8        | 0       | 0            |
| 5   | Q     | 12    | 0        | 8        | 0       | 0            |
| 5   | R     | 12    | 0        | 8        | 0       | 0            |
| 5   | S     | 12    | 0        | 8        | 1       | 0            |
| 5   | T     | 12    | 0        | 8        | 0       | 0            |
| 6   | A     | 17    | 0        | 0        | 6       | 0            |
| 6   | B     | 18    | 0        | 0        | 1       | 0            |
| 6   | C     | 13    | 0        | 0        | 0       | 0            |
| 6   | D     | 10    | 0        | 0        | 1       | 0            |
| 6   | E     | 13    | 0        | 0        | 0       | 0            |
| 6   | F     | 15    | 0        | 0        | 2       | 0            |
| 6   | G     | 16    | 0        | 0        | 2       | 0            |
| 6   | H     | 21    | 0        | 0        | 1       | 0            |
| 6   | I     | 20    | 0        | 0        | 5       | 0            |
| 6   | J     | 20    | 0        | 0        | 6       | 0            |
| 6   | K     | 17    | 0        | 0        | 2       | 0            |
| 6   | L     | 19    | 0        | 0        | 1       | 0            |
| 6   | M     | 16    | 0        | 0        | 1       | 0            |
| 6   | N     | 16    | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6   | O     | 16    | 0        | 0        | 0       | 0            |
| 6   | P     | 27    | 0        | 0        | 2       | 0            |
| 6   | Q     | 31    | 0        | 0        | 4       | 0            |
| 6   | R     | 28    | 0        | 0        | 0       | 0            |
| 6   | S     | 22    | 0        | 0        | 0       | 0            |
| 6   | T     | 16    | 0        | 0        | 0       | 0            |
| All | All   | 22511 | 0        | 22282    | 685     | 1            |

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 15.

All (685) 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:I:132:CYS:HB3  | 6:I:3102:HOH:O   | 1.42                     | 1.17              |
| 1:I:148:LEU:HD12 | 1:I:224:VAL:HG21 | 1.51                     | 0.91              |
| 1:B:148:LEU:HD12 | 1:B:224:VAL:HG21 | 1.51                     | 0.90              |
| 1:B:59:LEU:HB3   | 1:B:60:PRO:HD3   | 1.54                     | 0.90              |
| 1:J:148:LEU:HD12 | 1:J:224:VAL:HG21 | 1.51                     | 0.90              |
| 1:G:148:LEU:HD12 | 1:G:224:VAL:HG21 | 1.54                     | 0.90              |
| 1:D:148:LEU:HD12 | 1:D:224:VAL:HG21 | 1.54                     | 0.89              |
| 1:C:148:LEU:HD12 | 1:C:224:VAL:HG21 | 1.53                     | 0.88              |
| 1:A:148:LEU:HD12 | 1:A:224:VAL:HG21 | 1.57                     | 0.86              |
| 1:E:148:LEU:HD12 | 1:E:224:VAL:HG21 | 1.58                     | 0.86              |
| 1:F:148:LEU:HD12 | 1:F:224:VAL:HG21 | 1.57                     | 0.85              |
| 2:Q:43:ASN:H     | 2:Q:43:ASN:HD22  | 1.25                     | 0.83              |
| 1:H:148:LEU:HD12 | 1:H:224:VAL:HG21 | 1.62                     | 0.82              |
| 1:J:132:CYS:HB3  | 6:J:3107:HOH:O   | 1.79                     | 0.80              |
| 2:P:43:ASN:H     | 2:P:43:ASN:HD22  | 1.27                     | 0.80              |
| 1:I:138:PRO:O    | 1:I:202:MET:HB2  | 1.82                     | 0.80              |
| 2:R:43:ASN:HD22  | 2:R:43:ASN:H     | 1.27                     | 0.79              |
| 1:E:213:ASN:H    | 1:E:213:ASN:HD22 | 1.31                     | 0.79              |
| 2:M:43:ASN:HD22  | 2:M:43:ASN:H     | 1.31                     | 0.79              |
| 2:N:43:ASN:HD22  | 2:N:43:ASN:H     | 1.30                     | 0.79              |
| 1:H:213:ASN:HD22 | 1:H:213:ASN:H    | 1.31                     | 0.78              |
| 1:I:213:ASN:HD22 | 1:I:213:ASN:H    | 1.30                     | 0.78              |
| 2:K:43:ASN:HD22  | 2:K:43:ASN:H     | 1.31                     | 0.78              |
| 2:L:43:ASN:H     | 2:L:43:ASN:HD22  | 1.28                     | 0.78              |
| 2:S:43:ASN:HD22  | 2:S:43:ASN:H     | 1.29                     | 0.78              |
| 1:G:213:ASN:H    | 1:G:213:ASN:HD22 | 1.31                     | 0.78              |
| 1:J:132:CYS:SG   | 6:J:3107:HOH:O   | 2.43                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:138:PRO:O    | 1:H:202:MET:HB2  | 1.85                     | 0.77              |
| 1:E:138:PRO:O    | 1:E:202:MET:HB2  | 1.83                     | 0.77              |
| 1:G:111:ALA:HB3  | 1:G:158:LYS:HD3  | 1.65                     | 0.77              |
| 1:A:213:ASN:HD22 | 1:A:213:ASN:H    | 1.30                     | 0.77              |
| 2:Q:18:MET:HG2   | 6:Q:2017:HOH:O   | 1.85                     | 0.77              |
| 1:B:213:ASN:H    | 1:B:213:ASN:HD22 | 1.31                     | 0.76              |
| 1:C:213:ASN:H    | 1:C:213:ASN:HD22 | 1.31                     | 0.76              |
| 1:A:138:PRO:O    | 1:A:202:MET:HB2  | 1.85                     | 0.76              |
| 1:B:138:PRO:O    | 1:B:202:MET:HB2  | 1.85                     | 0.76              |
| 1:A:213:ASN:H    | 1:A:213:ASN:ND2  | 1.83                     | 0.76              |
| 1:I:203:CYS:HG   | 4:I:3101:ZN:ZN   | 0.96                     | 0.76              |
| 1:D:213:ASN:H    | 1:D:213:ASN:HD22 | 1.32                     | 0.75              |
| 1:I:213:ASN:H    | 1:I:213:ASN:ND2  | 1.85                     | 0.74              |
| 2:O:43:ASN:HD22  | 2:O:43:ASN:H     | 1.32                     | 0.74              |
| 1:B:213:ASN:ND2  | 1:B:213:ASN:H    | 1.84                     | 0.73              |
| 1:H:111:ALA:HB3  | 1:H:158:LYS:HD3  | 1.70                     | 0.73              |
| 1:H:59:LEU:HB3   | 1:H:60:PRO:HD3   | 1.69                     | 0.73              |
| 1:C:138:PRO:O    | 1:C:202:MET:HB2  | 1.88                     | 0.73              |
| 1:F:213:ASN:HD22 | 1:F:213:ASN:H    | 1.37                     | 0.73              |
| 1:B:107:VAL:HG22 | 1:B:161:ARG:HD3  | 1.70                     | 0.73              |
| 1:E:59:LEU:HB3   | 1:E:60:PRO:HD3   | 1.70                     | 0.73              |
| 1:F:111:ALA:HB3  | 1:F:158:LYS:HD3  | 1.71                     | 0.73              |
| 1:J:213:ASN:H    | 1:J:213:ASN:HD22 | 1.33                     | 0.72              |
| 2:T:43:ASN:H     | 2:T:43:ASN:HD22  | 1.35                     | 0.72              |
| 1:C:213:ASN:H    | 1:C:213:ASN:ND2  | 1.87                     | 0.72              |
| 1:A:54:ASP:HA    | 6:A:3110:HOH:O   | 1.89                     | 0.72              |
| 1:C:111:ALA:HB3  | 1:C:158:LYS:HD3  | 1.72                     | 0.71              |
| 1:H:213:ASN:N    | 1:H:213:ASN:HD22 | 1.88                     | 0.71              |
| 1:G:213:ASN:H    | 1:G:213:ASN:ND2  | 1.87                     | 0.71              |
| 1:J:138:PRO:O    | 1:J:202:MET:HB2  | 1.89                     | 0.71              |
| 1:E:213:ASN:H    | 1:E:213:ASN:ND2  | 1.87                     | 0.71              |
| 1:D:213:ASN:H    | 1:D:213:ASN:ND2  | 1.86                     | 0.71              |
| 1:C:112:ILE:HG21 | 1:C:152:GLN:HE21 | 1.55                     | 0.71              |
| 1:E:213:ASN:HD22 | 1:E:213:ASN:N    | 1.88                     | 0.70              |
| 1:J:213:ASN:ND2  | 1:J:213:ASN:H    | 1.89                     | 0.70              |
| 1:D:138:PRO:O    | 1:D:202:MET:HB2  | 1.91                     | 0.70              |
| 1:F:226:ARG:HD3  | 6:F:3116:HOH:O   | 1.90                     | 0.70              |
| 1:H:213:ASN:ND2  | 1:H:213:ASN:H    | 1.88                     | 0.70              |
| 1:I:111:ALA:H    | 1:I:158:LYS:HE3  | 1.56                     | 0.70              |
| 1:G:201:HIS:HD2  | 6:G:3115:HOH:O   | 1.76                     | 0.69              |
| 2:R:43:ASN:N     | 2:R:43:ASN:HD22  | 1.90                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:213:ASN:N    | 1:C:213:ASN:HD22 | 1.89                     | 0.69              |
| 1:D:111:ALA:HB3  | 1:D:158:LYS:HD3  | 1.74                     | 0.69              |
| 1:B:112:ILE:HG21 | 1:B:152:GLN:HE21 | 1.58                     | 0.69              |
| 1:I:213:ASN:HD22 | 1:I:213:ASN:N    | 1.88                     | 0.69              |
| 1:G:213:ASN:N    | 1:G:213:ASN:HD22 | 1.89                     | 0.69              |
| 1:J:132:CYS:CB   | 6:J:3107:HOH:O   | 2.37                     | 0.69              |
| 1:J:59:LEU:HB3   | 1:J:60:PRO:HD3   | 1.75                     | 0.68              |
| 2:L:43:ASN:N     | 2:L:43:ASN:HD22  | 1.90                     | 0.68              |
| 1:F:213:ASN:ND2  | 1:F:213:ASN:H    | 1.91                     | 0.68              |
| 1:I:59:LEU:HB3   | 1:I:60:PRO:HD3   | 1.75                     | 0.68              |
| 1:D:59:LEU:HB3   | 1:D:60:PRO:HD3   | 1.75                     | 0.68              |
| 1:A:213:ASN:HD22 | 1:A:213:ASN:N    | 1.87                     | 0.68              |
| 1:C:59:LEU:HB3   | 1:C:60:PRO:HD3   | 1.77                     | 0.67              |
| 1:H:111:ALA:H    | 1:H:158:LYS:HE3  | 1.59                     | 0.67              |
| 2:P:43:ASN:H     | 2:P:43:ASN:ND2   | 1.92                     | 0.67              |
| 2:N:43:ASN:HD22  | 2:N:43:ASN:N     | 1.91                     | 0.67              |
| 1:B:213:ASN:N    | 1:B:213:ASN:HD22 | 1.86                     | 0.67              |
| 1:G:138:PRO:O    | 1:G:202:MET:HB2  | 1.94                     | 0.67              |
| 1:G:59:LEU:HB3   | 1:G:60:PRO:HD3   | 1.74                     | 0.67              |
| 1:A:98:LYS:O     | 1:A:101:GLN:HG2  | 1.95                     | 0.67              |
| 1:H:107:VAL:HG22 | 1:H:161:ARG:HD3  | 1.77                     | 0.67              |
| 1:F:59:LEU:HB3   | 1:F:60:PRO:HD3   | 1.76                     | 0.67              |
| 2:S:43:ASN:N     | 2:S:43:ASN:HD22  | 1.91                     | 0.67              |
| 1:A:111:ALA:H    | 1:A:158:LYS:HE3  | 1.59                     | 0.67              |
| 1:J:213:ASN:HD22 | 1:J:213:ASN:N    | 1.90                     | 0.67              |
| 1:A:50:ARG:HB3   | 1:A:101:GLN:HB3  | 1.76                     | 0.67              |
| 1:E:111:ALA:HB3  | 1:E:158:LYS:HD3  | 1.75                     | 0.67              |
| 1:I:98:LYS:O     | 1:I:101:GLN:HG2  | 1.94                     | 0.66              |
| 1:I:111:ALA:HB3  | 1:I:158:LYS:HD3  | 1.75                     | 0.66              |
| 1:B:111:ALA:HB3  | 1:B:158:LYS:HD3  | 1.76                     | 0.66              |
| 1:J:111:ALA:HB3  | 1:J:158:LYS:HD3  | 1.76                     | 0.66              |
| 2:Q:43:ASN:H     | 2:Q:43:ASN:ND2   | 1.93                     | 0.66              |
| 1:G:98:LYS:O     | 1:G:101:GLN:HG2  | 1.96                     | 0.66              |
| 1:F:107:VAL:HG22 | 1:F:161:ARG:HD3  | 1.77                     | 0.66              |
| 1:F:138:PRO:O    | 1:F:202:MET:HB2  | 1.96                     | 0.66              |
| 1:C:98:LYS:O     | 1:C:101:GLN:HG2  | 1.94                     | 0.66              |
| 1:F:213:ASN:HD22 | 1:F:213:ASN:N    | 1.92                     | 0.66              |
| 2:L:43:ASN:H     | 2:L:43:ASN:ND2   | 1.93                     | 0.65              |
