



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:00 am GMT

PDB ID : 3TPU  
Title : 42F3 p5E8/H2-Ld complex  
Authors : Adams, J.J.; Kranz, D.M.; Garcia, K.C.  
Deposited on : 2011-09-08  
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

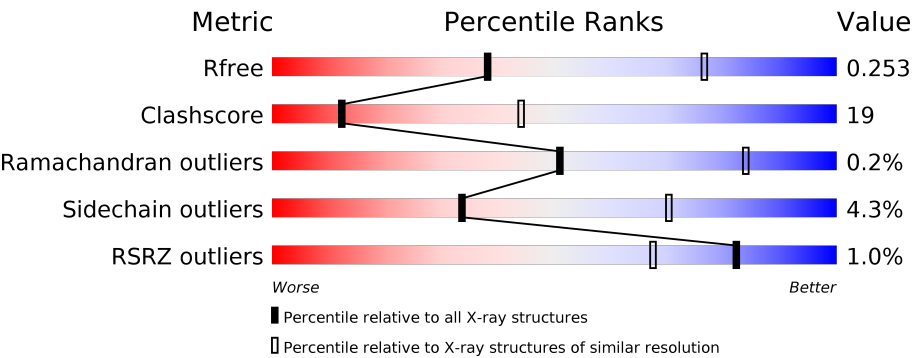
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 100719                      | 1001 (3.12-3.08)                                      |
| Clashscore            | 112137                      | 1099 (3.12-3.08)                                      |
| Ramachandran outliers | 110173                      | 1057 (3.12-3.08)                                      |
| Sidechain outliers    | 110143                      | 1057 (3.12-3.08)                                      |
| RSRZ outliers         | 101464                      | 1006 (3.12-3.08)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                              |
|-----|-------|--------|-----------------------------------------------|
| 1   | A     | 211    | <div><div></div><div>58%35% . .</div></div>   |
| 1   | C     | 211    | <div><div>%</div><div>60%35% . .</div></div>  |
| 1   | G     | 211    | <div><div>3%</div><div>63%31% . .</div></div> |
| 1   | M     | 211    | <div><div>2%</div><div>57%37% . .</div></div> |
| 2   | B     | 243    | <div><div></div><div>73%25% ..</div></div>    |
| 2   | D     | 243    | <div><div></div><div>69%28% ..</div></div>    |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | H     | 243    |                  |
| 2   | N     | 243    |                  |
| 3   | E     | 180    |                  |
| 3   | I     | 180    |                  |
| 3   | K     | 180    |                  |
| 3   | Q     | 180    |                  |
| 4   | F     | 9      |                  |
| 4   | J     | 9      |                  |
| 4   | L     | 9      |                  |
| 4   | R     | 9      |                  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 5   | SO4  | B     | 244 | -         | -        | -       | X                |
| 5   | SO4  | E     | 180 | -         | -        | X       | -                |
| 5   | SO4  | N     | 243 | -         | -        | X       | -                |

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20148 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 42F3 alpha.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1595  | 1007 | 264 | 316 | 8 |         |         |       |
| 1   | C     | 204      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1584  | 1000 | 262 | 314 | 8 |         |         |       |
| 1   | G     | 202      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1573  | 994  | 261 | 310 | 8 |         |         |       |
| 1   | M     | 204      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1587  | 1001 | 263 | 315 | 8 |         |         |       |

- Molecule 2 is a protein called 42F3 beta.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | B     | 240      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1900  | 1197 | 330 | 367 | 6 |         |         |       |
| 2   | D     | 240      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1900  | 1197 | 330 | 367 | 6 |         |         |       |
| 2   | H     | 240      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1900  | 1197 | 330 | 367 | 6 |         |         |       |
| 2   | N     | 240      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1900  | 1197 | 330 | 367 | 6 |         |         |       |

- Molecule 3 is a protein called H2-Ld SBM2.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3   | I     | 173      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1436  | 900 | 255 | 274 | 7 |         |         |       |
| 3   | E     | 175      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1449  | 907 | 258 | 277 | 7 |         |         |       |
| 3   | K     | 175      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1448  | 908 | 257 | 276 | 7 |         |         |       |
| 3   | Q     | 176      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1453  | 911 | 258 | 277 | 7 |         |         |       |

- Molecule 4 is a protein called p5E8 peptide.

| Mol | Chain | Residues | Atoms |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|---------|-------|
| 4   | J     | 9        | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 85    | 62 | 10 | 13 |         |         |       |
| 4   | F     | 9        | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 85    | 62 | 10 | 13 |         |         |       |
| 4   | L     | 9        | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 85    | 62 | 10 | 13 |         |         |       |
| 4   | R     | 9        | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 85    | 62 | 10 | 13 |         |         |       |

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 5   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | D     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | D     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 5   | G     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | K     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | K     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | N     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | N     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 5   | Q     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



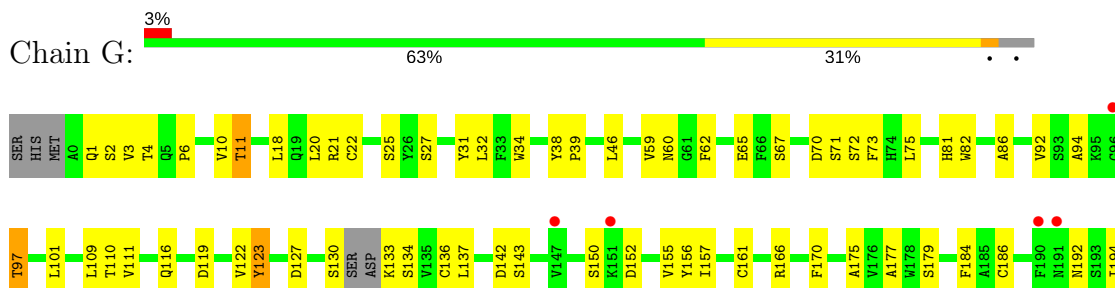
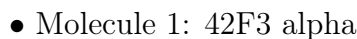
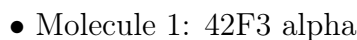
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 6   | N     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |

- Molecule 7 is water.

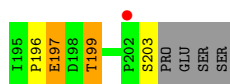
| Mol | Chain | Residues | Atoms      |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 7   | I     | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 7   | H     | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 7   | K     | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 7   | N     | 1        | Total<br>1 | O<br>1 | 0       | 0       |



- Molecule 1: 42F3 alpha



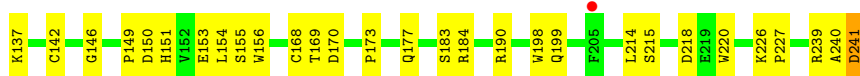




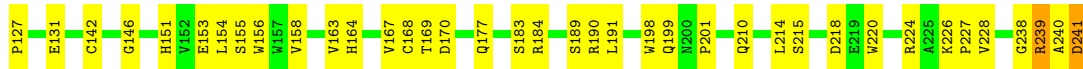
• Molecule 1: 42F3 alpha



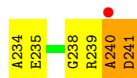
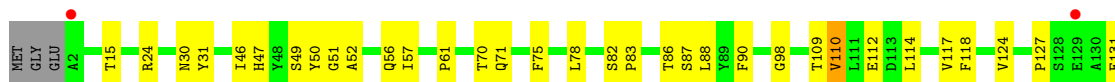
• Molecule 2: 42F3 beta



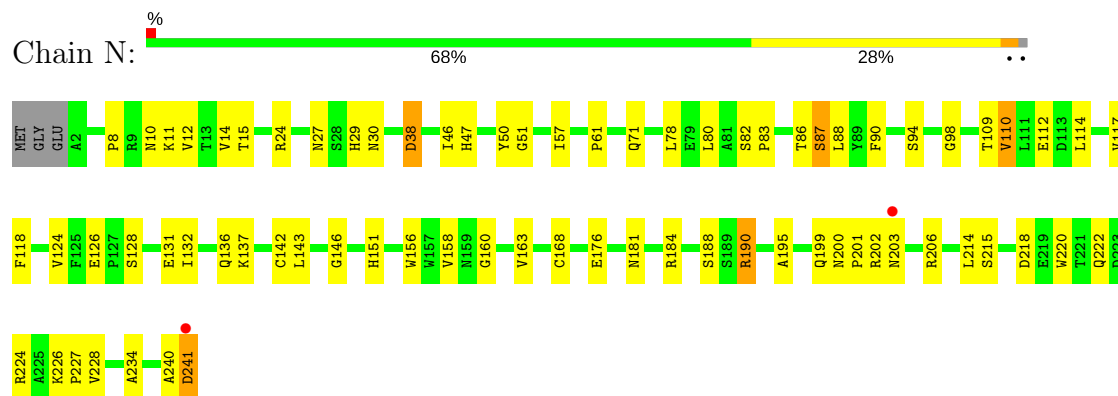
• Molecule 2: 42F3 beta



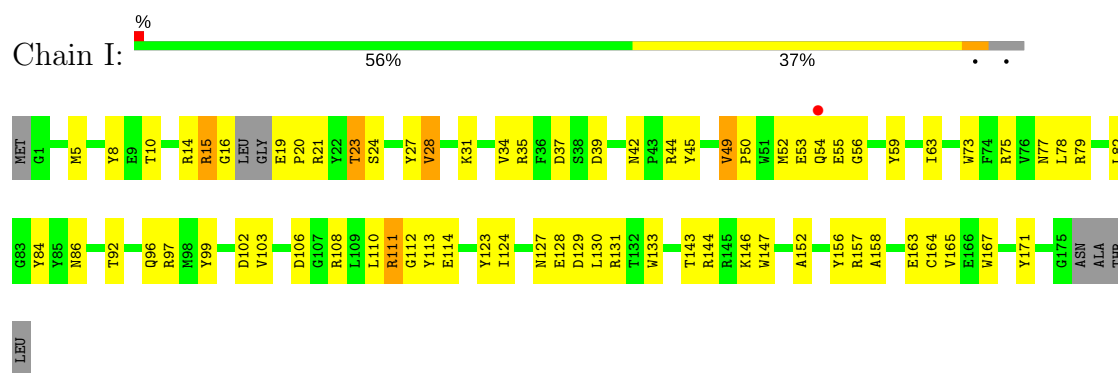
• Molecule 2: 42F3 beta



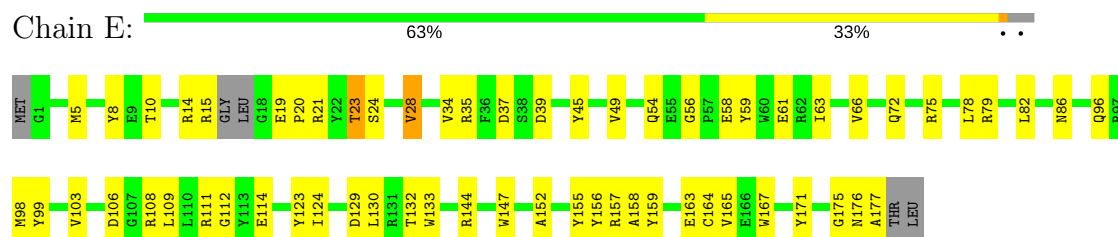
- Molecule 2: 42F3 beta



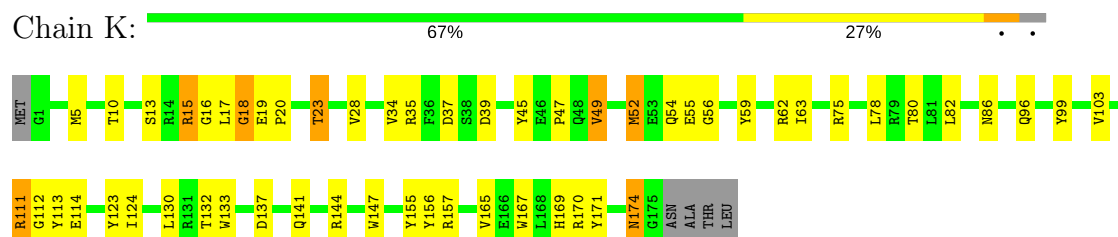
- Molecule 3: H2-Ld SBM2



- Molecule 3: H2-Ld SBM2

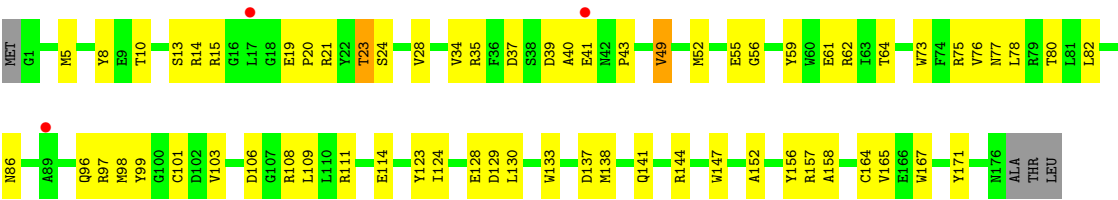


- Molecule 3: H2-Ld SBM2



- Molecule 3: H2-Ld SBM2





● Molecule 4: p5E8 peptide



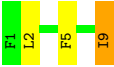
● Molecule 4: p5E8 peptide



● Molecule 4: p5E8 peptide



● Molecule 4: p5E8 peptide



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | H 3 2                                                       | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 291.33Å 291.33Å 291.24Å<br>90.00° 90.00° 120.00°            | Depositor        |
| Resolution (Å)                                                          | 45.31 – 3.10<br>45.31 – 3.10                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.7 (45.31-3.10)<br>99.6 (45.31-3.10)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.98 (at 3.12Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (phenix.refine: 1.7_650)                             | Depositor        |
| R, $R_{free}$                                                           | 0.231 , 0.258<br>0.224 , 0.253                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 4275 reflections (5.01%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 67.0                                                        | Xtriage          |
| Anisotropy                                                              | 0.432                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 45.3                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.91                                                        | EDS              |
| Total number of atoms                                                   | 20148                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 70.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% 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: SO4, EDO

