



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:47 AM UTC

PDB ID : 4AID / pdb\_00004aid  
Title : Crystal structure of C. crescentus PNPase bound to RNase E recognition peptide  
Authors : Hardwick, S.W.; Gubbey, T.; Hug, I.; Jenal, U.; Luisi, B.F.  
Deposited on : 2012-02-09  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

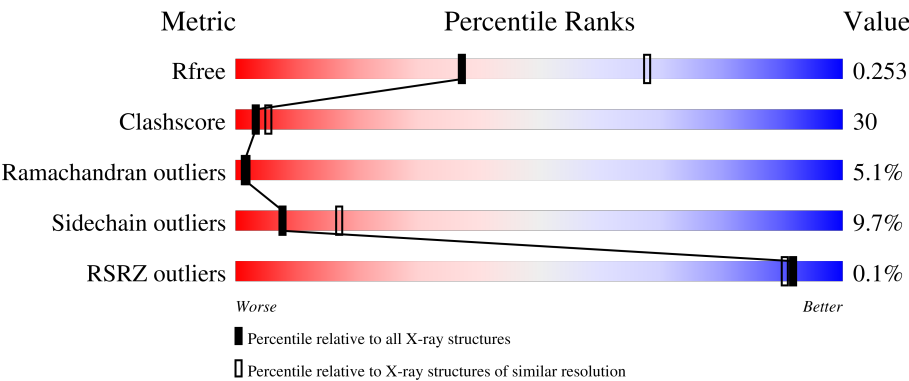
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| R <sub>free</sub>     | 180053                      | 4008 (2.60-2.60)                                      |
| Clashscore            | 190562                      | 4347 (2.60-2.60)                                      |
| Ramachandran outliers | 187476                      | 4277 (2.60-2.60)                                      |
| Sidechain outliers    | 187428                      | 4277 (2.60-2.60)                                      |
| RSRZ outliers         | 180081                      | 4008 (2.60-2.60)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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     | 726    | <div><div></div><div></div><div></div><div></div><div></div></div> <div>46%23%8%•21%</div>  |
| 1   | B     | 726    | <div><div></div><div></div><div></div><div></div><div></div></div> <div>43%23%9%•23%</div>  |
| 1   | C     | 726    | <div><div></div><div></div><div></div><div></div><div></div></div> <div>43%26%5%26%</div>   |
| 2   | F     | 14     | <div><div></div><div></div><div></div><div></div><div></div></div> <div>14%21%7%7%50%</div> |
| 2   | G     | 14     | <div><div></div><div></div><div></div><div></div><div></div></div> <div>29%21%7%43%</div>   |

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| Mol | Chain | Length | Quality of chain                                                                                                                            |
|-----|-------|--------|---------------------------------------------------------------------------------------------------------------------------------------------|
| 2   | H     | 14     |  <div> <div>29%</div> <div>7%</div> <div>64%</div> </div> |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12655 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 POLYRIBONUCLEOTIDE NUCLEOTIDYLTRANSFERASE.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 573      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 4248  | 2686 | 720 | 819 | 23 |         |         |       |
| 1   | B     | 558      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4170  | 2639 | 706 | 802 | 23 |         |         |       |
| 1   | C     | 539      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3836  | 2425 | 654 | 735 | 22 |         |         |       |

There are 42 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -13     | MET      | -      | expression tag | UNP Q9AC32 |
| A     | -12     | GLY      | -      | expression tag | UNP Q9AC32 |
| A     | -11     | SER      | -      | expression tag | UNP Q9AC32 |
| A     | -10     | SER      | -      | expression tag | UNP Q9AC32 |
| A     | -9      | HIS      | -      | expression tag | UNP Q9AC32 |
| A     | -8      | HIS      | -      | expression tag | UNP Q9AC32 |
| A     | -7      | HIS      | -      | expression tag | UNP Q9AC32 |
| A     | -6      | HIS      | -      | expression tag | UNP Q9AC32 |
| A     | -5      | HIS      | -      | expression tag | UNP Q9AC32 |
| A     | -4      | HIS      | -      | expression tag | UNP Q9AC32 |
| A     | -3      | SER      | -      | expression tag | UNP Q9AC32 |
| A     | -2      | GLN      | -      | expression tag | UNP Q9AC32 |
| A     | -1      | ASP      | -      | expression tag | UNP Q9AC32 |
| A     | 0       | PRO      | -      | expression tag | UNP Q9AC32 |
| B     | -13     | MET      | -      | expression tag | UNP Q9AC32 |
| B     | -12     | GLY      | -      | expression tag | UNP Q9AC32 |
| B     | -11     | SER      | -      | expression tag | UNP Q9AC32 |
| B     | -10     | SER      | -      | expression tag | UNP Q9AC32 |
| B     | -9      | HIS      | -      | expression tag | UNP Q9AC32 |
| B     | -8      | HIS      | -      | expression tag | UNP Q9AC32 |
| B     | -7      | HIS      | -      | expression tag | UNP Q9AC32 |
| B     | -6      | HIS      | -      | expression tag | UNP Q9AC32 |

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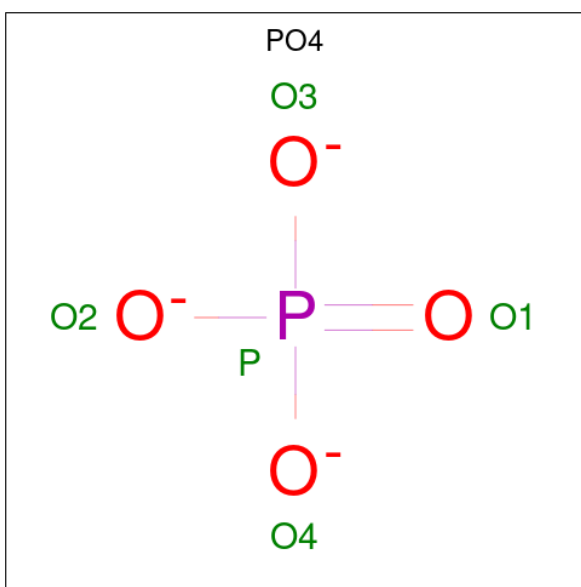
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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | -5      | HIS      | -      | expression tag | UNP Q9AC32 |
| B     | -4      | HIS      | -      | expression tag | UNP Q9AC32 |
| B     | -3      | SER      | -      | expression tag | UNP Q9AC32 |
| B     | -2      | GLN      | -      | expression tag | UNP Q9AC32 |
| B     | -1      | ASP      | -      | expression tag | UNP Q9AC32 |
| B     | 0       | PRO      | -      | expression tag | UNP Q9AC32 |
| C     | -13     | MET      | -      | expression tag | UNP Q9AC32 |
| C     | -12     | GLY      | -      | expression tag | UNP Q9AC32 |
| C     | -11     | SER      | -      | expression tag | UNP Q9AC32 |
| C     | -10     | SER      | -      | expression tag | UNP Q9AC32 |
| C     | -9      | HIS      | -      | expression tag | UNP Q9AC32 |
| C     | -8      | HIS      | -      | expression tag | UNP Q9AC32 |
| C     | -7      | HIS      | -      | expression tag | UNP Q9AC32 |
| C     | -6      | HIS      | -      | expression tag | UNP Q9AC32 |
| C     | -5      | HIS      | -      | expression tag | UNP Q9AC32 |
| C     | -4      | HIS      | -      | expression tag | UNP Q9AC32 |
| C     | -3      | SER      | -      | expression tag | UNP Q9AC32 |
| C     | -2      | GLN      | -      | expression tag | UNP Q9AC32 |
| C     | -1      | ASP      | -      | expression tag | UNP Q9AC32 |
| C     | 0       | PRO      | -      | expression tag | UNP Q9AC32 |

- Molecule 2 is a protein called RIBONUCLEASE, RNE/RNG FAMILY PROTEIN.

| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|---|---------|---------|-------|
| 2   | F     | 7        | Total | C  | N  | O | 0       | 0       | 0     |
|     |       |          | 66    | 44 | 15 | 7 |         |         |       |
| 2   | G     | 8        | Total | C  | N  | O | 0       | 0       | 0     |
|     |       |          | 77    | 50 | 19 | 8 |         |         |       |
| 2   | H     | 5        | Total | C  | N  | O | 0       | 0       | 0     |
|     |       |          | 42    | 30 | 7  | 5 |         |         |       |

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | A     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | B     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | C     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

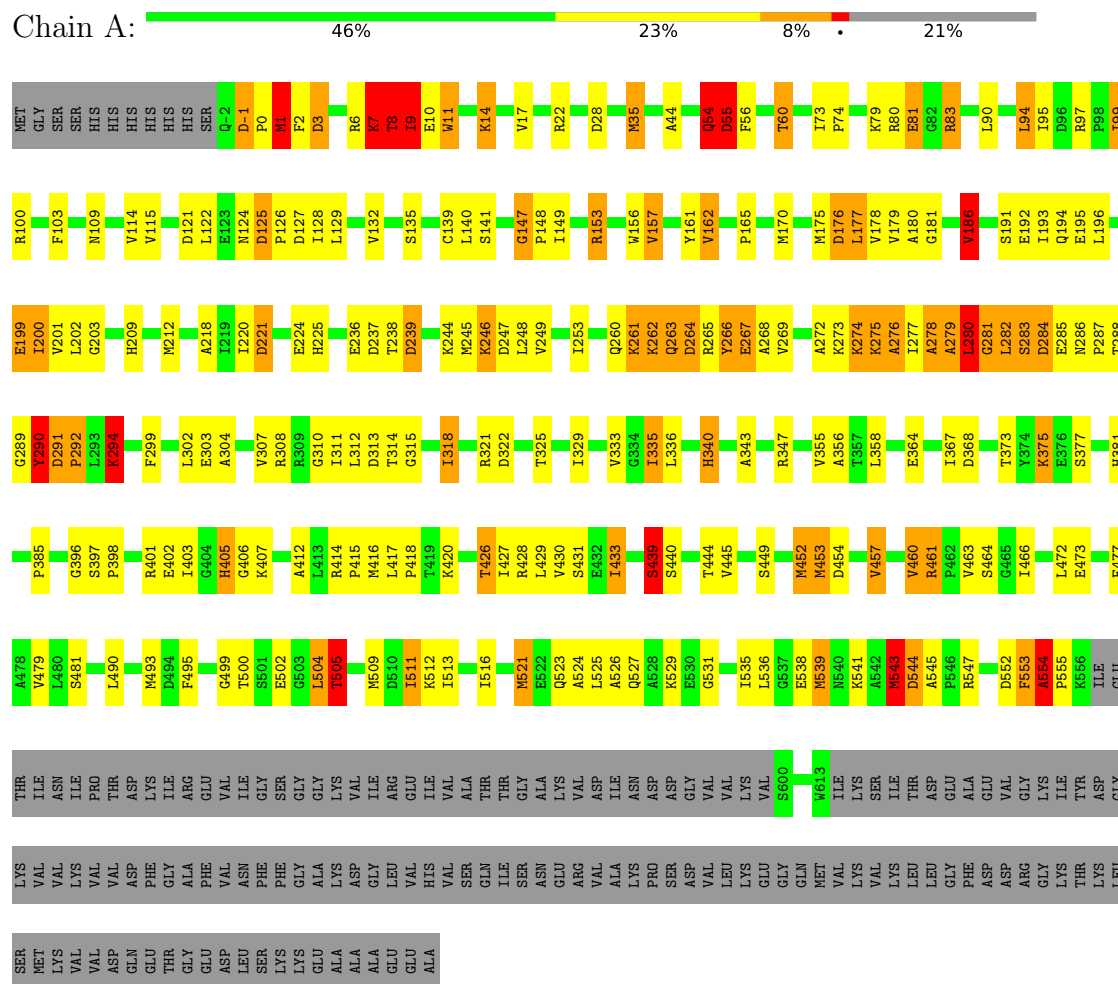
- Molecule 4 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | A     | 96       | Total | O  | 0       | 0       |
|     |       |          | 96    | 96 |         |         |
| 4   | B     | 80       | Total | O  | 0       | 0       |
|     |       |          | 80    | 80 |         |         |
| 4   | C     | 24       | Total | O  | 0       | 0       |
|     |       |          | 24    | 24 |         |         |
| 4   | G     | 1        | Total | O  | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

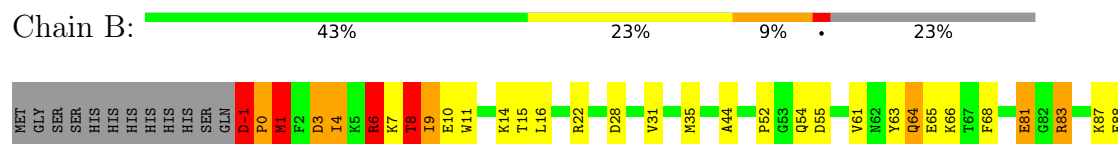
### 3 Residue-property plots

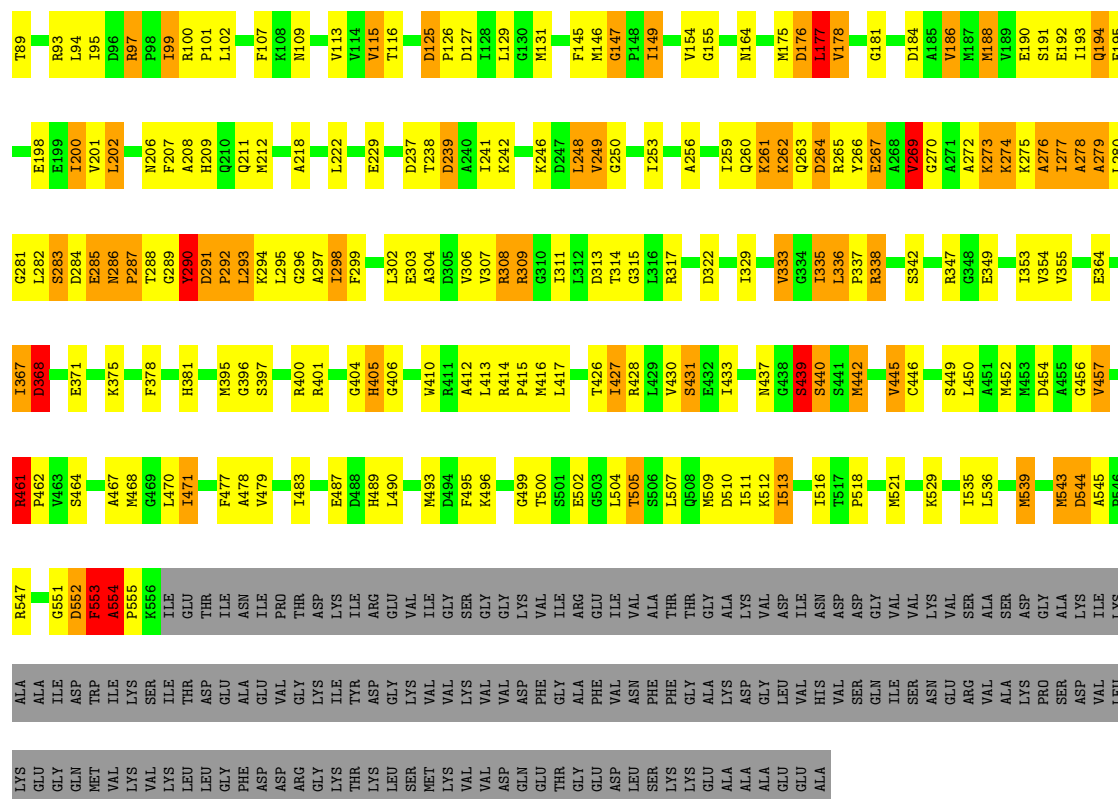
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: POLYRIBONUCLEOTIDE NUCLEOTIDYLTRANSFERASE



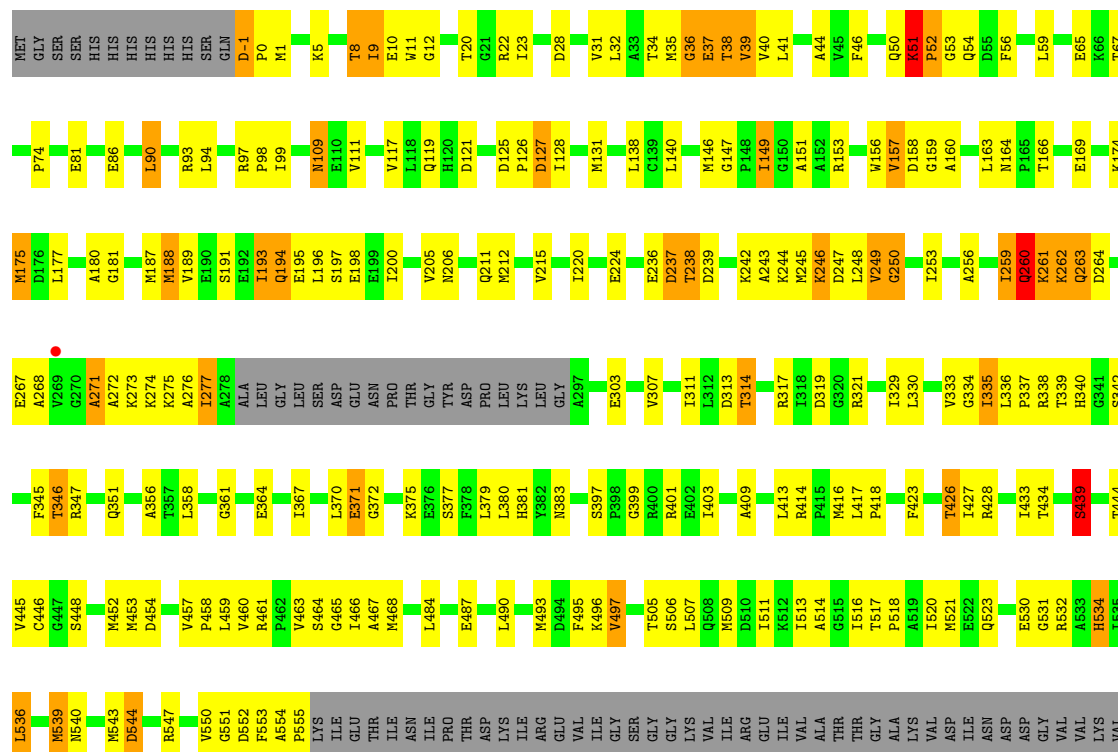
#### • Molecule 1: POLYRIBONUCLEOTIDE NUCLEOTIDYLTRANSFERASE