| 1:J:98:LYS:O     | 1:J:101:GLN:HG2  | 1.96                     | 0.65              |
| 1:H:234:GLU:HB2  | 6:H:3117:HOH:O   | 1.95                     | 0.65              |
| 1:A:157:SER:HB3  | 6:A:3114:HOH:O   | 1.96                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:59:LEU:HB3   | 1:A:60:PRO:HD3   | 1.79                     | 0.65              |
| 2:R:43:ASN:ND2   | 2:R:43:ASN:H     | 1.93                     | 0.65              |
| 1:C:107:VAL:HG22 | 1:C:161:ARG:HD3  | 1.78                     | 0.65              |
| 1:A:137:VAL:CG1  | 1:A:202:MET:HB3  | 2.28                     | 0.64              |
| 1:J:226:ARG:HD3  | 6:J:3113:HOH:O   | 1.97                     | 0.64              |
| 2:M:43:ASN:ND2   | 2:M:43:ASN:H     | 1.95                     | 0.64              |
| 1:J:107:VAL:HG22 | 1:J:161:ARG:HD3  | 1.79                     | 0.64              |
| 2:S:43:ASN:ND2   | 2:S:43:ASN:H     | 1.95                     | 0.64              |
| 2:P:43:ASN:N     | 2:P:43:ASN:HD22  | 1.89                     | 0.64              |
| 2:O:43:ASN:HD22  | 2:O:43:ASN:N     | 1.93                     | 0.64              |
| 1:B:137:VAL:HG12 | 1:B:202:MET:HB3  | 1.79                     | 0.63              |
| 2:N:43:ASN:H     | 2:N:43:ASN:ND2   | 1.95                     | 0.63              |
| 1:F:137:VAL:CG1  | 1:F:202:MET:HB3  | 2.27                     | 0.63              |
| 1:F:164:GLU:OE2  | 1:F:168:ARG:HD2  | 1.98                     | 0.63              |
| 1:A:137:VAL:HG12 | 1:A:202:MET:HB3  | 1.81                     | 0.63              |
| 2:K:43:ASN:H     | 2:K:43:ASN:ND2   | 1.95                     | 0.62              |
| 1:H:164:GLU:OE2  | 1:H:168:ARG:HD2  | 1.99                     | 0.62              |
| 1:D:137:VAL:CG1  | 1:D:202:MET:HB3  | 2.29                     | 0.62              |
| 1:G:107:VAL:HG22 | 1:G:161:ARG:HD3  | 1.81                     | 0.62              |
| 1:D:213:ASN:N    | 1:D:213:ASN:HD22 | 1.90                     | 0.61              |
| 1:J:111:ALA:H    | 1:J:158:LYS:HE3  | 1.64                     | 0.61              |
| 1:I:107:VAL:HG22 | 1:I:161:ARG:HD3  | 1.82                     | 0.61              |
| 1:C:76:ASP:OD2   | 1:C:78:GLN:HB2   | 2.00                     | 0.61              |
| 1:G:111:ALA:H    | 1:G:158:LYS:HE3  | 1.64                     | 0.61              |
| 2:T:43:ASN:H     | 2:T:43:ASN:ND2   | 1.99                     | 0.61              |
| 1:B:98:LYS:O     | 1:B:101:GLN:HG2  | 2.01                     | 0.61              |
| 1:H:98:LYS:O     | 1:H:101:GLN:HG2  | 2.01                     | 0.61              |
| 1:E:112:ILE:HG21 | 1:E:152:GLN:HE21 | 1.66                     | 0.61              |
| 1:I:137:VAL:HG12 | 1:I:202:MET:HB3  | 1.82                     | 0.60              |
| 1:A:57:LEU:HB2   | 6:A:3110:HOH:O   | 2.01                     | 0.60              |
| 1:G:164:GLU:OE2  | 1:G:168:ARG:HD2  | 2.01                     | 0.60              |
| 1:C:207:ARG:NH2  | 1:H:92:ALA:HA    | 2.16                     | 0.60              |
| 2:M:43:ASN:HD22  | 2:M:43:ASN:N     | 1.93                     | 0.60              |
| 2:T:43:ASN:N     | 2:T:43:ASN:HD22  | 1.94                     | 0.60              |
| 1:A:111:ALA:HB3  | 1:A:158:LYS:HD3  | 1.82                     | 0.60              |
| 1:A:124:LYS:NZ   | 1:A:241:SER:OG   | 2.31                     | 0.60              |
| 1:H:76:ASP:OD2   | 1:H:78:GLN:HB2   | 2.00                     | 0.60              |
| 2:Q:43:ASN:HD22  | 2:Q:43:ASN:N     | 1.90                     | 0.60              |
| 1:E:111:ALA:H    | 1:E:158:LYS:HE3  | 1.65                     | 0.60              |
| 1:I:201:HIS:HD2  | 6:I:3115:HOH:O   | 1.85                     | 0.60              |
| 1:B:137:VAL:CG1  | 1:B:202:MET:HB3  | 2.31                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:111:ALA:H    | 1:B:158:LYS:HE3  | 1.66                     | 0.60              |
| 2:R:2:PRO:HB2    | 2:R:82:HIS:CE1   | 2.37                     | 0.60              |
| 1:F:137:VAL:HG12 | 1:F:202:MET:HB3  | 1.83                     | 0.60              |
| 1:C:111:ALA:H    | 1:C:158:LYS:HE3  | 1.66                     | 0.59              |
| 2:K:43:ASN:HD22  | 2:K:43:ASN:N     | 1.92                     | 0.59              |
| 1:J:135:HIS:HB2  | 6:J:3107:HOH:O   | 2.02                     | 0.59              |
| 2:O:43:ASN:H     | 2:O:43:ASN:ND2   | 1.97                     | 0.59              |
| 1:A:76:ASP:OD2   | 1:A:78:GLN:HB2   | 2.01                     | 0.59              |
| 1:E:107:VAL:HG22 | 1:E:161:ARG:HD3  | 1.85                     | 0.59              |
| 1:A:112:ILE:HG21 | 1:A:152:GLN:HE21 | 1.68                     | 0.59              |
| 2:O:49:VAL:CG1   | 2:O:51:ASP:H     | 2.15                     | 0.59              |
| 1:I:137:VAL:CG1  | 1:I:202:MET:HB3  | 2.32                     | 0.59              |
| 1:F:111:ALA:H    | 1:F:158:LYS:HE3  | 1.67                     | 0.59              |
| 1:F:76:ASP:OD2   | 1:F:78:GLN:HB2   | 2.02                     | 0.58              |
| 1:C:115:GLU:OE1  | 1:C:115:GLU:HA   | 2.02                     | 0.58              |
| 1:G:137:VAL:CG1  | 1:G:202:MET:HB3  | 2.34                     | 0.58              |
| 1:A:116:ASP:OD1  | 1:A:151:LYS:HD2  | 2.03                     | 0.58              |
| 1:J:76:ASP:OD2   | 1:J:78:GLN:HB2   | 2.03                     | 0.58              |
| 2:R:49:VAL:CG1   | 2:R:51:ASP:H     | 2.17                     | 0.58              |
| 1:A:57:LEU:HD12  | 6:A:3110:HOH:O   | 2.02                     | 0.58              |
| 1:J:137:VAL:CG1  | 1:J:202:MET:HB3  | 2.34                     | 0.58              |
| 1:B:161:ARG:O    | 1:B:165:ILE:HG13 | 2.04                     | 0.57              |
| 1:C:112:ILE:HG21 | 1:C:152:GLN:NE2  | 2.18                     | 0.57              |
| 1:D:116:ASP:OD1  | 1:D:151:LYS:HD2  | 2.04                     | 0.57              |
| 1:J:115:GLU:HA   | 1:J:115:GLU:OE1  | 2.04                     | 0.57              |
| 1:D:137:VAL:HG12 | 1:D:202:MET:HB3  | 1.85                     | 0.57              |
| 1:F:50:ARG:HB3   | 1:F:101:GLN:HB3  | 1.86                     | 0.57              |
| 1:I:112:ILE:HG21 | 1:I:152:GLN:HE21 | 1.69                     | 0.57              |
| 1:H:137:VAL:HG12 | 1:H:202:MET:HB3  | 1.87                     | 0.57              |
| 1:G:158:LYS:HD2  | 1:G:158:LYS:N    | 2.20                     | 0.57              |
| 1:J:112:ILE:HG21 | 1:J:152:GLN:HE21 | 1.70                     | 0.57              |
| 1:B:115:GLU:OE1  | 1:B:115:GLU:HA   | 2.05                     | 0.57              |
| 1:H:112:ILE:HG21 | 1:H:152:GLN:HE21 | 1.70                     | 0.57              |
| 1:D:50:ARG:HB3   | 1:D:101:GLN:HB3  | 1.87                     | 0.57              |
| 1:H:137:VAL:CG1  | 1:H:202:MET:HB3  | 2.34                     | 0.56              |
| 1:A:107:VAL:HG22 | 1:A:161:ARG:HD3  | 1.85                     | 0.56              |
| 2:T:49:VAL:CG1   | 2:T:51:ASP:H     | 2.18                     | 0.56              |
| 1:A:58:ASN:HA    | 1:A:61:ASN:HD22  | 1.71                     | 0.56              |
| 1:E:76:ASP:OD2   | 1:E:78:GLN:HB2   | 2.05                     | 0.56              |
| 1:D:107:VAL:HG22 | 1:D:161:ARG:HD3  | 1.87                     | 0.56              |
| 2:R:49:VAL:HG13  | 2:R:51:ASP:H     | 1.71                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:112:ILE:HG21 | 1:G:152:GLN:HE21 | 1.71                     | 0.56              |
| 2:P:49:VAL:CG1   | 2:P:51:ASP:H     | 2.18                     | 0.56              |
| 2:L:2:PRO:HB2    | 2:L:82:HIS:CE1   | 2.41                     | 0.56              |
| 2:K:18:MET:CE    | 2:K:46:GLU:HB2   | 2.36                     | 0.56              |
| 2:P:2:PRO:HB2    | 2:P:82:HIS:CE1   | 2.41                     | 0.56              |
| 1:B:221:MET:O    | 1:B:226:ARG:HB2  | 2.06                     | 0.56              |
| 2:K:2:PRO:HB2    | 2:K:82:HIS:CE1   | 2.41                     | 0.55              |
| 1:D:164:GLU:OE2  | 1:D:168:ARG:HD2  | 2.06                     | 0.55              |
| 1:D:115:GLU:HA   | 1:D:115:GLU:OE1  | 2.06                     | 0.55              |
| 1:C:164:GLU:OE2  | 1:C:168:ARG:HD2  | 2.05                     | 0.55              |
| 1:D:111:ALA:H    | 1:D:158:LYS:HE3  | 1.70                     | 0.55              |
| 1:D:76:ASP:OD2   | 1:D:78:GLN:HB2   | 2.06                     | 0.55              |
| 1:I:115:GLU:HA   | 1:I:115:GLU:OE1  | 2.06                     | 0.55              |
| 1:F:98:LYS:O     | 1:F:101:GLN:HG2  | 2.07                     | 0.55              |
| 2:T:18:MET:HE1   | 2:T:46:GLU:HG3   | 1.88                     | 0.55              |
| 1:C:145:ILE:HD13 | 1:C:184:ILE:HD11 | 1.88                     | 0.55              |
| 1:B:50:ARG:HB3   | 1:B:101:GLN:HB3  | 1.88                     | 0.55              |
| 1:B:112:ILE:HG21 | 1:B:152:GLN:NE2  | 2.21                     | 0.55              |
| 1:E:158:LYS:HD2  | 1:E:158:LYS:N    | 2.20                     | 0.55              |
| 1:E:98:LYS:O     | 1:E:101:GLN:HG2  | 2.06                     | 0.55              |
| 2:N:49:VAL:CG1   | 2:N:51:ASP:H     | 2.19                     | 0.55              |
| 2:Q:49:VAL:HG13  | 2:Q:51:ASP:H     | 1.72                     | 0.55              |
| 2:M:49:VAL:HG13  | 2:M:51:ASP:H     | 1.72                     | 0.54              |
| 1:E:137:VAL:CG1  | 1:E:202:MET:HB3  | 2.38                     | 0.54              |
| 1:D:158:LYS:HD2  | 1:D:158:LYS:N    | 2.23                     | 0.54              |
| 1:A:140:VAL:HG12 | 1:A:141:GLY:N    | 2.23                     | 0.54              |
| 1:H:115:GLU:HA   | 1:H:115:GLU:OE1  | 2.07                     | 0.54              |
| 1:A:92:ALA:HA    | 1:J:207:ARG:NH2  | 2.23                     | 0.54              |
| 1:I:164:GLU:HG3  | 6:I:3112:HOH:O   | 2.08                     | 0.54              |
| 2:M:12:MET:HG2   | 6:M:2014:HOH:O   | 2.06                     | 0.54              |
| 1:H:124:LYS:NZ   | 1:H:241:SER:OG   | 2.30                     | 0.54              |
| 1:H:154:LEU:HB2  | 1:H:188:LEU:HD11 | 1.88                     | 0.54              |
| 1:F:115:GLU:HA   | 1:F:115:GLU:OE1  | 2.08                     | 0.54              |
| 1:D:103:THR:HA   | 6:D:3118:HOH:O   | 2.07                     | 0.54              |
| 1:B:164:GLU:OE2  | 1:B:168:ARG:HD2  | 2.07                     | 0.54              |
| 2:S:49:VAL:CG1   | 2:S:51:ASP:H     | 2.20                     | 0.54              |
| 1:C:137:VAL:HG12 | 1:C:202:MET:HB3  | 1.89                     | 0.53              |
| 2:Q:49:VAL:CG1   | 2:Q:51:ASP:H     | 2.21                     | 0.53              |
| 1:J:116:ASP:OD1  | 1:J:151:LYS:HD2  | 2.07                     | 0.53              |
| 2:N:22:GLU:HB2   | 6:N:2023:HOH:O   | 2.08                     | 0.53              |
| 2:S:2:PRO:HB2    | 2:S:82:HIS:CE1   | 2.43                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:50:ARG:HB3   | 1:G:101:GLN:HB3  | 1.89                     | 0.53              |
| 1:B:134:HIS:CG   | 6:I:3106:HOH:O   | 2.61                     | 0.53              |