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

| Mol | Chain | Bond lengths |                | Bond angles |                |
|-----|-------|--------------|----------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5        |
| 1   | A     | 0.59         | 0/1634         | 0.73        | 1/2214 (0.0%)  |
| 1   | C     | 0.57         | 0/1623         | 0.73        | 1/2200 (0.0%)  |
| 1   | G     | 0.64         | 0/1611         | 0.78        | 0/2182         |
| 1   | M     | 0.58         | 0/1626         | 0.81        | 0/2204         |
| 2   | B     | 0.61         | 0/1952         | 0.71        | 0/2662         |
| 2   | D     | 0.58         | 0/1952         | 0.71        | 1/2662 (0.0%)  |
| 2   | H     | 0.59         | 0/1952         | 0.74        | 2/2662 (0.1%)  |
| 2   | N     | 0.62         | 1/1952 (0.1%)  | 0.73        | 1/2662 (0.0%)  |
| 3   | E     | 0.59         | 1/1488 (0.1%)  | 0.70        | 0/2014         |
| 3   | I     | 0.59         | 0/1475         | 0.69        | 0/1996         |
| 3   | K     | 0.69         | 0/1488         | 0.73        | 1/2015 (0.0%)  |
| 3   | Q     | 0.57         | 0/1493         | 0.74        | 0/2022         |
| 4   | F     | 0.66         | 0/90           | 0.60        | 0/121          |
| 4   | J     | 0.68         | 0/90           | 0.67        | 0/121          |
| 4   | L     | 0.82         | 0/90           | 0.70        | 0/121          |
| 4   | R     | 1.02         | 0/90           | 0.76        | 0/121          |
| All | All   | 0.61         | 2/20606 (0.0%) | 0.73        | 7/27979 (0.0%) |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | N     | 8   | PRO  | N-CD   | -5.60 | 1.40        | 1.47     |
| 3   | E     | 72  | GLN  | CD-OE1 | 5.33  | 1.35        | 1.24     |