# ● Molecule 1: POLYRIBONUCLEOTIDE NUCLEOTIDYLTRANSFERASE

Chain C:





ARG  
ALA  
SER  
SER  
LYS  
GLY  
SER  
ALA  
LYS  
ILE  
LYS  
ALA  
ALA  
ILE  
ASP  
TRP  
ILE  
LYS  
SER  
ILE  
THR  
ASP  
GLU  
ALA  
GLU  
VAL  
GLY  
LYS  
ILE  
TYR  
LYS  
ASP  
GLY  
LYS  
VAL  
VAL  
LYS  
VAL  
ASP  
VAL  
PHE  
GLY  
ALA  
PHE  
VAL  
ASN  
PHE  
PHE  
LYS  
LYS  
GLU  
ALA  
LYS  
ASP  
GLY  
LEU  
VAL  
HIS  
VAL  
SER  
GLN  
ILE  
SER  
ASN  
GLU

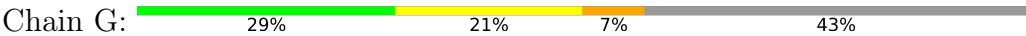
ARG  
VAL  
ALA  
SER  
PRO  
GLY  
SER  
ASP  
VAL  
LEU  
LYS  
GLY  
GLN  
MET  
VAL  
VAL  
LYS  
LYS  
LEU  
LEU  
GLY  
PHE  
ASP  
ASP  
ARG  
GLY  
LYS  
THR  
LYS  
LYS  
LEU  
SER  
MET  
LYS  
VAL  
VAL  
VAL  
GLN  
GLU  
THR  
GLY  
GLU  
ASP  
LEU  
SER  
LYS  
LYS  
GLU  
ALA  
ALA  
GLY  
GLU  
ALA

● Molecule 2: RIBONUCLEASE, RNE/RNG FAMILY PROTEIN



THR  
ALA  
PRO  
PRO  
GLU  
LYS  
P891  
R892  
R893  
G894  
W895  
W896  
R897  
ARG

● Molecule 2: RIBONUCLEASE, RNE/RNG FAMILY PROTEIN



THR  
ALA  
PRO  
PRO  
GLU  
LYS  
P890  
R892  
R893  
G894  
W895  
W896  
R897  
ARG

● Molecule 2: RIBONUCLEASE, RNE/RNG FAMILY PROTEIN



THR  
ALA  
PRO  
PRO  
GLU  
LYS  
PRO  
ARG  
R893  
W896  
R897  
ARG

## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | H 3                                                         | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 157.44Å 157.44Å 302.38Å<br>90.00° 90.00° 120.00°            | Depositor        |
| Resolution (Å)                                                          | 30.00 – 2.60<br>30.00 – 2.60                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 90.0 (30.00-2.60)<br>90.0 (30.00-2.60)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.22                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.92 (at 2.61Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.6.0117                                             | Depositor        |
| R, $R_{free}$                                                           | 0.209 , 0.254<br>0.209 , 0.253                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2587 reflections (3.01%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 46.7                                                        | Xtriage          |
| Anisotropy                                                              | 0.048                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 18.8                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$ | Xtriage          |
| Estimated twinning fraction                                             | 0.357 for h,-h-k,-l                                         | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 12655                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 60.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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     | 1.35         | 21/4324 (0.5%)  | 1.49        | 46/5859 (0.8%)   |
| 1   | B     | 1.39         | 18/4242 (0.4%)  | 1.51        | 65/5744 (1.1%)   |
| 1   | C     | 0.94         | 2/3900 (0.1%)   | 1.21        | 20/5305 (0.4%)   |
| 2   | F     | 1.49         | 1/70 (1.4%)     | 1.58        | 2/94 (2.1%)      |
| 2   | G     | 1.18         | 0/81            | 1.42        | 1/109 (0.9%)     |
| 2   | H     | 1.25         | 0/45            | 1.18        | 0/62             |
| All | All   | 1.25         | 42/12662 (0.3%) | 1.41        | 134/17173 (0.8%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 2                   |
| 1   | B     | 0                   | 3                   |
| 1   | C     | 0                   | 1                   |
| 2   | F     | 0                   | 1                   |
| All | All   | 0                   | 7                   |

All (42) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | B     | 164 | ASN  | C-O   | -11.03 | 1.18        | 1.23     |
| 1   | A     | 7   | LYS  | CA-C  | -9.33  | 1.43        | 1.52     |
| 1   | B     | 7   | LYS  | CA-C  | -8.39  | 1.42        | 1.52     |
| 1   | B     | 338 | ARG  | N-CA  | 7.59   | 1.55        | 1.46     |
| 1   | B     | 147 | GLY  | N-CA  | 7.25   | 1.54        | 1.44     |
| 1   | A     | 147 | GLY  | C-O   | -6.89  | 1.14        | 1.24     |
| 1   | B     | 440 | SER  | N-CA  | -6.74  | 1.37        | 1.46     |
| 1   | A     | 385 | PRO  | C-O   | -6.66  | 1.19        | 1.24     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 54  | GLN  | C-O     | -6.61 | 1.15        | 1.24     |
| 1   | B     | 405 | HIS  | ND1-CE1 | 6.54  | 1.39        | 1.32     |
| 1   | A     | -1  | ASP  | C-N     | 6.49  | 1.41        | 1.33     |
| 1   | A     | 156 | TRP  | CA-C    | -6.47 | 1.46        | 1.53     |
| 1   | B     | 286 | ASN  | C-O     | -6.45 | 1.16        | 1.24     |
| 1   | A     | 279 | ALA  | C-O     | -6.44 | 1.15        | 1.23     |
| 1   | C     | 259 | ILE  | C-O     | -6.19 | 1.15        | 1.24     |
| 1   | A     | 418 | PRO  | CA-C    | -6.12 | 1.46        | 1.52     |
| 1   | A     | 433 | ILE  | N-CA    | -6.03 | 1.39        | 1.46     |
| 1   | B     | 87  | LYS  | CA-C    | 5.82  | 1.60        | 1.52     |
| 1   | A     | 504 | LEU  | CA-C    | -5.70 | 1.45        | 1.53     |
| 1   | B     | 54  | GLN  | C-O     | -5.59 | 1.17        | 1.23     |
| 1   | A     | 176 | ASP  | C-O     | 5.56  | 1.30        | 1.23     |
| 1   | B     | 413 | LEU  | C-O     | -5.56 | 1.16        | 1.24     |
| 1   | A     | 11  | TRP  | CA-C    | -5.55 | 1.46        | 1.53     |
| 1   | B     | 405 | HIS  | CG-CD2  | 5.53  | 1.42        | 1.35     |
| 1   | A     | 439 | SER  | CA-C    | -5.49 | 1.45        | 1.52     |
| 1   | A     | 449 | SER  | CA-C    | -5.46 | 1.45        | 1.52     |
| 1   | A     | 405 | HIS  | CG-CD2  | 5.44  | 1.41        | 1.35     |
| 1   | A     | 225 | HIS  | CG-CD2  | 5.40  | 1.41        | 1.35     |
| 1   | B     | 442 | MET  | C-O     | 5.39  | 1.30        | 1.24     |
| 2   | F     | 896 | TRP  | CD2-CE2 | 5.30  | 1.50        | 1.41     |
| 1   | A     | 340 | HIS  | CG-ND1  | -5.30 | 1.32        | 1.38     |
| 1   | B     | 367 | ILE  | N-CA    | -5.26 | 1.39        | 1.46     |
| 1   | A     | 97  | ARG  | C-O     | -5.25 | 1.19        | 1.24     |
| 1   | A     | 505 | THR  | C-O     | -5.23 | 1.18        | 1.24     |
| 1   | B     | 333 | VAL  | C-O     | -5.22 | 1.18        | 1.23     |
| 1   | C     | 260 | GLN  | CA-C    | 5.21  | 1.59        | 1.52     |
| 1   | B     | 155 | GLY  | N-CA    | 5.19  | 1.49        | 1.44     |
| 1   | B     | 410 | TRP  | NE1-CE2 | -5.17 | 1.31        | 1.37     |
| 1   | B     | 249 | VAL  | CA-C    | 5.11  | 1.58        | 1.52     |
| 1   | B     | 378 | PHE  | N-CA    | -5.10 | 1.40        | 1.46     |
| 1   | A     | 343 | ALA  | CA-C    | -5.03 | 1.46        | 1.52     |
| 1   | A     | 186 | VAL  | C-O     | -5.01 | 1.18        | 1.24     |

All (134) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | A     | 7   | LYS  | N-CA-C | -12.51 | 96.71       | 112.72   |
| 1   | B     | 7   | LYS  | N-CA-C | -11.69 | 95.97       | 114.09   |
| 1   | A     | 9   | ILE  | N-CA-C | -11.46 | 85.50       | 109.34   |
| 1   | A     | 553 | PHE  | N-CA-C | -10.36 | 93.29       | 109.76   |

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| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 1   | C     | -1  | ASP  | CA-C-N   | -10.25 | 108.31      | 118.97   |
| 1   | C     | -1  | ASP  | C-N-CA   | -10.25 | 108.31      | 118.97   |
| 1   | A     | 73  | ILE  | CA-C-N   | -9.71  | 110.05      | 119.85   |
| 1   | A     | 73  | ILE  | C-N-CA   | -9.71  | 110.05      | 119.85   |
| 1   | A     | 8   | THR  | N-CA-C   | -9.09  | 97.18       | 110.64   |
| 1   | A     | 406 | GLY  | N-CA-C   | -8.96  | 101.98      | 112.73   |
| 1   | A     | 177 | LEU  | CA-C-N   | -8.58  | 112.55      | 123.19   |
| 1   | A     | 177 | LEU  | C-N-CA   | -8.58  | 112.55      | 123.19   |
| 1   | B     | 125 | ASP  | CA-C-N   | -8.57  | 111.06      | 121.00   |
| 1   | B     | 125 | ASP  | C-N-CA   | -8.57  | 111.06      | 121.00   |
| 1   | A     | 10  | GLU  | N-CA-C   | -8.26  | 97.58       | 109.96   |
| 1   | A     | 439 | SER  | N-CA-C   | 8.21   | 128.28      | 110.80   |
| 1   | C     | 346 | THR  | CB-CA-C  | 8.15   | 122.52      | 110.62   |
| 1   | A     | 505 | THR  | N-CA-C   | -8.14  | 105.33      | 114.62   |
| 1   | B     | 406 | GLY  | N-CA-C   | -7.99  | 103.14      | 112.73   |
| 1   | B     | -1  | ASP  | CA-C-N   | -7.82  | 110.33      | 118.85   |
| 1   | B     | -1  | ASP  | C-N-CA   | -7.82  | 110.33      | 118.85   |
| 1   | B     | 8   | THR  | N-CA-C   | -7.76  | 94.26       | 110.80   |
| 1   | B     | 457 | VAL  | N-CA-CB  | 7.60   | 118.36      | 110.23   |
| 1   | A     | -1  | ASP  | CA-C-N   | -7.51  | 112.95      | 120.31   |
| 1   | A     | -1  | ASP  | C-N-CA   | -7.51  | 112.95      | 120.31   |
| 1   | C     | 191 | SER  | N-CA-C   | 7.51   | 120.78      | 108.99   |
| 1   | B     | 461 | ARG  | CA-C-N   | -7.47  | 112.09      | 119.78   |
| 1   | B     | 461 | ARG  | C-N-CA   | -7.47  | 112.09      | 119.78   |
| 1   | A     | 99  | ILE  | CB-CA-C  | -7.40  | 102.00      | 112.22   |
| 1   | A     | 453 | MET  | N-CA-C   | -7.14  | 103.57      | 111.36   |
| 1   | B     | 553 | PHE  | N-CA-C   | -7.10  | 98.47       | 109.76   |
| 1   | B     | 439 | SER  | N-CA-C   | 7.06   | 125.84      | 110.80   |
| 2   | F     | 893 | ARG  | N-CA-C   | 7.03   | 122.72      | 113.30   |
| 1   | A     | 294 | LYS  | N-CA-C   | -6.86  | 96.19       | 110.80   |
| 1   | B     | 6   | ARG  | N-CA-C   | -6.78  | 97.23       | 108.34   |
| 2   | G     | 896 | TRP  | N-CA-C   | 6.74   | 120.72      | 112.23   |
| 1   | B     | 99  | ILE  | N-CA-C   | -6.62  | 105.38      | 111.67   |
| 1   | B     | 192 | GLU  | N-CA-C   | -6.62  | 96.97       | 108.69   |
| 1   | B     | 178 | VAL  | CB-CA-C  | 6.60   | 119.81      | 110.84   |
| 1   | A     | 385 | PRO  | CA-C-N   | 6.44   | 126.37      | 119.28   |
| 1   | A     | 385 | PRO  | C-N-CA   | 6.44   | 126.37      | 119.28   |
| 1   | B     | 8   | THR  | CB-CA-C  | 6.41   | 123.17      | 110.42   |
| 1   | B     | 539 | MET  | CG-SD-CE | -6.33  | 86.98       | 100.90   |
| 1   | C     | 439 | SER  | N-CA-C   | 6.31   | 124.25      | 110.80   |
| 1   | B     | 176 | ASP  | CA-C-N   | -6.29  | 113.90      | 122.77   |
| 1   | B     | 176 | ASP  | C-N-CA   | -6.29  | 113.90      | 122.77   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 449 | SER  | CB-CA-C   | -6.16 | 100.96      | 110.81   |
| 1   | A     | 445 | VAL  | N-CA-C    | -6.12 | 104.78      | 110.53   |
| 1   | B     | 194 | GLN  | CB-CA-C   | -6.11 | 102.63      | 111.91   |
| 1   | B     | 97  | ARG  | CA-C-N    | -6.04 | 113.74      | 120.45   |
| 1   | B     | 97  | ARG  | C-N-CA    | -6.04 | 113.74      | 120.45   |
| 1   | B     | 177 | LEU  | CB-CG-CD1 | -6.01 | 92.66       | 110.70   |
| 1   | C     | 238 | THR  | N-CA-C    | -6.00 | 106.05      | 113.19   |
| 1   | A     | 544 | ASP  | N-CA-CB   | -5.98 | 100.39      | 110.49   |
| 1   | B     | 177 | LEU  | CA-C-N    | -5.93 | 115.45      | 122.93   |
| 1   | B     | 177 | LEU  | C-N-CA    | -5.93 | 115.45      | 122.93   |
| 1   | B     | 3   | ASP  | N-CA-CB   | -5.93 | 100.97      | 110.63   |
| 1   | B     | 426 | THR  | CA-C-N    | -5.92 | 115.43      | 123.12   |
| 1   | B     | 426 | THR  | C-N-CA    | -5.92 | 115.43      | 123.12   |
| 1   | A     | 543 | MET  | CA-C-N    | -5.90 | 110.27      | 121.54   |
| 1   | A     | 543 | MET  | C-N-CA    | -5.90 | 110.27      | 121.54   |
| 1   | B     | 405 | HIS  | N-CA-C    | 5.89  | 118.45      | 111.33   |
| 1   | C     | 10  | GLU  | N-CA-C    | -5.88 | 100.94      | 109.59   |
| 1   | C     | 146 | MET  | N-CA-C    | 5.88  | 117.87      | 108.41   |
| 1   | B     | 164 | ASN  | CA-C-N    | -5.85 | 113.94      | 119.85   |
| 1   | B     | 164 | ASN  | C-N-CA    | -5.85 | 113.94      | 119.85   |
| 1   | C     | 506 | SER  | N-CA-C    | 5.84  | 117.98      | 108.76   |
| 1   | B     | 430 | VAL  | CA-C-N    | -5.81 | 114.80      | 122.99   |
| 1   | B     | 430 | VAL  | C-N-CA    | -5.81 | 114.80      | 122.99   |
| 1   | A     | 539 | MET  | CG-SD-CE  | -5.80 | 88.14       | 100.90   |
| 1   | B     | 554 | ALA  | CA-C-N    | -5.79 | 114.00      | 119.90   |
| 1   | B     | 554 | ALA  | C-N-CA    | -5.79 | 114.00      | 119.90   |
| 1   | A     | 335 | ILE  | N-CA-C    | 5.69  | 116.43      | 110.62   |
| 1   | A     | 186 | VAL  | N-CA-CB   | 5.66  | 117.27      | 110.31   |
| 1   | A     | 452 | MET  | CG-SD-CE  | -5.63 | 88.50       | 100.90   |
| 1   | B     | 184 | ASP  | N-CA-C    | 5.63  | 118.35      | 111.82   |
| 2   | F     | 894 | GLY  | N-CA-C    | 5.60  | 126.45      | 113.18   |
| 1   | C     | 544 | ASP  | N-CA-C    | 5.59  | 122.71      | 110.80   |
| 1   | A     | 291 | ASP  | CA-C-N    | -5.55 | 112.90      | 119.84   |
| 1   | A     | 291 | ASP  | C-N-CA    | -5.55 | 112.90      | 119.84   |
| 1   | A     | 461 | ARG  | CA-C-N    | -5.55 | 113.98      | 119.92   |
| 1   | A     | 461 | ARG  | C-N-CA    | -5.55 | 113.98      | 119.92   |
| 1   | B     | 95  | ILE  | N-CA-C    | -5.54 | 105.70      | 111.58   |
| 1   | B     | 10  | GLU  | N-CA-C    | -5.51 | 101.90      | 110.10   |
| 1   | B     | 0   | PRO  | N-CA-C    | -5.50 | 106.03      | 113.40   |
| 1   | C     | 127 | ASP  | N-CA-C    | 5.49  | 116.95      | 111.07   |
| 1   | B     | 147 | GLY  | N-CA-C    | -5.48 | 101.15      | 112.34   |
| 1   | A     | 115 | VAL  | CB-CA-C   | 5.47  | 117.80      | 110.42   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 555 | PRO  | N-CA-C     | 5.47  | 119.79      | 111.15   |
| 1   | B     | 283 | SER  | CA-C-O     | -5.45 | 115.22      | 121.54   |
| 1   | B     | 353 | ILE  | CB-CA-C    | -5.43 | 104.17      | 110.91   |
| 1   | A     | 426 | THR  | CB-CA-C    | 5.41  | 118.46      | 109.53   |
| 1   | B     | 194 | GLN  | CA-CB-CG   | 5.39  | 124.87      | 114.10   |
| 1   | B     | 239 | ASP  | N-CA-C     | 5.39  | 117.15      | 111.28   |
| 1   | B     | 54  | GLN  | CA-C-N     | -5.36 | 113.78      | 121.98   |
| 1   | B     | 54  | GLN  | C-N-CA     | -5.36 | 113.78      | 121.98   |
| 1   | B     | 483 | ILE  | CB-CA-C    | -5.36 | 103.11      | 111.26   |
| 1   | A     | 426 | THR  | OG1-CB-CG2 | -5.34 | 98.62       | 109.30   |
| 1   | A     | 367 | ILE  | CB-CA-C    | -5.34 | 103.19      | 110.77   |
| 1   | B     | 329 | ILE  | N-CA-C     | 5.33  | 116.40      | 108.46   |
| 1   | B     | 206 | ASN  | N-CA-C     | 5.32  | 117.16      | 111.36   |
| 1   | C     | 463 | VAL  | CB-CA-C    | -5.32 | 101.88      | 110.28   |
| 1   | C     | 536 | LEU  | N-CA-C     | -5.30 | 105.50      | 111.28   |
| 1   | A     | 55  | ASP  | CB-CA-C    | -5.29 | 99.90       | 110.42   |
| 1   | B     | 1   | MET  | CB-CA-C    | 5.28  | 118.46      | 109.75   |
| 1   | A     | 8   | THR  | N-CA-CB    | 5.23  | 117.24      | 109.19   |
| 1   | A     | 125 | ASP  | CA-C-N     | -5.23 | 114.65      | 120.45   |
| 1   | A     | 125 | ASP  | C-N-CA     | -5.23 | 114.65      | 120.45   |
| 1   | B     | 66  | LYS  | N-CA-C     | -5.21 | 100.02      | 108.52   |
| 1   | C     | 335 | ILE  | CB-CA-C    | -5.21 | 104.44      | 112.05   |
| 1   | B     | 513 | ILE  | N-CA-C     | 5.21  | 115.14      | 107.75   |
| 1   | B     | 427 | ILE  | CA-C-N     | -5.16 | 115.88      | 123.00   |
| 1   | B     | 427 | ILE  | C-N-CA     | -5.16 | 115.88      | 123.00   |
| 1   | B     | 229 | GLU  | CA-C-N     | -5.14 | 114.44      | 119.99   |
| 1   | B     | 229 | GLU  | C-N-CA     | -5.14 | 114.44      | 119.99   |
| 1   | B     | 1   | MET  | CB-CG-SD   | 5.13  | 128.10      | 112.70   |
| 1   | B     | 368 | ASP  | N-CA-CB    | 5.10  | 117.70      | 110.46   |
| 1   | C     | 5   | LYS  | N-CA-C     | 5.10  | 116.73      | 109.14   |
| 1   | B     | 81  | GLU  | CB-CA-C    | 5.09  | 118.83      | 109.46   |
| 1   | B     | 99  | ILE  | CB-CA-C    | -5.09 | 105.80      | 111.80   |
| 1   | B     | 186 | VAL  | N-CA-CB    | 5.07  | 116.54      | 110.31   |
| 1   | B     | 456 | GLY  | CA-C-N     | -5.06 | 114.25      | 121.23   |
| 1   | B     | 456 | GLY  | C-N-CA     | -5.06 | 114.25      | 121.23   |
| 1   | A     | 375 | LYS  | CA-C-N     | -5.05 | 114.95      | 122.74   |
| 1   | A     | 375 | LYS  | C-N-CA     | -5.05 | 114.95      | 122.74   |
| 1   | A     | 2   | PHE  | N-CA-CB    | -5.05 | 103.76      | 110.57   |
| 1   | C     | 51  | LYS  | CA-C-N     | -5.04 | 113.54      | 119.84   |
| 1   | C     | 51  | LYS  | C-N-CA     | -5.04 | 113.54      | 119.84   |
| 1   | A     | 94  | LEU  | N-CA-C     | 5.03  | 117.49      | 111.71   |
| 1   | C     | 539 | MET  | N-CA-C     | -5.03 | 105.46      | 112.45   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 375 | LYS  | N-CA-C  | 5.02  | 118.39      | 109.96   |
| 1   | A     | 81  | GLU  | CB-CA-C | 5.02  | 118.78      | 109.54   |
| 1   | C     | 37  | GLU  | CA-C-N  | -5.02 | 116.10      | 122.77   |
| 1   | C     | 37  | GLU  | C-N-CA  | -5.02 | 116.10      | 122.77   |