| 1:G:137:VAL:HG12 | 1:G:202:MET:HB3  | 1.88                     | 0.53              |
| 1:A:53:GLU:O     | 1:A:57:LEU:HG    | 2.08                     | 0.53              |
| 2:M:49:VAL:CG1   | 2:M:51:ASP:H     | 2.21                     | 0.53              |
| 2:O:65:PHE:CE2   | 2:O:83:LYS:HB2   | 2.44                     | 0.53              |
| 2:L:18:MET:HE1   | 2:L:46:GLU:HG3   | 1.90                     | 0.53              |
| 2:P:49:VAL:HG13  | 2:P:51:ASP:H     | 1.74                     | 0.53              |
| 1:J:158:LYS:N    | 1:J:158:LYS:HD2  | 2.24                     | 0.53              |
| 2:M:2:PRO:HB2    | 2:M:82:HIS:CE1   | 2.44                     | 0.53              |
| 1:B:148:LEU:HD12 | 1:B:224:VAL:CG2  | 2.32                     | 0.52              |
| 2:O:2:PRO:HB2    | 2:O:82:HIS:CE1   | 2.44                     | 0.52              |
| 1:E:58:ASN:HA    | 1:E:61:ASN:HD22  | 1.73                     | 0.52              |
| 1:B:158:LYS:N    | 1:B:158:LYS:HD2  | 2.24                     | 0.52              |
| 1:F:158:LYS:HD2  | 1:F:158:LYS:N    | 2.24                     | 0.52              |
| 2:R:65:PHE:CE2   | 2:R:83:LYS:HB2   | 2.44                     | 0.52              |
| 6:P:2019:HOH:O   | 2:Q:82:HIS:HD2   | 1.93                     | 0.52              |
| 1:F:145:ILE:HD13 | 1:F:184:ILE:HD11 | 1.92                     | 0.52              |
| 1:A:55:ASN:HA    | 1:A:94:GLN:HE22  | 1.75                     | 0.52              |
| 1:G:76:ASP:OD2   | 1:G:78:GLN:HB2   | 2.09                     | 0.52              |
| 2:Q:18:MET:CE    | 2:Q:46:GLU:HB2   | 2.40                     | 0.52              |
| 1:D:207:ARG:NH2  | 1:G:92:ALA:HA    | 2.25                     | 0.52              |
| 1:E:116:ASP:OD1  | 1:E:151:LYS:HD2  | 2.10                     | 0.52              |
| 1:D:154:LEU:HB2  | 1:D:188:LEU:HD11 | 1.91                     | 0.52              |
| 1:I:140:VAL:HG12 | 1:I:141:GLY:N    | 2.25                     | 0.52              |
| 1:E:50:ARG:HB3   | 1:E:101:GLN:HB3  | 1.90                     | 0.52              |
| 2:S:49:VAL:HG13  | 2:S:51:ASP:H     | 1.75                     | 0.52              |
| 1:D:112:ILE:HG21 | 1:D:152:GLN:HE21 | 1.74                     | 0.52              |
| 1:E:113:PHE:HZ   | 1:G:88:ARG:NH1   | 2.06                     | 0.52              |
| 1:E:137:VAL:HG12 | 1:E:202:MET:HB3  | 1.91                     | 0.52              |
| 1:A:207:ARG:NE   | 6:A:3103:HOH:O   | 2.43                     | 0.52              |
| 2:K:25:ASP:O     | 2:K:29:MET:HG2   | 2.10                     | 0.52              |
| 1:A:112:ILE:HG21 | 1:A:152:GLN:NE2  | 2.25                     | 0.51              |
| 2:K:49:VAL:CG1   | 2:K:51:ASP:H     | 2.22                     | 0.51              |
| 1:F:112:ILE:HG21 | 1:F:152:GLN:HE21 | 1.74                     | 0.51              |
| 2:N:49:VAL:HG13  | 2:N:51:ASP:H     | 1.75                     | 0.51              |
| 1:D:213:ASN:HD22 | 1:D:214:SER:H    | 1.59                     | 0.51              |
| 2:P:18:MET:CE    | 2:P:46:GLU:HB2   | 2.40                     | 0.51              |
| 1:E:115:GLU:OE1  | 1:E:115:GLU:HA   | 2.10                     | 0.51              |
| 2:P:1:MET:N      | 6:P:2025:HOH:O   | 2.43                     | 0.51              |
| 1:B:137:VAL:HB   | 1:B:203:CYS:HB3  | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:S:18:MET:HE1   | 2:S:46:GLU:HG3   | 1.92                     | 0.51              |
| 1:A:164:GLU:OE2  | 1:A:168:ARG:HD2  | 2.11                     | 0.51              |
| 1:A:230:LYS:HA   | 1:A:230:LYS:HE2  | 1.92                     | 0.51              |
| 1:I:240:ARG:HD2  | 6:J:3120:HOH:O   | 2.10                     | 0.51              |
| 1:G:115:GLU:HA   | 1:G:115:GLU:OE1  | 2.10                     | 0.51              |
| 1:G:140:VAL:HG12 | 1:G:141:GLY:N    | 2.26                     | 0.51              |
| 1:F:116:ASP:OD1  | 1:F:151:LYS:HD2  | 2.10                     | 0.51              |
| 2:O:49:VAL:HG13  | 2:O:51:ASP:H     | 1.76                     | 0.51              |
| 2:L:49:VAL:CG1   | 2:L:51:ASP:H     | 2.23                     | 0.51              |
| 1:F:213:ASN:ND2  | 1:F:213:ASN:N    | 2.55                     | 0.50              |
| 1:C:158:LYS:HD2  | 1:C:158:LYS:N    | 2.25                     | 0.50              |
| 1:A:140:VAL:HG11 | 1:J:212:MET:CE   | 2.42                     | 0.50              |
| 2:T:2:PRO:HB2    | 2:T:82:HIS:CE1   | 2.46                     | 0.50              |
| 1:A:158:LYS:N    | 1:A:158:LYS:HD2  | 2.27                     | 0.50              |
| 6:Q:2028:HOH:O   | 2:R:1:MET:HB3    | 2.11                     | 0.50              |
| 2:O:18:MET:CE    | 2:O:46:GLU:HB2   | 2.41                     | 0.50              |
| 2:N:2:PRO:HB2    | 2:N:82:HIS:CE1   | 2.46                     | 0.50              |
| 1:J:137:VAL:HG12 | 1:J:202:MET:HB3  | 1.92                     | 0.50              |
| 1:A:115:GLU:HA   | 1:A:115:GLU:OE1  | 2.11                     | 0.50              |
| 1:F:213:ASN:HD22 | 1:F:214:SER:H    | 1.59                     | 0.50              |
| 1:J:112:ILE:HG21 | 1:J:152:GLN:NE2  | 2.27                     | 0.50              |
| 2:O:18:MET:HE1   | 2:O:46:GLU:HG3   | 1.93                     | 0.50              |
| 1:I:154:LEU:HB2  | 1:I:188:LEU:HD11 | 1.94                     | 0.50              |
| 1:B:230:LYS:HE2  | 1:B:230:LYS:HA   | 1.93                     | 0.50              |
| 1:B:76:ASP:OD2   | 1:B:78:GLN:HB2   | 2.11                     | 0.50              |
| 2:Q:2:PRO:HB2    | 2:Q:82:HIS:CE1   | 2.46                     | 0.50              |
| 1:E:113:PHE:HZ   | 1:G:88:ARG:HH12  | 1.59                     | 0.50              |
| 1:H:50:ARG:HB3   | 1:H:101:GLN:HB3  | 1.93                     | 0.49              |
| 2:Q:65:PHE:CE2   | 2:Q:83:LYS:HB2   | 2.47                     | 0.49              |
| 1:G:58:ASN:HA    | 1:G:61:ASN:HD22  | 1.77                     | 0.49              |
| 2:N:43:ASN:N     | 2:N:43:ASN:ND2   | 2.58                     | 0.49              |
| 1:B:112:ILE:CG2  | 1:B:152:GLN:HE21 | 2.25                     | 0.49              |
| 2:K:49:VAL:HG13  | 2:K:51:ASP:H     | 1.77                     | 0.49              |
| 1:A:212:MET:CE   | 1:J:140:VAL:HG11 | 2.42                     | 0.49              |
| 1:E:161:ARG:O    | 1:E:165:ILE:HG13 | 2.11                     | 0.49              |
| 2:T:65:PHE:CE2   | 2:T:83:LYS:HB2   | 2.46                     | 0.49              |
| 1:E:137:VAL:HB   | 1:E:203:CYS:HB3  | 1.94                     | 0.49              |
| 2:Q:18:MET:HE1   | 2:Q:46:GLU:HG3   | 1.93                     | 0.49              |
| 2:L:49:VAL:HG13  | 2:L:51:ASP:H     | 1.76                     | 0.49              |
| 1:F:230:LYS:HA   | 1:F:230:LYS:HE2  | 1.93                     | 0.49              |
| 1:C:110:ASP:HB2  | 1:C:158:LYS:HE3  | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:234:GLU:OE2  | 1:J:232:ARG:HD3  | 2.12                     | 0.49              |
| 1:C:137:VAL:CG1  | 1:C:202:MET:HB3  | 2.42                     | 0.49              |
| 1:E:90:ALA:O     | 1:E:94:GLN:HG3   | 2.13                     | 0.49              |
| 1:H:116:ASP:OD1  | 1:H:151:LYS:HD2  | 2.12                     | 0.49              |
| 1:D:230:LYS:HE2  | 1:D:230:LYS:HA   | 1.95                     | 0.49              |
| 1:I:213:ASN:HD22 | 1:I:214:SER:H    | 1.61                     | 0.49              |
| 1:D:98:LYS:O     | 1:D:101:GLN:HG2  | 2.12                     | 0.49              |
| 1:H:137:VAL:HB   | 1:H:203:CYS:HB3  | 1.95                     | 0.49              |
| 1:C:112:ILE:CG2  | 1:C:152:GLN:HE21 | 2.24                     | 0.49              |
| 2:Q:54:ARG:NH1   | 2:R:21:ASP:OD1   | 2.41                     | 0.49              |
| 1:G:213:ASN:HD22 | 1:G:214:SER:H    | 1.59                     | 0.49              |
| 1:C:124:LYS:NZ   | 1:C:241:SER:OG   | 2.37                     | 0.49              |
| 2:K:65:PHE:CE2   | 2:K:83:LYS:HB2   | 2.47                     | 0.49              |
| 1:E:140:VAL:HG12 | 1:E:141:GLY:N    | 2.28                     | 0.49              |
| 2:L:58:ASP:OD1   | 2:M:2:PRO:HD2    | 2.13                     | 0.49              |
| 1:A:213:ASN:HD22 | 1:A:214:SER:H    | 1.61                     | 0.48              |
| 1:J:142:ARG:HG2  | 1:J:142:ARG:HH11 | 1.78                     | 0.48              |
| 1:G:53:GLU:O     | 1:G:57:LEU:HG    | 2.13                     | 0.48              |
| 1:D:92:ALA:HA    | 1:G:207:ARG:NH2  | 2.28                     | 0.48              |
| 1:E:124:LYS:NZ   | 1:E:241:SER:OG   | 2.36                     | 0.48              |
| 1:E:142:ARG:HG2  | 1:E:142:ARG:HH11 | 1.77                     | 0.48              |
| 2:T:18:MET:HE1   | 2:T:46:GLU:CG    | 2.42                     | 0.48              |
| 1:I:164:GLU:OE2  | 1:I:168:ARG:HD2  | 2.13                     | 0.48              |
| 1:B:107:VAL:HG22 | 1:B:161:ARG:CD   | 2.42                     | 0.48              |
| 1:G:232:ARG:HD3  | 1:H:234:GLU:OE2  | 2.12                     | 0.48              |
| 2:M:18:MET:CE    | 2:M:46:GLU:HB2   | 2.42                     | 0.48              |
| 1:B:116:ASP:OD1  | 1:B:151:LYS:HD2  | 2.13                     | 0.48              |
| 1:F:140:VAL:HG12 | 1:F:141:GLY:N    | 2.29                     | 0.48              |
| 1:B:154:LEU:HB2  | 1:B:188:LEU:HD11 | 1.96                     | 0.48              |
| 1:I:148:LEU:CD1  | 1:I:224:VAL:HG21 | 2.34                     | 0.48              |
| 1:E:112:ILE:HG21 | 1:E:152:GLN:NE2  | 2.27                     | 0.48              |
| 1:E:140:VAL:HG11 | 1:F:212:MET:CE   | 2.43                     | 0.48              |
| 1:A:71:ARG:HG3   | 1:A:77:PRO:HG2   | 1.96                     | 0.48              |
| 1:G:161:ARG:O    | 1:G:165:ILE:HG13 | 2.14                     | 0.48              |
| 1:B:79:ARG:NH1   | 6:B:3119:HOH:O   | 2.46                     | 0.48              |
| 1:G:110:ASP:HB2  | 1:G:158:LYS:HE3  | 1.96                     | 0.48              |
| 1:C:50:ARG:HB3   | 1:C:101:GLN:HB3  | 1.96                     | 0.48              |
| 2:O:18:MET:HE1   | 2:O:46:GLU:CG    | 2.44                     | 0.48              |
| 1:I:76:ASP:OD2   | 1:I:78:GLN:HB2   | 2.13                     | 0.48              |
| 1:E:148:LEU:CD1  | 1:E:224:VAL:HG21 | 2.39                     | 0.48              |
| 2:S:43:ASN:N     | 2:S:43:ASN:ND2   | 2.59                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:161:ARG:O    | 1:H:165:ILE:HG13 | 2.14                     | 0.48              |
| 1:E:164:GLU:O    | 1:E:168:ARG:HG3  | 2.14                     | 0.48              |
| 1:H:158:LYS:N    | 1:H:158:LYS:HD2  | 2.28                     | 0.47              |
| 1:F:236:LEU:O    | 1:F:240:ARG:HB2  | 2.14                     | 0.47              |
| 1:J:50:ARG:HB3   | 1:J:101:GLN:HB3  | 1.96                     | 0.47              |
| 2:N:73:VAL:O     | 5:N:1006:PHE:HB3 | 2.15                     | 0.47              |
| 1:D:58:ASN:HA    | 1:D:61:ASN:HD22  | 1.79                     | 0.47              |
| 1:G:137:VAL:HB   | 1:G:203:CYS:HB3  | 1.96                     | 0.47              |