All (7) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | D     | 4   | VAL  | N-CA-C  | -6.27 | 94.07       | 111.00   |
| 2   | H     | 240 | ALA  | N-CA-CB | 5.88  | 118.33      | 110.10   |
| 2   | N     | 203 | ASN  | N-CA-C  | 5.68  | 126.35      | 111.00   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | K     | 18  | GLY  | N-CA-C | -5.34 | 99.74       | 113.10   |
| 1   | C     | 142 | ASP  | N-CA-C | 5.21  | 125.07      | 111.00   |
| 2   | H     | 235 | GLU  | N-CA-C | 5.14  | 124.89      | 111.00   |
| 1   | A     | 181 | LYS  | N-CA-C | -5.03 | 97.42       | 111.00   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1595  | 0        | 1523     | 78      | 0            |
| 1   | C     | 1584  | 0        | 1509     | 70      | 0            |
| 1   | G     | 1573  | 0        | 1505     | 58      | 0            |
| 1   | M     | 1587  | 0        | 1515     | 67      | 1            |
| 2   | B     | 1900  | 0        | 1797     | 57      | 0            |
| 2   | D     | 1900  | 0        | 1797     | 72      | 0            |
| 2   | H     | 1900  | 0        | 1797     | 69      | 0            |
| 2   | N     | 1900  | 0        | 1796     | 67      | 1            |
| 3   | E     | 1449  | 0        | 1333     | 56      | 0            |
| 3   | I     | 1436  | 0        | 1322     | 73      | 0            |
| 3   | K     | 1448  | 0        | 1339     | 48      | 0            |
| 3   | Q     | 1453  | 0        | 1341     | 55      | 0            |
| 4   | F     | 85    | 0        | 77       | 8       | 0            |
| 4   | J     | 85    | 0        | 77       | 11      | 0            |
| 4   | L     | 85    | 0        | 77       | 8       | 0            |
| 4   | R     | 85    | 0        | 77       | 7       | 0            |
| 5   | A     | 5     | 0        | 0        | 0       | 0            |
| 5   | B     | 15    | 0        | 0        | 0       | 0            |
| 5   | D     | 10    | 0        | 0        | 1       | 0            |
| 5   | E     | 5     | 0        | 0        | 4       | 0            |
| 5   | G     | 5     | 0        | 0        | 0       | 0            |
| 5   | H     | 10    | 0        | 0        | 1       | 0            |
| 5   | K     | 10    | 0        | 0        | 0       | 0            |
| 5   | N     | 10    | 0        | 0        | 3       | 0            |
| 5   | Q     | 5     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6   | N     | 4     | 0        | 6        | 0       | 0            |
| 7   | H     | 1     | 0        | 0        | 0       | 0            |
| 7   | I     | 1     | 0        | 0        | 0       | 0            |
| 7   | K     | 1     | 0        | 0        | 0       | 0            |
| 7   | N     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 20148 | 0        | 18888    | 735     | 1            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (735) 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:161:CYS:HB3 | 2:B:168:CYS:SG   | 1.13                     | 1.69              |
| 1:G:161:CYS:HB3 | 2:H:168:CYS:SG   | 1.34                     | 1.63              |
| 1:C:161:CYS:HB3 | 2:D:168:CYS:SG   | 1.34                     | 1.62              |
| 1:A:161:CYS:CB  | 2:B:168:CYS:SG   | 2.08                     | 1.40              |
| 1:C:161:CYS:CB  | 2:D:168:CYS:SG   | 2.25                     | 1.25              |
| 1:G:161:CYS:CB  | 2:H:168:CYS:SG   | 2.27                     | 1.22              |
| 3:I:15:ARG:HD3  | 3:I:15:ARG:N     | 1.45                     | 1.15              |
| 3:I:15:ARG:HH11 | 3:I:15:ARG:N     | 1.47                     | 1.13              |
| 3:I:15:ARG:H    | 3:I:15:ARG:CD    | 1.60                     | 1.11              |
| 2:D:239:ARG:CG  | 2:D:239:ARG:HH11 | 1.64                     | 1.09              |
| 1:C:3:VAL:CG2   | 1:C:92:VAL:HG13  | 1.85                     | 1.06              |
| 2:N:86:THR:HG23 | 2:N:109:THR:HA   | 1.38                     | 1.05              |
| 2:D:239:ARG:HG3 | 2:D:239:ARG:HH11 | 1.16                     | 1.05              |
| 3:I:15:ARG:HD3  | 3:I:15:ARG:H     | 0.88                     | 1.05              |
| 1:M:67:SER:HB3  | 1:M:72:SER:HB3   | 1.35                     | 1.03              |
| 1:G:197:GLU:OE1 | 1:G:197:GLU:HA   | 1.60                     | 1.01              |
| 3:K:19:GLU:HG2  | 3:K:20:PRO:HD2   | 1.42                     | 0.99              |
| 3:I:19:GLU:HG2  | 3:I:20:PRO:HD2   | 1.45                     | 0.97              |
| 1:A:27:SER:O    | 1:A:30:PRO:HD3   | 1.64                     | 0.97              |
| 3:Q:19:GLU:HG2  | 3:Q:20:PRO:HD2   | 1.46                     | 0.97              |
| 1:M:142:ASP:OD1 | 1:M:143:SER:N    | 1.98                     | 0.97              |
| 1:M:1:GLN:OE1   | 1:M:94:ALA:HA    | 1.63                     | 0.97              |
| 3:E:19:GLU:HG2  | 3:E:20:PRO:HD2   | 1.48                     | 0.96              |
| 3:E:129:ASP:OD1 | 3:E:132:THR:HG23 | 1.67                     | 0.94              |
| 1:G:196:PRO:O   | 1:G:199:THR:HG23 | 1.70                     | 0.92              |
| 3:E:5:MET:HE2   | 3:E:164:CYS:SG   | 2.10                     | 0.91              |
| 4:L:1:PHE:HD1   | 4:L:1:PHE:O      | 1.53                     | 0.91              |
| 1:A:161:CYS:HB3 | 2:B:168:CYS:HG   | 1.35                     | 0.91              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:17:LEU:O     | 3:K:17:LEU:HD12  | 1.70                     | 0.90              |
| 3:E:130:LEU:HB3  | 3:E:157:ARG:HG3  | 1.53                     | 0.90              |
| 1:C:3:VAL:HG22   | 1:C:92:VAL:HG13  | 1.51                     | 0.89              |
| 1:M:136:CYS:HG   | 1:M:186:CYS:HG   | 0.90                     | 0.88              |
| 3:Q:130:LEU:HB3  | 3:Q:157:ARG:HG3  | 1.56                     | 0.88              |
| 3:K:130:LEU:HB3  | 3:K:157:ARG:HG3  | 1.55                     | 0.86              |
| 1:A:67:SER:HB3   | 1:A:72:SER:HB3   | 1.58                     | 0.86              |
| 4:F:1:PHE:O      | 4:F:1:PHE:HD1    | 1.59                     | 0.85              |
| 4:F:1:PHE:O      | 4:F:1:PHE:CD1    | 2.30                     | 0.84              |
| 3:E:5:MET:CE     | 3:E:164:CYS:SG   | 2.65                     | 0.84              |
| 1:A:136:CYS:HG   | 1:A:186:CYS:HG   | 0.85                     | 0.84              |
| 1:C:16:ALA:O     | 1:C:80:VAL:HG22  | 1.76                     | 0.84              |
| 4:L:1:PHE:CD1    | 4:L:1:PHE:O      | 2.30                     | 0.84              |
| 2:N:160:GLY:HA2  | 5:N:243:SO4:O3   | 1.79                     | 0.83              |
| 2:D:239:ARG:NH1  | 2:D:239:ARG:HG3  | 1.89                     | 0.83              |
| 3:I:111:ARG:NH1  | 3:I:128:GLU:HB2  | 1.94                     | 0.83              |
| 3:E:130:LEU:HD23 | 3:E:157:ARG:HG2  | 1.60                     | 0.83              |
| 1:A:161:CYS:CB   | 2:B:168:CYS:HG   | 1.86                     | 0.83              |
| 3:I:123:TYR:HD1  | 3:I:124:ILE:HG22 | 1.44                     | 0.83              |
| 2:D:239:ARG:CG   | 2:D:239:ARG:NH1  | 2.37                     | 0.82              |
| 3:Q:123:TYR:HD1  | 3:Q:124:ILE:HG22 | 1.44                     | 0.82              |
| 3:I:15:ARG:N     | 3:I:15:ARG:CD    | 2.29                     | 0.82              |
| 3:I:52:MET:O     | 3:I:55:GLU:HG3   | 1.77                     | 0.82              |
| 3:I:130:LEU:HB3  | 3:I:157:ARG:HG3  | 1.62                     | 0.81              |
| 2:N:88:LEU:HD21  | 2:N:90:PHE:CZ    | 2.15                     | 0.81              |
| 2:H:50:TYR:HE2   | 2:H:56:GLN:HG3   | 1.45                     | 0.80              |
| 1:G:101:LEU:HD13 | 2:H:98:GLY:HA2   | 1.64                     | 0.79              |
| 1:A:194:ILE:HG22 | 1:A:194:ILE:O    | 1.83                     | 0.79              |
| 2:D:83:PRO:HA    | 2:D:110:VAL:HG22 | 1.64                     | 0.79              |
| 2:H:86:THR:HG23  | 2:H:109:THR:HA   | 1.63                     | 0.79              |
| 1:M:51:SER:HB3   | 3:Q:158:ALA:HB2  | 1.63                     | 0.78              |
| 3:I:14:ARG:HB3   | 3:I:15:ARG:NH1   | 1.98                     | 0.78              |
| 1:M:3:VAL:CG2    | 1:M:22:CYS:SG    | 2.72                     | 0.78              |
| 3:E:123:TYR:HD1  | 3:E:124:ILE:HG22 | 1.47                     | 0.78              |
| 3:Q:101:CYS:CB   | 3:Q:164:CYS:HG   | 1.97                     | 0.77              |
| 3:Q:52:MET:O     | 3:Q:55:GLU:HG3   | 1.84                     | 0.77              |
| 3:K:52:MET:O     | 3:K:55:GLU:HG3   | 1.85                     | 0.77              |
| 1:M:81:HIS:O     | 1:M:111:VAL:HG11 | 1.83                     | 0.77              |
| 1:G:67:SER:HB3   | 1:G:72:SER:HB3   | 1.66                     | 0.76              |
| 2:D:75:PHE:CG    | 2:N:80:LEU:HD13  | 2.20                     | 0.76              |
| 3:I:5:MET:HE2    | 3:I:164:CYS:SG   | 2.26                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:15:ARG:NH1   | 3:I:15:ARG:H     | 1.83                     | 0.76              |
| 3:I:15:ARG:NH1   | 3:I:15:ARG:N     | 2.30                     | 0.76              |
| 2:H:78:LEU:HD12  | 2:H:78:LEU:N     | 2.01                     | 0.75              |
| 2:H:46:ILE:HG22  | 2:H:47:HIS:CD2   | 2.21                     | 0.75              |
| 3:K:111:ARG:HG3  | 3:K:112:GLY:N    | 2.02                     | 0.75              |
| 1:A:3:VAL:CG2    | 1:A:22:CYS:SG    | 2.75                     | 0.74              |
| 1:G:3:VAL:CG2    | 1:G:22:CYS:SG    | 2.75                     | 0.74              |
| 3:Q:49:VAL:HG12  | 3:Q:52:MET:HG2   | 1.69                     | 0.74              |
| 1:G:1:GLN:NE2    | 1:G:27:SER:HB2   | 2.02                     | 0.74              |
| 2:B:111:LEU:HD21 | 2:B:149:PRO:HG3  | 1.69                     | 0.74              |
| 1:M:194:ILE:O    | 1:M:194:ILE:HG22 | 1.87                     | 0.74              |
| 3:Q:101:CYS:CB   | 3:Q:164:CYS:SG   | 2.76                     | 0.73              |
| 3:I:111:ARG:HH11 | 3:I:128:GLU:HB2  | 1.51                     | 0.73              |
| 2:H:88:LEU:HD21  | 2:H:90:PHE:CZ    | 2.24                     | 0.73              |
| 3:K:54:GLN:HG3   | 3:K:54:GLN:O     | 1.87                     | 0.73              |
| 2:H:117:VAL:HG12 | 2:H:227:PRO:HB2  | 1.69                     | 0.73              |
| 3:I:5:MET:CE     | 3:I:164:CYS:SG   | 2.77                     | 0.72              |
| 2:N:195:ALA:O    | 2:N:199:GLN:HG3  | 1.88                     | 0.72              |
| 2:N:117:VAL:HG12 | 2:N:227:PRO:HB2  | 1.70                     | 0.72              |
| 2:D:27:ASN:HB3   | 2:D:29:HIS:CD2   | 2.25                     | 0.72              |
| 3:E:75:ARG:NH2   | 5:E:180:SO4:O2   | 2.23                     | 0.71              |
| 2:D:214:LEU:HD13 | 2:D:227:PRO:HG2  | 1.70                     | 0.71              |
| 3:E:37:ASP:OD1   | 3:E:39:ASP:HB2   | 1.89                     | 0.71              |
| 3:I:37:ASP:OD1   | 3:I:39:ASP:HB2   | 1.91                     | 0.71              |
| 1:A:151:LYS:CD   | 1:A:192:ASN:OD1  | 2.39                     | 0.71              |
| 2:D:199:GLN:HA   | 2:D:239:ARG:O    | 1.89                     | 0.71              |
| 2:D:117:VAL:O    | 2:D:224:ARG:NH2  | 2.23                     | 0.71              |
| 3:Q:103:VAL:HG11 | 3:Q:165:VAL:HG13 | 1.72                     | 0.71              |
| 1:C:183:ASP:C    | 1:C:183:ASP:OD1  | 2.30                     | 0.70              |
| 1:A:124:GLN:HB2  | 1:A:186:CYS:SG   | 2.31                     | 0.70              |
| 2:D:78:LEU:N     | 2:D:78:LEU:HD12  | 2.06                     | 0.70              |
| 3:Q:101:CYS:HB3  | 3:Q:164:CYS:SG   | 2.31                     | 0.70              |
| 2:D:46:ILE:HG22  | 2:D:47:HIS:CD2   | 2.26                     | 0.70              |
| 1:C:151:LYS:HG3  | 1:C:152:ASP:N    | 2.06                     | 0.70              |
| 2:H:156:TRP:HD1  | 2:H:167:VAL:HG11 | 1.56                     | 0.70              |
| 1:C:136:CYS:SG   | 1:C:184:PHE:CE2  | 2.85                     | 0.70              |
| 1:C:3:VAL:HG22   | 1:C:92:VAL:CG1   | 2.20                     | 0.69              |
| 2:B:86:THR:HG23  | 2:B:109:THR:HA   | 1.75                     | 0.69              |
| 3:E:103:VAL:HG11 | 3:E:165:VAL:HG13 | 1.72                     | 0.69              |
| 2:N:88:LEU:HD23  | 2:N:90:PHE:CE2   | 2.27                     | 0.69              |
| 1:A:183:ASP:O    | 1:A:184:PHE:CB   | 2.40                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:194:ILE:O    | 1:G:194:ILE:HG22 | 1.93                     | 0.69              |
| 3:E:176:ASN:O    | 3:E:177:ALA:O    | 2.10                     | 0.69              |
| 2:B:46:ILE:HG22  | 2:B:47:HIS:CD2   | 2.26                     | 0.69              |
| 1:C:194:ILE:O    | 1:C:194:ILE:HG22 | 1.93                     | 0.69              |
| 1:G:81:HIS:O     | 1:G:111:VAL:HG11 | 1.93                     | 0.69              |
| 2:N:200:ASN:OD1  | 2:N:201:PRO:HD2  | 1.92                     | 0.69              |
| 1:C:6:PRO:HG3    | 1:C:21:ARG:HB2   | 1.74                     | 0.69              |
| 2:H:50:TYR:CE2   | 2:H:56:GLN:HG3   | 2.28                     | 0.69              |
| 1:C:161:CYS:HB3  | 2:D:168:CYS:HG   | 1.54                     | 0.69              |
| 3:I:103:VAL:HG11 | 3:I:165:VAL:HG13 | 1.75                     | 0.68              |
| 1:M:123:TYR:CE1  | 2:N:131:GLU:HA   | 2.27                     | 0.68              |
| 1:A:183:ASP:C    | 1:A:183:ASP:OD1  | 2.30                     | 0.68              |
| 3:E:10:THR:HG22  | 3:E:96:GLN:HG3   | 1.75                     | 0.68              |
| 2:D:2:ALA:HB2    | 2:D:101:TYR:HD1  | 1.58                     | 0.68              |
| 2:D:82:SER:C     | 2:D:110:VAL:HG21 | 2.14                     | 0.68              |
| 3:I:15:ARG:HH11  | 3:I:15:ARG:H     | 1.15                     | 0.68              |
| 1:M:3:VAL:HG21   | 1:M:22:CYS:SG    | 2.33                     | 0.68              |
| 3:Q:130:LEU:HB3  | 3:Q:157:ARG:CG   | 2.24                     | 0.68              |
| 1:A:3:VAL:HG21   | 1:A:22:CYS:SG    | 2.34                     | 0.68              |
| 2:H:156:TRP:CD1  | 2:H:167:VAL:HG11 | 2.28                     | 0.67              |
| 2:H:117:VAL:O    | 2:H:224:ARG:NH2  | 2.28                     | 0.67              |
| 2:D:117:VAL:HG12 | 2:D:227:PRO:HB2  | 1.76                     | 0.67              |
| 1:A:81:HIS:O     | 1:A:111:VAL:HG11 | 1.94                     | 0.67              |
| 2:B:78:LEU:N     | 2:B:78:LEU:HD12  | 2.10                     | 0.67              |
| 3:Q:37:ASP:OD1   | 3:Q:39:ASP:HB2   | 1.93                     | 0.67              |
| 4:L:1:PHE:C      | 4:L:1:PHE:CD1    | 2.68                     | 0.67              |
| 2:D:83:PRO:HA    | 2:D:110:VAL:CG2  | 2.23                     | 0.67              |
| 3:K:37:ASP:OD1   | 3:K:39:ASP:HB2   | 1.95                     | 0.67              |
| 1:M:124:GLN:HB2  | 1:M:186:CYS:SG   | 2.35                     | 0.67              |
| 2:D:146:GLY:O    | 2:D:184:ARG:HD2  | 1.95                     | 0.66              |
| 1:G:3:VAL:HG21   | 1:G:22:CYS:SG    | 2.36                     | 0.66              |
| 1:M:6:PRO:HG3    | 1:M:21:ARG:HB2   | 1.76                     | 0.66              |
| 3:I:129:ASP:O    | 3:I:131:ARG:NH1  | 2.27                     | 0.66              |
| 3:E:54:GLN:HG2   | 3:E:54:GLN:O     | 1.95                     | 0.66              |
| 1:A:6:PRO:HG3    | 1:A:21:ARG:HB2   | 1.78                     | 0.66              |
| 3:K:123:TYR:HD1  | 3:K:124:ILE:HG22 | 1.59                     | 0.66              |
| 1:G:142:ASP:C    | 1:G:142:ASP:OD2  | 2.33                     | 0.66              |
| 2:H:214:LEU:HD13 | 2:H:227:PRO:HG2  | 1.78                     | 0.65              |
| 2:N:214:LEU:HD13 | 2:N:227:PRO:HG2  | 1.77                     | 0.65              |
| 2:N:46:ILE:HG22  | 2:N:47:HIS:CD2   | 2.30                     | 0.65              |
| 1:A:183:ASP:OD1  | 1:A:184:PHE:N    | 2.30                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:88:LEU:CD2   | 2:H:90:PHE:CE2   | 2.79                     | 0.65              |
| 3:K:103:VAL:HG11 | 3:K:165:VAL:HG13 | 1.79                     | 0.65              |
| 2:D:239:ARG:HD3  | 2:D:241:ASP:OD2  | 1.96                     | 0.65              |
| 2:H:156:TRP:CD1  | 2:H:167:VAL:CG1  | 2.80                     | 0.65              |
| 3:Q:128:GLU:O    | 3:Q:130:LEU:HD13 | 1.97                     | 0.65              |
| 1:A:5:GLN:O      | 1:A:105:LYS:HE3  | 1.97                     | 0.65              |
| 2:D:239:ARG:HG2  | 2:D:239:ARG:HH11 | 1.58                     | 0.65              |
| 3:E:129:ASP:OD1  | 3:E:132:THR:CG2  | 2.43                     | 0.65              |