There are no chirality outliers.

All (7) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 554 | ALA  | Peptide |
| 1   | A     | 8   | THR  | Peptide |
| 1   | B     | 554 | ALA  | Peptide |
| 1   | B     | 6   | ARG  | Peptide |
| 1   | B     | 9   | ILE  | Peptide |
| 1   | C     | 35  | MET  | Peptide |
| 2   | F     | 892 | ARG  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 4248  | 0        | 4212     | 290     | 1            |
| 1   | B     | 4170  | 0        | 4161     | 275     | 1            |
| 1   | C     | 3836  | 0        | 3670     | 190     | 2            |
| 2   | F     | 66    | 0        | 58       | 2       | 0            |
| 2   | G     | 77    | 0        | 70       | 3       | 0            |
| 2   | H     | 42    | 0        | 26       | 1       | 0            |
| 3   | A     | 5     | 0        | 0        | 1       | 0            |
| 3   | B     | 5     | 0        | 0        | 1       | 0            |
| 3   | C     | 5     | 0        | 0        | 1       | 0            |
| 4   | A     | 96    | 0        | 0        | 6       | 0            |
| 4   | B     | 80    | 0        | 0        | 1       | 0            |
| 4   | C     | 24    | 0        | 0        | 3       | 0            |
| 4   | G     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 12655 | 0        | 12197    | 750     | 2            |

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 30.