| 2:S:18:MET:CE    | 2:S:46:GLU:HB2   | 2.43                     | 0.47              |
| 1:F:71:ARG:HG3   | 1:F:77:PRO:HG2   | 1.96                     | 0.47              |
| 1:F:205:VAL:HA   | 1:F:211:LYS:HB3  | 1.95                     | 0.47              |
| 2:O:43:ASN:N     | 2:O:43:ASN:ND2   | 2.61                     | 0.47              |
| 1:E:212:MET:CE   | 1:F:140:VAL:HG11 | 2.44                     | 0.47              |
| 2:K:53:PRO:HG2   | 6:K:2009:HOH:O   | 2.14                     | 0.47              |
| 2:S:65:PHE:CE2   | 2:S:83:LYS:HB2   | 2.50                     | 0.47              |
| 2:Q:18:MET:HE1   | 2:Q:46:GLU:CG    | 2.45                     | 0.47              |
| 1:I:148:LEU:HD12 | 1:I:224:VAL:CG2  | 2.36                     | 0.47              |
| 1:F:239:ILE:HG13 | 1:F:240:ARG:N    | 2.30                     | 0.47              |
| 2:L:65:PHE:CE2   | 2:L:83:LYS:HB2   | 2.49                     | 0.47              |
| 2:K:18:MET:HE1   | 2:K:46:GLU:HG3   | 1.97                     | 0.47              |
| 2:T:25:ASP:O     | 2:T:29:MET:HG2   | 2.15                     | 0.47              |
| 2:L:60:LEU:HD23  | 2:L:81:LEU:HD22  | 1.97                     | 0.47              |
| 1:G:148:LEU:HD12 | 1:G:224:VAL:CG2  | 2.36                     | 0.47              |
| 1:J:140:VAL:HG12 | 1:J:141:GLY:N    | 2.30                     | 0.47              |
| 1:A:154:LEU:HB2  | 1:A:188:LEU:HD11 | 1.97                     | 0.47              |
| 2:O:75:GLN:OE1   | 5:O:1008:PHE:N   | 2.48                     | 0.47              |
| 1:C:116:ASP:OD1  | 1:C:151:LYS:HD2  | 2.15                     | 0.47              |
| 1:D:112:ILE:HG21 | 1:D:152:GLN:NE2  | 2.30                     | 0.47              |
| 1:H:112:ILE:HG21 | 1:H:152:GLN:NE2  | 2.31                     | 0.46              |
| 2:L:18:MET:HE1   | 2:L:46:GLU:CG    | 2.44                     | 0.46              |
| 1:A:188:LEU:O    | 1:A:189:GLN:C    | 2.54                     | 0.46              |
| 1:J:154:LEU:HB2  | 1:J:188:LEU:HD11 | 1.97                     | 0.46              |
| 2:M:73:VAL:O     | 2:M:73:VAL:HG13  | 2.15                     | 0.46              |
| 1:F:90:ALA:O     | 1:F:94:GLN:HG3   | 2.15                     | 0.46              |
| 1:I:112:ILE:HG21 | 1:I:152:GLN:NE2  | 2.30                     | 0.46              |
| 1:G:154:LEU:HB2  | 1:G:188:LEU:HD11 | 1.97                     | 0.46              |
| 5:S:1004:PHE:HB3 | 2:T:73:VAL:O     | 2.15                     | 0.46              |
| 1:C:154:LEU:HB2  | 1:C:188:LEU:HD11 | 1.96                     | 0.46              |
| 1:F:112:ILE:HG21 | 1:F:152:GLN:NE2  | 2.30                     | 0.46              |
| 1:I:145:ILE:HD13 | 1:I:184:ILE:HD11 | 1.97                     | 0.46              |
| 1:C:142:ARG:HH11 | 1:C:142:ARG:HG2  | 1.80                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:65:PHE:CE2   | 2:N:83:LYS:HB2   | 2.51                     | 0.46              |
| 1:B:59:LEU:CB    | 1:B:60:PRO:HD3   | 2.35                     | 0.46              |
| 1:I:158:LYS:HD2  | 1:I:158:LYS:N    | 2.31                     | 0.46              |
| 1:J:205:VAL:HA   | 1:J:211:LYS:HB3  | 1.97                     | 0.46              |
| 1:F:137:VAL:HB   | 1:F:203:CYS:HB3  | 1.98                     | 0.46              |
| 1:C:90:ALA:O     | 1:C:94:GLN:HG3   | 2.16                     | 0.46              |
| 1:J:236:LEU:O    | 1:J:240:ARG:HB2  | 2.15                     | 0.46              |
| 1:G:116:ASP:OD1  | 1:G:151:LYS:HD2  | 2.15                     | 0.46              |
| 1:G:226:ARG:HD3  | 6:G:3112:HOH:O   | 2.14                     | 0.46              |
| 1:J:110:ASP:CB   | 1:J:158:LYS:HE3  | 2.46                     | 0.46              |
| 1:E:207:ARG:NH2  | 1:F:92:ALA:HA    | 2.31                     | 0.46              |
| 1:G:236:LEU:O    | 1:G:240:ARG:HB2  | 2.15                     | 0.46              |
| 1:A:161:ARG:O    | 1:A:165:ILE:HG13 | 2.16                     | 0.46              |
| 1:J:107:VAL:HG12 | 1:J:158:LYS:HG3  | 1.98                     | 0.46              |
| 1:C:113:PHE:HZ   | 6:I:3106:HOH:O   | 1.99                     | 0.46              |
| 2:R:18:MET:CE    | 2:R:46:GLU:HB2   | 2.45                     | 0.46              |
| 1:H:142:ARG:HH11 | 1:H:142:ARG:HG2  | 1.80                     | 0.46              |
| 1:B:212:MET:CE   | 1:I:140:VAL:HG11 | 2.46                     | 0.45              |
| 1:G:52:GLU:O     | 1:G:56:GLU:HG3   | 2.16                     | 0.45              |
| 1:A:232:ARG:HD3  | 1:B:234:GLU:OE2  | 2.16                     | 0.45              |
| 2:L:18:MET:CE    | 2:L:46:GLU:HB2   | 2.46                     | 0.45              |
| 1:D:239:ILE:HG13 | 1:D:240:ARG:N    | 2.31                     | 0.45              |
| 2:R:18:MET:HE1   | 2:R:46:GLU:HG3   | 1.98                     | 0.45              |
| 1:F:154:LEU:HB2  | 1:F:188:LEU:HD11 | 1.98                     | 0.45              |
| 1:E:239:ILE:HG13 | 1:E:240:ARG:N    | 2.32                     | 0.45              |
| 1:J:174:GLU:H    | 1:J:174:GLU:CD   | 2.18                     | 0.45              |
| 1:B:205:VAL:HA   | 1:B:211:LYS:HB3  | 1.98                     | 0.45              |
| 2:L:25:ASP:O     | 2:L:29:MET:HG2   | 2.16                     | 0.45              |
| 1:J:148:LEU:HD12 | 1:J:224:VAL:CG2  | 2.36                     | 0.45              |
| 1:A:137:VAL:HB   | 1:A:203:CYS:HB3  | 1.97                     | 0.45              |
| 1:I:189:GLN:N    | 1:I:190:PRO:HD3  | 2.32                     | 0.45              |
| 1:A:150:ASN:HD22 | 1:A:150:ASN:HA   | 1.62                     | 0.45              |
| 1:C:221:MET:O    | 1:C:226:ARG:HB2  | 2.17                     | 0.45              |
| 1:E:92:ALA:HA    | 1:F:207:ARG:NH2  | 2.32                     | 0.45              |
| 1:D:189:GLN:N    | 1:D:190:PRO:HD3  | 2.31                     | 0.45              |
| 1:G:71:ARG:HG2   | 1:G:71:ARG:HH11  | 1.81                     | 0.45              |
| 1:E:148:LEU:HD12 | 1:E:224:VAL:CG2  | 2.38                     | 0.45              |
| 1:F:205:VAL:HA   | 1:F:211:LYS:CB   | 2.47                     | 0.45              |
| 2:O:25:ASP:O     | 2:O:29:MET:HG2   | 2.16                     | 0.45              |
| 2:S:73:VAL:O     | 2:S:73:VAL:HG13  | 2.16                     | 0.45              |
| 1:B:148:LEU:CD1  | 1:B:224:VAL:HG21 | 2.36                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:213:ASN:ND2  | 1:B:213:ASN:N    | 2.49                     | 0.45              |
| 1:A:110:ASP:HB2  | 1:A:158:LYS:HE3  | 1.98                     | 0.45              |
| 1:J:205:VAL:HA   | 1:J:211:LYS:CB   | 2.46                     | 0.45              |
| 2:S:25:ASP:O     | 2:S:29:MET:HG2   | 2.17                     | 0.45              |
| 2:P:65:PHE:CE2   | 2:P:83:LYS:HB2   | 2.52                     | 0.45              |
| 2:K:60:LEU:HD23  | 2:K:81:LEU:HD22  | 1.99                     | 0.45              |
| 1:H:52:GLU:O     | 1:H:56:GLU:HG3   | 2.16                     | 0.45              |
| 1:I:137:VAL:HB   | 1:I:203:CYS:HB3  | 1.98                     | 0.45              |
| 1:B:232:ARG:HD3  | 1:C:234:GLU:OE2  | 2.16                     | 0.45              |
| 1:D:140:VAL:HG12 | 1:D:141:GLY:N    | 2.32                     | 0.45              |
| 2:S:54:ARG:NH1   | 2:T:21:ASP:OD2   | 2.50                     | 0.45              |
| 2:Q:73:VAL:HG13  | 2:Q:73:VAL:O     | 2.16                     | 0.45              |
| 1:I:110:ASP:HB2  | 1:I:158:LYS:HE3  | 1.99                     | 0.45              |
| 1:E:150:ASN:HA   | 1:E:150:ASN:HD22 | 1.62                     | 0.45              |
| 2:N:83:LYS:HG2   | 2:N:84:GLU:N     | 2.32                     | 0.45              |
| 1:G:110:ASP:CB   | 1:G:158:LYS:HE3  | 2.47                     | 0.44              |
| 1:E:164:GLU:OE2  | 1:E:168:ARG:HD2  | 2.17                     | 0.44              |
| 1:E:62:LEU:HD21  | 1:F:72:SER:HB2   | 1.99                     | 0.44              |
| 1:I:142:ARG:HH11 | 1:I:142:ARG:HG2  | 1.81                     | 0.44              |
| 1:C:230:LYS:HE2  | 1:C:230:LYS:HA   | 1.99                     | 0.44              |
| 2:R:73:VAL:O     | 2:R:73:VAL:HG13  | 2.17                     | 0.44              |
| 1:H:71:ARG:HG3   | 1:H:77:PRO:HG2   | 1.99                     | 0.44              |
| 1:G:230:LYS:HD2  | 6:Q:2031:HOH:O   | 2.17                     | 0.44              |
| 1:C:110:ASP:CB   | 1:C:158:LYS:HE3  | 2.47                     | 0.44              |
| 1:J:239:ILE:HG13 | 1:J:240:ARG:N    | 2.32                     | 0.44              |
| 1:C:140:VAL:HG12 | 1:C:141:GLY:N    | 2.32                     | 0.44              |
| 1:I:174:GLU:CD   | 1:I:174:GLU:H    | 2.21                     | 0.44              |
| 1:G:148:LEU:CD1  | 1:G:224:VAL:HG21 | 2.39                     | 0.44              |
| 1:H:107:VAL:HG22 | 1:H:161:ARG:CD   | 2.46                     | 0.44              |
| 6:Q:2008:HOH:O   | 2:R:1:MET:HB3    | 2.18                     | 0.44              |
| 1:I:189:GLN:N    | 1:I:190:PRO:CD   | 2.81                     | 0.44              |
| 2:M:60:LEU:HD23  | 2:M:81:LEU:HD22  | 1.99                     | 0.44              |
| 1:F:88:ARG:HD3   | 6:F:3119:HOH:O   | 2.18                     | 0.44              |
| 1:H:213:ASN:ND2  | 1:H:213:ASN:N    | 2.53                     | 0.44              |
| 1:C:137:VAL:HB   | 1:C:203:CYS:HB3  | 1.99                     | 0.44              |
| 2:L:38:ARG:NE    | 6:L:2012:HOH:O   | 2.46                     | 0.44              |
| 1:H:58:ASN:HA    | 1:H:61:ASN:HD22  | 1.83                     | 0.44              |
| 2:R:14:VAL:HG22  | 2:R:15:GLY:N     | 2.33                     | 0.44              |
| 2:R:25:ASP:O     | 2:R:29:MET:HG2   | 2.17                     | 0.44              |
| 1:D:189:GLN:N    | 1:D:190:PRO:CD   | 2.80                     | 0.44              |
| 1:B:140:VAL:HG11 | 1:I:212:MET:CE   | 2.48                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:52:GLU:O     | 1:E:56:GLU:HG3   | 2.18                     | 0.44              |
| 1:D:124:LYS:NZ   | 1:D:241:SER:OG   | 2.38                     | 0.44              |
| 2:T:43:ASN:N     | 2:T:43:ASN:ND2   | 2.61                     | 0.44              |
| 1:I:50:ARG:HB3   | 1:I:101:GLN:HB3  | 1.99                     | 0.44              |
| 1:E:113:PHE:CD1  | 1:E:113:PHE:N    | 2.86                     | 0.44              |
| 2:R:72:GLY:HA3   | 2:S:73:VAL:HB    | 2.00                     | 0.44              |
| 1:A:72:SER:HB2   | 1:J:62:LEU:HD21  | 1.99                     | 0.44              |
| 1:H:148:LEU:HD12 | 1:H:224:VAL:CG2  | 2.41                     | 0.44              |
| 1:J:137:VAL:HB   | 1:J:203:CYS:HB3  | 2.00                     | 0.44              |
| 1:A:107:VAL:CG1  | 1:A:158:LYS:HG3  | 2.48                     | 0.44              |
| 1:H:239:ILE:HG13 | 1:H:240:ARG:N    | 2.32                     | 0.44              |
| 1:B:213:ASN:HD22 | 1:B:214:SER:H    | 1.65                     | 0.44              |
| 1:D:150:ASN:O    | 1:D:151:LYS:HB2  | 2.18                     | 0.44              |