| 3:Q:101:CYS:HG   | 3:Q:164:CYS:HG   | 0.66                     | 0.65              |
| 1:G:136:CYS:SG   | 1:G:186:CYS:HA   | 2.37                     | 0.64              |
| 2:B:87:SER:OG    | 2:B:88:LEU:N     | 2.30                     | 0.64              |
| 3:E:130:LEU:HB3  | 3:E:157:ARG:CG   | 2.27                     | 0.64              |
| 3:I:123:TYR:CD1  | 3:I:124:ILE:HG22 | 2.31                     | 0.64              |
| 1:A:51:SER:HB3   | 3:I:158:ALA:HB2  | 1.79                     | 0.64              |
| 2:N:87:SER:OG    | 2:N:88:LEU:N     | 2.30                     | 0.64              |
| 2:N:88:LEU:CD2   | 2:N:90:PHE:CE2   | 2.80                     | 0.64              |
| 3:K:10:THR:HG22  | 3:K:96:GLN:HG3   | 1.79                     | 0.64              |
| 2:H:88:LEU:HD23  | 2:H:90:PHE:CE2   | 2.32                     | 0.64              |
| 1:M:146:ASN:OD1  | 1:M:146:ASN:N    | 2.30                     | 0.63              |
| 3:K:130:LEU:HB3  | 3:K:157:ARG:CG   | 2.27                     | 0.63              |
| 3:E:123:TYR:CD1  | 3:E:124:ILE:HG22 | 2.31                     | 0.63              |
| 2:B:146:GLY:O    | 2:B:184:ARG:HD2  | 1.98                     | 0.63              |
| 2:H:24:ARG:HG3   | 2:H:24:ARG:HH11  | 1.64                     | 0.63              |
| 3:Q:123:TYR:CD1  | 3:Q:124:ILE:HG22 | 2.29                     | 0.63              |
| 1:A:202:PRO:O    | 1:A:206:SER:N    | 2.29                     | 0.63              |
| 2:H:146:GLY:O    | 2:H:184:ARG:HD2  | 1.99                     | 0.63              |
| 2:H:164:HIS:O    | 2:H:167:VAL:HG23 | 1.98                     | 0.63              |
| 3:I:10:THR:HG22  | 3:I:96:GLN:HG3   | 1.80                     | 0.63              |
| 3:I:15:ARG:HD2   | 3:I:92:THR:OG1   | 1.99                     | 0.63              |
| 1:C:32:LEU:CD2   | 1:C:92:VAL:HG12  | 2.28                     | 0.62              |
| 2:D:118:PHE:CD2  | 2:D:184:ARG:HD3  | 2.33                     | 0.62              |
| 3:I:5:MET:SD     | 3:I:167:TRP:CE3  | 2.93                     | 0.62              |
| 3:K:16:GLY:H     | 3:K:17:LEU:HA    | 1.64                     | 0.62              |
| 3:E:5:MET:SD     | 3:E:167:TRP:CE3  | 2.92                     | 0.62              |
| 1:A:181:LYS:HB2  | 1:A:183:ASP:O    | 2.00                     | 0.62              |
| 2:B:47:HIS:CE1   | 2:B:61:PRO:CB    | 2.82                     | 0.62              |
| 2:D:47:HIS:ND1   | 2:D:57:ILE:HA    | 2.15                     | 0.62              |
| 2:H:118:PHE:CD2  | 2:H:184:ARG:HD3  | 2.33                     | 0.62              |
| 2:H:47:HIS:CE1   | 2:H:61:PRO:CB    | 2.83                     | 0.62              |
| 3:E:79:ARG:NH1   | 5:E:180:SO4:O4   | 2.26                     | 0.62              |
| 1:M:38:TYR:CD1   | 1:M:86:ALA:HB2   | 2.35                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:6:PRO:HG3    | 1:G:21:ARG:HB2   | 1.81                     | 0.62              |
| 3:I:99:TYR:HB3   | 3:I:114:GLU:OE2  | 1.99                     | 0.62              |
| 3:K:156:TYR:OH   | 4:L:5:PHE:HA     | 2.00                     | 0.62              |
| 3:Q:10:THR:HG22  | 3:Q:96:GLN:HG3   | 1.80                     | 0.62              |
| 1:A:183:ASP:O    | 1:A:184:PHE:HB3  | 1.99                     | 0.62              |
| 1:C:29:THR:HG23  | 3:E:163:GLU:OE2  | 2.00                     | 0.62              |
| 3:E:75:ARG:NE    | 5:E:180:SO4:O2   | 2.32                     | 0.61              |
| 2:H:177:GLN:O    | 2:H:183:SER:HB2  | 2.00                     | 0.61              |
| 3:K:59:TYR:CD1   | 3:K:62:ARG:NH2   | 2.68                     | 0.61              |
| 2:N:88:LEU:CD2   | 2:N:90:PHE:CZ    | 2.83                     | 0.61              |
| 1:G:127:ASP:HB2  | 1:G:133:LYS:HB2  | 1.83                     | 0.61              |
| 1:M:38:TYR:HD1   | 1:M:86:ALA:HB2   | 1.65                     | 0.61              |
| 3:I:106:ASP:OD2  | 3:I:108:ARG:HG3  | 2.00                     | 0.61              |
| 2:N:47:HIS:CE1   | 2:N:61:PRO:CB    | 2.84                     | 0.61              |
| 2:B:214:LEU:HD13 | 2:B:227:PRO:HG2  | 1.82                     | 0.61              |
| 3:E:99:TYR:HB3   | 3:E:114:GLU:OE2  | 2.01                     | 0.60              |
| 3:K:59:TYR:CE1   | 3:K:62:ARG:NH2   | 2.68                     | 0.60              |
| 3:K:80:THR:HG21  | 4:L:9:ILE:HG22   | 1.83                     | 0.60              |
| 3:I:131:ARG:HG3  | 3:I:131:ARG:HH11 | 1.66                     | 0.60              |
| 3:I:146:LYS:HD2  | 4:J:9:ILE:OXT    | 2.01                     | 0.60              |
| 2:H:88:LEU:HD23  | 2:H:90:PHE:HE2   | 1.65                     | 0.60              |
| 1:G:122:VAL:HG12 | 1:G:122:VAL:O    | 1.99                     | 0.60              |
| 1:M:32:LEU:CD2   | 1:M:92:VAL:HG12  | 2.32                     | 0.60              |
| 2:N:47:HIS:ND1   | 2:N:57:ILE:HA    | 2.16                     | 0.60              |
| 2:H:47:HIS:CE1   | 2:H:61:PRO:HB3   | 2.37                     | 0.60              |
| 2:N:78:LEU:HD12  | 2:N:78:LEU:N     | 2.17                     | 0.60              |
| 2:H:47:HIS:ND1   | 2:H:57:ILE:HA    | 2.16                     | 0.60              |
| 2:D:24:ARG:HH11  | 2:D:24:ARG:HG3   | 1.67                     | 0.60              |
| 3:Q:137:ASP:O    | 3:Q:141:GLN:HG2  | 2.02                     | 0.60              |
| 1:A:123:TYR:CE1  | 2:B:131:GLU:HA   | 2.37                     | 0.59              |
| 1:G:70:ASP:HB3   | 1:G:72:SER:HB2   | 1.84                     | 0.59              |
| 2:N:88:LEU:HD23  | 2:N:90:PHE:HE2   | 1.66                     | 0.59              |
| 1:A:170:PHE:CE2  | 2:B:137:LYS:HE3  | 2.38                     | 0.59              |
| 2:B:47:HIS:CE1   | 2:B:61:PRO:HB3   | 2.37                     | 0.59              |
| 3:I:130:LEU:HB3  | 3:I:157:ARG:CG   | 2.31                     | 0.59              |
| 2:H:82:SER:C     | 2:H:110:VAL:HG21 | 2.23                     | 0.59              |
| 3:I:75:ARG:NH1   | 3:I:79:ARG:HH12  | 2.00                     | 0.59              |
| 2:D:50:TYR:HE2   | 2:D:56:GLN:HG3   | 1.68                     | 0.59              |
| 3:K:141:GLN:OE1  | 3:K:144:ARG:NH2  | 2.35                     | 0.59              |
| 1:M:178:TRP:CD2  | 2:N:143:LEU:HD21 | 2.38                     | 0.59              |
| 2:H:154:LEU:HD23 | 2:H:155:SER:N    | 2.17                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:E:28:VAL:HG21  | 3:E:171:TYR:CE2  | 2.38                     | 0.59              |
| 3:Q:99:TYR:HB3   | 3:Q:114:GLU:OE2  | 2.03                     | 0.59              |
| 1:M:70:ASP:HB3   | 1:M:72:SER:HB2   | 1.84                     | 0.58              |
| 2:N:82:SER:C     | 2:N:110:VAL:HG21 | 2.24                     | 0.58              |
| 1:A:70:ASP:HB3   | 1:A:72:SER:HB2   | 1.85                     | 0.58              |
| 1:A:32:LEU:CD2   | 1:A:92:VAL:HG12  | 2.33                     | 0.58              |
| 1:A:95:LYS:NZ    | 4:J:1:PHE:CE2    | 2.62                     | 0.58              |
| 2:D:86:THR:HG23  | 2:D:109:THR:HA   | 1.85                     | 0.58              |
| 1:A:194:ILE:CG2  | 1:A:194:ILE:O    | 2.51                     | 0.58              |
| 1:C:149:GLN:HG3  | 1:C:150:SER:N    | 2.19                     | 0.58              |
| 2:N:222:GLN:HG2  | 2:N:224:ARG:NH1  | 2.19                     | 0.58              |
| 1:A:94:ALA:HB3   | 1:A:97:THR:HB    | 1.86                     | 0.58              |
| 3:E:21:ARG:NE    | 3:E:39:ASP:OD2   | 2.37                     | 0.58              |
| 4:F:1:PHE:CD1    | 4:F:1:PHE:C      | 2.77                     | 0.58              |
| 2:B:215:SER:HB3  | 2:B:218:ASP:OD1  | 2.03                     | 0.57              |
| 3:E:34:VAL:HG22  | 3:E:35:ARG:N     | 2.18                     | 0.57              |
| 2:B:82:SER:C     | 2:B:110:VAL:HG21 | 2.25                     | 0.57              |
| 1:G:150:SER:HB3  | 1:G:157:ILE:HD12 | 1.84                     | 0.57              |
| 3:I:28:VAL:HG21  | 3:I:171:TYR:CE2  | 2.40                     | 0.57              |
| 1:C:17:SER:HA    | 1:C:78:ALA:O     | 2.04                     | 0.57              |
| 1:C:24:TYR:HH    | 1:C:66:PHE:HE1   | 1.51                     | 0.57              |
| 2:N:118:PHE:CD2  | 2:N:184:ARG:HD3  | 2.40                     | 0.57              |
| 1:G:32:LEU:CD2   | 1:G:92:VAL:HG12  | 2.35                     | 0.57              |
| 3:Q:156:TYR:OH   | 4:R:5:PHE:HA     | 2.05                     | 0.57              |
| 2:B:30:ASN:HB3   | 2:B:50:TYR:O     | 2.04                     | 0.57              |
| 2:D:10:ASN:OD1   | 2:D:151:HIS:NE2  | 2.28                     | 0.57              |
| 3:E:176:ASN:O    | 3:E:177:ALA:C    | 2.42                     | 0.57              |
| 3:I:133:TRP:HB2  | 3:I:144:ARG:HG3  | 1.87                     | 0.57              |
| 1:M:1:GLN:OE1    | 1:M:94:ALA:CA    | 2.46                     | 0.56              |
| 3:Q:34:VAL:HG22  | 3:Q:35:ARG:N     | 2.20                     | 0.56              |
| 3:E:19:GLU:HG3   | 3:E:75:ARG:HH11  | 1.70                     | 0.56              |
| 1:M:155:VAL:HG22 | 1:M:179:SER:HB2  | 1.86                     | 0.56              |
| 1:M:82:TRP:HD1   | 1:M:111:VAL:O    | 1.89                     | 0.56              |
| 1:M:120:PRO:HB2  | 1:M:199:THR:HA   | 1.87                     | 0.56              |
| 3:Q:21:ARG:NE    | 3:Q:39:ASP:OD2   | 2.37                     | 0.56              |
| 1:A:120:PRO:HB2  | 1:A:199:THR:HB   | 1.87                     | 0.56              |
| 3:E:156:TYR:OH   | 4:F:5:PHE:HA     | 2.06                     | 0.56              |
| 2:H:83:PRO:HA    | 2:H:110:VAL:CG2  | 2.36                     | 0.56              |
| 3:I:73:TRP:CE2   | 3:I:77:ASN:ND2   | 2.74                     | 0.56              |
| 1:M:115:ILE:HG22 | 1:M:118:PRO:HD3  | 1.87                     | 0.56              |
| 2:D:9:ARG:NH1    | 2:D:153:GLU:OE2  | 2.38                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:Q:14:ARG:HD2   | 3:Q:19:GLU:O     | 2.05                     | 0.56              |
| 1:A:95:LYS:NZ    | 3:I:163:GLU:OE1  | 2.39                     | 0.55              |
| 2:B:50:TYR:HE2   | 2:B:56:GLN:HG3   | 1.71                     | 0.55              |
| 1:C:136:CYS:SG   | 1:C:184:PHE:CZ   | 2.99                     | 0.55              |
| 1:G:127:ASP:HB3  | 1:G:130:SER:O    | 2.06                     | 0.55              |
| 1:G:123:TYR:CE1  | 2:H:131:GLU:HA   | 2.41                     | 0.55              |
| 3:K:137:ASP:O    | 3:K:141:GLN:HG2  | 2.06                     | 0.55              |
| 1:M:70:ASP:CB    | 1:M:72:SER:HB2   | 2.37                     | 0.55              |
| 2:N:14:VAL:HG22  | 2:N:114:LEU:HD21 | 1.88                     | 0.55              |
| 2:D:47:HIS:CE1   | 2:D:61:PRO:CB    | 2.90                     | 0.55              |
| 2:N:201:PRO:CD   | 2:N:202:ARG:H    | 2.20                     | 0.55              |
| 3:Q:28:VAL:HG21  | 3:Q:171:TYR:CE2  | 2.41                     | 0.55              |
| 2:H:215:SER:HB3  | 2:H:218:ASP:OD1  | 2.07                     | 0.55              |
| 3:I:84:TYR:HE2   | 4:J:9:ILE:HG22   | 1.71                     | 0.55              |
| 1:G:127:ASP:OD2  | 1:G:133:LYS:HD3  | 2.07                     | 0.55              |
| 1:M:2:SER:H      | 1:M:25:SER:HB2   | 1.72                     | 0.55              |
| 2:N:47:HIS:CE1   | 2:N:61:PRO:HB3   | 2.41                     | 0.55              |
| 1:G:197:GLU:OE1  | 1:G:197:GLU:CA   | 2.42                     | 0.55              |
| 1:A:181:LYS:CB   | 1:A:183:ASP:O    | 2.56                     | 0.54              |
| 1:C:32:LEU:HD23  | 1:C:92:VAL:HG12  | 1.89                     | 0.54              |
| 1:G:137:LEU:HD12 | 1:G:175:ALA:O    | 2.06                     | 0.54              |
| 1:A:161:CYS:SG   | 2:B:168:CYS:SG   | 3.06                     | 0.54              |
| 1:M:122:VAL:O    | 1:M:122:VAL:HG12 | 2.07                     | 0.54              |
| 1:C:95:LYS:NZ    | 4:F:3:SER:HA     | 2.23                     | 0.54              |
| 3:I:21:ARG:NE    | 3:I:39:ASP:OD2   | 2.38                     | 0.54              |
| 1:M:194:ILE:O    | 1:M:194:ILE:CG2  | 2.54                     | 0.54              |
| 3:Q:106:ASP:OD2  | 3:Q:108:ARG:HG3  | 2.07                     | 0.54              |
| 1:A:59:VAL:HG22  | 1:A:60:ASN:N     | 2.23                     | 0.54              |
| 2:D:87:SER:OG    | 2:D:88:LEU:N     | 2.41                     | 0.54              |
| 1:G:59:VAL:HG22  | 1:G:60:ASN:N     | 2.22                     | 0.54              |
| 3:Q:109:LEU:HD11 | 3:Q:111:ARG:O    | 2.07                     | 0.54              |
| 2:H:24:ARG:NH1   | 2:H:24:ARG:HG3   | 2.22                     | 0.54              |
| 3:I:143:THR:HA   | 4:J:9:ILE:OXT    | 2.08                     | 0.54              |
| 1:A:11:THR:HG23  | 1:A:110:THR:HB   | 1.91                     | 0.53              |
| 3:E:75:ARG:CZ    | 5:E:180:SO4:O2   | 2.57                     | 0.53              |
| 1:A:152:ASP:O    | 1:A:154:ASP:N    | 2.34                     | 0.53              |
| 1:A:203:SER:N    | 1:A:204:PRO:HD2  | 2.23                     | 0.53              |
| 3:K:59:TYR:HD1   | 3:K:62:ARG:HH22  | 1.57                     | 0.53              |
| 3:E:15:ARG:NH1   | 3:Q:61:GLU:HB2   | 2.24                     | 0.53              |
| 2:D:78:LEU:N     | 2:D:78:LEU:CD1   | 2.72                     | 0.53              |
| 3:I:102:ASP:O    | 3:I:110:LEU:HB3  | 2.08                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:2:SER:H      | 1:M:25:SER:CB    | 2.20                     | 0.53              |
| 3:K:99:TYR:HB3   | 3:K:114:GLU:OE2  | 2.09                     | 0.53              |
| 3:K:130:LEU:HD23 | 3:K:157:ARG:HG2  | 1.91                     | 0.53              |
| 2:D:215:SER:HB3  | 2:D:218:ASP:OD1  | 2.07                     | 0.53              |
| 3:E:109:LEU:HD11 | 3:E:111:ARG:O    | 2.09                     | 0.53              |
| 1:G:196:PRO:O    | 1:G:199:THR:CG2  | 2.51                     | 0.53              |
| 3:I:34:VAL:HG22  | 3:I:35:ARG:N     | 2.24                     | 0.53              |
| 1:A:32:LEU:HD13  | 1:A:73:PHE:HB2   | 1.91                     | 0.53              |
| 2:D:177:GLN:O    | 2:D:183:SER:HB2  | 2.09                     | 0.53              |
| 2:D:167:VAL:HG22 | 2:D:191:LEU:HD13 | 1.91                     | 0.53              |
| 3:I:49:VAL:O     | 3:I:53:GLU:HG3   | 2.09                     | 0.53              |
| 2:N:160:GLY:CA   | 5:N:243:SO4:O3   | 2.55                     | 0.53              |
| 2:D:47:HIS:CE1   | 2:D:61:PRO:HB3   | 2.44                     | 0.53              |
| 3:I:14:ARG:HB3   | 3:I:15:ARG:HH12  | 1.74                     | 0.52              |
| 2:N:88:LEU:HD21  | 2:N:90:PHE:HZ    | 1.70                     | 0.52              |
| 3:Q:19:GLU:HG3   | 3:Q:75:ARG:HH11  | 1.74                     | 0.52              |
| 3:E:106:ASP:OD2  | 3:E:108:ARG:HG3  | 2.09                     | 0.52              |
| 3:I:130:LEU:CD1  | 3:I:130:LEU:N    | 2.71                     | 0.52              |
| 2:N:83:PRO:HA    | 2:N:110:VAL:HG22 | 1.91                     | 0.52              |
| 1:M:136:CYS:SG   | 1:M:186:CYS:HA   | 2.49                     | 0.52              |
| 2:N:27:ASN:HB3   | 2:N:29:HIS:CD2   | 2.44                     | 0.52              |
| 3:E:14:ARG:HD2   | 3:E:19:GLU:O     | 2.09                     | 0.52              |
| 1:G:155:VAL:HG22 | 1:G:179:SER:HB2  | 1.89                     | 0.52              |
| 2:D:142:CYS:HB2  | 2:D:156:TRP:CH2  | 2.44                     | 0.52              |
| 4:J:9:ILE:HG22   | 4:J:9:ILE:O      | 2.10                     | 0.52              |
| 2:H:46:ILE:HG22  | 2:H:47:HIS:HD2   | 1.73                     | 0.52              |
| 3:K:111:ARG:HG2  | 3:K:113:TYR:CZ   | 2.45                     | 0.52              |
| 3:K:34:VAL:HG22  | 3:K:35:ARG:N     | 2.24                     | 0.52              |
| 2:N:215:SER:HB3  | 2:N:218:ASP:OD1  | 2.09                     | 0.52              |
| 2:N:15:THR:HG23  | 2:N:83:PRO:HD3   | 1.90                     | 0.52              |
| 1:G:82:TRP:HD1   | 1:G:111:VAL:O    | 1.92                     | 0.52              |
| 2:H:51:GLY:O     | 2:H:52:ALA:C     | 2.47                     | 0.52              |
| 3:K:132:THR:HG22 | 3:K:133:TRP:N    | 2.25                     | 0.52              |
| 2:N:146:GLY:O    | 2:N:184:ARG:HD2  | 2.10                     | 0.52              |
| 2:N:206:ARG:NH2  | 5:N:243:SO4:O2   | 2.42                     | 0.52              |
| 2:D:2:ALA:HB2    | 2:D:101:TYR:CD1  | 2.43                     | 0.52              |