All (750) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:287:PRO:HB2 | 1:A:288:THR:CG2  | 1.29                     | 1.60              |
| 1:A:287:PRO:CB  | 1:A:288:THR:CG2  | 1.84                     | 1.53              |
| 1:A:282:LEU:HA  | 1:A:292:PRO:CG   | 1.44                     | 1.43              |
| 1:A:281:GLY:CA  | 1:A:289:GLY:O    | 1.68                     | 1.37              |
| 1:A:493:MET:CE  | 1:A:509:MET:HE3  | 1.55                     | 1.34              |
| 1:B:274:LYS:HA  | 1:B:277:ILE:CG2  | 1.57                     | 1.34              |
| 1:B:291:ASP:O   | 1:B:293:LEU:N    | 1.61                     | 1.29              |
| 1:A:282:LEU:CA  | 1:A:292:PRO:HG3  | 1.66                     | 1.25              |
| 1:A:287:PRO:CB  | 1:A:288:THR:HG22 | 1.56                     | 1.21              |
| 1:A:464:SER:CB  | 1:A:539:MET:HE1  | 1.71                     | 1.21              |
| 1:B:278:ALA:O   | 1:B:282:LEU:HD23 | 1.37                     | 1.18              |
| 1:A:274:LYS:O   | 1:A:277:ILE:HG22 | 1.43                     | 1.14              |
| 1:A:274:LYS:HE2 | 1:A:274:LYS:HA   | 1.29                     | 1.13              |
| 1:A:277:ILE:O   | 1:A:282:LEU:HD12 | 1.46                     | 1.13              |
| 1:A:277:ILE:C   | 1:A:282:LEU:HD12 | 1.71                     | 1.13              |
| 1:B:279:ALA:O   | 1:B:282:LEU:CD2  | 1.97                     | 1.13              |
| 1:A:287:PRO:CB  | 1:A:288:THR:HG23 | 1.57                     | 1.13              |
| 1:B:274:LYS:CD  | 1:B:277:ILE:HG21 | 1.80                     | 1.12              |
| 1:B:274:LYS:CD  | 1:B:277:ILE:HD13 | 1.80                     | 1.12              |
| 1:A:287:PRO:CA  | 1:A:288:THR:CG2  | 2.28                     | 1.10              |
| 1:A:416:MET:HE2 | 1:A:500:THR:HG21 | 1.27                     | 1.10              |
| 1:A:543:MET:O   | 1:A:544:ASP:HB3  | 1.36                     | 1.09              |
| 1:B:279:ALA:O   | 1:B:282:LEU:HD21 | 1.53                     | 1.09              |
| 1:B:274:LYS:HA  | 1:B:277:ILE:HG22 | 1.30                     | 1.09              |
| 1:B:274:LYS:HA  | 1:B:277:ILE:HG21 | 1.28                     | 1.08              |
| 1:A:281:GLY:HA2 | 1:A:289:GLY:O    | 0.90                     | 1.08              |
| 1:A:464:SER:HB2 | 1:A:539:MET:HE1  | 1.36                     | 1.07              |
| 1:C:338:ARG:HA  | 1:C:553:PHE:HE1  | 1.05                     | 1.07              |
| 1:A:287:PRO:CA  | 1:A:288:THR:HG22 | 1.85                     | 1.06              |
| 1:B:287:PRO:HB2 | 1:B:288:THR:HA   | 1.08                     | 1.05              |
| 1:A:453:MET:HB3 | 1:A:543:MET:CE   | 1.86                     | 1.05              |
| 1:A:493:MET:HE1 | 1:A:509:MET:HE3  | 1.08                     | 1.04              |
| 1:C:249:VAL:CG1 | 1:C:272:ALA:HB1  | 1.87                     | 1.04              |
| 1:A:181:GLY:CA  | 1:A:212:MET:HE1  | 1.87                     | 1.03              |
| 1:A:493:MET:CE  | 1:A:509:MET:CE   | 2.36                     | 1.03              |
| 1:C:338:ARG:HA  | 1:C:553:PHE:CE1  | 1.93                     | 1.02              |
| 1:B:279:ALA:O   | 1:B:282:LEU:CG   | 2.07                     | 1.02              |
| 1:C:52:PRO:O    | 1:C:54:GLN:N     | 1.92                     | 1.01              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:303:GLU:O    | 1:B:306:VAL:HG12 | 1.61                     | 1.00              |
| 1:C:340:HIS:HD2  | 1:C:358:LEU:H    | 1.05                     | 0.98              |
| 1:A:381:HIS:HD2  | 1:A:428:ARG:NH1  | 1.62                     | 0.98              |
| 1:B:287:PRO:CB   | 1:B:288:THR:HA   | 1.94                     | 0.98              |
| 1:B:354:VAL:HG22 | 1:B:431:SER:HB2  | 1.42                     | 0.98              |
| 1:B:416:MET:CE   | 1:B:461:ARG:HB2  | 1.93                     | 0.97              |
| 1:C:128:ILE:HD11 | 1:C:153:ARG:HB2  | 1.44                     | 0.97              |
| 1:B:97:ARG:NH2   | 1:B:190:GLU:OE1  | 1.96                     | 0.97              |
| 1:A:340:HIS:HD2  | 1:A:358:LEU:H    | 1.13                     | 0.97              |
| 1:B:83:ARG:HB2   | 1:B:83:ARG:HH11  | 1.28                     | 0.97              |
| 1:B:275:LYS:O    | 1:B:277:ILE:N    | 1.97                     | 0.97              |
| 1:B:464:SER:HB2  | 1:B:539:MET:HE1  | 1.45                     | 0.97              |
| 1:A:381:HIS:CD2  | 1:A:428:ARG:HH11 | 1.82                     | 0.97              |
| 1:A:281:GLY:O    | 1:A:290:TYR:O    | 1.82                     | 0.97              |
| 1:A:54:GLN:O     | 1:A:55:ASP:HB2   | 1.62                     | 0.96              |
| 1:A:181:GLY:HA3  | 1:A:212:MET:HE1  | 1.46                     | 0.96              |
| 1:C:99:ILE:HG22  | 1:C:149:ILE:HD12 | 1.47                     | 0.96              |
| 1:B:263:GLN:HG3  | 1:B:264:ASP:H    | 1.28                     | 0.96              |
| 1:A:364:GLU:HG2  | 1:A:426:THR:HG21 | 1.47                     | 0.95              |
| 1:A:493:MET:HE3  | 1:A:509:MET:CE   | 1.97                     | 0.95              |
| 1:A:464:SER:HB3  | 1:A:539:MET:HE1  | 1.45                     | 0.94              |
| 1:A:287:PRO:HB3  | 1:A:288:THR:HG22 | 1.49                     | 0.93              |
| 1:B:364:GLU:OE1  | 1:B:375:LYS:HE3  | 1.68                     | 0.93              |
| 1:B:263:GLN:O    | 1:B:266:TYR:N    | 2.01                     | 0.93              |
| 1:B:93:ARG:HH11  | 1:B:404:GLY:HA3  | 1.34                     | 0.93              |
| 1:B:97:ARG:CZ    | 1:B:188:MET:HE3  | 1.97                     | 0.93              |
| 1:A:8:THR:O      | 1:A:9:ILE:HG12   | 1.68                     | 0.93              |
| 1:B:279:ALA:O    | 1:B:282:LEU:HG   | 1.66                     | 0.93              |
| 1:A:493:MET:HG3  | 1:A:511:ILE:HG13 | 1.52                     | 0.92              |
| 1:B:9:ILE:HG13   | 1:B:218:ALA:HB2  | 1.50                     | 0.92              |
| 1:A:452:MET:HE2  | 1:A:457:VAL:HG21 | 1.51                     | 0.92              |
| 1:B:181:GLY:CA   | 1:B:212:MET:HE1  | 2.00                     | 0.92              |
| 1:B:282:LEU:HB3  | 1:B:287:PRO:O    | 1.70                     | 0.92              |
| 1:C:39:VAL:HG12  | 1:C:119:GLN:HB3  | 1.53                     | 0.91              |
| 1:B:283:SER:HB2  | 1:B:287:PRO:HB3  | 1.52                     | 0.91              |
| 1:B:102:LEU:HD12 | 1:B:149:ILE:HD11 | 1.51                     | 0.91              |
| 1:A:60:THR:HG23  | 4:A:2012:HOH:O   | 1.69                     | 0.91              |
| 1:A:543:MET:O    | 1:A:544:ASP:CB   | 2.11                     | 0.91              |
| 1:C:67:THR:HG21  | 1:C:74:PRO:HG3   | 1.52                     | 0.91              |
| 1:A:276:ALA:O    | 1:A:280:LEU:CB   | 2.19                     | 0.91              |
| 1:B:287:PRO:HB2  | 1:B:288:THR:CA   | 1.99                     | 0.90              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:1:MET:HG2    | 1:B:22:ARG:HA    | 1.54                     | 0.90              |
| 1:C:94:LEU:HD12  | 1:C:97:ARG:NH2   | 1.87                     | 0.90              |
| 1:A:281:GLY:O    | 1:A:292:PRO:HD3  | 1.73                     | 0.89              |
| 1:C:249:VAL:HG13 | 1:C:272:ALA:HB1  | 1.54                     | 0.89              |
| 1:A:416:MET:CE   | 1:A:500:THR:HG21 | 2.03                     | 0.89              |
| 1:A:282:LEU:CA   | 1:A:292:PRO:CG   | 2.38                     | 0.89              |
| 1:B:284:ASP:HA   | 1:B:285:GLU:HB3  | 1.51                     | 0.89              |
| 1:A:274:LYS:HE2  | 1:A:277:ILE:HG21 | 1.52                     | 0.89              |
| 1:B:274:LYS:CA   | 1:B:277:ILE:CG2  | 2.47                     | 0.88              |
| 1:A:287:PRO:HB2  | 1:A:288:THR:HG23 | 0.89                     | 0.88              |
| 1:A:282:LEU:HA   | 1:A:292:PRO:HG2  | 1.56                     | 0.88              |
| 1:B:470:LEU:HD12 | 1:B:478:ALA:O    | 1.72                     | 0.88              |
| 1:A:416:MET:HE2  | 1:A:500:THR:CG2  | 2.03                     | 0.88              |
| 1:C:340:HIS:CD2  | 1:C:358:LEU:H    | 1.92                     | 0.88              |
| 1:B:275:LYS:HG2  | 1:B:276:ALA:N    | 1.87                     | 0.87              |
| 1:C:337:PRO:O    | 1:C:338:ARG:HB2  | 1.72                     | 0.87              |
| 1:B:427:ILE:HG21 | 1:B:452:MET:HE3  | 1.56                     | 0.87              |
| 1:A:287:PRO:HB2  | 1:A:288:THR:HG21 | 1.53                     | 0.87              |
| 1:B:93:ARG:NH1   | 1:B:404:GLY:HA3  | 1.88                     | 0.86              |
| 1:A:493:MET:HE1  | 1:A:509:MET:CE   | 2.00                     | 0.86              |
| 1:A:381:HIS:HD2  | 1:A:428:ARG:HH11 | 0.91                     | 0.86              |
| 1:C:493:MET:HE2  | 1:C:495:PHE:CD1  | 2.11                     | 0.86              |
| 1:A:416:MET:CE   | 1:A:461:ARG:HB2  | 2.06                     | 0.86              |
| 1:A:277:ILE:C    | 1:A:282:LEU:CD1  | 2.49                     | 0.85              |
| 1:B:274:LYS:CA   | 1:B:277:ILE:HG22 | 2.03                     | 0.85              |
| 1:C:39:VAL:CG1   | 1:C:119:GLN:HB3  | 2.05                     | 0.85              |
| 1:B:181:GLY:HA3  | 1:B:212:MET:HE1  | 1.58                     | 0.85              |
| 1:B:277:ILE:O    | 1:B:278:ALA:C    | 2.20                     | 0.85              |
| 1:A:274:LYS:C    | 1:A:277:ILE:HG22 | 2.00                     | 0.85              |
| 1:B:291:ASP:C    | 1:B:293:LEU:N    | 2.32                     | 0.85              |
| 1:B:275:LYS:HG2  | 1:B:276:ALA:H    | 1.39                     | 0.84              |
| 1:C:338:ARG:CA   | 1:C:553:PHE:HE1  | 1.87                     | 0.84              |
| 1:B:464:SER:CB   | 1:B:539:MET:HE1  | 2.06                     | 0.84              |
| 1:C:409:ALA:O    | 1:C:413:LEU:HG   | 1.77                     | 0.83              |
| 1:A:249:VAL:CG2  | 1:A:276:ALA:HB2  | 2.08                     | 0.82              |
| 1:A:502:GLU:OE2  | 1:B:529:LYS:HE2  | 1.78                     | 0.82              |
| 1:B:-1:ASP:HB3   | 1:B:0:PRO:HD3    | 1.61                     | 0.82              |
| 1:B:97:ARG:CZ    | 1:B:188:MET:CE   | 2.57                     | 0.82              |
| 1:A:493:MET:HE3  | 1:A:509:MET:HE3  | 1.53                     | 0.82              |
| 1:A:8:THR:HG22   | 1:A:9:ILE:HD13   | 1.59                     | 0.82              |
| 1:B:263:GLN:HG3  | 1:B:264:ASP:N    | 1.95                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:200:ILE:HD11 | 1:B:200:ILE:HD11 | 1.62                     | 0.81              |
| 1:A:276:ALA:O    | 1:A:280:LEU:HB3  | 1.80                     | 0.81              |
| 1:C:125:ASP:OD1  | 1:C:126:PRO:HD2  | 1.81                     | 0.81              |
| 1:C:131:MET:HE2  | 1:C:151:ALA:CB   | 2.11                     | 0.81              |
| 1:C:268:ALA:O    | 1:C:271:ALA:HB3  | 1.81                     | 0.81              |
| 1:A:453:MET:HB3  | 1:A:543:MET:HE3  | 1.62                     | 0.81              |
| 1:A:464:SER:HB2  | 1:A:539:MET:CE   | 2.10                     | 0.81              |
| 1:B:283:SER:HB2  | 1:B:287:PRO:CB   | 2.11                     | 0.81              |
| 1:A:177:LEU:HD12 | 1:A:191:SER:HB3  | 1.62                     | 0.81              |
| 1:B:275:LYS:C    | 1:B:277:ILE:H    | 1.87                     | 0.81              |
| 1:C:509:MET:HE1  | 1:C:521:MET:SD   | 2.21                     | 0.80              |
| 1:A:364:GLU:OE1  | 1:A:375:LYS:HE3  | 1.80                     | 0.80              |
| 1:B:309:ARG:HG3  | 1:B:309:ARG:HH11 | 1.46                     | 0.80              |
| 1:A:274:LYS:HA   | 1:A:274:LYS:CE   | 2.10                     | 0.80              |
| 1:B:277:ILE:HG23 | 1:B:278:ALA:H    | 1.46                     | 0.80              |
| 1:B:-1:ASP:HB3   | 1:B:0:PRO:CD     | 2.11                     | 0.80              |
| 1:C:338:ARG:HG2  | 1:C:553:PHE:CZ   | 2.17                     | 0.80              |
| 1:B:433:ILE:HD12 | 1:B:440:SER:HB2  | 1.63                     | 0.80              |
| 1:A:287:PRO:C    | 1:A:288:THR:HG23 | 2.07                     | 0.79              |
| 1:A:175:MET:HE3  | 1:A:196:LEU:HD12 | 1.64                     | 0.79              |
| 1:A:287:PRO:HA   | 1:A:288:THR:HG22 | 1.62                     | 0.79              |
| 1:C:381:HIS:HD2  | 1:C:428:ARG:HH11 | 1.30                     | 0.79              |
| 1:A:83:ARG:HG3   | 1:A:83:ARG:HH11  | 1.46                     | 0.79              |
| 1:C:131:MET:HE2  | 1:C:151:ALA:HB2  | 1.63                     | 0.79              |
| 1:A:276:ALA:O    | 1:A:280:LEU:HB2  | 1.81                     | 0.79              |
| 1:A:95:ILE:O     | 1:A:99:ILE:HG12  | 1.82                     | 0.79              |
| 1:B:338:ARG:HA   | 1:B:553:PHE:HE1  | 1.48                     | 0.79              |
| 1:B:249:VAL:O    | 1:B:253:ILE:HG12 | 1.82                     | 0.79              |
| 1:A:7:LYS:O      | 1:A:8:THR:C      | 2.26                     | 0.79              |
| 1:A:249:VAL:CG1  | 1:A:272:ALA:HB1  | 2.11                     | 0.79              |
| 1:A:287:PRO:CA   | 1:A:288:THR:HG23 | 2.00                     | 0.79              |
| 1:B:464:SER:HB2  | 1:B:539:MET:CE   | 2.12                     | 0.79              |
| 1:A:274:LYS:O    | 1:A:277:ILE:CG2  | 2.30                     | 0.78              |
| 1:B:278:ALA:O    | 1:B:282:LEU:CD2  | 2.28                     | 0.78              |
| 1:C:319:ASP:OD2  | 1:C:321:ARG:NH1  | 2.16                     | 0.78              |
| 1:B:274:LYS:CA   | 1:B:277:ILE:HG21 | 2.11                     | 0.77              |
| 1:A:277:ILE:HG12 | 1:A:282:LEU:HD11 | 1.64                     | 0.77              |
| 1:C:181:GLY:N    | 1:C:212:MET:HE1  | 2.00                     | 0.77              |
| 1:A:284:ASP:OD1  | 1:A:285:GLU:N    | 2.18                     | 0.77              |
| 1:A:282:LEU:HA   | 1:A:292:PRO:HG3  | 0.77                     | 0.77              |
| 1:C:249:VAL:CG2  | 1:C:276:ALA:HB2  | 2.15                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:291:ASP:O    | 1:B:292:PRO:C    | 2.27                     | 0.76              |
| 1:A:236:GLU:HB3  | 1:A:238:THR:HG23 | 1.66                     | 0.76              |
| 1:B:283:SER:CB   | 1:B:287:PRO:HB3  | 2.15                     | 0.76              |
| 1:A:83:ARG:HH11  | 1:A:83:ARG:CG    | 1.98                     | 0.75              |
| 1:B:416:MET:HE2  | 1:B:500:THR:HG21 | 1.68                     | 0.75              |
| 1:C:249:VAL:O    | 1:C:253:ILE:HG12 | 1.86                     | 0.75              |
| 1:C:383:ASN:O    | 1:C:433:ILE:HG12 | 1.86                     | 0.75              |
| 1:A:536:LEU:HA   | 1:A:539:MET:HE3  | 1.68                     | 0.75              |
| 1:A:401:ARG:NE   | 1:A:405:HIS:HE1  | 1.85                     | 0.75              |
| 1:A:308:ARG:O    | 1:A:312:LEU:HD12 | 1.87                     | 0.74              |
| 1:C:236:GLU:O    | 1:C:238:THR:N    | 2.20                     | 0.74              |
| 1:A:287:PRO:HB3  | 1:A:288:THR:CG2  | 2.07                     | 0.74              |
| 1:B:286:ASN:N    | 1:B:287:PRO:O    | 2.20                     | 0.74              |
| 1:C:99:ILE:HG22  | 1:C:149:ILE:CD1  | 2.16                     | 0.74              |
| 1:C:181:GLY:CA   | 1:C:212:MET:HE1  | 2.18                     | 0.74              |
| 1:A:340:HIS:CD2  | 1:A:358:LEU:H    | 2.01                     | 0.74              |
| 1:C:12:GLY:HA3   | 1:C:163:LEU:HD23 | 1.67                     | 0.74              |
| 1:A:202:LEU:HD11 | 1:A:525:LEU:HD12 | 1.70                     | 0.74              |
| 1:B:412:ALA:HA   | 1:B:505:THR:HG23 | 1.70                     | 0.74              |
| 1:A:417:LEU:CD2  | 1:A:452:MET:HE1  | 2.17                     | 0.74              |
| 1:A:281:GLY:O    | 1:A:292:PRO:CD   | 2.35                     | 0.74              |
| 1:B:290:TYR:O    | 1:B:292:PRO:N    | 2.21                     | 0.74              |
| 1:A:181:GLY:N    | 1:A:212:MET:HE1  | 2.03                     | 0.73              |
| 1:C:536:LEU:HA   | 1:C:539:MET:HE2  | 1.70                     | 0.73              |
| 1:A:249:VAL:HG11 | 1:A:272:ALA:HB1  | 1.69                     | 0.73              |
| 1:C:67:THR:HG21  | 1:C:74:PRO:CG    | 2.19                     | 0.73              |