| 2:T:49:VAL:HG13  | 2:T:51:ASP:H     | 1.80                     | 0.44              |
| 1:B:212:MET:HE2  | 1:I:140:VAL:HG11 | 2.00                     | 0.44              |
| 2:K:75:GLN:OE1   | 5:K:1009:PHE:N   | 2.51                     | 0.44              |
| 2:M:73:VAL:O     | 5:M:1010:PHE:HB3 | 2.18                     | 0.43              |
| 1:A:76:ASP:C     | 1:A:78:GLN:H     | 2.21                     | 0.43              |
| 1:A:78:GLN:O     | 1:A:79:ARG:C     | 2.57                     | 0.43              |
| 1:C:71:ARG:HG3   | 1:C:77:PRO:HG2   | 2.00                     | 0.43              |
| 1:J:71:ARG:HG3   | 1:J:77:PRO:HG2   | 2.00                     | 0.43              |
| 1:D:90:ALA:O     | 1:D:94:GLN:HG3   | 2.18                     | 0.43              |
| 1:G:205:VAL:HA   | 1:G:211:LYS:HB3  | 2.00                     | 0.43              |
| 2:P:73:VAL:O     | 2:P:73:VAL:HG13  | 2.18                     | 0.43              |
| 1:I:150:ASN:HA   | 1:I:150:ASN:HD22 | 1.59                     | 0.43              |
| 1:A:113:PHE:CD1  | 1:A:113:PHE:N    | 2.86                     | 0.43              |
| 1:D:198:GLU:HA   | 1:D:216:THR:O    | 2.18                     | 0.43              |
| 1:F:148:LEU:HD12 | 1:F:224:VAL:CG2  | 2.39                     | 0.43              |
| 1:H:148:LEU:HA   | 1:H:148:LEU:HD23 | 1.81                     | 0.43              |
| 1:B:150:ASN:HD22 | 1:B:150:ASN:HA   | 1.60                     | 0.43              |
| 2:N:54:ARG:NH1   | 2:O:21:ASP:OD1   | 2.48                     | 0.43              |
| 1:F:123:VAL:HG12 | 1:F:126:ILE:HD11 | 2.00                     | 0.43              |
| 1:B:148:LEU:HD23 | 1:B:148:LEU:HA   | 1.82                     | 0.43              |
| 1:A:110:ASP:CB   | 1:A:158:LYS:HE3  | 2.47                     | 0.43              |
| 1:B:140:VAL:HG12 | 1:B:141:GLY:N    | 2.34                     | 0.43              |
| 1:F:58:ASN:HA    | 1:F:61:ASN:HD22  | 1.83                     | 0.43              |
| 1:H:180:ILE:O    | 1:H:184:ILE:HG13 | 2.19                     | 0.43              |
| 2:M:83:LYS:HG2   | 2:M:84:GLU:N     | 2.33                     | 0.43              |
| 1:J:230:LYS:HA   | 1:J:230:LYS:HE2  | 2.01                     | 0.43              |
| 1:A:158:LYS:HD3  | 6:A:3114:HOH:O   | 2.17                     | 0.43              |
| 2:O:83:LYS:HG2   | 2:O:84:GLU:N     | 2.34                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:212:MET:HE1  | 1:J:140:VAL:HG11 | 2.00                     | 0.43              |
| 2:T:83:LYS:HG2   | 2:T:84:GLU:N     | 2.34                     | 0.43              |
| 1:H:236:LEU:O    | 1:H:240:ARG:HB2  | 2.17                     | 0.43              |
| 1:C:205:VAL:HA   | 1:C:211:LYS:HB3  | 2.00                     | 0.43              |
| 1:I:58:ASN:HA    | 1:I:61:ASN:HD22  | 1.83                     | 0.43              |
| 6:K:2022:HOH:O   | 2:L:82:HIS:HD2   | 2.02                     | 0.43              |
| 2:K:18:MET:HE1   | 2:K:46:GLU:CG    | 2.49                     | 0.43              |
| 1:J:150:ASN:HA   | 1:J:150:ASN:HD22 | 1.57                     | 0.43              |
| 1:I:116:ASP:OD1  | 1:I:151:LYS:HD2  | 2.19                     | 0.43              |
| 1:J:150:ASN:O    | 1:J:151:LYS:HB2  | 2.18                     | 0.43              |
| 2:R:54:ARG:NH1   | 2:S:21:ASP:OD1   | 2.47                     | 0.43              |
| 1:J:90:ALA:O     | 1:J:94:GLN:HG3   | 2.19                     | 0.43              |
| 1:C:92:ALA:HA    | 1:H:207:ARG:NH2  | 2.34                     | 0.43              |
| 1:D:52:GLU:O     | 1:D:56:GLU:HG3   | 2.19                     | 0.43              |
| 1:E:140:VAL:HG11 | 1:F:212:MET:HE2  | 2.00                     | 0.43              |
| 2:O:73:VAL:O     | 2:O:73:VAL:HG13  | 2.18                     | 0.43              |
| 1:A:107:VAL:HG12 | 1:A:158:LYS:HG3  | 2.00                     | 0.43              |
| 1:A:205:VAL:HA   | 1:A:211:LYS:HB3  | 1.99                     | 0.43              |
| 1:H:140:VAL:HG12 | 1:H:141:GLY:N    | 2.34                     | 0.43              |
| 2:O:32:LEU:HD11  | 2:O:60:LEU:HD11  | 2.01                     | 0.43              |
| 2:M:25:ASP:O     | 2:M:29:MET:HG2   | 2.19                     | 0.43              |
| 1:D:205:VAL:HA   | 1:D:211:LYS:CB   | 2.49                     | 0.43              |
| 2:S:43:ASN:ND2   | 2:S:44:PHE:HD2   | 2.17                     | 0.43              |
| 1:B:110:ASP:HB2  | 1:B:158:LYS:HE3  | 2.01                     | 0.43              |
| 2:O:49:VAL:HG12  | 2:O:51:ASP:H     | 1.82                     | 0.43              |
| 1:E:205:VAL:HA   | 1:E:211:LYS:HB3  | 2.01                     | 0.43              |
| 1:G:175:ARG:O    | 1:G:179:GLN:HG3  | 2.19                     | 0.43              |
| 2:L:83:LYS:HG2   | 2:L:84:GLU:N     | 2.34                     | 0.42              |
| 1:J:70:LEU:HB3   | 1:J:77:PRO:HG3   | 2.01                     | 0.42              |
| 1:B:113:PHE:CD1  | 1:B:113:PHE:N    | 2.87                     | 0.42              |
| 2:P:18:MET:HE1   | 2:P:46:GLU:HG3   | 2.02                     | 0.42              |
| 2:P:83:LYS:HG2   | 2:P:84:GLU:N     | 2.34                     | 0.42              |
| 1:H:205:VAL:HA   | 1:H:211:LYS:HB3  | 2.00                     | 0.42              |
| 1:I:205:VAL:HA   | 1:I:211:LYS:HB3  | 2.00                     | 0.42              |
| 2:N:18:MET:CE    | 2:N:46:GLU:HB2   | 2.49                     | 0.42              |
| 1:G:213:ASN:O    | 1:G:215:LYS:NZ   | 2.52                     | 0.42              |
| 1:E:112:ILE:CG2  | 1:E:152:GLN:HE21 | 2.31                     | 0.42              |
| 1:G:112:ILE:HG21 | 1:G:152:GLN:NE2  | 2.33                     | 0.42              |
| 1:A:140:VAL:HG11 | 1:J:212:MET:HE2  | 2.00                     | 0.42              |
| 1:H:205:VAL:HA   | 1:H:211:LYS:CB   | 2.49                     | 0.42              |
| 1:E:154:LEU:HB2  | 1:E:188:LEU:HD11 | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:110:ASP:HB2  | 1:J:158:LYS:HE3  | 1.99                     | 0.42              |
| 1:E:142:ARG:HG2  | 1:E:142:ARG:NH1  | 2.34                     | 0.42              |
| 1:A:71:ARG:HH11  | 1:A:71:ARG:HG2   | 1.84                     | 0.42              |
| 1:B:150:ASN:O    | 1:B:151:LYS:HB2  | 2.20                     | 0.42              |
| 1:E:212:MET:HE2  | 1:F:140:VAL:HG11 | 2.00                     | 0.42              |
| 2:P:25:ASP:O     | 2:P:29:MET:HG2   | 2.20                     | 0.42              |
| 1:F:148:LEU:HD23 | 1:F:148:LEU:HA   | 1.88                     | 0.42              |
| 1:E:213:ASN:HD22 | 1:E:214:SER:H    | 1.66                     | 0.42              |
| 2:T:18:MET:CE    | 2:T:46:GLU:HB2   | 2.49                     | 0.42              |
| 1:E:150:ASN:O    | 1:E:151:LYS:HB2  | 2.20                     | 0.42              |
| 1:F:150:ASN:O    | 1:F:151:LYS:HB2  | 2.20                     | 0.42              |
| 1:D:205:VAL:HA   | 1:D:211:LYS:HB3  | 2.01                     | 0.42              |
| 2:N:9:GLN:O      | 2:N:11:ARG:N     | 2.48                     | 0.42              |
| 1:H:213:ASN:HD22 | 1:H:214:SER:H    | 1.67                     | 0.42              |
| 1:E:76:ASP:C     | 1:E:78:GLN:H     | 2.23                     | 0.42              |
| 2:O:65:PHE:CD2   | 2:O:83:LYS:HB2   | 2.55                     | 0.42              |
| 2:K:83:LYS:HG2   | 2:K:84:GLU:N     | 2.35                     | 0.42              |
| 1:J:189:GLN:N    | 1:J:190:PRO:CD   | 2.82                     | 0.42              |
| 1:H:232:ARG:HD3  | 1:I:234:GLU:OE2  | 2.19                     | 0.42              |
| 1:C:236:LEU:O    | 1:C:240:ARG:HB2  | 2.20                     | 0.42              |
| 1:B:207:ARG:NH2  | 1:I:92:ALA:HA    | 2.34                     | 0.42              |
| 1:H:111:ALA:HB3  | 1:H:158:LYS:CD   | 2.46                     | 0.42              |
| 1:G:98:LYS:HE3   | 1:G:168:ARG:HD3  | 2.02                     | 0.42              |
| 2:R:65:PHE:CD2   | 2:R:83:LYS:HB2   | 2.55                     | 0.42              |
| 1:C:232:ARG:HD3  | 1:D:234:GLU:OE2  | 2.19                     | 0.42              |
| 1:F:161:ARG:O    | 1:F:165:ILE:HG13 | 2.19                     | 0.42              |
| 1:A:205:VAL:C    | 1:A:207:ARG:H    | 2.24                     | 0.42              |
| 2:L:73:VAL:O     | 2:L:73:VAL:HG13  | 2.20                     | 0.42              |
| 2:M:65:PHE:CE2   | 2:M:83:LYS:HB2   | 2.54                     | 0.42              |
| 1:F:113:PHE:CD1  | 1:F:113:PHE:N    | 2.88                     | 0.42              |
| 1:H:164:GLU:O    | 1:H:168:ARG:HG3  | 2.20                     | 0.42              |
| 1:H:113:PHE:N    | 1:H:113:PHE:CD1  | 2.87                     | 0.42              |
| 1:D:148:LEU:HA   | 1:D:148:LEU:HD23 | 1.83                     | 0.41              |
| 1:G:164:GLU:O    | 1:G:168:ARG:HG3  | 2.20                     | 0.41              |
| 1:E:50:ARG:O     | 1:E:101:GLN:CB   | 2.68                     | 0.41              |
| 1:J:188:LEU:O    | 1:J:189:GLN:C    | 2.58                     | 0.41              |
| 1:G:150:ASN:O    | 1:G:151:LYS:HB2  | 2.20                     | 0.41              |
| 2:N:25:ASP:O     | 2:N:29:MET:HG2   | 2.20                     | 0.41              |
| 1:G:63:ALA:O     | 1:G:86:PRO:HB3   | 2.19                     | 0.41              |
| 1:J:198:GLU:HA   | 1:J:216:THR:O    | 2.20                     | 0.41              |
| 1:D:174:GLU:H    | 1:D:174:GLU:CD   | 2.23                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:110:ASP:CB   | 1:H:158:LYS:HE3  | 2.50                     | 0.41              |
| 1:B:110:ASP:CB   | 1:B:158:LYS:HE3  | 2.50                     | 0.41              |
| 1:I:205:VAL:HA   | 1:I:211:LYS:CB   | 2.50                     | 0.41              |
| 1:B:90:ALA:O     | 1:B:94:GLN:HG3   | 2.20                     | 0.41              |
| 1:B:71:ARG:HG3   | 1:B:77:PRO:HG2   | 2.02                     | 0.41              |
| 1:B:59:LEU:HB3   | 1:B:60:PRO:CD    | 2.36                     | 0.41              |
| 2:R:83:LYS:HG2   | 2:R:84:GLU:N     | 2.36                     | 0.41              |
| 2:S:18:MET:HE1   | 2:S:46:GLU:CG    | 2.50                     | 0.41              |
| 1:E:145:ILE:HD13 | 1:E:184:ILE:HD11 | 2.01                     | 0.41              |
| 1:D:113:PHE:CD1  | 1:D:113:PHE:N    | 2.88                     | 0.41              |
| 2:K:21:ASP:OD1   | 2:O:54:ARG:NH1   | 2.50                     | 0.41              |
| 2:S:83:LYS:HG2   | 2:S:84:GLU:N     | 2.34                     | 0.41              |
| 2:M:32:LEU:HD11  | 2:M:60:LEU:HD11  | 2.02                     | 0.41              |
| 1:B:145:ILE:HD13 | 1:B:184:ILE:HD11 | 2.01                     | 0.41              |
| 1:F:189:GLN:N    | 1:F:190:PRO:HD3  | 2.34                     | 0.41              |
| 1:G:135:HIS:O    | 1:G:136:LEU:HB2  | 2.20                     | 0.41              |
| 1:H:110:ASP:HB2  | 1:H:158:LYS:HE3  | 2.01                     | 0.41              |
| 1:I:107:VAL:CG1  | 1:I:158:LYS:HG3  | 2.51                     | 0.41              |
| 1:J:107:VAL:CG1  | 1:J:158:LYS:HG3  | 2.50                     | 0.41              |