| 2:D:50:TYR:CE2   | 2:D:56:GLN:HG3   | 2.44                     | 0.52              |
| 2:B:150:ASP:OD1  | 2:B:150:ASP:C    | 2.47                     | 0.51              |
| 2:B:24:ARG:HH11  | 2:B:24:ARG:HG3   | 1.74                     | 0.51              |
| 1:M:127:ASP:HB3  | 1:M:130:SER:O    | 2.10                     | 0.51              |
| 2:N:11:LYS:HG3   | 2:N:12:VAL:N     | 2.25                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:15:THR:HG23  | 2:B:83:PRO:HD3   | 1.91                     | 0.51              |
| 1:M:32:LEU:HD13  | 1:M:73:PHE:HB2   | 1.92                     | 0.51              |
| 1:C:82:TRP:HD1   | 1:C:111:VAL:O    | 1.93                     | 0.51              |
| 1:M:119:ASP:O    | 1:M:140:ASP:HB2  | 2.11                     | 0.51              |
| 3:I:131:ARG:NH1  | 3:I:131:ARG:HG3  | 2.25                     | 0.51              |
| 1:M:18:LEU:HD11  | 1:M:20:LEU:HG    | 1.92                     | 0.51              |
| 2:N:30:ASN:HB3   | 2:N:50:TYR:O     | 2.10                     | 0.51              |
| 1:C:3:VAL:HG23   | 1:C:92:VAL:HG13  | 1.88                     | 0.51              |
| 3:E:111:ARG:HG3  | 3:E:112:GLY:H    | 1.75                     | 0.51              |
| 2:H:117:VAL:HG11 | 2:H:214:LEU:CD1  | 2.40                     | 0.51              |
| 3:I:5:MET:SD     | 3:I:167:TRP:HE3  | 2.33                     | 0.51              |
| 2:B:149:PRO:O    | 2:B:151:HIS:N    | 2.44                     | 0.51              |
| 3:E:111:ARG:HG3  | 3:E:112:GLY:N    | 2.25                     | 0.51              |
| 3:E:129:ASP:O    | 3:E:130:LEU:HB2  | 2.11                     | 0.51              |
| 3:K:17:LEU:HD11  | 3:K:75:ARG:HH21  | 1.76                     | 0.51              |
| 2:D:2:ALA:HB1    | 2:D:101:TYR:HB3  | 1.93                     | 0.51              |
| 3:Q:130:LEU:HD12 | 3:Q:130:LEU:N    | 2.25                     | 0.51              |
| 1:C:137:LEU:HD11 | 1:C:174:SER:OG   | 2.11                     | 0.51              |
| 2:B:27:ASN:HB3   | 2:B:29:HIS:CD2   | 2.46                     | 0.51              |
| 3:E:133:TRP:HB2  | 3:E:144:ARG:HG3  | 1.92                     | 0.51              |
| 3:E:5:MET:SD     | 3:E:167:TRP:HE3  | 2.34                     | 0.51              |
| 3:I:111:ARG:HG3  | 3:I:112:GLY:N    | 2.25                     | 0.51              |
| 1:A:151:LYS:HD3  | 1:A:192:ASN:OD1  | 2.10                     | 0.50              |
| 1:A:120:PRO:HB2  | 1:A:199:THR:HA   | 1.93                     | 0.50              |
| 1:C:136:CYS:SG   | 1:C:184:PHE:HE2  | 2.33                     | 0.50              |
| 1:M:158:THR:HG21 | 2:N:188:SER:OG   | 2.12                     | 0.50              |
| 3:K:147:TRP:NE1  | 4:L:8:ASP:O      | 2.38                     | 0.50              |
| 1:C:98:GLY:HA3   | 4:F:6:TRP:NE1    | 2.26                     | 0.50              |
| 2:H:199:GLN:HA   | 2:H:239:ARG:O    | 2.12                     | 0.50              |
| 1:C:101:LEU:HD13 | 2:D:98:GLY:HA2   | 1.93                     | 0.50              |
| 2:H:134:HIS:HD2  | 2:H:134:HIS:O    | 1.94                     | 0.50              |
| 1:G:150:SER:HB3  | 1:G:157:ILE:CD1  | 2.40                     | 0.50              |
| 2:H:83:PRO:HA    | 2:H:110:VAL:HG22 | 1.94                     | 0.50              |
| 4:J:1:PHE:CG     | 4:J:2:LEU:N      | 2.80                     | 0.50              |
| 2:B:150:ASP:O    | 2:B:150:ASP:OD1  | 2.30                     | 0.50              |
| 2:B:114:LEU:HD22 | 2:B:214:LEU:HD21 | 1.93                     | 0.50              |
| 2:H:78:LEU:CD1   | 2:H:78:LEU:N     | 2.70                     | 0.50              |
| 3:I:15:ARG:NH1   | 3:I:16:GLY:H     | 2.09                     | 0.50              |
| 2:H:82:SER:O     | 2:H:110:VAL:HG21 | 2.12                     | 0.50              |
| 1:M:198:ASP:OD2  | 1:M:198:ASP:C    | 2.50                     | 0.50              |
| 2:B:83:PRO:HA    | 2:B:110:VAL:HG22 | 1.93                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:32:LEU:HD13  | 1:C:73:PHE:HB2   | 1.93                     | 0.50              |
| 2:B:114:LEU:HD13 | 2:B:214:LEU:CD2  | 2.43                     | 0.49              |
| 3:K:19:GLU:CG    | 3:K:20:PRO:HD2   | 2.30                     | 0.49              |
| 1:M:82:TRP:HA    | 1:M:111:VAL:CG1  | 2.41                     | 0.49              |
| 1:M:24:TYR:HH    | 1:M:66:PHE:HE1   | 1.59                     | 0.49              |
| 1:A:26:TYR:C     | 1:A:26:TYR:CD2   | 2.81                     | 0.49              |
| 1:A:70:ASP:O     | 1:A:71:SER:HB2   | 2.11                     | 0.49              |
| 1:G:1:GLN:NE2    | 1:G:27:SER:CB    | 2.73                     | 0.49              |
| 2:H:206:ARG:NE   | 5:H:243:SO4:O3   | 2.44                     | 0.49              |
| 3:K:56:GLY:O     | 3:K:59:TYR:HB3   | 2.13                     | 0.49              |
| 1:M:150:SER:HB3  | 1:M:157:ILE:CD1  | 2.43                     | 0.49              |
| 2:N:38:ASP:OD1   | 2:N:87:SER:HB2   | 2.12                     | 0.49              |
| 2:B:118:PHE:CD2  | 2:B:184:ARG:HD3  | 2.48                     | 0.49              |
| 2:B:240:ALA:O    | 2:B:241:ASP:C    | 2.51                     | 0.49              |
| 2:D:24:ARG:HG3   | 2:D:24:ARG:NH1   | 2.26                     | 0.49              |
| 2:N:195:ALA:O    | 2:N:199:GLN:CG   | 2.59                     | 0.49              |
| 2:B:117:VAL:HG12 | 2:B:227:PRO:HB2  | 1.94                     | 0.49              |
| 2:H:154:LEU:HD23 | 2:H:154:LEU:C    | 2.32                     | 0.49              |
| 3:K:80:THR:CG2   | 4:L:9:ILE:HG22   | 2.42                     | 0.49              |
| 1:M:150:SER:HB3  | 1:M:157:ILE:HD12 | 1.94                     | 0.49              |
| 1:A:18:LEU:HD11  | 1:A:20:LEU:HG    | 1.95                     | 0.49              |
| 2:H:30:ASN:HB3   | 2:H:50:TYR:O     | 2.12                     | 0.49              |
| 1:M:97:THR:O     | 1:M:97:THR:OG1   | 2.30                     | 0.49              |
| 1:A:101:LEU:HD13 | 2:B:98:GLY:HA2   | 1.94                     | 0.49              |
| 1:A:196:PRO:O    | 1:A:199:THR:CG2  | 2.61                     | 0.49              |
| 1:C:18:LEU:HD11  | 1:C:20:LEU:HG    | 1.93                     | 0.49              |
| 1:G:2:SER:H      | 1:G:25:SER:CB    | 2.26                     | 0.49              |
| 1:M:136:CYS:HG   | 1:M:186:CYS:CB   | 2.26                     | 0.49              |
| 1:A:152:ASP:O    | 1:A:152:ASP:OD1  | 2.30                     | 0.49              |
| 1:A:32:LEU:HD23  | 1:A:92:VAL:HG12  | 1.95                     | 0.49              |
| 1:C:151:LYS:CG   | 1:C:152:ASP:N    | 2.75                     | 0.49              |
| 1:C:3:VAL:HG13   | 1:C:22:CYS:SG    | 2.53                     | 0.49              |
| 2:N:86:THR:O     | 2:N:87:SER:CB    | 2.60                     | 0.49              |
| 2:B:134:HIS:O    | 2:B:134:HIS:HD2  | 1.96                     | 0.49              |
| 1:C:1:GLN:HA     | 1:C:25:SER:HB3   | 1.95                     | 0.48              |
| 3:K:123:TYR:CD1  | 3:K:124:ILE:HG22 | 2.45                     | 0.48              |
| 1:A:151:LYS:HD2  | 1:A:192:ASN:OD1  | 2.12                     | 0.48              |
| 2:B:199:GLN:HA   | 2:B:239:ARG:O    | 2.13                     | 0.48              |
| 2:H:127:PRO:HD2  | 2:H:198:TRP:CZ2  | 2.48                     | 0.48              |
| 2:H:134:HIS:CD2  | 2:H:134:HIS:O    | 2.66                     | 0.48              |
| 3:I:147:TRP:NE1  | 4:J:8:ASP:O      | 2.37                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:201:PRO:HD2  | 2:N:202:ARG:H    | 1.77                     | 0.48              |
| 1:A:155:VAL:HG22 | 1:A:179:SER:HB2  | 1.95                     | 0.48              |
| 2:D:142:CYS:HB2  | 2:D:156:TRP:CZ2  | 2.48                     | 0.48              |
| 2:N:83:PRO:HA    | 2:N:110:VAL:CG2  | 2.43                     | 0.48              |
| 2:N:14:VAL:CG2   | 2:N:114:LEU:HD21 | 2.42                     | 0.48              |
| 3:Q:80:THR:OG1   | 4:R:9:ILE:HG21   | 2.12                     | 0.48              |
| 1:G:152:ASP:OD1  | 1:G:152:ASP:O    | 2.30                     | 0.48              |
| 2:H:88:LEU:HD21  | 2:H:90:PHE:CE2   | 2.48                     | 0.48              |
| 3:K:28:VAL:HG21  | 3:K:171:TYR:CE2  | 2.48                     | 0.48              |
| 3:Q:78:LEU:O     | 3:Q:82:LEU:HD13  | 2.13                     | 0.48              |
| 1:C:6:PRO:CG     | 1:C:21:ARG:HB2   | 2.42                     | 0.48              |
| 3:Q:130:LEU:HD23 | 3:Q:157:ARG:HG2  | 1.96                     | 0.48              |
| 1:A:194:ILE:HD11 | 2:N:224:ARG:CA   | 2.44                     | 0.48              |
| 3:K:78:LEU:O     | 3:K:82:LEU:HD13  | 2.12                     | 0.48              |
| 1:A:24:TYR:HH    | 1:A:66:PHE:HE1   | 1.61                     | 0.48              |
| 2:B:83:PRO:HA    | 2:B:110:VAL:CG2  | 2.44                     | 0.48              |
| 1:C:149:GLN:HG3  | 1:C:150:SER:H    | 1.79                     | 0.48              |
| 1:C:194:ILE:CG2  | 1:C:194:ILE:O    | 2.61                     | 0.48              |
| 3:E:159:TYR:CZ   | 3:E:164:CYS:HB2  | 2.49                     | 0.48              |
| 3:I:42:ASN:ND2   | 3:I:44:ARG:HD2   | 2.29                     | 0.48              |
| 1:M:10:VAL:HG12  | 1:M:109:LEU:HD12 | 1.95                     | 0.48              |
| 1:A:196:PRO:HB2  | 1:A:199:THR:HG22 | 1.95                     | 0.48              |
| 3:Q:130:LEU:N    | 3:Q:130:LEU:CD1  | 2.76                     | 0.48              |
| 1:A:196:PRO:O    | 1:A:199:THR:HG23 | 2.14                     | 0.48              |
| 3:E:111:ARG:CG   | 3:E:112:GLY:N    | 2.77                     | 0.48              |
| 1:G:70:ASP:O     | 1:G:71:SER:HB2   | 2.14                     | 0.47              |
| 3:I:128:GLU:O    | 3:I:130:LEU:HD13 | 2.14                     | 0.47              |
| 1:M:59:VAL:HG22  | 1:M:60:ASN:N     | 2.29                     | 0.47              |
| 1:G:18:LEU:HD11  | 1:G:20:LEU:HG    | 1.96                     | 0.47              |
| 2:H:142:CYS:HB2  | 2:H:156:TRP:CH2  | 2.49                     | 0.47              |
| 2:D:80:LEU:HD13  | 2:H:75:PHE:CG    | 2.49                     | 0.47              |
| 1:A:28:ALA:HA    | 1:A:29:THR:HA    | 1.68                     | 0.47              |
| 1:C:82:TRP:HA    | 1:C:111:VAL:CG1  | 2.44                     | 0.47              |
| 1:C:155:VAL:HG22 | 1:C:179:SER:HB2  | 1.96                     | 0.47              |
| 1:G:199:THR:O    | 1:G:199:THR:OG1  | 2.30                     | 0.47              |
| 2:B:134:HIS:O    | 2:B:134:HIS:CD2  | 2.68                     | 0.47              |
| 3:Q:56:GLY:O     | 3:Q:59:TYR:HB3   | 2.14                     | 0.47              |
| 3:Q:96:GLN:HG2   | 3:Q:97:ARG:N     | 2.29                     | 0.47              |
| 3:I:27:TYR:HA    | 3:I:31:LYS:O     | 2.15                     | 0.47              |
| 1:M:70:ASP:O     | 1:M:71:SER:HB2   | 2.14                     | 0.47              |
| 2:N:29:HIS:HB3   | 2:N:94:SER:O     | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:202:PRO:HG2  | 1:A:205:GLU:HB2  | 1.97                     | 0.47              |
| 2:B:78:LEU:N     | 2:B:78:LEU:CD1   | 2.76                     | 0.47              |
| 3:E:159:TYR:CE2  | 3:E:164:CYS:HB2  | 2.49                     | 0.47              |
| 2:N:117:VAL:HG11 | 2:N:214:LEU:CD1  | 2.45                     | 0.47              |
| 1:A:82:TRP:HD1   | 1:A:111:VAL:O    | 1.98                     | 0.47              |
| 1:C:123:TYR:CE1  | 2:D:131:GLU:HA   | 2.50                     | 0.47              |
| 1:C:70:ASP:O     | 1:C:71:SER:HB2   | 2.14                     | 0.47              |
| 2:N:142:CYS:HB2  | 2:N:156:TRP:CH2  | 2.50                     | 0.47              |
| 1:A:142:ASP:OD1  | 1:A:145:THR:OG1  | 2.28                     | 0.47              |
| 1:C:1:GLN:OE1    | 1:C:27:SER:HB2   | 2.14                     | 0.47              |
| 2:D:117:VAL:HG11 | 2:D:214:LEU:CD1  | 2.45                     | 0.47              |
| 3:E:56:GLY:O     | 3:E:59:TYR:HB3   | 2.14                     | 0.47              |
| 1:G:32:LEU:HD23  | 1:G:92:VAL:HG12  | 1.97                     | 0.47              |
| 2:N:240:ALA:O    | 2:N:241:ASP:C    | 2.53                     | 0.47              |
| 1:G:194:ILE:CG2  | 1:G:194:ILE:O    | 2.61                     | 0.46              |
| 1:M:32:LEU:HD23  | 1:M:92:VAL:HG12  | 1.97                     | 0.46              |
| 1:A:122:VAL:O    | 1:A:122:VAL:HG12 | 2.13                     | 0.46              |
| 1:C:59:VAL:HG22  | 1:C:60:ASN:N     | 2.30                     | 0.46              |
| 2:D:127:PRO:HD2  | 2:D:198:TRP:CZ2  | 2.50                     | 0.46              |
| 2:D:30:ASN:HB3   | 2:D:50:TYR:O     | 2.15                     | 0.46              |
| 1:G:170:PHE:CE2  | 2:H:137:LYS:HE3  | 2.49                     | 0.46              |
| 2:H:47:HIS:CE1   | 2:H:61:PRO:HB2   | 2.51                     | 0.46              |
| 2:B:150:ASP:O    | 2:B:150:ASP:CG   | 2.53                     | 0.46              |
| 2:H:15:THR:HG23  | 2:H:83:PRO:HD3   | 1.97                     | 0.46              |
| 3:I:130:LEU:HD12 | 3:I:130:LEU:N    | 2.29                     | 0.46              |
| 2:N:86:THR:O     | 2:N:87:SER:HB2   | 2.15                     | 0.46              |
| 1:A:97:THR:O     | 1:A:97:THR:HG22  | 2.14                     | 0.46              |
| 1:C:95:LYS:NZ    | 4:F:2:LEU:O      | 2.32                     | 0.46              |
| 1:M:170:PHE:CE2  | 2:N:137:LYS:HE3  | 2.50                     | 0.46              |
| 3:E:14:ARG:CD    | 3:E:19:GLU:O     | 2.64                     | 0.46              |
| 2:D:62:ASP:HB3   | 2:H:70:THR:HG22  | 1.96                     | 0.46              |
| 3:Q:133:TRP:HB2  | 3:Q:144:ARG:HG3  | 1.98                     | 0.46              |
| 1:C:26:TYR:CD2   | 1:C:26:TYR:C     | 2.88                     | 0.46              |
| 3:K:13:SER:HB3   | 3:K:78:LEU:HD13  | 1.97                     | 0.46              |
| 1:C:137:LEU:HD12 | 1:C:175:ALA:O    | 2.16                     | 0.46              |
| 3:E:19:GLU:HG3   | 3:E:75:ARG:NH1   | 2.30                     | 0.46              |
| 3:K:167:TRP:CE2  | 4:L:1:PHE:HB3    | 2.51                     | 0.46              |
| 1:M:29:THR:OG1   | 1:M:29:THR:O     | 2.30                     | 0.46              |
| 1:A:62:PHE:CD2   | 1:A:75:LEU:HD11  | 2.50                     | 0.46              |
| 2:D:83:PRO:CA    | 2:D:110:VAL:CG2  | 2.92                     | 0.46              |
| 1:G:46:LEU:HA    | 1:G:46:LEU:HD12  | 1.71                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:Q:138:MET:O    | 3:Q:141:GLN:HB2  | 2.15                     | 0.46              |
| 1:C:10:VAL:HG12  | 1:C:109:LEU:HD12 | 1.98                     | 0.46              |
| 1:C:127:ASP:HB3  | 1:C:130:SER:O    | 2.16                     | 0.46              |
| 2:D:82:SER:O     | 2:D:110:VAL:HG21 | 2.15                     | 0.46              |
| 3:E:147:TRP:HB3  | 3:E:152:ALA:HB3  | 1.98                     | 0.46              |
| 1:G:2:SER:H      | 1:G:25:SER:HB3   | 1.81                     | 0.46              |
| 2:H:31:TYR:HA    | 2:H:49:SER:O     | 2.16                     | 0.46              |
| 1:M:128:SER:HB2  | 2:N:126:GLU:OE2  | 2.16                     | 0.46              |
| 2:B:169:THR:O    | 2:B:170:ASP:C    | 2.54                     | 0.45              |
| 2:D:71:GLN:HG3   | 2:D:71:GLN:O     | 2.13                     | 0.45              |
| 1:G:82:TRP:HA    | 1:G:111:VAL:CG1  | 2.46                     | 0.45              |
| 2:H:124:VAL:HG23 | 2:H:234:ALA:HB3  | 1.97                     | 0.45              |
| 3:I:15:ARG:CZ    | 3:I:15:ARG:H     | 2.30                     | 0.45              |
| 1:M:47:LEU:HB2   | 1:M:56:VAL:HG11  | 1.98                     | 0.45              |
| 2:N:47:HIS:CE1   | 2:N:61:PRO:HB2   | 2.51                     | 0.45              |
| 3:Q:14:ARG:CD    | 3:Q:19:GLU:O     | 2.65                     | 0.45              |
| 1:A:116:GLN:CD   | 1:A:116:GLN:H    | 2.20                     | 0.45              |
| 2:B:177:GLN:O    | 2:B:183:SER:HB2  | 2.17                     | 0.45              |
| 1:G:10:VAL:HG12  | 1:G:109:LEU:HD12 | 1.98                     | 0.45              |
| 2:H:167:VAL:HG22 | 2:H:191:LEU:HD13 | 1.99                     | 0.45              |
| 1:C:51:SER:HB3   | 3:E:158:ALA:HB2  | 1.97                     | 0.45              |
| 2:D:220:TRP:HB2  | 2:D:226:LYS:HG3  | 1.99                     | 0.45              |
| 3:I:45:TYR:CE2   | 3:I:63:ILE:HG22  | 2.51                     | 0.45              |