| 1:A:417:LEU:HD22 | 1:A:452:MET:HE1  | 1.71                     | 0.73              |
| 1:A:454:ASP:OD1  | 1:A:547:ARG:NH1  | 2.20                     | 0.73              |
| 1:A:303:GLU:O    | 1:A:307:VAL:HG23 | 1.88                     | 0.73              |
| 1:B:97:ARG:HD2   | 1:B:510:ASP:OD1  | 1.88                     | 0.73              |
| 1:B:83:ARG:HH11  | 1:B:83:ARG:CB    | 1.99                     | 0.73              |
| 1:A:499:GLY:HA2  | 1:A:505:THR:HB   | 1.71                     | 0.73              |
| 1:B:304:ALA:O    | 1:B:308:ARG:HG3  | 1.89                     | 0.73              |
| 1:A:8:THR:O      | 1:A:9:ILE:CG1    | 2.37                     | 0.72              |
| 1:B:417:LEU:CD2  | 1:B:452:MET:HE1  | 2.19                     | 0.72              |
| 1:B:337:PRO:O    | 1:B:338:ARG:HB2  | 1.90                     | 0.72              |
| 1:C:128:ILE:HD11 | 1:C:153:ARG:CB   | 2.17                     | 0.72              |
| 1:B:416:MET:CE   | 1:B:461:ARG:CB   | 2.67                     | 0.72              |
| 1:B:454:ASP:OD1  | 1:B:547:ARG:NH1  | 2.22                     | 0.72              |
| 1:B:253:ILE:CG2  | 1:B:306:VAL:HG11 | 2.20                     | 0.71              |
| 1:B:260:GLN:O    | 1:B:261:LYS:CB   | 2.35                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:176:ASP:O    | 1:B:191:SER:HA   | 1.90                     | 0.71              |
| 1:B:274:LYS:C    | 1:B:277:ILE:HG22 | 2.15                     | 0.71              |
| 1:A:401:ARG:CZ   | 1:A:405:HIS:HE1  | 2.05                     | 0.70              |
| 1:B:238:THR:O    | 1:B:241:ILE:HG22 | 1.91                     | 0.70              |
| 1:A:209:HIS:HD2  | 1:A:212:MET:HE2  | 1.56                     | 0.70              |
| 1:B:175:MET:SD   | 1:B:177:LEU:HD23 | 2.32                     | 0.70              |
| 1:B:416:MET:HE1  | 1:B:461:ARG:HB2  | 1.70                     | 0.70              |
| 1:B:439:SER:HA   | 3:B:1557:PO4:O4  | 1.91                     | 0.70              |
| 1:B:417:LEU:HD21 | 1:B:452:MET:HE1  | 1.74                     | 0.70              |
| 1:A:54:GLN:O     | 1:A:55:ASP:CB    | 2.36                     | 0.70              |
| 1:A:377:SER:HB2  | 1:A:426:THR:HG22 | 1.74                     | 0.69              |
| 1:A:493:MET:HE3  | 1:A:509:MET:HE2  | 1.73                     | 0.69              |
| 1:A:277:ILE:O    | 1:A:282:LEU:CD1  | 2.34                     | 0.69              |
| 1:C:249:VAL:HG11 | 1:C:272:ALA:HB1  | 1.72                     | 0.69              |
| 1:A:278:ALA:HA   | 1:A:282:LEU:HD13 | 1.74                     | 0.69              |
| 1:C:157:VAL:O    | 1:C:159:GLY:N    | 2.25                     | 0.69              |
| 1:C:452:MET:O    | 1:C:457:VAL:HG22 | 1.93                     | 0.69              |
| 1:B:277:ILE:HG23 | 1:B:278:ALA:N    | 2.08                     | 0.69              |
| 1:C:177:LEU:HD11 | 1:C:189:VAL:HG13 | 1.74                     | 0.69              |
| 1:B:261:LYS:O    | 1:B:262:LYS:O    | 2.11                     | 0.69              |
| 1:A:266:TYR:O    | 1:A:267:GLU:C    | 2.36                     | 0.68              |
| 1:C:8:THR:O      | 1:C:9:ILE:HB     | 1.93                     | 0.68              |
| 1:C:39:VAL:O     | 1:C:40:VAL:HG23  | 1.91                     | 0.68              |
| 1:C:109:ASN:N    | 1:C:109:ASN:HD22 | 1.91                     | 0.68              |
| 1:A:281:GLY:C    | 1:A:289:GLY:O    | 2.36                     | 0.68              |
| 1:A:433:ILE:HD12 | 1:A:440:SER:HB2  | 1.75                     | 0.68              |
| 1:B:275:LYS:CG   | 1:B:276:ALA:N    | 2.55                     | 0.68              |
| 1:C:364:GLU:OE2  | 1:C:375:LYS:HE3  | 1.93                     | 0.68              |
| 1:B:277:ILE:O    | 1:B:279:ALA:N    | 2.26                     | 0.68              |
| 1:C:94:LEU:HD12  | 1:C:97:ARG:HH21  | 1.56                     | 0.68              |
| 1:B:209:HIS:HD2  | 1:B:212:MET:HE2  | 1.58                     | 0.68              |
| 1:B:291:ASP:OD1  | 1:B:293:LEU:HB2  | 1.93                     | 0.68              |
| 1:B:364:GLU:OE1  | 1:B:375:LYS:CE   | 2.42                     | 0.68              |
| 1:A:275:LYS:HG2  | 1:A:276:ALA:N    | 2.09                     | 0.67              |
| 1:A:479:VAL:HG23 | 1:A:527:GLN:CD   | 2.19                     | 0.67              |
| 1:A:175:MET:HE3  | 1:A:196:LEU:CD1  | 2.24                     | 0.67              |
| 1:A:416:MET:HE1  | 1:A:461:ARG:HB2  | 1.77                     | 0.67              |
| 1:A:453:MET:CB   | 1:A:543:MET:CE   | 2.70                     | 0.67              |
| 1:A:153:ARG:HD3  | 1:A:176:ASP:OD1  | 1.95                     | 0.67              |
| 1:B:309:ARG:HG3  | 1:B:309:ARG:NH1  | 2.09                     | 0.67              |
| 1:B:97:ARG:NH2   | 1:B:188:MET:HE1  | 2.09                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:543:MET:HE1  | 1:C:547:ARG:CZ   | 2.25                     | 0.67              |
| 1:C:340:HIS:HB2  | 1:C:356:ALA:O    | 1.95                     | 0.67              |
| 1:C:417:LEU:HD22 | 1:C:452:MET:HE1  | 1.76                     | 0.66              |
| 1:A:401:ARG:HD2  | 4:A:2078:HOH:O   | 1.95                     | 0.66              |
| 1:B:263:GLN:O    | 1:B:267:GLU:N    | 2.26                     | 0.66              |
| 1:B:9:ILE:HG13   | 1:B:218:ALA:CB   | 2.26                     | 0.66              |
| 1:B:83:ARG:HB2   | 1:B:83:ARG:NH1   | 2.06                     | 0.66              |
| 1:B:97:ARG:NH1   | 1:B:188:MET:HE3  | 2.10                     | 0.66              |
| 1:A:401:ARG:NE   | 1:A:405:HIS:CE1  | 2.63                     | 0.66              |
| 1:C:338:ARG:HG2  | 1:C:553:PHE:HZ   | 1.60                     | 0.66              |
| 1:A:381:HIS:CD2  | 1:A:428:ARG:NH1  | 2.54                     | 0.65              |
| 1:B:97:ARG:NH1   | 1:B:188:MET:CE   | 2.59                     | 0.65              |
| 1:B:303:GLU:O    | 1:B:307:VAL:HG23 | 1.95                     | 0.65              |
| 1:A:249:VAL:HG21 | 1:A:276:ALA:HB2  | 1.76                     | 0.65              |
| 1:B:9:ILE:HG22   | 1:B:11:TRP:HB2   | 1.79                     | 0.65              |
| 1:C:249:VAL:HG12 | 1:C:253:ILE:HG12 | 1.79                     | 0.65              |
| 1:A:181:GLY:CA   | 1:A:212:MET:CE   | 2.72                     | 0.65              |
| 1:A:265:ARG:HH22 | 1:A:318:ILE:HA   | 1.61                     | 0.65              |
| 1:C:189:VAL:HG11 | 1:C:507:LEU:HD12 | 1.77                     | 0.64              |
| 1:A:277:ILE:HG12 | 1:A:282:LEU:CD1  | 2.27                     | 0.64              |
| 1:B:509:MET:HE3  | 1:B:511:ILE:HD11 | 1.80                     | 0.64              |
| 1:B:535:ILE:HG22 | 1:B:539:MET:HE3  | 1.79                     | 0.64              |
| 1:B:381:HIS:HD2  | 1:B:428:ARG:HE   | 1.45                     | 0.64              |
| 1:C:39:VAL:CG1   | 1:C:119:GLN:CB   | 2.76                     | 0.64              |
| 1:C:181:GLY:H    | 1:C:212:MET:HE1  | 1.63                     | 0.64              |
| 1:A:135:SER:HB2  | 1:A:149:ILE:HG12 | 1.80                     | 0.63              |
| 1:A:311:ILE:O    | 1:A:314:THR:O    | 2.16                     | 0.63              |
| 1:A:427:ILE:HD13 | 1:A:452:MET:CE   | 2.27                     | 0.63              |
| 1:A:502:GLU:O    | 4:A:2091:HOH:O   | 2.15                     | 0.63              |
| 1:B:286:ASN:HB2  | 1:B:287:PRO:O    | 1.98                     | 0.63              |
| 1:B:249:VAL:HG13 | 1:B:272:ALA:HB1  | 1.81                     | 0.63              |
| 1:B:535:ILE:HG22 | 1:B:539:MET:CE   | 2.27                     | 0.63              |
| 1:B:9:ILE:CG1    | 1:B:218:ALA:HB2  | 2.24                     | 0.62              |
| 1:C:417:LEU:CD2  | 1:C:452:MET:HE1  | 2.29                     | 0.62              |
| 1:B:468:MET:HB2  | 1:B:495:PHE:CE1  | 2.35                     | 0.62              |
| 1:C:40:VAL:HG22  | 1:C:117:VAL:HA   | 1.80                     | 0.62              |
| 1:C:175:MET:HB2  | 1:C:193:ILE:HG23 | 1.82                     | 0.62              |
| 1:C:468:MET:HB2  | 1:C:495:PHE:CE2  | 2.34                     | 0.62              |
| 1:A:509:MET:HE1  | 1:A:521:MET:SD   | 2.39                     | 0.62              |
| 1:B:303:GLU:O    | 1:B:306:VAL:CG1  | 2.44                     | 0.62              |
| 1:B:337:PRO:O    | 1:B:338:ARG:CB   | 2.42                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:260:GLN:O    | 1:A:261:LYS:C    | 2.42                     | 0.62              |
| 1:C:340:HIS:HD2  | 1:C:358:LEU:N    | 1.87                     | 0.61              |
| 1:A:262:LYS:O    | 1:A:263:GLN:C    | 2.42                     | 0.61              |
| 1:C:381:HIS:CD2  | 1:C:428:ARG:HD2  | 2.35                     | 0.61              |
| 1:A:427:ILE:HD13 | 1:A:452:MET:HE3  | 1.81                     | 0.61              |
| 1:B:442:MET:HA   | 1:B:445:VAL:HG13 | 1.81                     | 0.61              |
| 1:A:200:ILE:HD11 | 1:B:200:ILE:CD1  | 2.31                     | 0.61              |
| 1:A:236:GLU:C    | 1:A:238:THR:H    | 2.08                     | 0.61              |
| 1:B:303:GLU:C    | 1:B:306:VAL:HG12 | 2.23                     | 0.61              |
| 1:A:161:TYR:OH   | 1:A:203:GLY:HA3  | 2.00                     | 0.61              |
| 1:B:269:VAL:HG12 | 1:B:270:GLY:N    | 2.15                     | 0.61              |
| 1:B:381:HIS:CD2  | 1:B:428:ARG:HE   | 2.19                     | 0.61              |
| 1:C:423:PHE:CZ   | 1:C:457:VAL:HG12 | 2.35                     | 0.61              |
| 1:C:256:ALA:O    | 1:C:259:ILE:CB   | 2.49                     | 0.60              |
| 1:B:253:ILE:HG22 | 1:B:306:VAL:HG11 | 1.83                     | 0.60              |
| 1:A:495:PHE:HB3  | 1:A:509:MET:HG2  | 1.83                     | 0.60              |
| 1:C:337:PRO:O    | 1:C:338:ARG:CB   | 2.41                     | 0.60              |
| 1:A:249:VAL:HG23 | 1:A:276:ALA:HB2  | 1.83                     | 0.60              |
| 1:B:279:ALA:C    | 1:B:282:LEU:HD21 | 2.26                     | 0.60              |
| 1:B:259:ILE:O    | 1:B:265:ARG:NH1  | 2.34                     | 0.60              |
| 1:A:245:MET:CE   | 1:A:299:PHE:HA   | 2.31                     | 0.60              |
| 1:A:340:HIS:CE1  | 1:A:554:ALA:HB3  | 2.36                     | 0.60              |
| 1:B:181:GLY:N    | 1:B:212:MET:HE1  | 2.17                     | 0.60              |
| 1:A:238:THR:HG22 | 1:A:290:TYR:OH   | 2.02                     | 0.60              |
| 1:C:246:LYS:O    | 1:C:247:ASP:C    | 2.43                     | 0.60              |
| 1:A:364:GLU:HG2  | 1:A:426:THR:CG2  | 2.28                     | 0.59              |
| 1:B:3:ASP:O      | 1:B:4:ILE:HG13   | 2.01                     | 0.59              |
| 1:C:67:THR:HG21  | 1:C:74:PRO:CD    | 2.32                     | 0.59              |
| 1:A:304:ALA:O    | 1:A:308:ARG:HG3  | 2.03                     | 0.59              |
| 1:A:261:LYS:O    | 1:A:262:LYS:C    | 2.45                     | 0.59              |
| 1:B:287:PRO:HD2  | 1:B:288:THR:HG23 | 1.82                     | 0.59              |
| 1:C:543:MET:HE1  | 1:C:547:ARG:NH1  | 2.17                     | 0.59              |
| 1:B:275:LYS:C    | 1:B:277:ILE:N    | 2.53                     | 0.59              |
| 1:B:284:ASP:CA   | 1:B:285:GLU:HB3  | 2.29                     | 0.59              |
| 1:A:315:GLY:O    | 1:A:322:ASP:HA   | 2.03                     | 0.59              |
| 1:A:401:ARG:CZ   | 1:A:405:HIS:CE1  | 2.85                     | 0.59              |
| 1:C:264:ASP:O    | 1:C:267:GLU:N    | 2.36                     | 0.59              |
| 1:A:412:ALA:O    | 1:A:505:THR:HG21 | 2.03                     | 0.59              |
| 1:B:64:GLN:HE21  | 1:B:116:THR:HG23 | 1.68                     | 0.59              |
| 1:B:99:ILE:HD13  | 1:B:149:ILE:CD1  | 2.32                     | 0.58              |
| 1:C:550:VAL:HG21 | 1:C:555:PRO:HB3  | 1.85                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:1:MET:HE3    | 1:B:22:ARG:HG3   | 1.85                     | 0.58              |
| 1:B:274:LYS:CD   | 1:B:277:ILE:CG2  | 2.70                     | 0.58              |
| 1:B:260:GLN:HA   | 1:B:265:ARG:NH1  | 2.18                     | 0.58              |
| 1:B:470:LEU:HD13 | 1:B:479:VAL:HG13 | 1.85                     | 0.58              |
| 1:A:6:ARG:HD3    | 1:A:221:ASP:HB3  | 1.85                     | 0.58              |
| 1:C:67:THR:HG21  | 1:C:74:PRO:HD3   | 1.85                     | 0.58              |
| 1:C:531:GLY:HA3  | 4:C:2020:HOH:O   | 2.03                     | 0.58              |
| 1:A:275:LYS:O    | 1:A:278:ALA:N    | 2.36                     | 0.58              |
| 1:A:535:ILE:HG22 | 1:A:539:MET:HE2  | 1.86                     | 0.58              |
| 1:A:412:ALA:HA   | 1:A:505:THR:CG2  | 2.34                     | 0.58              |
| 1:A:83:ARG:HG3   | 1:A:83:ARG:NH1   | 2.12                     | 0.58              |
| 1:B:277:ILE:O    | 1:B:280:LEU:N    | 2.37                     | 0.58              |
| 1:B:253:ILE:HG21 | 1:B:306:VAL:HG11 | 1.84                     | 0.58              |
| 1:C:509:MET:CE   | 1:C:521:MET:SD   | 2.91                     | 0.58              |
| 1:B:303:GLU:HA   | 1:B:306:VAL:HG12 | 1.86                     | 0.57              |
| 1:A:176:ASP:O    | 1:A:191:SER:HA   | 2.04                     | 0.57              |
| 1:A:479:VAL:HG23 | 1:A:527:GLN:NE2  | 2.19                     | 0.57              |
| 1:B:4:ILE:HG22   | 1:B:222:LEU:HD11 | 1.87                     | 0.57              |
| 2:G:896:TRP:N    | 2:G:897:ARG:HA   | 2.19                     | 0.57              |
| 1:A:245:MET:HE1  | 1:A:299:PHE:CA   | 2.34                     | 0.57              |
| 1:B:499:GLY:HA2  | 1:B:505:THR:HB   | 1.87                     | 0.57              |
| 1:C:317:ARG:HG3  | 1:C:321:ARG:O    | 2.04                     | 0.57              |
| 1:A:200:ILE:CD1  | 1:B:200:ILE:HD11 | 2.32                     | 0.56              |
| 1:A:274:LYS:NZ   | 1:A:277:ILE:HD13 | 2.20                     | 0.56              |
| 1:A:333:VAL:HG11 | 1:A:543:MET:HG3  | 1.86                     | 0.56              |
| 1:C:93:ARG:HH12  | 1:C:401:ARG:HA   | 1.69                     | 0.56              |
| 1:B:414:ARG:N    | 1:B:415:PRO:CD   | 2.67                     | 0.56              |
| 1:A:277:ILE:HG23 | 1:A:278:ALA:N    | 2.20                     | 0.56              |
| 1:B:64:GLN:NE2   | 1:B:116:THR:HG23 | 2.20                     | 0.56              |
| 1:B:282:LEU:CB   | 1:B:287:PRO:O    | 2.50                     | 0.56              |
| 1:B:147:GLY:HA2  | 2:G:896:TRP:O    | 2.06                     | 0.56              |
| 1:A:125:ASP:OD1  | 1:A:126:PRO:HD2  | 2.05                     | 0.56              |
| 1:B:97:ARG:NH2   | 1:B:188:MET:CE   | 2.68                     | 0.56              |
| 1:A:285:GLU:O    | 1:A:286:ASN:ND2  | 2.40                     | 0.55              |
| 1:B:28:ASP:HB2   | 1:B:44:ALA:O     | 2.07                     | 0.55              |
| 1:B:282:LEU:HA   | 1:B:284:ASP:O    | 2.05                     | 0.55              |
| 1:B:293:LEU:C    | 1:B:295:LEU:H    | 2.14                     | 0.55              |
| 1:B:315:GLY:O    | 1:B:322:ASP:HA   | 2.07                     | 0.55              |
| 1:A:266:TYR:O    | 1:A:269:VAL:N    | 2.39                     | 0.55              |
| 1:B:291:ASP:O    | 1:B:293:LEU:CA   | 2.52                     | 0.55              |
| 1:C:333:VAL:HG11 | 1:C:543:MET:CE   | 2.37                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:310:GLY:O    | 1:A:313:ASP:O    | 2.24                     | 0.55              |
| 1:C:439:SER:HB2  | 1:C:467:ALA:HB2  | 1.88                     | 0.55              |
| 1:C:86:GLU:O     | 1:C:90:LEU:HB2   | 2.07                     | 0.55              |
| 1:B:284:ASP:HA   | 1:B:285:GLU:CB   | 2.16                     | 0.55              |
| 1:B:381:HIS:CD2  | 1:B:428:ARG:HH21 | 2.25                     | 0.55              |
| 1:C:493:MET:SD   | 1:C:516:ILE:HD13 | 2.47                     | 0.55              |
| 1:B:193:ILE:HD13 | 1:B:201:VAL:HG21 | 1.89                     | 0.55              |
| 1:A:277:ILE:CG2  | 1:A:278:ALA:N    | 2.70                     | 0.54              |