| 1:J:205:VAL:C    | 1:J:207:ARG:H    | 2.24                     | 0.41              |
| 1:G:188:LEU:O    | 1:G:189:GLN:C    | 2.58                     | 0.41              |
| 1:B:140:VAL:HG11 | 1:I:212:MET:HE1  | 2.03                     | 0.41              |
| 5:K:1009:PHE:HB3 | 2:L:73:VAL:O     | 2.20                     | 0.41              |
| 1:A:174:GLU:CD   | 1:A:174:GLU:H    | 2.23                     | 0.41              |
| 1:I:65:ALA:O     | 1:I:69:ILE:HG13  | 2.20                     | 0.41              |
| 1:F:213:ASN:HD22 | 1:F:214:SER:N    | 2.19                     | 0.41              |
| 2:S:6:ILE:HA     | 2:S:18:MET:O     | 2.20                     | 0.41              |
| 2:O:60:LEU:HD23  | 2:O:81:LEU:HD22  | 2.03                     | 0.41              |
| 1:B:206:MET:O    | 1:B:207:ARG:HG3  | 2.21                     | 0.41              |
| 1:A:239:ILE:HG13 | 1:A:240:ARG:N    | 2.35                     | 0.41              |
| 1:D:111:ALA:HB3  | 1:D:158:LYS:CD   | 2.48                     | 0.41              |
| 1:J:189:GLN:N    | 1:J:190:PRO:HD3  | 2.36                     | 0.41              |
| 2:T:14:VAL:HG22  | 2:T:15:GLY:N     | 2.36                     | 0.41              |
| 1:F:174:GLU:H    | 1:F:174:GLU:CD   | 2.23                     | 0.41              |
| 1:J:113:PHE:N    | 1:J:113:PHE:CD1  | 2.89                     | 0.41              |
| 1:I:71:ARG:HG3   | 1:I:77:PRO:HG2   | 2.03                     | 0.41              |
| 1:D:148:LEU:HD12 | 1:D:224:VAL:CG2  | 2.38                     | 0.41              |
| 1:A:150:ASN:O    | 1:A:151:LYS:HB2  | 2.20                     | 0.41              |
| 1:D:161:ARG:O    | 1:D:165:ILE:HG13 | 2.21                     | 0.41              |
| 1:H:188:LEU:O    | 1:H:189:GLN:C    | 2.59                     | 0.41              |
| 1:G:71:ARG:HG3   | 1:G:77:PRO:HG2   | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:43:ASN:ND2   | 2:R:44:PHE:HD2   | 2.19                     | 0.41              |
| 1:G:107:VAL:CG1  | 1:G:158:LYS:HG3  | 2.51                     | 0.41              |
| 1:H:98:LYS:HE3   | 1:H:168:ARG:HD3  | 2.02                     | 0.41              |
| 2:T:49:VAL:HG12  | 2:T:51:ASP:H     | 1.83                     | 0.41              |
| 1:E:205:VAL:C    | 1:E:207:ARG:H    | 2.24                     | 0.41              |
| 1:D:174:GLU:HB3  | 1:E:117:HIS:CE1  | 2.56                     | 0.41              |
| 2:M:14:VAL:HG22  | 2:M:15:GLY:N     | 2.36                     | 0.41              |
| 1:A:93:MET:HG3   | 1:J:73:LEU:HD21  | 2.03                     | 0.41              |
| 1:F:52:GLU:O     | 1:F:56:GLU:HG3   | 2.21                     | 0.41              |
| 1:E:238:LEU:HA   | 1:E:238:LEU:HD12 | 1.92                     | 0.41              |
| 1:J:213:ASN:HD22 | 1:J:214:SER:H    | 1.69                     | 0.41              |
| 1:G:205:VAL:HA   | 1:G:211:LYS:CB   | 2.51                     | 0.41              |
| 2:Q:60:LEU:HA    | 2:Q:60:LEU:HD12  | 1.88                     | 0.41              |
| 1:G:113:PHE:CD1  | 1:G:113:PHE:N    | 2.89                     | 0.41              |
| 2:N:60:LEU:HD23  | 2:N:81:LEU:HD22  | 2.03                     | 0.41              |
| 1:C:62:LEU:HD21  | 1:H:72:SER:HB2   | 2.03                     | 0.41              |
| 1:E:148:LEU:HA   | 1:E:148:LEU:HD23 | 1.90                     | 0.40              |
| 2:M:43:ASN:ND2   | 2:M:44:PHE:HD2   | 2.18                     | 0.40              |
| 1:C:213:ASN:HD22 | 1:C:214:SER:H    | 1.67                     | 0.40              |
| 1:C:207:ARG:HH22 | 1:H:92:ALA:HA    | 1.85                     | 0.40              |
| 1:A:140:VAL:HG11 | 1:J:212:MET:HE1  | 2.03                     | 0.40              |
| 1:I:236:LEU:O    | 1:I:240:ARG:HB2  | 2.21                     | 0.40              |
| 1:F:71:ARG:HG2   | 1:F:71:ARG:HH11  | 1.86                     | 0.40              |
| 2:N:18:MET:HE1   | 2:N:46:GLU:HG3   | 2.04                     | 0.40              |
| 1:I:113:PHE:N    | 1:I:113:PHE:CD1  | 2.89                     | 0.40              |
| 1:E:230:LYS:HA   | 1:E:230:LYS:HE2  | 2.02                     | 0.40              |
| 1:A:72:SER:HB2   | 1:J:62:LEU:CD2   | 2.51                     | 0.40              |
| 1:H:205:VAL:C    | 1:H:207:ARG:H    | 2.25                     | 0.40              |
| 1:I:238:LEU:HA   | 1:I:238:LEU:HD12 | 1.90                     | 0.40              |
| 1:G:228:ASP:HA   | 1:G:229:PRO:HD2  | 1.98                     | 0.40              |
| 2:N:43:ASN:ND2   | 2:N:44:PHE:HD2   | 2.19                     | 0.40              |
| 1:G:189:GLN:N    | 1:G:190:PRO:HD3  | 2.36                     | 0.40              |
| 1:G:238:LEU:HD12 | 1:G:238:LEU:HA   | 1.90                     | 0.40              |
| 2:O:13:GLU:CD    | 2:O:13:GLU:H     | 2.24                     | 0.40              |
| 1:H:150:ASN:O    | 1:H:151:LYS:HB2  | 2.21                     | 0.40              |
| 2:T:73:VAL:O     | 2:T:73:VAL:HG13  | 2.22                     | 0.40              |
| 1:D:175:ARG:O    | 1:D:179:GLN:HG3  | 2.22                     | 0.40              |
| 1:F:53:GLU:O     | 1:F:57:LEU:HG    | 2.20                     | 0.40              |
| 2:O:14:VAL:HG22  | 2:O:15:GLY:N     | 2.37                     | 0.40              |
| 1:J:238:LEU:HD12 | 1:J:238:LEU:HA   | 1.89                     | 0.40              |
| 1:G:107:VAL:HG12 | 1:G:158:LYS:HG3  | 2.02                     | 0.40              |

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| Atom-1        | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|-----------------|--------------------------|-------------------|
| 1:C:113:PHE:N | 1:C:113:PHE:CD1 | 2.89                     | 0.40              |
| 2:P:13:GLU:CD | 2:P:13:GLU:H    | 2.25                     | 0.40              |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1        | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|-----------------------|--------------------------|-------------------|
| 2:Q:45:TYR:OH | 2:S:30:GLN:NE2[2_645] | 2.07                     | 0.13              |

## 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     | 188/230 (82%) | 177 (94%) | 9 (5%)  | 2 (1%)   | 17          | 42  |
| 1   | B     | 188/230 (82%) | 178 (95%) | 8 (4%)  | 2 (1%)   | 17          | 42  |
| 1   | C     | 188/230 (82%) | 177 (94%) | 9 (5%)  | 2 (1%)   | 17          | 42  |
| 1   | D     | 188/230 (82%) | 177 (94%) | 9 (5%)  | 2 (1%)   | 17          | 42  |
| 1   | E     | 188/230 (82%) | 177 (94%) | 9 (5%)  | 2 (1%)   | 17          | 42  |
| 1   | F     | 188/230 (82%) | 177 (94%) | 9 (5%)  | 2 (1%)   | 17          | 42  |
| 1   | G     | 188/230 (82%) | 179 (95%) | 7 (4%)  | 2 (1%)   | 17          | 42  |
| 1   | H     | 188/230 (82%) | 177 (94%) | 9 (5%)  | 2 (1%)   | 17          | 42  |
| 1   | I     | 188/230 (82%) | 178 (95%) | 8 (4%)  | 2 (1%)   | 17          | 42  |
| 1   | J     | 188/230 (82%) | 177 (94%) | 9 (5%)  | 2 (1%)   | 17          | 42  |
| 2   | K     | 82/84 (98%)   | 78 (95%)  | 4 (5%)  | 0        | 100         | 100 |
| 2   | L     | 82/84 (98%)   | 79 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 2   | M     | 82/84 (98%)   | 79 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 2   | N     | 82/84 (98%)   | 78 (95%)  | 4 (5%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 2   | O     | 82/84 (98%)     | 79 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 2   | P     | 82/84 (98%)     | 78 (95%)   | 4 (5%)   | 0        | 100         | 100 |
| 2   | Q     | 82/84 (98%)     | 79 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 2   | R     | 82/84 (98%)     | 79 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 2   | S     | 82/84 (98%)     | 79 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 2   | T     | 82/84 (98%)     | 78 (95%)   | 4 (5%)   | 0        | 100         | 100 |
| All | All   | 2700/3140 (86%) | 2560 (95%) | 120 (4%) | 20 (1%)  | 26          | 55  |

All (20) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 110 | ASP  |
| 1   | B     | 108 | LEU  |
| 1   | B     | 110 | ASP  |
| 1   | C     | 110 | ASP  |
| 1   | D     | 110 | ASP  |
| 1   | E     | 110 | ASP  |
| 1   | F     | 110 | ASP  |
| 1   | G     | 108 | LEU  |
| 1   | G     | 110 | ASP  |
| 1   | H     | 110 | ASP  |
| 1   | I     | 110 | ASP  |
| 1   | J     | 110 | ASP  |
| 1   | A     | 108 | LEU  |
| 1   | C     | 108 | LEU  |
| 1   | D     | 108 | LEU  |
| 1   | E     | 108 | LEU  |
| 1   | F     | 108 | LEU  |
| 1   | H     | 108 | LEU  |
| 1   | I     | 108 | LEU  |
| 1   | J     | 108 | LEU  |

### 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     | 169/196 (86%)   | 157 (93%)  | 12 (7%)  | 18          | 41 |
| 1   | B     | 169/196 (86%)   | 156 (92%)  | 13 (8%)  | 16          | 36 |
| 1   | C     | 169/196 (86%)   | 158 (94%)  | 11 (6%)  | 21          | 46 |
| 1   | D     | 169/196 (86%)   | 158 (94%)  | 11 (6%)  | 21          | 46 |
| 1   | E     | 169/196 (86%)   | 157 (93%)  | 12 (7%)  | 18          | 41 |
| 1   | F     | 169/196 (86%)   | 158 (94%)  | 11 (6%)  | 21          | 46 |
| 1   | G     | 169/196 (86%)   | 158 (94%)  | 11 (6%)  | 21          | 46 |
| 1   | H     | 169/196 (86%)   | 158 (94%)  | 11 (6%)  | 21          | 46 |
| 1   | I     | 169/196 (86%)   | 158 (94%)  | 11 (6%)  | 21          | 46 |
| 1   | J     | 169/196 (86%)   | 157 (93%)  | 12 (7%)  | 18          | 41 |
| 2   | K     | 76/76 (100%)    | 71 (93%)   | 5 (7%)   | 21          | 45 |
| 2   | L     | 76/76 (100%)    | 71 (93%)   | 5 (7%)   | 21          | 45 |
| 2   | M     | 76/76 (100%)    | 71 (93%)   | 5 (7%)   | 21          | 45 |
| 2   | N     | 76/76 (100%)    | 71 (93%)   | 5 (7%)   | 21          | 45 |
| 2   | O     | 76/76 (100%)    | 71 (93%)   | 5 (7%)   | 21          | 45 |
| 2   | P     | 76/76 (100%)    | 71 (93%)   | 5 (7%)   | 21          | 45 |
| 2   | Q     | 76/76 (100%)    | 71 (93%)   | 5 (7%)   | 21          | 45 |
| 2   | R     | 76/76 (100%)    | 71 (93%)   | 5 (7%)   | 21          | 45 |
| 2   | S     | 76/76 (100%)    | 71 (93%)   | 5 (7%)   | 21          | 45 |
| 2   | T     | 76/76 (100%)    | 72 (95%)   | 4 (5%)   | 28          | 57 |
| All | All   | 2450/2720 (90%) | 2286 (93%) | 164 (7%) | 20          | 44 |

All (164) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 70  | LEU  |
| 1   | A     | 82  | LEU  |
| 1   | A     | 84  | LYS  |
| 1   | A     | 115 | GLU  |
| 1   | A     | 128 | MET  |
| 1   | A     | 150 | ASN  |
| 1   | A     | 154 | LEU  |
| 1   | A     | 168 | ARG  |
| 1   | A     | 193 | VAL  |
| 1   | A     | 202 | MET  |
| 1   | A     | 213 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 238 | LEU  |
| 1   | B     | 60  | PRO  |
| 1   | B     | 70  | LEU  |
| 1   | B     | 82  | LEU  |
| 1   | B     | 84  | LYS  |
| 1   | B     | 115 | GLU  |
| 1   | B     | 128 | MET  |
| 1   | B     | 150 | ASN  |
| 1   | B     | 154 | LEU  |
| 1   | B     | 168 | ARG  |
| 1   | B     | 193 | VAL  |
| 1   | B     | 202 | MET  |
| 1   | B     | 213 | ASN  |
| 1   | B     | 238 | LEU  |
| 1   | C     | 70  | LEU  |
| 1   | C     | 82  | LEU  |
| 1   | C     | 84  | LYS  |