| 3:I:78:LEU:O     | 3:I:82:LEU:HD13  | 2.16                     | 0.45              |
| 2:B:114:LEU:HD13 | 2:B:214:LEU:HD21 | 1.98                     | 0.45              |
| 2:D:114:LEU:HD22 | 2:D:214:LEU:HD21 | 1.98                     | 0.45              |
| 3:K:174:ASN:N    | 3:K:174:ASN:OD1  | 2.50                     | 0.45              |
| 2:B:24:ARG:NH1   | 2:B:24:ARG:HG3   | 2.32                     | 0.45              |
| 1:A:120:PRO:CB   | 1:A:199:THR:HB   | 2.45                     | 0.45              |
| 2:B:220:TRP:CB   | 2:B:226:LYS:HG3  | 2.47                     | 0.45              |
| 1:G:116:GLN:CD   | 1:G:116:GLN:H    | 2.20                     | 0.45              |
| 2:H:201:PRO:HB3  | 2:H:238:GLY:O    | 2.16                     | 0.45              |
| 3:Q:23:THR:HG23  | 3:Q:24:SER:N     | 2.31                     | 0.45              |
| 3:Q:8:TYR:CE1    | 3:Q:98:MET:HG3   | 2.52                     | 0.45              |
| 1:A:120:PRO:HB2  | 1:A:199:THR:CA   | 2.47                     | 0.45              |
| 3:E:15:ARG:HD3   | 3:Q:61:GLU:HG2   | 1.99                     | 0.45              |
| 3:E:175:GLY:O    | 3:E:176:ASN:ND2  | 2.50                     | 0.45              |
| 3:I:54:GLN:O     | 3:I:55:GLU:HG2   | 2.16                     | 0.45              |
| 1:A:10:VAL:HG12  | 1:A:109:LEU:HD12 | 1.98                     | 0.45              |
| 2:N:24:ARG:HG3   | 2:N:24:ARG:HH11  | 1.82                     | 0.45              |
| 1:C:96:GLY:HA2   | 3:E:66:VAL:HG13  | 1.98                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:169:THR:HG23 | 2:D:189:SER:HB2  | 1.99                     | 0.44              |
| 3:I:49:VAL:HG12  | 3:I:52:MET:HG3   | 1.99                     | 0.44              |
| 3:I:156:TYR:OH   | 4:J:5:PHE:HA     | 2.18                     | 0.44              |
| 1:M:198:ASP:OD2  | 1:M:198:ASP:O    | 2.35                     | 0.44              |
| 2:N:158:VAL:HB   | 2:N:163:VAL:HG11 | 1.98                     | 0.44              |
| 1:A:105:LYS:HG3  | 1:A:106:GLY:N    | 2.32                     | 0.44              |
| 1:M:133:LYS:HD2  | 1:M:133:LYS:HA   | 1.67                     | 0.44              |
| 2:H:220:TRP:CB   | 2:H:226:LYS:HG3  | 2.48                     | 0.44              |
| 1:C:122:VAL:O    | 1:C:122:VAL:HG12 | 2.16                     | 0.44              |
| 2:D:167:VAL:CG2  | 2:D:191:LEU:HD13 | 2.48                     | 0.44              |
| 2:H:132:ILE:HG23 | 2:H:195:ALA:CB   | 2.47                     | 0.44              |
| 2:H:87:SER:OG    | 2:H:88:LEU:N     | 2.50                     | 0.44              |
| 1:M:152:ASP:OD2  | 1:M:154:ASP:HB2  | 2.18                     | 0.44              |
| 1:M:46:LEU:HD12  | 1:M:46:LEU:HA    | 1.72                     | 0.44              |
| 1:M:49:TYR:CE2   | 1:M:66:PHE:CD2   | 3.05                     | 0.44              |
| 2:N:10:ASN:OD1   | 2:N:151:HIS:NE2  | 2.39                     | 0.44              |
| 2:N:220:TRP:HB2  | 2:N:226:LYS:HG3  | 1.99                     | 0.44              |
| 3:Q:73:TRP:CE2   | 3:Q:77:ASN:ND2   | 2.85                     | 0.44              |
| 1:A:137:LEU:HD12 | 1:A:175:ALA:O    | 2.18                     | 0.44              |
| 1:C:156:TYR:O    | 1:C:177:ALA:HA   | 2.18                     | 0.44              |
| 3:E:78:LEU:O     | 3:E:82:LEU:HD13  | 2.18                     | 0.44              |
| 1:G:11:THR:HG23  | 1:G:110:THR:HB   | 1.99                     | 0.44              |
| 3:I:77:ASN:OD1   | 4:J:9:ILE:HG12   | 2.18                     | 0.44              |
| 1:M:116:GLN:CD   | 1:M:116:GLN:H    | 2.21                     | 0.44              |
| 1:A:120:PRO:HB2  | 1:A:199:THR:CB   | 2.47                     | 0.44              |
| 1:A:128:SER:HB3  | 2:B:126:GLU:HG3  | 2.00                     | 0.44              |
| 2:B:50:TYR:CE2   | 2:B:56:GLN:HG3   | 2.50                     | 0.44              |
| 1:G:156:TYR:O    | 1:G:177:ALA:HA   | 2.18                     | 0.44              |
| 1:C:1:GLN:OE1    | 1:C:27:SER:CB    | 2.66                     | 0.44              |
| 1:G:62:PHE:CD2   | 1:G:75:LEU:HD11  | 2.52                     | 0.44              |
| 3:I:49:VAL:HG12  | 3:I:52:MET:CG    | 2.48                     | 0.44              |
| 1:M:137:LEU:HG   | 1:M:137:LEU:O    | 2.18                     | 0.44              |
| 3:Q:40:ALA:O     | 3:Q:41:GLU:C     | 2.53                     | 0.44              |
| 2:B:9:ARG:NH2    | 2:B:153:GLU:OE2  | 2.35                     | 0.44              |
| 1:C:149:GLN:CG   | 1:C:150:SER:N    | 2.80                     | 0.44              |
| 3:K:47:PRO:HB3   | 3:K:52:MET:HB3   | 1.98                     | 0.44              |
| 1:M:123:TYR:HB3  | 2:N:128:SER:CB   | 2.48                     | 0.44              |
| 2:B:154:LEU:HD23 | 2:B:155:SER:N    | 2.33                     | 0.44              |
| 1:C:49:TYR:CE2   | 1:C:66:PHE:CD2   | 3.06                     | 0.44              |
| 2:H:156:TRP:CD1  | 2:H:167:VAL:HG13 | 2.52                     | 0.44              |
| 1:G:119:ASP:C    | 1:G:119:ASP:OD1  | 2.56                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:240:ALA:O    | 2:H:241:ASP:C    | 2.56                     | 0.43              |
| 3:I:19:GLU:CG    | 3:I:20:PRO:HD2   | 2.33                     | 0.43              |
| 3:Q:156:TYR:HH   | 4:R:5:PHE:HA     | 1.83                     | 0.43              |
| 2:H:220:TRP:HB2  | 2:H:226:LYS:HG3  | 2.00                     | 0.43              |
| 3:I:147:TRP:CZ2  | 4:J:5:PHE:CZ     | 3.06                     | 0.43              |
| 3:I:56:GLY:O     | 3:I:59:TYR:HB3   | 2.18                     | 0.43              |
| 1:M:95:LYS:NZ    | 4:R:2:LEU:O      | 2.51                     | 0.43              |
| 1:C:0:ALA:O      | 1:C:1:GLN:C      | 2.53                     | 0.43              |
| 1:G:32:LEU:HD13  | 1:G:73:PHE:HB2   | 2.01                     | 0.43              |
| 3:I:147:TRP:CZ2  | 4:J:5:PHE:HZ     | 2.35                     | 0.43              |
| 3:Q:129:ASP:O    | 3:Q:130:LEU:HB2  | 2.17                     | 0.43              |
| 2:B:47:HIS:CE1   | 2:B:61:PRO:HB2   | 2.52                     | 0.43              |
| 2:D:240:ALA:O    | 2:D:241:ASP:C    | 2.56                     | 0.43              |
| 3:K:54:GLN:CG    | 3:K:54:GLN:O     | 2.59                     | 0.43              |
| 3:Q:80:THR:OG1   | 4:R:9:ILE:CG2    | 2.66                     | 0.43              |
| 1:C:33:PHE:CZ    | 2:D:98:GLY:HA3   | 2.53                     | 0.43              |
| 1:G:192:ASN:O    | 1:G:192:ASN:ND2  | 2.51                     | 0.43              |
| 3:I:49:VAL:HA    | 3:I:50:PRO:HD3   | 1.93                     | 0.43              |
| 3:K:15:ARG:HG3   | 3:K:15:ARG:H     | 1.51                     | 0.43              |
| 1:M:16:ALA:O     | 1:M:80:VAL:HG22  | 2.17                     | 0.43              |
| 1:C:62:PHE:CD2   | 1:C:75:LEU:HD11  | 2.53                     | 0.43              |
| 1:C:95:LYS:HZ2   | 4:F:3:SER:HA     | 1.83                     | 0.43              |
| 3:I:8:TYR:O      | 3:I:24:SER:HA    | 2.19                     | 0.43              |
| 2:N:168:CYS:HB3  | 2:N:190:ARG:HD2  | 2.01                     | 0.43              |
| 1:M:33:PHE:CZ    | 2:N:98:GLY:HA3   | 2.54                     | 0.43              |
| 3:Q:61:GLU:O     | 3:Q:62:ARG:C     | 2.57                     | 0.43              |
| 1:C:97:THR:O     | 1:C:97:THR:OG1   | 2.36                     | 0.43              |
| 2:N:201:PRO:CD   | 2:N:202:ARG:N    | 2.82                     | 0.43              |
| 1:A:197:GLU:HB3  | 2:D:228:VAL:HG21 | 2.00                     | 0.43              |
| 2:D:114:LEU:HD13 | 2:D:214:LEU:HD21 | 2.00                     | 0.43              |
| 1:M:6:PRO:CG     | 1:M:21:ARG:HB2   | 2.44                     | 0.43              |
| 2:N:132:ILE:HG23 | 2:N:195:ALA:CB   | 2.48                     | 0.43              |
| 3:K:17:LEU:CD1   | 3:K:75:ARG:HH21  | 2.31                     | 0.42              |
| 4:R:9:ILE:HD12   | 4:R:9:ILE:HA     | 1.65                     | 0.42              |
| 2:B:127:PRO:HD2  | 2:B:198:TRP:CZ2  | 2.54                     | 0.42              |
| 3:E:23:THR:HG22  | 3:E:23:THR:O     | 2.19                     | 0.42              |
| 1:G:31:TYR:CE2   | 3:K:155:TYR:CE1  | 3.08                     | 0.42              |
| 3:K:23:THR:O     | 3:K:23:THR:HG22  | 2.18                     | 0.42              |
| 1:A:6:PRO:CG     | 1:A:21:ARG:HB2   | 2.46                     | 0.42              |
| 2:B:86:THR:O     | 2:B:87:SER:HB2   | 2.20                     | 0.42              |
| 1:C:46:LEU:HD12  | 1:C:46:LEU:HA    | 1.72                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:127:ASN:O    | 3:I:130:LEU:HD12 | 2.19                     | 0.42              |
| 1:A:203:SER:HB2  | 1:A:204:PRO:CD   | 2.50                     | 0.42              |
| 1:C:116:GLN:H    | 1:C:116:GLN:CD   | 2.22                     | 0.42              |
| 1:C:163:LEU:HB3  | 2:D:168:CYS:HB2  | 2.01                     | 0.42              |
| 2:D:169:THR:O    | 2:D:170:ASP:C    | 2.55                     | 0.42              |
| 3:I:96:GLN:HG2   | 3:I:97:ARG:N     | 2.34                     | 0.42              |
| 3:K:49:VAL:HG12  | 3:K:52:MET:HG2   | 2.02                     | 0.42              |
| 3:Q:5:MET:CE     | 3:Q:167:TRP:CE3  | 3.02                     | 0.42              |
| 1:A:152:ASP:O    | 1:A:153:SER:OG   | 2.30                     | 0.42              |
| 1:A:70:ASP:CB    | 1:A:72:SER:HB2   | 2.48                     | 0.42              |
| 2:B:150:ASP:OD2  | 2:B:173:PRO:HG3  | 2.19                     | 0.42              |
| 2:D:158:VAL:HB   | 2:D:163:VAL:HG11 | 2.01                     | 0.42              |
| 1:G:34:TRP:CE2   | 1:G:75:LEU:HB2   | 2.55                     | 0.42              |
| 2:H:175:LYS:HD3  | 2:H:183:SER:HB3  | 2.02                     | 0.42              |
| 3:K:16:GLY:HA3   | 3:K:18:GLY:N     | 2.35                     | 0.42              |
| 2:B:31:TYR:HA    | 2:B:49:SER:O     | 2.19                     | 0.42              |
| 1:C:29:THR:CG2   | 3:E:163:GLU:HB2  | 2.49                     | 0.42              |
| 2:H:114:LEU:HD22 | 2:H:214:LEU:HD21 | 2.02                     | 0.42              |
| 3:I:129:ASP:O    | 3:I:130:LEU:HB2  | 2.19                     | 0.42              |
| 2:N:51:GLY:HA3   | 3:Q:76:VAL:HG21  | 2.02                     | 0.42              |
| 2:N:78:LEU:CD1   | 2:N:78:LEU:N     | 2.82                     | 0.42              |
| 3:K:169:HIS:O    | 3:K:170:ARG:C    | 2.57                     | 0.42              |
| 1:M:17:SER:HA    | 1:M:78:ALA:O     | 2.20                     | 0.42              |
| 3:Q:19:GLU:CG    | 3:Q:20:PRO:HD2   | 2.34                     | 0.42              |
| 1:A:138:PHE:HB2  | 1:A:190:PHE:CZ   | 2.55                     | 0.42              |
| 1:C:149:GLN:CG   | 1:C:150:SER:H    | 2.32                     | 0.42              |
| 1:C:24:TYR:OH    | 1:C:66:PHE:HE1   | 2.02                     | 0.42              |
| 2:H:169:THR:HG23 | 2:H:189:SER:HB2  | 2.02                     | 0.42              |
| 3:I:23:THR:HG23  | 3:I:24:SER:N     | 2.33                     | 0.42              |
| 1:A:127:ASP:HB2  | 1:A:133:LYS:HB2  | 2.00                     | 0.41              |
| 3:E:155:TYR:CD2  | 3:E:156:TYR:CE2  | 3.08                     | 0.41              |
| 2:H:231:ILE:HG22 | 2:H:232:VAL:N    | 2.35                     | 0.41              |
| 3:K:171:TYR:CD2  | 3:K:171:TYR:C    | 2.93                     | 0.41              |
| 1:M:141:PHE:CZ   | 1:M:173:ASN:HB3  | 2.55                     | 0.41              |
| 3:Q:13:SER:HB3   | 3:Q:78:LEU:HD13  | 2.01                     | 0.41              |
| 1:G:6:PRO:CG     | 1:G:21:ARG:HB2   | 2.49                     | 0.41              |
| 3:I:111:ARG:HG2  | 3:I:113:TYR:CZ   | 2.55                     | 0.41              |
| 2:N:142:CYS:HB2  | 2:N:156:TRP:CZ2  | 2.55                     | 0.41              |
| 2:B:57:ILE:CG1   | 2:B:61:PRO:HG3   | 2.51                     | 0.41              |
| 2:D:15:THR:HG23  | 2:D:83:PRO:HD3   | 2.01                     | 0.41              |
| 3:Q:147:TRP:HB3  | 3:Q:152:ALA:HB3  | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:220:TRP:CB   | 2:D:226:LYS:HG3  | 2.50                     | 0.41              |
| 2:H:169:THR:O    | 2:H:170:ASP:C    | 2.58                     | 0.41              |
| 2:D:117:VAL:HG11 | 2:D:214:LEU:HD12 | 2.03                     | 0.41              |
| 1:G:166:ARG:HB2  | 1:G:166:ARG:HE   | 1.61                     | 0.41              |
| 1:G:70:ASP:CB    | 1:G:72:SER:HB2   | 2.48                     | 0.41              |
| 2:N:181:ASN:N    | 2:N:181:ASN:OD1  | 2.53                     | 0.41              |
| 1:A:133:LYS:HD2  | 1:A:133:LYS:HA   | 1.76                     | 0.41              |
| 2:D:101:TYR:CD2  | 2:D:101:TYR:N    | 2.89                     | 0.41              |
| 1:M:125:LEU:HB3  | 2:N:126:GLU:O    | 2.21                     | 0.41              |
| 2:N:220:TRP:CB   | 2:N:226:LYS:HG3  | 2.51                     | 0.41              |
| 3:Q:61:GLU:O     | 3:Q:64:THR:N     | 2.53                     | 0.41              |
| 1:A:82:TRP:HA    | 1:A:111:VAL:CG1  | 2.50                     | 0.41              |
| 1:C:133:LYS:HD2  | 1:C:133:LYS:HA   | 1.72                     | 0.41              |
| 2:D:201:PRO:HB3  | 2:D:238:GLY:O    | 2.21                     | 0.41              |
| 3:E:8:TYR:CE1    | 3:E:98:MET:HG3   | 2.56                     | 0.41              |
| 1:G:136:CYS:SG   | 1:G:184:PHE:CE2  | 3.13                     | 0.41              |
| 3:I:147:TRP:HB3  | 3:I:152:ALA:HB3  | 2.03                     | 0.41              |
| 1:A:113:PRO:O    | 1:A:143:SER:OG   | 2.39                     | 0.41              |
| 2:B:220:TRP:HB2  | 2:B:226:LYS:HG3  | 2.02                     | 0.41              |
| 1:M:62:PHE:CD2   | 1:M:75:LEU:HD11  | 2.55                     | 0.41              |
| 2:N:124:VAL:HG23 | 2:N:234:ALA:HB3  | 2.03                     | 0.41              |
| 2:B:82:SER:O     | 2:B:110:VAL:HG21 | 2.20                     | 0.41              |
| 1:C:183:ASP:O    | 1:C:183:ASP:OD1  | 2.38                     | 0.41              |
| 2:D:154:LEU:HD23 | 2:D:155:SER:N    | 2.36                     | 0.41              |
| 1:C:3:VAL:CG1    | 1:C:22:CYS:SG    | 3.09                     | 0.40              |
| 1:G:59:VAL:HG22  | 1:G:60:ASN:H     | 1.86                     | 0.40              |
| 2:H:220:TRP:CG   | 2:H:226:LYS:HG3  | 2.56                     | 0.40              |
| 3:K:45:TYR:CE2   | 3:K:63:ILE:HG22  | 2.56                     | 0.40              |
| 1:M:34:TRP:CE2   | 1:M:75:LEU:HB2   | 2.56                     | 0.40              |
| 3:E:58:GLU:HA    | 3:E:61:GLU:HB2   | 2.03                     | 0.40              |
| 2:B:142:CYS:HB2  | 2:B:156:TRP:CH2  | 2.57                     | 0.40              |
| 1:C:115:ILE:O    | 1:C:118:PRO:HD3  | 2.22                     | 0.40              |
| 3:E:23:THR:HG23  | 3:E:24:SER:N     | 2.36                     | 0.40              |
| 2:H:86:THR:O     | 2:H:87:SER:HB2   | 2.22                     | 0.40              |
| 3:I:130:LEU:HD23 | 3:I:157:ARG:HG2  | 2.02                     | 0.40              |
| 1:C:119:ASP:O    | 1:C:140:ASP:HB2  | 2.21                     | 0.40              |
| 1:C:38:TYR:CD1   | 1:C:86:ALA:HB2   | 2.56                     | 0.40              |
| 2:D:126:GLU:HA   | 2:D:127:PRO:HD3  | 1.89                     | 0.40              |
| 2:D:164:HIS:N    | 5:D:242:SO4:O2   | 2.52                     | 0.40              |
| 1:G:38:TYR:CD1   | 1:G:86:ALA:HB2   | 2.57                     | 0.40              |
| 3:K:78:LEU:HA    | 3:K:78:LEU:HD23  | 1.92                     | 0.40              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:M:127:ASP:HB2 | 1:M:133:LYS:HB2 | 2.03                     | 0.40              |
| 3:Q:5:MET:SD    | 3:Q:167:TRP:CE3 | 3.15                     | 0.40              |
| 4:R:2:LEU:HA    | 4:R:2:LEU:HD23  | 1.75                     | 0.40              |
| 1:C:192:ASN:O   | 1:C:192:ASN:ND2 | 2.54                     | 0.40              |
| 2:D:9:ARG:HH12  | 2:D:153:GLU:CD  | 2.22                     | 0.40              |
| 3:E:45:TYR:CE2  | 3:E:63:ILE:HG22 | 2.56                     | 0.40              |
| 1:G:97:THR:O    | 1:G:97:THR:OG1  | 2.35                     | 0.40              |
| 3:K:133:TRP:HB2 | 3:K:144:ARG:HG3 | 2.03                     | 0.40              |
| 3:Q:34:VAL:CG2  | 3:Q:35:ARG:N    | 2.85                     | 0.40              |
| 3:Q:78:LEU:HD23 | 3:Q:78:LEU:HA   | 1.91                     | 0.40              |