| 1:C:490:LEU:O    | 1:C:490:LEU:HG   | 2.06                     | 0.54              |
| 1:A:209:HIS:CD2  | 1:A:212:MET:HE2  | 2.38                     | 0.54              |
| 1:B:263:GLN:O    | 1:B:265:ARG:N    | 2.41                     | 0.54              |
| 1:C:416:MET:HE2  | 1:C:461:ARG:HB2  | 1.88                     | 0.54              |
| 1:B:439:SER:HB2  | 1:B:467:ALA:HB2  | 1.90                     | 0.54              |
| 1:C:370:LEU:C    | 1:C:372:GLY:H    | 2.15                     | 0.54              |
| 1:A:275:LYS:O    | 1:A:277:ILE:N    | 2.40                     | 0.54              |
| 1:A:261:LYS:O    | 1:A:262:LYS:O    | 2.25                     | 0.54              |
| 1:B:102:LEU:CD1  | 1:B:149:ILE:HD11 | 2.33                     | 0.54              |
| 1:B:286:ASN:H    | 1:B:287:PRO:C    | 2.14                     | 0.54              |
| 1:A:249:VAL:HG21 | 1:A:276:ALA:CB   | 2.38                     | 0.54              |
| 1:A:368:ASP:N    | 1:A:368:ASP:OD1  | 2.37                     | 0.54              |
| 1:C:36:GLY:O     | 1:C:37:GLU:HB2   | 2.08                     | 0.54              |
| 1:C:98:PRO:HD3   | 1:C:188:MET:HG2  | 1.89                     | 0.54              |
| 1:A:281:GLY:N    | 1:A:289:GLY:O    | 2.39                     | 0.54              |
| 1:A:431:SER:OG   | 1:A:444:THR:CG2  | 2.56                     | 0.54              |
| 1:C:377:SER:HA   | 1:C:426:THR:HG23 | 1.89                     | 0.54              |
| 1:B:100:ARG:HB3  | 1:B:101:PRO:HD3  | 1.90                     | 0.54              |
| 1:C:20:THR:HG21  | 1:C:140:LEU:HD21 | 1.89                     | 0.54              |
| 1:A:127:ASP:OD1  | 1:A:128:ILE:N    | 2.41                     | 0.54              |
| 1:A:427:ILE:HG21 | 1:A:452:MET:HE3  | 1.90                     | 0.54              |
| 1:A:263:GLN:O    | 1:A:264:ASP:C    | 2.52                     | 0.53              |
| 1:C:330:LEU:O    | 1:C:346:THR:HG22 | 2.09                     | 0.53              |
| 1:A:274:LYS:HA   | 1:A:277:ILE:HG21 | 1.91                     | 0.53              |
| 1:A:529:LYS:HE2  | 1:B:502:GLU:OE2  | 2.08                     | 0.53              |
| 1:C:22:ARG:HG2   | 1:C:23:ILE:HG13  | 1.91                     | 0.53              |
| 1:C:333:VAL:HG11 | 1:C:543:MET:HE3  | 1.89                     | 0.53              |
| 1:B:246:LYS:O    | 1:B:250:GLY:N    | 2.41                     | 0.53              |
| 1:C:93:ARG:NH1   | 1:C:401:ARG:HA   | 2.24                     | 0.53              |
| 1:A:245:MET:HE3  | 1:A:299:PHE:HA   | 1.90                     | 0.53              |
| 1:B:551:GLY:O    | 1:B:552:ASP:C    | 2.51                     | 0.53              |
| 1:B:8:THR:O      | 1:B:9:ILE:C      | 2.48                     | 0.53              |
| 1:B:145:PHE:HZ   | 1:B:149:ILE:HD12 | 1.74                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:470:LEU:HD13 | 1:B:479:VAL:CG1  | 2.39                     | 0.53              |
| 1:B:493:MET:HE3  | 1:B:509:MET:HE3  | 1.90                     | 0.53              |
| 1:C:32:LEU:HD11  | 1:C:39:VAL:CG2   | 2.39                     | 0.53              |
| 1:A:195:GLU:HA   | 1:A:504:LEU:O    | 2.09                     | 0.53              |
| 1:A:287:PRO:HA   | 1:A:288:THR:CG2  | 2.25                     | 0.53              |
| 1:C:131:MET:HE2  | 1:C:151:ALA:HB1  | 1.91                     | 0.53              |
| 1:A:401:ARG:CD   | 4:A:2078:HOH:O   | 2.55                     | 0.53              |
| 1:A:329:ILE:CG1  | 1:A:347:ARG:HG3  | 2.39                     | 0.52              |
| 1:B:416:MET:HE2  | 1:B:461:ARG:CB   | 2.37                     | 0.52              |
| 1:C:259:ILE:O    | 1:C:260:GLN:O    | 2.27                     | 0.52              |
| 1:A:157:VAL:HG13 | 1:A:162:VAL:HG11 | 1.90                     | 0.52              |
| 1:A:509:MET:HE2  | 1:A:511:ILE:HD11 | 1.91                     | 0.52              |
| 1:B:313:ASP:O    | 1:B:314:THR:OG1  | 2.13                     | 0.52              |
| 1:C:531:GLY:O    | 1:C:534:HIS:HB3  | 2.09                     | 0.52              |
| 1:A:181:GLY:C    | 1:A:212:MET:CE   | 2.82                     | 0.52              |
| 1:A:274:LYS:CE   | 1:A:277:ILE:HG21 | 2.34                     | 0.52              |
| 1:B:193:ILE:HD13 | 1:B:201:VAL:CG2  | 2.39                     | 0.52              |
| 1:C:-1:ASP:O     | 1:C:0:PRO:C      | 2.49                     | 0.52              |
| 1:C:163:LEU:HD13 | 1:C:211:GLN:HG2  | 1.91                     | 0.52              |
| 1:A:253:ILE:HD11 | 1:A:299:PHE:HE1  | 1.75                     | 0.52              |
| 1:A:440:SER:O    | 1:A:444:THR:HG23 | 2.10                     | 0.52              |
| 1:A:8:THR:C      | 1:A:9:ILE:HD13   | 2.35                     | 0.52              |
| 1:A:412:ALA:O    | 1:A:505:THR:CG2  | 2.58                     | 0.52              |
| 1:B:280:LEU:N    | 1:B:280:LEU:HD12 | 2.24                     | 0.51              |
| 1:B:317:ARG:HD2  | 1:B:487:GLU:OE2  | 2.11                     | 0.51              |
| 1:C:249:VAL:CG2  | 1:C:276:ALA:CB   | 2.88                     | 0.51              |
| 1:A:453:MET:HB3  | 1:A:543:MET:HE1  | 1.87                     | 0.51              |
| 1:A:479:VAL:CG2  | 1:A:527:GLN:OE1  | 2.58                     | 0.51              |
| 1:B:263:GLN:O    | 1:B:266:TYR:CA   | 2.58                     | 0.51              |
| 1:A:35:MET:HB2   | 1:A:129:LEU:HD13 | 1.92                     | 0.51              |
| 1:A:157:VAL:CG1  | 1:A:162:VAL:HG11 | 2.40                     | 0.51              |
| 1:A:429:LEU:HD21 | 1:A:452:MET:HG3  | 1.92                     | 0.51              |
| 1:A:502:GLU:OE2  | 1:B:529:LYS:CE   | 2.55                     | 0.51              |
| 1:A:175:MET:CE   | 1:A:196:LEU:HD12 | 2.39                     | 0.51              |
| 1:B:89:THR:HG23  | 1:B:400:ARG:HG2  | 1.93                     | 0.51              |
| 1:A:479:VAL:HG23 | 1:A:527:GLN:OE1  | 2.11                     | 0.51              |
| 1:B:298:ILE:N    | 1:B:298:ILE:HD13 | 2.25                     | 0.51              |
| 1:A:321:ARG:HB3  | 1:A:325:THR:HB   | 1.91                     | 0.51              |
| 1:B:261:LYS:C    | 1:B:262:LYS:O    | 2.52                     | 0.51              |
| 1:C:416:MET:CE   | 1:C:461:ARG:HB2  | 2.41                     | 0.51              |
| 1:A:28:ASP:HB2   | 1:A:44:ALA:O     | 2.10                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:260:GLN:O    | 1:A:261:LYS:O    | 2.28                     | 0.51              |
| 1:A:265:ARG:O    | 1:A:266:TYR:C    | 2.52                     | 0.51              |
| 1:C:551:GLY:O    | 1:C:552:ASP:C    | 2.52                     | 0.51              |
| 1:B:266:TYR:CD1  | 1:B:266:TYR:C    | 2.89                     | 0.50              |
| 1:A:265:ARG:O    | 1:A:266:TYR:O    | 2.29                     | 0.50              |
| 1:B:256:ALA:O    | 1:B:259:ILE:HB   | 2.11                     | 0.50              |
| 1:B:274:LYS:CD   | 1:B:277:ILE:CD1  | 2.72                     | 0.50              |
| 1:C:358:LEU:HD21 | 1:C:457:VAL:HG11 | 1.94                     | 0.50              |
| 1:C:39:VAL:HG13  | 1:C:119:GLN:HB3  | 1.90                     | 0.50              |
| 1:A:236:GLU:CB   | 1:A:238:THR:HG23 | 2.38                     | 0.50              |
| 1:B:311:ILE:O    | 1:B:314:THR:O    | 2.29                     | 0.50              |
| 1:B:416:MET:CE   | 1:B:500:THR:HG21 | 2.41                     | 0.50              |
| 1:C:249:VAL:HG22 | 1:C:276:ALA:HB2  | 1.91                     | 0.50              |
| 1:B:154:VAL:CG2  | 1:B:208:ALA:HB2  | 2.42                     | 0.50              |
| 1:C:329:ILE:CG1  | 1:C:347:ARG:HG3  | 2.41                     | 0.50              |
| 1:B:99:ILE:HD13  | 1:B:149:ILE:HD12 | 1.94                     | 0.50              |
| 1:C:340:HIS:HE1  | 1:C:554:ALA:H    | 1.59                     | 0.50              |
| 1:A:464:SER:CB   | 1:A:539:MET:CE   | 2.64                     | 0.50              |
| 1:A:523:GLN:O    | 1:A:526:ALA:N    | 2.44                     | 0.50              |
| 1:B:381:HIS:HD2  | 1:B:428:ARG:HH21 | 1.59                     | 0.50              |
| 1:C:439:SER:HA   | 3:C:1556:PO4:P   | 2.51                     | 0.50              |
| 1:A:401:ARG:HE   | 1:A:405:HIS:HE1  | 1.59                     | 0.50              |
| 1:A:535:ILE:HG22 | 1:A:539:MET:CE   | 2.42                     | 0.50              |
| 1:A:453:MET:CB   | 1:A:543:MET:HE2  | 2.42                     | 0.50              |
| 1:C:38:THR:OG1   | 1:C:121:ASP:N    | 2.34                     | 0.49              |
| 1:C:416:MET:CE   | 1:C:460:VAL:HB   | 2.42                     | 0.49              |
| 1:B:308:ARG:HB3  | 1:B:471:ILE:HG21 | 1.93                     | 0.49              |
| 1:C:39:VAL:HG13  | 1:C:119:GLN:CB   | 2.42                     | 0.49              |
| 1:A:275:LYS:C    | 1:A:277:ILE:N    | 2.70                     | 0.49              |
| 1:B:68:PHE:CD1   | 1:B:68:PHE:C     | 2.90                     | 0.49              |
| 1:A:7:LYS:C      | 1:A:8:THR:O      | 2.50                     | 0.49              |
| 1:A:245:MET:HE1  | 1:A:299:PHE:HA   | 1.95                     | 0.49              |
| 1:A:284:ASP:C    | 1:A:286:ASN:H    | 2.20                     | 0.49              |
| 1:B:35:MET:HE3   | 1:B:129:LEU:HB2  | 1.94                     | 0.49              |
| 1:B:9:ILE:HG21   | 1:B:16:LEU:HD23  | 1.93                     | 0.49              |
| 1:B:264:ASP:HA   | 1:B:267:GLU:CB   | 2.42                     | 0.49              |
| 1:C:237:ASP:C    | 1:C:239:ASP:H    | 2.19                     | 0.49              |
| 1:A:274:LYS:HA   | 1:A:277:ILE:CG2  | 2.43                     | 0.49              |
| 1:A:278:ALA:CA   | 1:A:282:LEU:HD13 | 2.42                     | 0.49              |
| 1:A:403:ILE:HA   | 4:A:2080:HOH:O   | 2.12                     | 0.49              |
| 1:A:340:HIS:HB2  | 1:A:356:ALA:O    | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:99:ILE:CG2   | 1:A:103:PHE:HE1  | 2.26                     | 0.48              |
| 1:A:460:VAL:O    | 1:A:461:ARG:HG3  | 2.13                     | 0.48              |
| 1:B:237:ASP:OD1  | 1:B:239:ASP:HB2  | 2.12                     | 0.48              |
| 1:B:279:ALA:C    | 1:B:280:LEU:HD12 | 2.37                     | 0.48              |
| 1:B:283:SER:N    | 1:B:284:ASP:C    | 2.71                     | 0.48              |
| 1:B:416:MET:HE2  | 1:B:500:THR:CG2  | 2.39                     | 0.48              |
| 1:B:446:CYS:SG   | 1:B:539:MET:HE2  | 2.53                     | 0.48              |
| 1:C:330:LEU:O    | 1:C:346:THR:CG2  | 2.61                     | 0.48              |
| 1:B:281:GLY:O    | 1:B:289:GLY:O    | 2.32                     | 0.48              |
| 1:C:193:ILE:CG2  | 1:C:196:LEU:HB2  | 2.43                     | 0.48              |
| 1:C:531:GLY:CA   | 4:C:2020:HOH:O   | 2.58                     | 0.48              |
| 1:A:377:SER:CB   | 1:A:426:THR:HG22 | 2.41                     | 0.48              |
| 1:B:209:HIS:CD2  | 1:B:212:MET:HE2  | 2.44                     | 0.48              |
| 1:A:165:PRO:HG2  | 1:A:170:MET:SD   | 2.53                     | 0.48              |
| 1:C:333:VAL:HG12 | 1:C:334:GLY:N    | 2.28                     | 0.48              |
| 1:A:245:MET:HE1  | 1:A:299:PHE:N    | 2.29                     | 0.48              |
| 1:A:414:ARG:N    | 1:A:415:PRO:HD2  | 2.28                     | 0.48              |
| 1:C:370:LEU:O    | 1:C:372:GLY:N    | 2.47                     | 0.48              |
| 1:C:468:MET:HB2  | 1:C:495:PHE:CZ   | 2.48                     | 0.48              |
| 1:A:313:ASP:O    | 1:A:314:THR:OG1  | 2.29                     | 0.48              |
| 1:C:195:GLU:OE2  | 1:C:461:ARG:NH1  | 2.47                     | 0.48              |
| 1:A:282:LEU:N    | 1:A:292:PRO:HG3  | 2.25                     | 0.47              |
| 1:B:468:MET:HB2  | 1:B:495:PHE:CZ   | 2.48                     | 0.47              |
| 1:A:220:ILE:HG12 | 2:F:896:TRP:CD1  | 2.50                     | 0.47              |
| 1:A:263:GLN:O    | 1:A:265:ARG:N    | 2.47                     | 0.47              |
| 1:B:4:ILE:HG22   | 1:B:222:LEU:CD1  | 2.43                     | 0.47              |
| 1:A:273:LYS:HB2  | 1:A:299:PHE:CE2  | 2.50                     | 0.47              |
| 1:A:335:ILE:HG13 | 1:A:336:LEU:N    | 2.28                     | 0.47              |
| 1:B:303:GLU:CA   | 1:B:306:VAL:HG12 | 2.43                     | 0.47              |
| 1:C:336:LEU:HB2  | 1:C:342:SER:HB3  | 1.97                     | 0.47              |
| 1:C:516:ILE:HG22 | 1:C:521:MET:HG3  | 1.96                     | 0.47              |
| 1:A:401:ARG:NH2  | 1:A:405:HIS:HE1  | 2.12                     | 0.47              |
| 1:C:464:SER:HB3  | 1:C:539:MET:HE1  | 1.95                     | 0.47              |
| 1:B:414:ARG:N    | 1:B:415:PRO:HD2  | 2.29                     | 0.47              |
| 1:C:346:THR:HB   | 1:C:351:GLN:HG3  | 1.96                     | 0.47              |
| 1:C:513:ILE:HD12 | 1:C:514:ALA:O    | 2.13                     | 0.47              |
| 1:A:277:ILE:HG23 | 1:A:282:LEU:HD11 | 1.96                     | 0.47              |
| 1:B:125:ASP:OD1  | 1:B:126:PRO:HD2  | 2.14                     | 0.47              |
| 1:B:295:LEU:HA   | 1:B:298:ILE:HG12 | 1.97                     | 0.47              |
| 1:B:543:MET:O    | 1:B:545:ALA:N    | 2.45                     | 0.47              |
| 1:C:54:GLN:NE2   | 1:C:56:PHE:CE1   | 2.82                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:197:SER:H    | 1:C:200:ILE:HD12 | 1.79                     | 0.47              |
| 1:C:338:ARG:HG2  | 1:C:553:PHE:CE1  | 2.50                     | 0.47              |
| 1:C:8:THR:O      | 1:C:9:ILE:CB     | 2.63                     | 0.47              |
| 1:C:65:GLU:HB3   | 1:C:370:LEU:HD11 | 1.95                     | 0.47              |
| 1:B:8:THR:HG23   | 1:B:9:ILE:H      | 1.80                     | 0.47              |
| 1:C:446:CYS:SG   | 4:C:2015:HOH:O   | 2.50                     | 0.46              |
| 1:B:99:ILE:O     | 1:B:100:ARG:C    | 2.58                     | 0.46              |
| 1:B:273:LYS:C    | 1:B:275:LYS:H    | 2.23                     | 0.46              |
| 1:A:0:PRO:O      | 1:A:1:MET:HB2    | 2.15                     | 0.46              |
| 1:B:274:LYS:CB   | 1:B:277:ILE:HG21 | 2.44                     | 0.46              |
| 1:B:279:ALA:C    | 1:B:282:LEU:CD2  | 2.79                     | 0.46              |
| 1:C:381:HIS:CD2  | 1:C:428:ARG:HH11 | 2.22                     | 0.46              |
| 1:C:418:PRO:HG3  | 1:C:458:PRO:HD2  | 1.96                     | 0.46              |
| 1:C:466:ILE:HG12 | 1:C:467:ALA:N    | 2.31                     | 0.46              |
| 1:A:9:ILE:HG22   | 1:A:11:TRP:HB2   | 1.98                     | 0.46              |
| 1:A:139:CYS:HA   | 4:A:2030:HOH:O   | 2.15                     | 0.46              |
| 1:B:89:THR:CG2   | 1:B:400:ARG:HG2  | 2.46                     | 0.46              |
| 1:B:207:PHE:O    | 1:B:211:GLN:HG2  | 2.15                     | 0.46              |
| 1:C:416:MET:HE3  | 1:C:460:VAL:HB   | 1.98                     | 0.46              |
| 1:A:8:THR:C      | 1:A:9:ILE:CG1    | 2.89                     | 0.46              |
| 1:B:280:LEU:N    | 1:B:280:LEU:CD1  | 2.79                     | 0.46              |
| 1:B:544:ASP:OD1  | 1:B:544:ASP:C    | 2.59                     | 0.46              |
| 1:A:109:ASN:N    | 1:A:109:ASN:HD22 | 2.14                     | 0.46              |
| 1:A:299:PHE:O    | 1:A:302:LEU:N    | 2.48                     | 0.46              |
| 1:C:163:LEU:O    | 1:C:164:ASN:C    | 2.59                     | 0.46              |
| 1:A:90:LEU:HD13  | 1:A:407:LYS:HG2  | 1.97                     | 0.46              |
| 1:C:127:ASP:OD1  | 1:C:128:ILE:N    | 2.47                     | 0.46              |
| 1:C:31:VAL:O     | 1:C:41:LEU:HD12  | 2.16                     | 0.46              |
| 1:A:181:GLY:O    | 1:A:212:MET:HE3  | 2.16                     | 0.46              |
| 1:B:55:ASP:OD1   | 1:B:55:ASP:N     | 2.48                     | 0.46              |
| 1:C:311:ILE:O    | 1:C:314:THR:O    | 2.33                     | 0.46              |
| 1:C:330:LEU:HB3  | 1:C:346:THR:HG23 | 1.98                     | 0.46              |