| 1   | C     | 115 | GLU  |
| 1   | C     | 128 | MET  |
| 1   | C     | 150 | ASN  |
| 1   | C     | 154 | LEU  |
| 1   | C     | 193 | VAL  |
| 1   | C     | 202 | MET  |
| 1   | C     | 213 | ASN  |
| 1   | C     | 238 | LEU  |
| 1   | D     | 70  | LEU  |
| 1   | D     | 82  | LEU  |
| 1   | D     | 84  | LYS  |
| 1   | D     | 115 | GLU  |
| 1   | D     | 128 | MET  |
| 1   | D     | 150 | ASN  |
| 1   | D     | 154 | LEU  |
| 1   | D     | 193 | VAL  |
| 1   | D     | 202 | MET  |
| 1   | D     | 213 | ASN  |
| 1   | D     | 238 | LEU  |
| 1   | E     | 70  | LEU  |
| 1   | E     | 82  | LEU  |
| 1   | E     | 84  | LYS  |
| 1   | E     | 115 | GLU  |
| 1   | E     | 128 | MET  |
| 1   | E     | 150 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 154 | LEU  |
| 1   | E     | 168 | ARG  |
| 1   | E     | 193 | VAL  |
| 1   | E     | 202 | MET  |
| 1   | E     | 213 | ASN  |
| 1   | E     | 238 | LEU  |
| 1   | F     | 70  | LEU  |
| 1   | F     | 82  | LEU  |
| 1   | F     | 84  | LYS  |
| 1   | F     | 115 | GLU  |
| 1   | F     | 128 | MET  |
| 1   | F     | 150 | ASN  |
| 1   | F     | 154 | LEU  |
| 1   | F     | 193 | VAL  |
| 1   | F     | 202 | MET  |
| 1   | F     | 213 | ASN  |
| 1   | F     | 238 | LEU  |
| 1   | G     | 70  | LEU  |
| 1   | G     | 82  | LEU  |
| 1   | G     | 84  | LYS  |
| 1   | G     | 115 | GLU  |
| 1   | G     | 128 | MET  |
| 1   | G     | 150 | ASN  |
| 1   | G     | 154 | LEU  |
| 1   | G     | 193 | VAL  |
| 1   | G     | 202 | MET  |
| 1   | G     | 213 | ASN  |
| 1   | G     | 238 | LEU  |
| 1   | H     | 70  | LEU  |
| 1   | H     | 82  | LEU  |
| 1   | H     | 84  | LYS  |
| 1   | H     | 115 | GLU  |
| 1   | H     | 128 | MET  |
| 1   | H     | 150 | ASN  |
| 1   | H     | 154 | LEU  |
| 1   | H     | 193 | VAL  |
| 1   | H     | 202 | MET  |
| 1   | H     | 213 | ASN  |
| 1   | H     | 238 | LEU  |
| 1   | I     | 70  | LEU  |
| 1   | I     | 82  | LEU  |
| 1   | I     | 84  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 115 | GLU  |
| 1   | I     | 128 | MET  |
| 1   | I     | 150 | ASN  |
| 1   | I     | 154 | LEU  |
| 1   | I     | 193 | VAL  |
| 1   | I     | 202 | MET  |
| 1   | I     | 213 | ASN  |
| 1   | I     | 238 | LEU  |
| 1   | J     | 70  | LEU  |
| 1   | J     | 82  | LEU  |
| 1   | J     | 84  | LYS  |
| 1   | J     | 115 | GLU  |
| 1   | J     | 128 | MET  |
| 1   | J     | 150 | ASN  |
| 1   | J     | 154 | LEU  |
| 1   | J     | 168 | ARG  |
| 1   | J     | 193 | VAL  |
| 1   | J     | 202 | MET  |
| 1   | J     | 213 | ASN  |
| 1   | J     | 238 | LEU  |
| 2   | K     | 40  | LEU  |
| 2   | K     | 43  | ASN  |
| 2   | K     | 49  | VAL  |
| 2   | K     | 60  | LEU  |
| 2   | K     | 84  | GLU  |
| 2   | L     | 40  | LEU  |
| 2   | L     | 43  | ASN  |
| 2   | L     | 49  | VAL  |
| 2   | L     | 60  | LEU  |
| 2   | L     | 84  | GLU  |
| 2   | M     | 40  | LEU  |
| 2   | M     | 43  | ASN  |
| 2   | M     | 49  | VAL  |
| 2   | M     | 60  | LEU  |
| 2   | M     | 84  | GLU  |
| 2   | N     | 40  | LEU  |
| 2   | N     | 43  | ASN  |
| 2   | N     | 49  | VAL  |
| 2   | N     | 60  | LEU  |
| 2   | N     | 84  | GLU  |
| 2   | O     | 40  | LEU  |
| 2   | O     | 43  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | O     | 49  | VAL  |
| 2   | O     | 60  | LEU  |
| 2   | O     | 84  | GLU  |
| 2   | P     | 40  | LEU  |
| 2   | P     | 43  | ASN  |
| 2   | P     | 49  | VAL  |
| 2   | P     | 60  | LEU  |
| 2   | P     | 84  | GLU  |
| 2   | Q     | 40  | LEU  |
| 2   | Q     | 43  | ASN  |
| 2   | Q     | 49  | VAL  |
| 2   | Q     | 60  | LEU  |
| 2   | Q     | 84  | GLU  |
| 2   | R     | 40  | LEU  |
| 2   | R     | 43  | ASN  |
| 2   | R     | 49  | VAL  |
| 2   | R     | 60  | LEU  |
| 2   | R     | 84  | GLU  |
| 2   | S     | 40  | LEU  |
| 2   | S     | 43  | ASN  |
| 2   | S     | 49  | VAL  |
| 2   | S     | 60  | LEU  |
| 2   | S     | 84  | GLU  |
| 2   | T     | 40  | LEU  |
| 2   | T     | 43  | ASN  |
| 2   | T     | 49  | VAL  |
| 2   | T     | 60  | LEU  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 61  | ASN  |
| 1   | A     | 94  | GLN  |
| 1   | A     | 150 | ASN  |
| 1   | A     | 152 | GLN  |
| 1   | A     | 213 | ASN  |
| 1   | B     | 61  | ASN  |
| 1   | B     | 150 | ASN  |
| 1   | B     | 152 | GLN  |
| 1   | B     | 201 | HIS  |
| 1   | B     | 213 | ASN  |
| 1   | C     | 61  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 94  | GLN  |
| 1   | C     | 150 | ASN  |
| 1   | C     | 152 | GLN  |
| 1   | C     | 213 | ASN  |
| 1   | D     | 61  | ASN  |
| 1   | D     | 94  | GLN  |
| 1   | D     | 150 | ASN  |
| 1   | D     | 152 | GLN  |
| 1   | D     | 201 | HIS  |
| 1   | D     | 213 | ASN  |
| 1   | E     | 61  | ASN  |
| 1   | E     | 94  | GLN  |
| 1   | E     | 150 | ASN  |
| 1   | E     | 152 | GLN  |
| 1   | E     | 213 | ASN  |
| 1   | F     | 61  | ASN  |
| 1   | F     | 94  | GLN  |
| 1   | F     | 150 | ASN  |
| 1   | F     | 152 | GLN  |
| 1   | F     | 201 | HIS  |
| 1   | F     | 213 | ASN  |
| 1   | G     | 61  | ASN  |
| 1   | G     | 94  | GLN  |
| 1   | G     | 150 | ASN  |
| 1   | G     | 152 | GLN  |
| 1   | G     | 201 | HIS  |
| 1   | G     | 213 | ASN  |
| 1   | H     | 61  | ASN  |
| 1   | H     | 150 | ASN  |
| 1   | H     | 152 | GLN  |
| 1   | H     | 201 | HIS  |
| 1   | H     | 213 | ASN  |
| 1   | I     | 61  | ASN  |
| 1   | I     | 150 | ASN  |
| 1   | I     | 152 | GLN  |
| 1   | I     | 201 | HIS  |
| 1   | I     | 213 | ASN  |
| 1   | J     | 61  | ASN  |
| 1   | J     | 94  | GLN  |
| 1   | J     | 150 | ASN  |
| 1   | J     | 152 | GLN  |
| 1   | J     | 201 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 213 | ASN  |
| 2   | K     | 42  | ASN  |
| 2   | K     | 43  | ASN  |
| 2   | K     | 75  | GLN  |
| 2   | K     | 82  | HIS  |
| 2   | L     | 9   | GLN  |
| 2   | L     | 42  | ASN  |
| 2   | L     | 43  | ASN  |
| 2   | L     | 75  | GLN  |
| 2   | L     | 82  | HIS  |
| 2   | M     | 42  | ASN  |
| 2   | M     | 43  | ASN  |
| 2   | M     | 75  | GLN  |
| 2   | M     | 82  | HIS  |
| 2   | N     | 42  | ASN  |
| 2   | N     | 43  | ASN  |
| 2   | N     | 75  | GLN  |
| 2   | N     | 82  | HIS  |
| 2   | O     | 42  | ASN  |
| 2   | O     | 43  | ASN  |
| 2   | O     | 75  | GLN  |
| 2   | O     | 82  | HIS  |
| 2   | P     | 42  | ASN  |
| 2   | P     | 43  | ASN  |
| 2   | P     | 75  | GLN  |
| 2   | P     | 82  | HIS  |
| 2   | Q     | 42  | ASN  |
| 2   | Q     | 43  | ASN  |
| 2   | Q     | 75  | GLN  |
| 2   | Q     | 82  | HIS  |
| 2   | R     | 9   | GLN  |
| 2   | R     | 42  | ASN  |
| 2   | R     | 43  | ASN  |
| 2   | R     | 75  | GLN  |
| 2   | R     | 82  | HIS  |
| 2   | S     | 9   | GLN  |
| 2   | S     | 42  | ASN  |
| 2   | S     | 43  | ASN  |
| 2   | S     | 75  | GLN  |
| 2   | S     | 82  | HIS  |
| 2   | T     | 42  | ASN  |
| 2   | T     | 43  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | T     | 75  | GLN  |

### 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](#)

Of 30 ligands modelled in this entry, 20 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 5   | PHE  | K     | 1009 | -    | 9,12,12      | 0.27 | 0           | 9,15,15     | 0.16 | 0           |
| 5   | PHE  | M     | 1010 | -    | 9,12,12      | 0.77 | 0           | 9,15,15     | 0.20 | 0           |
| 5   | PHE  | N     | 1006 | -    | 9,12,12      | 0.47 | 0           | 9,15,15     | 0.23 | 0           |
| 5   | PHE  | N     | 1007 | -    | 9,12,12      | 0.51 | 0           | 9,15,15     | 0.15 | 0           |
| 5   | PHE  | O     | 1008 | -    | 9,12,12      | 0.28 | 0           | 9,15,15     | 0.20 | 0           |
| 5   | PHE  | P     | 1003 | -    | 9,12,12      | 0.46 | 0           | 9,15,15     | 0.29 | 0           |
| 5   | PHE  | Q     | 1001 | -    | 9,12,12      | 0.39 | 0           | 9,15,15     | 0.27 | 0           |
| 5   | PHE  | R     | 1002 | -    | 9,12,12      | 0.71 | 0           | 9,15,15     | 0.37 | 0           |
| 5   | PHE  | S     | 1004 | -    | 9,12,12      | 0.46 | 0           | 9,15,15     | 0.28 | 0           |
| 5   | PHE  | T     | 1005 | -    | 9,12,12      | 0.28 | 0           | 9,15,15     | 0.22 | 0           |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings   |
|-----|------|-------|------|------|---------|----------|---------|
| 5   | PHE  | K     | 1009 | -    | -       | 0/4/8/8  | 0/1/1/1 |
| 5   | PHE  | M     | 1010 | -    | -       | 0/4/8/8  | 0/1/1/1 |
| 5   | PHE  | N     | 1006 | -    | -       | 0/4/8/8  | 0/1/1/1 |
| 5   | PHE  | N     | 1007 | -    | -       | 0/4/8/8  | 0/1/1/1 |
| 5   | PHE  | O     | 1008 | -    | -       | 0/4/8/8  | 0/1/1/1 |
| 5   | PHE  | P     | 1003 | -    | -       | 0/4/8/8  | 0/1/1/1 |
| 5   | PHE  | Q     | 1001 | -    | -       | 0/4/8/8  | 0/1/1/1 |
| 5   | PHE  | R     | 1002 | -    | -       | 0/4/8/8  | 0/1/1/1 |
| 5   | PHE  | S     | 1004 | -    | -       | 0/4/8/8  | 0/1/1/1 |
| 5   | PHE  | T     | 1005 | -    | -       | 0/4/8/8  | 0/1/1/1 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 5   | K     | 1009 | PHE  | 2       | 0            |
| 5   | M     | 1010 | PHE  | 1       | 0            |
| 5   | N     | 1006 | PHE  | 1       | 0            |
| 5   | O     | 1008 | PHE  | 1       | 0            |
| 5   | S     | 1004 | PHE  | 1       | 0            |

## 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     | 192/230 (83%)   | 0.48   | 26 (13%) 4 3   | 18, 38, 89, 107       | 0     |
| 1   | B     | 192/230 (83%)   | 0.12   | 13 (6%) 20 19  | 17, 36, 88, 107       | 0     |
| 1   | C     | 192/230 (83%)   | 0.17   | 16 (8%) 14 11  | 16, 38, 88, 108       | 0     |
| 1   | D     | 192/230 (83%)   | 0.21   | 17 (8%) 12 9   | 18, 39, 89, 108       | 0     |
| 1   | E     | 192/230 (83%)   | 0.19   | 12 (6%) 23 22  | 19, 40, 89, 107       | 0     |
| 1   | F     | 192/230 (83%)   | 0.22   | 13 (6%) 20 19  | 17, 39, 88, 107       | 0     |
| 1   | G     | 192/230 (83%)   | 0.31   | 22 (11%) 6 5   | 16, 39, 88, 108       | 0     |
| 1   | H     | 192/230 (83%)   | 0.15   | 12 (6%) 23 22  | 15, 38, 89, 107       | 0     |
| 1   | I     | 192/230 (83%)   | 0.16   | 12 (6%) 23 22  | 15, 35, 88, 107       | 0     |
| 1   | J     | 192/230 (83%)   | 0.18   | 16 (8%) 14 11  | 16, 38, 90, 108       | 0     |
| 2   | K     | 84/84 (100%)    | -0.12  | 0 100 100      | 22, 41, 57, 78        | 0     |
| 2   | L     | 84/84 (100%)    | -0.18  | 2 (2%) 62 62   | 21, 42, 56, 78        | 0     |
| 2   | M     | 84/84 (100%)    | -0.05  | 2 (2%) 62 62   | 20, 41, 58, 77        | 0     |
| 2   | N     | 84/84 (100%)    | 0.07   | 5 (5%) 25 24   | 21, 41, 58, 79        | 0     |
| 2   | O     | 84/84 (100%)    | -0.11  | 3 (3%) 46 46   | 21, 41, 59, 78        | 0     |
| 2   | P     | 84/84 (100%)    | -0.28  | 1 (1%) 81 81   | 18, 40, 58, 78        | 0     |
| 2   | Q     | 84/84 (100%)    | -0.14  | 0 100 100      | 18, 38, 56, 77        | 0     |
| 2   | R     | 84/84 (100%)    | -0.19  | 2 (2%) 62 62   | 19, 39, 57, 79        | 0     |
| 2   | S     | 84/84 (100%)    | -0.19  | 1 (1%) 81 81   | 18, 38, 57, 78        | 0     |
| 2   | T     | 84/84 (100%)    | -0.13  | 3 (3%) 46 46   | 18, 39, 58, 79        | 0     |