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

| Atom-1        | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|------------------------|--------------------------|-------------------|
| 1:M:167:SER:O | 2:N:136:GLN:NE2[2_555] | 2.03                     | 0.17              |

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 201/211 (95%) | 183 (91%) | 16 (8%) | 2 (1%)   | 18          | 57  |
| 1   | C     | 202/211 (96%) | 184 (91%) | 18 (9%) | 0        | 100         | 100 |
| 1   | G     | 198/211 (94%) | 181 (91%) | 15 (8%) | 2 (1%)   | 18          | 57  |
| 1   | M     | 202/211 (96%) | 189 (94%) | 13 (6%) | 0        | 100         | 100 |
| 2   | B     | 238/243 (98%) | 223 (94%) | 15 (6%) | 0        | 100         | 100 |
| 2   | D     | 238/243 (98%) | 225 (94%) | 13 (6%) | 0        | 100         | 100 |
| 2   | H     | 238/243 (98%) | 224 (94%) | 14 (6%) | 0        | 100         | 100 |
| 2   | N     | 238/243 (98%) | 226 (95%) | 11 (5%) | 1 (0%)   | 38          | 75  |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 3   | E     | 171/180 (95%)   | 160 (94%)  | 11 (6%)  | 0        | 100         | 100 |
| 3   | I     | 169/180 (94%)   | 158 (94%)  | 11 (6%)  | 0        | 100         | 100 |
| 3   | K     | 173/180 (96%)   | 158 (91%)  | 15 (9%)  | 0        | 100         | 100 |
| 3   | Q     | 174/180 (97%)   | 161 (92%)  | 12 (7%)  | 1 (1%)   | 28          | 67  |
| 4   | F     | 7/9 (78%)       | 7 (100%)   | 0        | 0        | 100         | 100 |
| 4   | J     | 7/9 (78%)       | 7 (100%)   | 0        | 0        | 100         | 100 |
| 4   | L     | 7/9 (78%)       | 7 (100%)   | 0        | 0        | 100         | 100 |
| 4   | R     | 7/9 (78%)       | 6 (86%)    | 1 (14%)  | 0        | 100         | 100 |
| All | All   | 2470/2572 (96%) | 2299 (93%) | 165 (7%) | 6 (0%)   | 51          | 84  |

All (6) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 184 | PHE  |
| 3   | Q     | 43  | PRO  |
| 2   | N     | 87  | SER  |
| 1   | G     | 94  | ALA  |
| 1   | A     | 39  | PRO  |
| 1   | G     | 39  | 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     | 180/186 (97%) | 169 (94%) | 11 (6%)  | 22          | 58 |
| 1   | C     | 178/186 (96%) | 166 (93%) | 12 (7%)  | 19          | 54 |
| 1   | G     | 177/186 (95%) | 167 (94%) | 10 (6%)  | 25          | 61 |
| 1   | M     | 179/186 (96%) | 171 (96%) | 8 (4%)   | 32          | 68 |
| 2   | B     | 206/208 (99%) | 199 (97%) | 7 (3%)   | 42          | 77 |
| 2   | D     | 206/208 (99%) | 198 (96%) | 8 (4%)   | 37          | 73 |
| 2   | H     | 206/208 (99%) | 200 (97%) | 6 (3%)   | 48          | 80 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 2   | N     | 206/208 (99%)   | 198 (96%)  | 8 (4%)   | 37          | 73  |
| 3   | E     | 144/148 (97%)   | 140 (97%)  | 4 (3%)   | 49          | 81  |
| 3   | I     | 143/148 (97%)   | 137 (96%)  | 6 (4%)   | 34          | 71  |
| 3   | K     | 144/148 (97%)   | 136 (94%)  | 8 (6%)   | 25          | 61  |
| 3   | Q     | 144/148 (97%)   | 140 (97%)  | 4 (3%)   | 49          | 81  |
| 4   | F     | 9/9 (100%)      | 9 (100%)   | 0        | 100         | 100 |
| 4   | J     | 9/9 (100%)      | 9 (100%)   | 0        | 100         | 100 |
| 4   | L     | 9/9 (100%)      | 9 (100%)   | 0        | 100         | 100 |
| 4   | R     | 9/9 (100%)      | 8 (89%)    | 1 (11%)  | 7           | 29  |
| All | All   | 2149/2204 (98%) | 2056 (96%) | 93 (4%)  | 33          | 70  |