| 1:B:83:ARG:HH11  | 1:B:83:ARG:CG    | 2.28                     | 0.45              |
| 1:B:286:ASN:N    | 1:B:287:PRO:CA   | 2.79                     | 0.45              |
| 1:B:512:LYS:C    | 1:B:513:ILE:HG23 | 2.41                     | 0.45              |
| 1:B:127:ASP:O    | 1:B:131:MET:HG3  | 2.16                     | 0.45              |
| 1:A:74:PRO:O     | 1:A:79:LYS:HD3   | 2.16                     | 0.45              |
| 1:A:224:GLU:O    | 2:F:892:ARG:HD3  | 2.16                     | 0.45              |
| 1:A:9:ILE:HG13   | 1:A:218:ALA:HB2  | 1.98                     | 0.45              |
| 1:B:295:LEU:HG   | 1:B:295:LEU:O    | 2.16                     | 0.45              |
| 1:C:174:LYS:O    | 1:C:194:GLN:HG3  | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:61:VAL:HG22  | 1:B:113:VAL:CG1  | 2.47                     | 0.45              |
| 1:B:462:PRO:HB2  | 1:B:536:LEU:HD11 | 1.99                     | 0.45              |
| 1:C:157:VAL:C    | 1:C:159:GLY:H    | 2.24                     | 0.45              |
| 1:A:466:ILE:HD12 | 1:A:531:GLY:HA3  | 1.99                     | 0.45              |
| 1:B:3:ASP:HB2    | 4:B:2002:HOH:O   | 2.17                     | 0.45              |
| 1:A:373:THR:O    | 1:A:373:THR:CG2  | 2.63                     | 0.45              |
| 1:B:237:ASP:C    | 1:B:239:ASP:H    | 2.25                     | 0.45              |
| 1:B:260:GLN:HA   | 1:B:265:ARG:HH12 | 1.82                     | 0.45              |
| 1:A:14:LYS:HD3   | 1:A:124:ASN:OD1  | 2.17                     | 0.45              |
| 1:C:484:LEU:HB2  | 1:C:487:GLU:HG3  | 1.98                     | 0.45              |
| 1:A:179:VAL:HG12 | 1:A:180:ALA:N    | 2.32                     | 0.45              |
| 1:B:147:GLY:HA2  | 2:G:896:TRP:CA   | 2.47                     | 0.45              |
| 1:B:198:GLU:O    | 1:B:202:LEU:HB2  | 2.17                     | 0.45              |
| 1:B:273:LYS:O    | 1:B:275:LYS:N    | 2.50                     | 0.45              |
| 1:C:147:GLY:H    | 2:H:896:TRP:HA   | 1.82                     | 0.45              |
| 1:C:189:VAL:HB   | 1:C:509:MET:HB2  | 1.99                     | 0.45              |
| 1:A:202:LEU:HD23 | 1:A:202:LEU:HA   | 1.82                     | 0.45              |
| 1:A:414:ARG:N    | 1:A:415:PRO:CD   | 2.80                     | 0.45              |
| 1:B:414:ARG:C    | 1:B:416:MET:N    | 2.74                     | 0.45              |
| 1:A:236:GLU:O    | 1:A:238:THR:N    | 2.49                     | 0.44              |
| 1:B:286:ASN:N    | 1:B:287:PRO:HA   | 2.31                     | 0.44              |
| 1:C:44:ALA:HB1   | 1:C:138:LEU:HD23 | 1.99                     | 0.44              |
| 1:B:274:LYS:CG   | 1:B:277:ILE:HG21 | 2.46                     | 0.44              |
| 1:C:206:ASN:OD1  | 1:C:518:PRO:HG3  | 2.18                     | 0.44              |
| 1:A:420:LYS:HA   | 1:A:420:LYS:HD3  | 1.77                     | 0.44              |
| 1:C:157:VAL:C    | 1:C:159:GLY:N    | 2.75                     | 0.44              |
| 1:C:166:THR:HG23 | 1:C:169:GLU:OE2  | 2.18                     | 0.44              |
| 1:A:3:ASP:N      | 1:A:3:ASP:OD1    | 2.50                     | 0.44              |
| 1:A:266:TYR:O    | 1:A:268:ALA:N    | 2.51                     | 0.44              |
| 1:B:368:ASP:OD1  | 1:B:368:ASP:N    | 2.50                     | 0.44              |
| 1:C:39:VAL:C     | 1:C:40:VAL:HG23  | 2.41                     | 0.44              |
| 1:A:181:GLY:HA3  | 1:A:212:MET:CE   | 2.32                     | 0.44              |
| 1:B:63:TYR:HD2   | 1:B:115:VAL:HG22 | 1.82                     | 0.44              |
| 1:B:401:ARG:HH21 | 1:B:405:HIS:HE1  | 1.65                     | 0.44              |
| 1:B:94:LEU:HD12  | 1:B:94:LEU:HA    | 1.75                     | 0.44              |
| 1:B:401:ARG:NH2  | 1:B:405:HIS:HE1  | 2.14                     | 0.44              |
| 1:B:303:GLU:HA   | 1:B:306:VAL:CG1  | 2.48                     | 0.44              |
| 1:B:347:ARG:NH2  | 1:B:439:SER:O    | 2.51                     | 0.44              |
| 1:B:427:ILE:HD13 | 1:B:452:MET:CE   | 2.48                     | 0.44              |
| 1:A:1:MET:HG2    | 1:A:22:ARG:HA    | 1.99                     | 0.44              |
| 1:A:472:LEU:HD12 | 1:A:477:PHE:HB3  | 1.99                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:246:LYS:HA   | 1:B:302:LEU:HD21 | 2.00                     | 0.43              |
| 1:B:307:VAL:O    | 1:B:311:ILE:HG13 | 2.18                     | 0.43              |
| 1:C:414:ARG:C    | 1:C:416:MET:H    | 2.26                     | 0.43              |
| 1:C:427:ILE:HD13 | 1:C:452:MET:HE3  | 2.00                     | 0.43              |
| 1:A:7:LYS:O      | 1:A:9:ILE:N      | 2.50                     | 0.43              |
| 1:A:55:ASP:HB3   | 1:A:56:PHE:HD1   | 1.83                     | 0.43              |
| 1:A:177:LEU:CD1  | 1:A:191:SER:HB3  | 2.40                     | 0.43              |
| 1:A:285:GLU:C    | 1:A:286:ASN:ND2  | 2.76                     | 0.43              |
| 1:C:553:PHE:O    | 1:C:553:PHE:CD1  | 2.71                     | 0.43              |
| 1:B:248:LEU:HG   | 1:B:249:VAL:HG23 | 1.99                     | 0.43              |
| 1:B:296:GLY:O    | 1:B:297:ALA:C    | 2.61                     | 0.43              |
| 1:B:336:LEU:C    | 1:B:337:PRO:O    | 2.59                     | 0.43              |
| 1:C:246:LYS:O    | 1:C:250:GLY:N    | 2.50                     | 0.43              |
| 1:A:194:GLN:O    | 1:A:195:GLU:C    | 2.61                     | 0.43              |
| 1:C:181:GLY:C    | 1:C:212:MET:HE1  | 2.42                     | 0.43              |
| 1:C:198:GLU:OE2  | 1:C:532:ARG:NH2  | 2.47                     | 0.43              |
| 1:A:516:ILE:HG22 | 1:A:521:MET:HG2  | 2.01                     | 0.43              |
| 1:C:50:GLN:C     | 1:C:51:LYS:O     | 2.60                     | 0.43              |
| 1:A:275:LYS:CG   | 1:A:276:ALA:N    | 2.76                     | 0.43              |
| 1:B:263:GLN:CG   | 1:B:264:ASP:H    | 2.04                     | 0.43              |
| 1:B:277:ILE:C    | 1:B:279:ALA:N    | 2.76                     | 0.43              |
| 1:B:414:ARG:C    | 1:B:416:MET:H    | 2.26                     | 0.43              |
| 1:C:256:ALA:O    | 1:C:259:ILE:N    | 2.50                     | 0.43              |
| 1:C:345:PHE:O    | 1:C:351:GLN:HA   | 2.19                     | 0.43              |
| 1:A:281:GLY:C    | 1:A:292:PRO:HG3  | 2.43                     | 0.43              |
| 1:B:181:GLY:CA   | 1:B:212:MET:CE   | 2.87                     | 0.43              |
| 1:B:551:GLY:O    | 1:B:552:ASP:O    | 2.37                     | 0.43              |
| 1:C:329:ILE:HG13 | 1:C:347:ARG:HG3  | 2.00                     | 0.43              |
| 1:B:107:PHE:CZ   | 1:B:109:ASN:HB2  | 2.54                     | 0.43              |
| 1:B:282:LEU:C    | 1:B:284:ASP:C    | 2.86                     | 0.43              |
| 1:B:283:SER:N    | 1:B:285:GLU:N    | 2.67                     | 0.43              |
| 1:B:338:ARG:HA   | 1:B:553:PHE:CE1  | 2.38                     | 0.43              |
| 1:C:180:ALA:O    | 1:C:187:MET:N    | 2.42                     | 0.43              |
| 1:C:303:GLU:O    | 1:C:307:VAL:HG12 | 2.18                     | 0.43              |
| 1:C:339:THR:O    | 1:C:340:HIS:C    | 2.61                     | 0.43              |
| 1:C:262:LYS:O    | 1:C:263:GLN:C    | 2.62                     | 0.43              |
| 1:A:7:LYS:HG2    | 1:A:17:VAL:HG13  | 2.01                     | 0.42              |
| 1:A:181:GLY:C    | 1:A:212:MET:HE3  | 2.44                     | 0.42              |
| 1:B:65:GLU:HG3   | 1:B:88:GLU:HG2   | 2.01                     | 0.42              |
| 1:A:543:MET:O    | 1:A:545:ALA:N    | 2.44                     | 0.42              |
| 1:B:416:MET:HE2  | 1:B:461:ARG:HB3  | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:242:LYS:O    | 1:C:243:ALA:C    | 2.62                     | 0.42              |
| 1:C:329:ILE:HG12 | 1:C:347:ARG:HG3  | 2.01                     | 0.42              |
| 1:C:509:MET:HE3  | 1:C:511:ILE:HD11 | 2.01                     | 0.42              |
| 1:A:249:VAL:HG12 | 1:A:253:ILE:HG13 | 2.00                     | 0.42              |
| 1:A:280:LEU:C    | 1:A:282:LEU:H    | 2.27                     | 0.42              |
| 1:B:145:PHE:CZ   | 1:B:149:ILE:HD12 | 2.54                     | 0.42              |
| 1:B:381:HIS:HD2  | 1:B:428:ARG:NE   | 2.12                     | 0.42              |
| 1:B:395:MET:HE3  | 1:B:395:MET:HB3  | 1.96                     | 0.42              |
| 1:A:199:GLU:CD   | 1:A:199:GLU:H    | 2.26                     | 0.42              |
| 1:B:490:LEU:HG   | 1:B:490:LEU:O    | 2.20                     | 0.42              |
| 1:C:94:LEU:HD12  | 1:C:97:ARG:HH22  | 1.80                     | 0.42              |
| 1:C:466:ILE:CG1  | 1:C:467:ALA:N    | 2.83                     | 0.42              |
| 1:A:543:MET:HE3  | 1:A:543:MET:HB3  | 1.88                     | 0.42              |
| 1:B:109:ASN:N    | 1:B:109:ASN:HD22 | 2.17                     | 0.42              |
| 1:B:195:GLU:HA   | 1:B:504:LEU:O    | 2.19                     | 0.42              |
| 1:A:201:VAL:HG21 | 1:A:504:LEU:HD12 | 2.02                     | 0.42              |
| 1:B:286:ASN:CA   | 1:B:287:PRO:O    | 2.68                     | 0.42              |
| 1:B:477:PHE:CD1  | 1:B:477:PHE:C    | 2.98                     | 0.42              |
| 1:C:177:LEU:HD21 | 1:C:205:VAL:HG23 | 2.01                     | 0.42              |
| 1:C:361:GLY:O    | 1:C:364:GLU:HG2  | 2.20                     | 0.42              |
| 1:C:465:GLY:HA2  | 1:C:497:VAL:O    | 2.20                     | 0.42              |
| 1:A:246:LYS:O    | 1:A:247:ASP:C    | 2.62                     | 0.42              |
| 1:A:265:ARG:HH22 | 1:A:318:ILE:CA   | 2.32                     | 0.42              |
| 1:A:274:LYS:CE   | 1:A:274:LYS:CA   | 2.92                     | 0.42              |
| 1:C:128:ILE:CD1  | 1:C:153:ARG:CB   | 2.95                     | 0.42              |
| 1:A:121:ASP:O    | 1:A:122:LEU:HB2  | 2.20                     | 0.41              |
| 1:A:274:LYS:HZ1  | 1:A:277:ILE:HD13 | 1.85                     | 0.41              |
| 1:A:453:MET:C    | 1:A:543:MET:CE   | 2.93                     | 0.41              |
| 1:B:468:MET:CB   | 1:B:495:PHE:CZ   | 3.03                     | 0.41              |
| 1:C:189:VAL:HB   | 1:C:509:MET:CB   | 2.50                     | 0.41              |
| 1:C:370:LEU:C    | 1:C:372:GLY:N    | 2.78                     | 0.41              |
| 1:A:1:MET:HB2    | 1:A:1:MET:HE2    | 1.92                     | 0.41              |
| 1:B:286:ASN:CA   | 1:B:287:PRO:C    | 2.93                     | 0.41              |
| 1:C:11:TRP:CZ3   | 1:C:215:VAL:HG21 | 2.56                     | 0.41              |
| 1:C:28:ASP:HB2   | 1:C:44:ALA:O     | 2.20                     | 0.41              |
| 1:C:453:MET:HG3  | 1:C:459:LEU:HD12 | 2.02                     | 0.41              |
| 1:A:512:LYS:C    | 1:A:513:ILE:HG23 | 2.46                     | 0.41              |
| 1:A:525:LEU:HD23 | 1:A:525:LEU:HA   | 1.81                     | 0.41              |
| 1:C:156:TRP:HA   | 1:C:160:ALA:O    | 2.19                     | 0.41              |
| 1:C:317:ARG:NH2  | 1:C:321:ARG:NH2  | 2.67                     | 0.41              |
| 1:A:192:GLU:C    | 1:A:193:ILE:HG13 | 2.46                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:286:ASN:H     | 1:B:287:PRO:HA   | 1.85                     | 0.41              |
| 1:C:163:LEU:HD22  | 1:C:211:GLN:HG2  | 2.02                     | 0.41              |
| 1:C:193:ILE:O     | 1:C:505:THR:HG22 | 2.20                     | 0.41              |
| 1:C:380:LEU:HD21  | 1:C:444:THR:HG21 | 2.01                     | 0.41              |
| 1:C:399:GLY:O     | 1:C:403:ILE:HG13 | 2.20                     | 0.41              |
| 1:A:135:SER:HB2   | 1:A:149:ILE:CG1  | 2.48                     | 0.41              |
| 1:B:35:MET:HB2    | 1:B:129:LEU:HD13 | 2.01                     | 0.41              |
| 1:B:287:PRO:CB    | 1:B:288:THR:CA   | 2.77                     | 0.41              |
| 1:B:553:PHE:HA    | 1:B:554:ALA:HA   | 1.72                     | 0.41              |
| 1:C:553:PHE:O     | 1:C:553:PHE:HD1  | 2.03                     | 0.41              |
| 1:B:263:GLN:C     | 1:B:265:ARG:N    | 2.77                     | 0.41              |
| 1:C:334:GLY:HA2   | 1:C:342:SER:OG   | 2.20                     | 0.41              |
| 1:A:127:ASP:OD1   | 1:A:128:ILE:HG12 | 2.21                     | 0.41              |
| 1:A:277:ILE:CG2   | 1:A:278:ALA:H    | 2.34                     | 0.41              |
| 1:A:401:ARG:NH2   | 1:A:405:HIS:CE1  | 2.87                     | 0.41              |
| 1:B:177:LEU:HD12  | 1:B:177:LEU:C    | 2.45                     | 0.41              |
| 1:A:253:ILE:HD11  | 1:A:299:PHE:CE1  | 2.53                     | 0.41              |
| 1:A:281:GLY:O     | 1:A:292:PRO:CG   | 2.69                     | 0.41              |
| 1:A:397[A]:SER:HA | 1:A:398:PRO:HD2  | 1.93                     | 0.41              |
| 1:B:296:GLY:C     | 1:B:298:ILE:N    | 2.78                     | 0.41              |
| 1:B:450:LEU:HD23  | 1:B:450:LEU:HA   | 1.94                     | 0.41              |
| 1:A:186:VAL:O     | 1:A:511:ILE:HD13 | 2.20                     | 0.41              |
| 1:A:281:GLY:O     | 1:A:292:PRO:HG3  | 2.21                     | 0.41              |
| 1:B:261:LYS:O     | 1:B:262:LYS:C    | 2.63                     | 0.41              |
| 1:B:273:LYS:HD2   | 1:B:299:PHE:CD2  | 2.55                     | 0.41              |
| 1:C:261:LYS:O     | 1:C:262:LYS:C    | 2.64                     | 0.41              |
| 1:A:28:ASP:HB3    | 1:A:141:SER:HB2  | 2.03                     | 0.41              |
| 1:A:147:GLY:HA3   | 1:A:148:PRO:HA   | 1.86                     | 0.41              |
| 1:A:538:GLU:HA    | 1:A:541:LYS:HD2  | 2.03                     | 0.41              |
| 1:B:286:ASN:H     | 1:B:287:PRO:CA   | 2.34                     | 0.41              |
| 1:C:46:PHE:CB     | 1:C:111:VAL:HG22 | 2.51                     | 0.41              |
| 1:C:177:LEU:HD21  | 1:C:205:VAL:CG2  | 2.51                     | 0.41              |
| 1:C:381:HIS:HD2   | 1:C:428:ARG:HD2  | 1.80                     | 0.41              |
| 1:A:99:ILE:O      | 1:A:100:ARG:C    | 2.62                     | 0.40              |
| 1:A:495:PHE:CZ    | 1:A:524:ALA:HB1  | 2.56                     | 0.40              |
| 1:B:263:GLN:CG    | 1:B:264:ASP:N    | 2.70                     | 0.40              |
| 1:A:308:ARG:NH2   | 1:A:473:GLU:OE2  | 2.55                     | 0.40              |
| 1:B:146:MET:C     | 1:B:147:GLY:O    | 2.61                     | 0.40              |
| 1:B:191:SER:OG    | 1:B:507:LEU:O    | 2.40                     | 0.40              |
| 1:B:308:ARG:CZ    | 1:B:471:ILE:HG23 | 2.51                     | 0.40              |
| 1:C:256:ALA:HB1   | 1:C:268:ALA:HB3  | 2.02                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:99:ILE:HD13  | 1:B:99:ILE:HA    | 1.91                     | 0.40              |
| 1:C:256:ALA:HB2  | 1:C:268:ALA:HB1  | 2.03                     | 0.40              |
| 1:A:279:ALA:O    | 1:A:280:LEU:HD22 | 2.21                     | 0.40              |
| 1:A:439:SER:HA   | 3:A:1614:PO4:O1  | 2.22                     | 0.40              |
| 1:A:464:SER:HB3  | 1:A:539:MET:CE   | 2.33                     | 0.40              |
| 1:B:15:THR:O     | 1:B:35:MET:HA    | 2.21                     | 0.40              |
| 1:B:238:THR:HG22 | 1:B:290:TYR:OH   | 2.22                     | 0.40              |
| 1:C:256:ALA:CB   | 1:C:268:ALA:HB1  | 2.51                     | 0.40              |
| 1:C:274:LYS:O    | 1:C:277:ILE:CB   | 2.70                     | 0.40              |
| 1:A:291:ASP:O    | 1:A:294:LYS:HB3  | 2.21                     | 0.40              |
| 1:B:335:ILE:HG13 | 1:B:342:SER:OG   | 2.21                     | 0.40              |
| 1:B:349:GLU:OE1  | 1:B:437:ASN:ND2  | 2.54                     | 0.40              |
| 1:C:313:ASP:C    | 1:C:314:THR:O    | 2.63                     | 0.40              |
| 1:C:333:VAL:HG13 | 1:C:454:ASP:HB2  | 2.03                     | 0.40              |
| 1:C:517:THR:OG1  | 1:C:520:ILE:HG12 | 2.21                     | 0.40              |