| All | All   | 2760/3140 (87%) | 0.11   | 178 (6%) 23 21 | 15, 39, 84, 108       | 0     |

All (178) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | H     | 109 | ASN  | 10.5 |
| 1   | J     | 108 | LEU  | 9.7  |
| 1   | J     | 109 | ASN  | 9.6  |
| 1   | B     | 108 | LEU  | 9.4  |
| 1   | F     | 112 | ILE  | 8.5  |
| 1   | H     | 111 | ALA  | 8.1  |
| 1   | G     | 108 | LEU  | 7.9  |
| 1   | G     | 109 | ASN  | 7.6  |
| 1   | E     | 108 | LEU  | 7.3  |
| 1   | A     | 112 | ILE  | 7.2  |
| 1   | C     | 112 | ILE  | 7.1  |
| 1   | D     | 112 | ILE  | 7.1  |
| 1   | A     | 55  | ASN  | 7.0  |
| 1   | A     | 103 | THR  | 6.7  |
| 1   | G     | 110 | ASP  | 6.6  |
| 1   | G     | 112 | ILE  | 6.6  |
| 1   | A     | 106 | ASP  | 6.4  |
| 1   | D     | 108 | LEU  | 6.4  |
| 1   | G     | 113 | PHE  | 6.3  |
| 1   | F     | 108 | LEU  | 6.2  |
| 2   | N     | 84  | GLU  | 6.2  |
| 2   | R     | 84  | GLU  | 6.2  |
| 1   | H     | 110 | ASP  | 6.2  |
| 1   | E     | 107 | VAL  | 6.0  |
| 1   | I     | 110 | ASP  | 6.0  |
| 1   | I     | 112 | ILE  | 5.9  |
| 1   | B     | 109 | ASN  | 5.8  |
| 1   | I     | 113 | PHE  | 5.8  |
| 1   | C     | 113 | PHE  | 5.7  |
| 1   | J     | 48  | ARG  | 5.6  |
| 1   | D     | 106 | ASP  | 5.6  |
| 1   | A     | 50  | ARG  | 5.6  |
| 1   | G     | 107 | VAL  | 5.4  |
| 1   | A     | 52  | GLU  | 5.4  |
| 1   | I     | 109 | ASN  | 5.3  |
| 1   | C     | 208 | GLY  | 5.3  |
| 1   | G     | 111 | ALA  | 5.3  |
| 1   | B     | 112 | ILE  | 5.2  |
| 1   | H     | 108 | LEU  | 5.1  |
| 1   | J     | 110 | ASP  | 5.1  |
| 1   | F     | 109 | ASN  | 4.9  |
| 1   | D     | 109 | ASN  | 4.9  |
| 1   | C     | 114 | ASP  | 4.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 51  | SER  | 4.7  |
| 1   | J     | 105 | SER  | 4.7  |
| 1   | D     | 111 | ALA  | 4.7  |
| 1   | E     | 112 | ILE  | 4.7  |
| 1   | E     | 109 | ASN  | 4.7  |
| 1   | B     | 111 | ALA  | 4.6  |
| 1   | E     | 111 | ALA  | 4.5  |
| 1   | A     | 114 | ASP  | 4.4  |
| 1   | F     | 48  | ARG  | 4.4  |
| 1   | E     | 106 | ASP  | 4.4  |
| 1   | A     | 108 | LEU  | 4.4  |
| 1   | H     | 112 | ILE  | 4.3  |
| 1   | A     | 208 | GLY  | 4.3  |
| 1   | D     | 114 | ASP  | 4.3  |
| 1   | A     | 56  | GLU  | 4.2  |
| 1   | A     | 48  | ARG  | 4.2  |
| 1   | J     | 103 | THR  | 4.1  |
| 1   | G     | 106 | ASP  | 4.1  |
| 2   | P     | 84  | GLU  | 4.1  |
| 1   | I     | 116 | ASP  | 4.1  |
| 1   | E     | 208 | GLY  | 4.0  |
| 1   | C     | 108 | LEU  | 4.0  |
| 1   | B     | 106 | ASP  | 4.0  |
| 1   | C     | 213 | ASN  | 4.0  |
| 1   | C     | 111 | ALA  | 4.0  |
| 1   | I     | 111 | ALA  | 4.0  |
| 1   | G     | 52  | GLU  | 3.9  |
| 1   | B     | 205 | VAL  | 3.9  |
| 1   | A     | 59  | LEU  | 3.9  |
| 1   | D     | 113 | PHE  | 3.9  |
| 1   | I     | 48  | ARG  | 3.9  |
| 1   | G     | 51  | SER  | 3.8  |
| 1   | A     | 109 | ASN  | 3.8  |
| 1   | F     | 113 | PHE  | 3.8  |
| 2   | O     | 84  | GLU  | 3.8  |
| 1   | D     | 213 | ASN  | 3.8  |
| 1   | C     | 116 | ASP  | 3.7  |
| 2   | S     | 84  | GLU  | 3.6  |
| 2   | L     | 84  | GLU  | 3.6  |
| 1   | H     | 48  | ARG  | 3.6  |
| 1   | B     | 212 | MET  | 3.6  |
| 1   | J     | 212 | MET  | 3.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 111 | ALA  | 3.5  |
| 1   | A     | 110 | ASP  | 3.5  |
| 1   | F     | 212 | MET  | 3.5  |
| 1   | E     | 212 | MET  | 3.5  |
| 2   | T     | 84  | GLU  | 3.5  |
| 1   | A     | 212 | MET  | 3.4  |
| 1   | A     | 111 | ALA  | 3.3  |
| 1   | D     | 48  | ARG  | 3.3  |
| 1   | I     | 114 | ASP  | 3.3  |
| 1   | H     | 241 | SER  | 3.2  |
| 1   | J     | 205 | VAL  | 3.2  |
| 1   | F     | 110 | ASP  | 3.2  |
| 1   | H     | 113 | PHE  | 3.2  |
| 1   | H     | 212 | MET  | 3.2  |
| 1   | A     | 213 | ASN  | 3.1  |
| 1   | C     | 204 | MET  | 3.1  |
| 2   | T     | 23  | HIS  | 3.1  |
| 2   | M     | 84  | GLU  | 3.1  |
| 1   | F     | 105 | SER  | 3.1  |
| 1   | B     | 107 | VAL  | 3.0  |
| 1   | G     | 50  | ARG  | 3.0  |
| 1   | F     | 115 | GLU  | 3.0  |
| 1   | J     | 106 | ASP  | 3.0  |
| 1   | B     | 103 | THR  | 2.9  |
| 1   | B     | 113 | PHE  | 2.9  |
| 1   | I     | 213 | ASN  | 2.9  |
| 1   | I     | 212 | MET  | 2.9  |
| 2   | O     | 1   | MET  | 2.8  |
| 1   | G     | 56  | GLU  | 2.8  |
| 1   | I     | 115 | GLU  | 2.8  |
| 1   | B     | 110 | ASP  | 2.8  |
| 1   | A     | 116 | ASP  | 2.8  |
| 1   | C     | 109 | ASN  | 2.8  |
| 1   | G     | 241 | SER  | 2.7  |
| 1   | I     | 108 | LEU  | 2.7  |
| 2   | N     | 23  | HIS  | 2.7  |
| 1   | A     | 113 | PHE  | 2.7  |
| 1   | A     | 205 | VAL  | 2.7  |
| 1   | G     | 55  | ASN  | 2.7  |
| 1   | G     | 80  | GLN  | 2.6  |
| 2   | T     | 1   | MET  | 2.6  |
| 1   | G     | 213 | ASN  | 2.6  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | E            | 56         | GLU         | 2.6         |
| 1          | A            | 206        | MET         | 2.6         |
| 1          | E            | 103        | THR         | 2.6         |
| 1          | D            | 104        | ILE         | 2.5         |
| 1          | A            | 115        | GLU         | 2.5         |
| 1          | J            | 213        | ASN         | 2.5         |
| 1          | H            | 80         | GLN         | 2.5         |
| 1          | A            | 107        | VAL         | 2.4         |
| 1          | J            | 52         | GLU         | 2.4         |
| 1          | D            | 80         | GLN         | 2.4         |
| 1          | E            | 241        | SER         | 2.4         |
| 1          | C            | 110        | ASP         | 2.4         |
| 1          | D            | 110        | ASP         | 2.4         |
| 1          | G            | 48         | ARG         | 2.4         |
| 1          | G            | 212        | MET         | 2.4         |
| 1          | E            | 110        | ASP         | 2.4         |
| 1          | D            | 212        | MET         | 2.3         |
| 1          | G            | 207        | ARG         | 2.3         |
| 1          | A            | 60         | PRO         | 2.3         |
| 2          | N            | 2          | PRO         | 2.3         |
| 2          | M            | 35         | SER         | 2.3         |
| 2          | R            | 1          | MET         | 2.3         |
| 1          | J            | 80         | GLN         | 2.3         |
| 1          | D            | 56         | GLU         | 2.3         |
| 1          | C            | 103        | THR         | 2.3         |
| 1          | D            | 204        | MET         | 2.3         |
| 1          | B            | 213        | ASN         | 2.3         |
| 1          | H            | 116        | ASP         | 2.2         |
| 1          | D            | 103        | THR         | 2.2         |
| 1          | J            | 57         | LEU         | 2.2         |
| 1          | J            | 107        | VAL         | 2.2         |
| 1          | G            | 118        | ASP         | 2.2         |
| 1          | C            | 214        | SER         | 2.2         |
| 1          | C            | 207        | ARG         | 2.2         |
| 2          | N            | 1          | MET         | 2.2         |
| 1          | A            | 53         | GLU         | 2.2         |
| 1          | B            | 80         | GLN         | 2.1         |
| 1          | C            | 241        | SER         | 2.1         |
| 1          | F            | 57         | LEU         | 2.1         |
| 2          | L            | 83         | LYS         | 2.1         |
| 1          | C            | 80         | GLN         | 2.1         |
| 1          | F            | 206        | MET         | 2.1         |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 53  | GLU  | 2.1  |
| 1   | G     | 116 | ASP  | 2.1  |
| 1   | J     | 206 | MET  | 2.1  |
| 1   | F     | 52  | GLU  | 2.1  |
| 1   | H     | 208 | GLY  | 2.1  |
| 1   | J     | 56  | GLU  | 2.1  |
| 2   | O     | 62  | CYS  | 2.1  |
| 2   | N     | 83  | LYS  | 2.0  |
| 1   | D     | 53  | GLU  | 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 5   | PHE  | N     | 1007 | 12/12 | 0.94 | 0.16 | 1.20  | 33,35,37,38                | 0     |
| 5   | PHE  | R     | 1002 | 12/12 | 0.96 | 0.14 | 0.58  | 19,21,23,24                | 0     |
| 5   | PHE  | Q     | 1001 | 12/12 | 0.96 | 0.12 | 0.04  | 18,21,25,28                | 0     |
| 5   | PHE  | M     | 1010 | 12/12 | 0.96 | 0.12 | -0.18 | 21,24,26,28                | 0     |
| 5   | PHE  | N     | 1006 | 12/12 | 0.96 | 0.12 | -0.28 | 24,28,29,30                | 0     |
| 5   | PHE  | K     | 1009 | 12/12 | 0.97 | 0.10 | -0.91 | 17,21,25,26                | 0     |
| 5   | PHE  | P     | 1003 | 12/12 | 0.97 | 0.10 | -0.94 | 18,20,25,26                | 0     |
| 5   | PHE  | O     | 1008 | 12/12 | 0.97 | 0.10 | -1.09 | 21,23,24,25                | 0     |
| 5   | PHE  | T     | 1005 | 12/12 | 0.98 | 0.10 | -1.29 | 16,18,21,24                | 0     |
| 3   | K    | Q     | 2005 | 1/1   | 0.97 | 0.08 | -1.74 | 23,23,23,23                | 0     |
| 3   | K    | N     | 2009 | 1/1   | 0.97 | 0.08 | -1.84 | 36,36,36,36                | 0     |
| 3   | K    | O     | 2010 | 1/1   | 0.97 | 0.09 | -1.88 | 35,35,35,35                | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 3   | K    | T     | 2003 | 1/1   | 0.99 | 0.08 | -1.98 | 30,30,30,30                 | 0     |
| 5   | PHE  | S     | 1004 | 12/12 | 0.98 | 0.08 | -1.98 | 9,13,15,17                  | 0     |
| 3   | K    | M     | 2008 | 1/1   | 0.98 | 0.05 | -2.50 | 32,32,32,32                 | 0     |
| 3   | K    | K     | 2006 | 1/1   | 0.96 | 0.05 | -2.99 | 27,27,27,27                 | 0     |
| 3   | K    | L     | 2007 | 1/1   | 0.98 | 0.06 | -3.00 | 29,29,29,29                 | 0     |
| 3   | K    | R     | 2001 | 1/1   | 0.98 | 0.04 | -3.71 | 23,23,23,23                 | 0     |
| 3   | K    | S     | 2002 | 1/1   | 0.98 | 0.07 | -3.81 | 23,23,23,23                 | 0     |
| 3   | K    | P     | 2004 | 1/1   | 0.99 | 0.04 | -3.81 | 28,28,28,28                 | 0     |
| 4   | ZN   | C     | 3107 | 1/1   | 0.99 | 0.06 | -     | 55,55,55,55                 | 0     |
| 4   | ZN   | J     | 3106 | 1/1   | 0.97 | 0.05 | -     | 53,53,53,53                 | 0     |
| 4   | ZN   | A     | 3102 | 1/1   | 0.98 | 0.05 | -     | 53,53,53,53                 | 0     |
| 4   | ZN   | B     | 3109 | 1/1   | 0.97 | 0.04 | -     | 54,54,54,54                 | 0     |
| 4   | ZN   | D     | 3108 | 1/1   | 0.93 | 0.07 | -     | 73,73,73,73                 | 0     |
| 4   | ZN   | H     | 3104 | 1/1   | 0.99 | 0.04 | -     | 49,49,49,49                 | 0     |
| 4   | ZN   | F     | 3110 | 1/1   | 0.99 | 0.03 | -     | 62,62,62,62                 | 0     |
| 4   | ZN   | I     | 3101 | 1/1   | 0.95 | 0.08 | -     | 50,50,50,50                 | 0     |
| 4   | ZN   | G     | 3103 | 1/1   | 0.99 | 0.04 | -     | 56,56,56,56                 | 0     |
| 4   | ZN   | E     | 3105 | 1/1   | 0.96 | 0.03 | -     | 57,57,57,57                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.