All (93) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 4   | THR  |
| 1   | A     | 11  | THR  |
| 1   | A     | 26  | TYR  |
| 1   | A     | 65  | GLU  |
| 1   | A     | 99  | SER  |
| 1   | A     | 123 | TYR  |
| 1   | A     | 182 | SER  |
| 1   | A     | 183 | ASP  |
| 1   | A     | 199 | THR  |
| 1   | A     | 205 | GLU  |
| 1   | A     | 206 | SER  |
| 2   | B     | 9   | ARG  |
| 2   | B     | 38  | ASP  |
| 2   | B     | 71  | GLN  |
| 2   | B     | 110 | VAL  |
| 2   | B     | 112 | GLU  |
| 2   | B     | 190 | ARG  |
| 2   | B     | 241 | ASP  |
| 3   | I     | 15  | ARG  |
| 3   | I     | 23  | THR  |
| 3   | I     | 28  | VAL  |
| 3   | I     | 49  | VAL  |
| 3   | I     | 86  | ASN  |
| 3   | I     | 111 | ARG  |
| 1   | C     | 4   | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 26  | TYR  |
| 1   | C     | 29  | THR  |
| 1   | C     | 65  | GLU  |
| 1   | C     | 81  | HIS  |
| 1   | C     | 95  | LYS  |
| 1   | C     | 97  | THR  |
| 1   | C     | 135 | VAL  |
| 1   | C     | 138 | PHE  |
| 1   | C     | 151 | LYS  |
| 1   | C     | 153 | SER  |
| 1   | C     | 186 | CYS  |
| 2   | D     | 9   | ARG  |
| 2   | D     | 71  | GLN  |
| 2   | D     | 110 | VAL  |
| 2   | D     | 112 | GLU  |
| 2   | D     | 190 | ARG  |
| 2   | D     | 210 | GLN  |
| 2   | D     | 239 | ARG  |
| 2   | D     | 241 | ASP  |
| 3   | E     | 23  | THR  |
| 3   | E     | 28  | VAL  |
| 3   | E     | 49  | VAL  |
| 3   | E     | 86  | ASN  |
| 1   | G     | 4   | THR  |
| 1   | G     | 11  | THR  |
| 1   | G     | 65  | GLU  |
| 1   | G     | 97  | THR  |
| 1   | G     | 123 | TYR  |
| 1   | G     | 134 | SER  |
| 1   | G     | 143 | SER  |
| 1   | G     | 197 | GLU  |
| 1   | G     | 199 | THR  |
| 1   | G     | 203 | SER  |
| 2   | H     | 71  | GLN  |
| 2   | H     | 110 | VAL  |
| 2   | H     | 112 | GLU  |
| 2   | H     | 187 | LEU  |
| 2   | H     | 190 | ARG  |
| 2   | H     | 241 | ASP  |
| 3   | K     | 5   | MET  |
| 3   | K     | 15  | ARG  |
| 3   | K     | 23  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | K     | 49  | VAL  |
| 3   | K     | 52  | MET  |
| 3   | K     | 86  | ASN  |
| 3   | K     | 111 | ARG  |
| 3   | K     | 174 | ASN  |
| 1   | M     | 4   | THR  |
| 1   | M     | 65  | GLU  |
| 1   | M     | 95  | LYS  |
| 1   | M     | 97  | THR  |
| 1   | M     | 131 | SER  |
| 1   | M     | 146 | ASN  |
| 1   | M     | 149 | GLN  |
| 1   | M     | 198 | ASP  |
| 2   | N     | 38  | ASP  |
| 2   | N     | 71  | GLN  |
| 2   | N     | 110 | VAL  |
| 2   | N     | 112 | GLU  |
| 2   | N     | 176 | GLU  |
| 2   | N     | 190 | ARG  |
| 2   | N     | 228 | VAL  |
| 2   | N     | 241 | ASP  |
| 3   | Q     | 15  | ARG  |
| 3   | Q     | 23  | THR  |
| 3   | Q     | 49  | VAL  |
| 3   | Q     | 86  | ASN  |
| 4   | R     | 9   | ILE  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 47  | HIS  |
| 2   | B     | 134 | HIS  |
| 2   | B     | 177 | GLN  |
| 3   | I     | 127 | ASN  |
| 3   | E     | 176 | ASN  |
| 2   | H     | 47  | HIS  |
| 2   | H     | 134 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

16 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 | $\# Z  > 2$ |
| 5   | SO4  | A     | 208 | -    | 4,4,4        | 0.18 | 0           | 6,6,6       | 0.67 | 0           |
| 5   | SO4  | B     | 242 | -    | 4,4,4        | 0.25 | 0           | 6,6,6       | 0.44 | 0           |
| 5   | SO4  | B     | 243 | -    | 4,4,4        | 0.36 | 0           | 6,6,6       | 0.45 | 0           |
| 5   | SO4  | B     | 244 | -    | 4,4,4        | 0.20 | 0           | 6,6,6       | 0.36 | 0           |
| 5   | SO4  | D     | 242 | -    | 4,4,4        | 0.08 | 0           | 6,6,6       | 0.48 | 0           |
| 5   | SO4  | D     | 243 | -    | 4,4,4        | 0.22 | 0           | 6,6,6       | 0.36 | 0           |
| 5   | SO4  | E     | 180 | -    | 4,4,4        | 0.18 | 0           | 6,6,6       | 0.19 | 0           |
| 5   | SO4  | G     | 208 | -    | 4,4,4        | 0.23 | 0           | 6,6,6       | 0.20 | 0           |
| 5   | SO4  | H     | 242 | -    | 4,4,4        | 0.19 | 0           | 6,6,6       | 0.34 | 0           |
| 5   | SO4  | H     | 243 | -    | 4,4,4        | 0.35 | 0           | 6,6,6       | 0.51 | 0           |
| 5   | SO4  | K     | 180 | -    | 4,4,4        | 0.23 | 0           | 6,6,6       | 0.37 | 0           |
| 5   | SO4  | K     | 181 | -    | 4,4,4        | 1.01 | 0           | 6,6,6       | 1.58 | 1 (16%)     |
| 5   | SO4  | N     | 242 | -    | 4,4,4        | 0.13 | 0           | 6,6,6       | 0.05 | 0           |
| 5   | SO4  | N     | 243 | -    | 4,4,4        | 0.17 | 0           | 6,6,6       | 0.59 | 0           |
| 6   | EDO  | N     | 244 | -    | 3,3,3        | 0.40 | 0           | 2,2,2       | 0.41 | 0           |
| 5   | SO4  | Q     | 180 | -    | 4,4,4        | 0.28 | 0           | 6,6,6       | 0.32 | 0           |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 5   | SO4  | A     | 208 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 5   | SO4  | B     | 242 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 5   | SO4  | B     | 243 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 5   | SO4  | B     | 244 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 5   | SO4  | D     | 242 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 5   | SO4  | D     | 243 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 5   | SO4  | E     | 180 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 5   | SO4  | G     | 208 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 5   | SO4  | H     | 242 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 5   | SO4  | H     | 243 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 5   | SO4  | K     | 180 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 5   | SO4  | K     | 181 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 5   | SO4  | N     | 242 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 5   | SO4  | N     | 243 | -    | -       | 0/0/0/0  | 0/0/0/0 |
| 6   | EDO  | N     | 244 | -    | -       | 0/1/1/1  | 0/0/0/0 |
| 5   | SO4  | Q     | 180 | -    | -       | 0/0/0/0  | 0/0/0/0 |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 5   | K     | 181 | SO4  | O4-S-O3 | 3.65 | 125.39      | 108.96   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5   | D     | 242 | SO4  | 1       | 0            |
| 5   | E     | 180 | SO4  | 4       | 0            |
| 5   | H     | 243 | SO4  | 1       | 0            |
| 5   | N     | 243 | SO4  | 3       | 0            |

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2                                 | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|-----------------------------------------|-----------------------|-------|
| 1   | A     | 205/211 (97%)   | -0.02  | 0 <span>100</span> <span>100</span>     | 42, 77, 113, 124      | 0     |
| 1   | C     | 204/211 (96%)   | 0.21   | 2 (0%) <span>82</span> <span>67</span>  | 24, 81, 114, 125      | 0     |
| 1   | G     | 202/211 (95%)   | 0.35   | 6 (2%) <span>51</span> <span>27</span>  | 44, 80, 119, 130      | 0     |
| 1   | M     | 204/211 (96%)   | 0.36   | 4 (1%) <span>65</span> <span>44</span>  | 49, 82, 119, 140      | 0     |
| 2   | B     | 240/243 (98%)   | -0.34  | 1 (0%) <span>92</span> <span>84</span>  | 34, 54, 94, 130       | 0     |
| 2   | D     | 240/243 (98%)   | -0.40  | 0 <span>100</span> <span>100</span>     | 32, 55, 95, 133       | 0     |
| 2   | H     | 240/243 (98%)   | -0.18  | 5 (2%) <span>64</span> <span>43</span>  | 33, 56, 100, 131      | 0     |
| 2   | N     | 240/243 (98%)   | -0.18  | 2 (0%) <span>86</span> <span>71</span>  | 34, 55, 100, 133      | 0     |
| 3   | E     | 175/180 (97%)   | -0.24  | 0 <span>100</span> <span>100</span>     | 44, 61, 109, 155      | 0     |
| 3   | I     | 173/180 (96%)   | -0.22  | 1 (0%) <span>89</span> <span>77</span>  | 46, 64, 111, 154      | 0     |
| 3   | K     | 175/180 (97%)   | -0.18  | 0 <span>100</span> <span>100</span>     | 43, 59, 113, 153      | 0     |
| 3   | Q     | 176/180 (97%)   | -0.17  | 3 (1%) <span>70</span> <span>49</span>  | 46, 64, 119, 137      | 0     |
| 4   | F     | 9/9 (100%)      | -0.28  | 0 <span>100</span> <span>100</span>     | 45, 50, 55, 58        | 0     |
| 4   | J     | 9/9 (100%)      | -0.26  | 0 <span>100</span> <span>100</span>     | 49, 54, 70, 71        | 0     |
| 4   | L     | 9/9 (100%)      | -0.16  | 0 <span>100</span> <span>100</span>     | 39, 45, 52, 53        | 0     |
| 4   | R     | 9/9 (100%)      | -0.30  | 0 <span>100</span> <span>100</span>     | 49, 55, 62, 65        | 0     |
| All | All   | 2510/2572 (97%) | -0.09  | 24 (0%) <span>82</span> <span>67</span> | 24, 66, 111, 155      | 0     |

All (24) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 202 | PRO  | 3.5  |
| 3   | Q     | 17  | LEU  | 3.5  |
| 1   | G     | 191 | ASN  | 3.4  |
| 2   | H     | 240 | ALA  | 3.2  |
| 2   | N     | 203 | ASN  | 2.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | H     | 2   | ALA  | 2.6  |
| 2   | H     | 180 | LEU  | 2.6  |
| 2   | H     | 129 | GLU  | 2.6  |
| 1   | G     | 151 | LYS  | 2.5  |
| 1   | C     | 194 | ILE  | 2.5  |
| 3   | Q     | 41  | GLU  | 2.5  |
| 1   | G     | 190 | PHE  | 2.4  |
| 1   | M     | 132 | ASP  | 2.4  |
| 1   | M     | 150 | SER  | 2.4  |
| 3   | I     | 54  | GLN  | 2.3  |
| 2   | H     | 132 | ILE  | 2.2  |
| 1   | C     | 152 | ASP  | 2.2  |
| 3   | Q     | 89  | ALA  | 2.1  |
| 1   | M     | 190 | PHE  | 2.1  |
| 1   | G     | 147 | VAL  | 2.1  |
| 1   | G     | 96  | GLY  | 2.1  |
| 2   | N     | 241 | ASP  | 2.1  |
| 2   | B     | 205 | PHE  | 2.0  |
| 1   | M     | 194 | ILE  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|----------------------------|-------|
| 5   | SO4  | B     | 244 | 5/5   | 0.86 | 0.30 | 2.11 | 49,62,74,75                | 5     |
| 6   | EDO  | N     | 244 | 4/4   | 0.94 | 0.27 | 0.92 | 60,62,75,79                | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|-----------------------------|-------|
| 5   | SO4  | A     | 208 | 5/5   | 0.80 | 0.25 | 0.44  | 78,93,101,101               | 5     |
| 5   | SO4  | B     | 243 | 5/5   | 0.90 | 0.20 | 0.05  | 79,83,100,128               | 0     |
| 5   | SO4  | N     | 243 | 5/5   | 0.85 | 0.25 | -0.57 | 91,98,118,124               | 5     |
| 5   | SO4  | H     | 243 | 5/5   | 0.90 | 0.12 | -2.19 | 86,88,91,118                | 0     |
| 5   | SO4  | G     | 208 | 5/5   | 0.92 | 0.17 | -3.70 | 45,56,62,76                 | 5     |
| 5   | SO4  | D     | 243 | 5/5   | 0.97 | 0.14 | -5.68 | 45,68,82,97                 | 5     |
| 5   | SO4  | K     | 180 | 5/5   | 0.95 | 0.10 | -     | 59,68,72,82                 | 5     |
| 5   | SO4  | N     | 242 | 5/5   | 0.96 | 0.14 | -     | 96,97,97,98                 | 5     |
| 5   | SO4  | Q     | 180 | 5/5   | 0.93 | 0.17 | -     | 79,86,105,119               | 5     |
| 5   | SO4  | D     | 242 | 5/5   | 0.94 | 0.11 | -     | 63,72,93,94                 | 0     |
| 5   | SO4  | K     | 181 | 5/5   | 0.94 | 0.22 | -     | 88,91,95,97                 | 5     |
| 5   | SO4  | H     | 242 | 5/5   | 0.95 | 0.10 | -     | 77,89,102,117               | 0     |
| 5   | SO4  | B     | 242 | 5/5   | 0.96 | 0.11 | -     | 57,71,84,89                 | 0     |
| 5   | SO4  | E     | 180 | 5/5   | 0.92 | 0.19 | -     | 60,68,75,77                 | 5     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.