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

| Atom-1        | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|------------------------|--------------------------|-------------------|
| 1:A:8:THR:OG1 | 1:C:540:ASN:O[2_555]   | 1.87                     | 0.33              |
| 1:B:6:ARG:NH2 | 1:C:224:GLU:OE2[3_565] | 2.10                     | 0.10              |

## 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     | 570/726 (78%) | 502 (88%) | 37 (6%) | 31 (5%)  | <b>1</b> <b>1</b> |
| 1   | B     | 556/726 (77%) | 490 (88%) | 41 (7%) | 25 (4%)  | <b>2</b> <b>2</b> |
| 1   | C     | 535/726 (74%) | 476 (89%) | 32 (6%) | 27 (5%)  | <b>1</b> <b>2</b> |
| 2   | F     | 5/14 (36%)    | 4 (80%)   | 0       | 1 (20%)  | <b>0</b> <b>0</b> |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 2   | G     | 6/14 (43%)      | 5 (83%)    | 0        | 1 (17%)  | 0           | 0   |
| 2   | H     | 3/14 (21%)      | 2 (67%)    | 1 (33%)  | 0        | 100         | 100 |
| All | All   | 1675/2220 (76%) | 1479 (88%) | 111 (7%) | 85 (5%)  | 1           | 2   |

All (85) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 9   | ILE  |
| 1   | A     | 55  | ASP  |
| 1   | A     | 239 | ASP  |
| 1   | A     | 248 | LEU  |
| 1   | A     | 262 | LYS  |
| 1   | A     | 263 | GLN  |
| 1   | A     | 266 | TYR  |
| 1   | A     | 275 | LYS  |
| 1   | A     | 294 | LYS  |
| 1   | A     | 554 | ALA  |
| 1   | B     | 248 | LEU  |
| 1   | B     | 264 | ASP  |
| 1   | B     | 276 | ALA  |
| 1   | B     | 278 | ALA  |
| 1   | B     | 287 | PRO  |
| 1   | B     | 290 | TYR  |
| 1   | B     | 291 | ASP  |
| 1   | B     | 292 | PRO  |
| 1   | B     | 552 | ASP  |
| 1   | B     | 554 | ALA  |
| 1   | C     | 8   | THR  |
| 1   | C     | 53  | GLY  |
| 1   | C     | 158 | ASP  |
| 1   | C     | 237 | ASP  |
| 1   | C     | 244 | LYS  |
| 1   | C     | 248 | LEU  |
| 1   | C     | 262 | LYS  |
| 1   | C     | 271 | ALA  |
| 1   | C     | 275 | LYS  |
| 1   | C     | 277 | ILE  |
| 1   | C     | 397 | SER  |
| 1   | C     | 544 | ASP  |
| 1   | A     | 54  | GLN  |
| 1   | A     | 246 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 261 | LYS  |
| 1   | A     | 264 | ASP  |
| 1   | A     | 267 | GLU  |
| 1   | A     | 276 | ALA  |
| 1   | A     | 278 | ALA  |
| 1   | A     | 284 | ASP  |
| 1   | A     | 318 | ILE  |
| 1   | A     | 396 | GLY  |
| 1   | B     | 261 | LYS  |
| 1   | B     | 262 | LYS  |
| 1   | B     | 269 | VAL  |
| 1   | B     | 273 | LYS  |
| 1   | B     | 274 | LYS  |
| 1   | B     | 277 | ILE  |
| 1   | B     | 396 | GLY  |
| 1   | B     | 439 | SER  |
| 1   | C     | 1   | MET  |
| 1   | C     | 9   | ILE  |
| 1   | C     | 36  | GLY  |
| 1   | C     | 52  | PRO  |
| 1   | C     | 260 | GLN  |
| 1   | C     | 261 | LYS  |
| 1   | C     | 263 | GLN  |
| 1   | C     | 371 | GLU  |
| 1   | C     | 439 | SER  |
| 1   | A     | 244 | LYS  |
| 1   | A     | 280 | LEU  |
| 1   | A     | 283 | SER  |
| 1   | A     | 290 | TYR  |
| 1   | B     | 279 | ALA  |
| 1   | B     | 285 | GLU  |
| 1   | B     | 371 | GLU  |
| 1   | C     | 246 | LYS  |
| 1   | B     | 294 | LYS  |
| 1   | C     | 245 | MET  |
| 1   | C     | 273 | LYS  |
| 1   | C     | 314 | THR  |
| 2   | G     | 894 | GLY  |
| 1   | A     | 237 | ASP  |
| 1   | A     | 292 | PRO  |
| 1   | A     | 439 | SER  |
| 1   | A     | 552 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 267 | GLU  |
| 1   | B     | 397 | SER  |
| 2   | F     | 892 | ARG  |
| 1   | A     | 1   | MET  |
| 1   | A     | 281 | GLY  |
| 1   | B     | 52  | PRO  |
| 1   | C     | 51  | LYS  |
| 1   | C     | 250 | GLY  |
| 1   | A     | 555 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |     |
|-----|-------|-----------------|------------|-----------|-------------|-----|
| 1   | A     | 432/578 (75%)   | 389 (90%)  | 43 (10%)  | 7           | 16  |
| 1   | B     | 428/578 (74%)   | 382 (89%)  | 46 (11%)  | 6           | 14  |
| 1   | C     | 364/578 (63%)   | 336 (92%)  | 28 (8%)   | 12          | 27  |
| 2   | F     | 5/12 (42%)      | 3 (60%)    | 2 (40%)   | 0           | 0   |
| 2   | G     | 6/12 (50%)      | 5 (83%)    | 1 (17%)   | 2           | 4   |
| 2   | H     | 2/12 (17%)      | 2 (100%)   | 0         | 100         | 100 |
| All | All   | 1237/1770 (70%) | 1117 (90%) | 120 (10%) | 8           | 17  |

All (120) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | -1  | ASP  |
| 1   | A     | 1   | MET  |
| 1   | A     | 3   | ASP  |
| 1   | A     | 7   | LYS  |
| 1   | A     | 14  | LYS  |
| 1   | A     | 35  | MET  |
| 1   | A     | 54  | GLN  |
| 1   | A     | 55  | ASP  |
| 1   | A     | 60  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 80  | ARG  |
| 1   | A     | 81  | GLU  |
| 1   | A     | 83  | ARG  |
| 1   | A     | 94  | LEU  |
| 1   | A     | 114 | VAL  |
| 1   | A     | 132 | VAL  |
| 1   | A     | 140 | LEU  |
| 1   | A     | 153 | ARG  |
| 1   | A     | 157 | VAL  |
| 1   | A     | 162 | VAL  |
| 1   | A     | 178 | VAL  |
| 1   | A     | 186 | VAL  |
| 1   | A     | 199 | GLU  |
| 1   | A     | 200 | ILE  |
| 1   | A     | 221 | ASP  |
| 1   | A     | 239 | ASP  |
| 1   | A     | 274 | LYS  |
| 1   | A     | 280 | LEU  |
| 1   | A     | 282 | LEU  |
| 1   | A     | 283 | SER  |
| 1   | A     | 290 | TYR  |
| 1   | A     | 355 | VAL  |
| 1   | A     | 402 | GLU  |
| 1   | A     | 430 | VAL  |
| 1   | A     | 457 | VAL  |
| 1   | A     | 460 | VAL  |
| 1   | A     | 463 | VAL  |
| 1   | A     | 481 | SER  |
| 1   | A     | 490 | LEU  |
| 1   | A     | 505 | THR  |
| 1   | A     | 511 | ILE  |
| 1   | A     | 521 | MET  |
| 1   | A     | 543 | MET  |
| 1   | A     | 553 | PHE  |
| 1   | B     | -1  | ASP  |
| 1   | B     | 1   | MET  |
| 1   | B     | 4   | ILE  |
| 1   | B     | 8   | THR  |
| 1   | B     | 14  | LYS  |
| 1   | B     | 31  | VAL  |
| 1   | B     | 64  | GLN  |
| 1   | B     | 81  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 83  | ARG  |
| 1   | B     | 115 | VAL  |
| 1   | B     | 149 | ILE  |
| 1   | B     | 177 | LEU  |
| 1   | B     | 178 | VAL  |
| 1   | B     | 186 | VAL  |
| 1   | B     | 188 | MET  |
| 1   | B     | 194 | GLN  |
| 1   | B     | 200 | ILE  |
| 1   | B     | 202 | LEU  |
| 1   | B     | 242 | LYS  |
| 1   | B     | 269 | VAL  |
| 1   | B     | 290 | TYR  |
| 1   | B     | 293 | LEU  |
| 1   | B     | 298 | ILE  |
| 1   | B     | 308 | ARG  |
| 1   | B     | 309 | ARG  |
| 1   | B     | 333 | VAL  |
| 1   | B     | 335 | ILE  |
| 1   | B     | 336 | LEU  |
| 1   | B     | 355 | VAL  |
| 1   | B     | 367 | ILE  |
| 1   | B     | 368 | ASP  |
| 1   | B     | 431 | SER  |
| 1   | B     | 445 | VAL  |
| 1   | B     | 449 | SER  |
| 1   | B     | 457 | VAL  |
| 1   | B     | 461 | ARG  |
| 1   | B     | 471 | ILE  |
| 1   | B     | 489 | HIS  |
| 1   | B     | 496 | LYS  |
| 1   | B     | 505 | THR  |
| 1   | B     | 516 | ILE  |
| 1   | B     | 518 | PRO  |
| 1   | B     | 521 | MET  |
| 1   | B     | 543 | MET  |
| 1   | B     | 544 | ASP  |
| 1   | B     | 553 | PHE  |
| 1   | C     | 34  | THR  |
| 1   | C     | 38  | THR  |
| 1   | C     | 39  | VAL  |
| 1   | C     | 59  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 81  | GLU  |
| 1   | C     | 90  | LEU  |
| 1   | C     | 109 | ASN  |
| 1   | C     | 149 | ILE  |
| 1   | C     | 157 | VAL  |
| 1   | C     | 175 | MET  |
| 1   | C     | 188 | MET  |
| 1   | C     | 193 | ILE  |
| 1   | C     | 194 | GLN  |
| 1   | C     | 220 | ILE  |
| 1   | C     | 249 | VAL  |
| 1   | C     | 335 | ILE  |
| 1   | C     | 367 | ILE  |
| 1   | C     | 371 | GLU  |
| 1   | C     | 379 | LEU  |
| 1   | C     | 426 | THR  |
| 1   | C     | 434 | THR  |
| 1   | C     | 445 | VAL  |
| 1   | C     | 448 | SER  |
| 1   | C     | 496 | LYS  |
| 1   | C     | 497 | VAL  |
| 1   | C     | 523 | GLN  |
| 1   | C     | 530 | GLU  |
| 1   | C     | 534 | HIS  |
| 2   | F     | 892 | ARG  |
| 2   | F     | 897 | ARG  |
| 2   | G     | 892 | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 62  | ASN  |
| 1   | A     | 109 | ASN  |
| 1   | A     | 112 | GLN  |
| 1   | A     | 209 | HIS  |
| 1   | A     | 225 | HIS  |
| 1   | A     | 286 | ASN  |
| 1   | A     | 340 | HIS  |
| 1   | A     | 381 | HIS  |
| 1   | A     | 405 | HIS  |
| 1   | A     | 508 | GLN  |
| 1   | B     | 62  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 64  | GLN  |
| 1   | B     | 109 | ASN  |
| 1   | B     | 112 | GLN  |
| 1   | B     | 206 | ASN  |
| 1   | B     | 209 | HIS  |
| 1   | B     | 381 | HIS  |
| 1   | B     | 405 | HIS  |
| 1   | C     | 62  | ASN  |
| 1   | C     | 109 | ASN  |
| 1   | C     | 112 | GLN  |
| 1   | C     | 225 | HIS  |
| 1   | C     | 340 | HIS  |
| 1   | C     | 381 | HIS  |
| 1   | C     | 523 | 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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 | $\# Z  > 2$ |
| 3   | PO4  | B     | 1557 | -    | 4,4,4        | 0.73 | 0           | 6,6,6       | 0.81 | 0           |
| 3   | PO4  | A     | 1614 | -    | 4,4,4        | 0.92 | 0           | 6,6,6       | 1.37 | 1 (16%)     |
| 3   | PO4  | C     | 1556 | -    | 4,4,4        | 0.81 | 0           | 6,6,6       | 1.02 | 1 (16%)     |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|------|-------------|----------|
| 3   | A     | 1614 | PO4  | O4-P-O3 | 2.38 | 115.30      | 107.91   |
| 3   | C     | 1556 | PO4  | O4-P-O2 | 2.26 | 114.96      | 107.91   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | B     | 1557 | PO4  | 1       | 0            |
| 3   | A     | 1614 | PO4  | 1       | 0            |
| 3   | C     | 1556 | PO4  | 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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     | 573/726 (78%)   | -1.55  | 0 100 100    | 24, 34, 123, 161      | 1 (0%) |
| 1   | B     | 558/726 (76%)   | -1.58  | 0 100 100    | 24, 33, 109, 147      | 0      |
| 1   | C     | 539/726 (74%)   | -0.78  | 1 (0%) 91 90 | 53, 87, 184, 253      | 0      |
| 2   | F     | 7/14 (50%)      | -1.07  | 0 100 100    | 40, 67, 84, 94        | 0      |
| 2   | G     | 8/14 (57%)      | -1.30  | 0 100 100    | 37, 68, 86, 93        | 0      |
| 2   | H     | 5/14 (35%)      | -0.75  | 0 100 100    | 82, 97, 103, 107      | 0      |
| All | All   | 1690/2220 (76%) | -1.31  | 1 (0%) 92 90 | 24, 49, 135, 253      | 1 (0%) |

All (1) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 269 | VAL  | 2.5  |

### 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 oligosaccharides 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. 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  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 3   | PO4  | C     | 1556 | 5/5   | 0.98 | 0.10 | 86,89,109,117               | 0     |
| 3   | PO4  | B     | 1557 | 5/5   | 0.99 | 0.05 | 76,82,92,104                | 0     |
| 3   | PO4  | A     | 1614 | 5/5   | 0.99 | 0.04 | 58,60,69,75                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.