



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:29 PM UTC

PDB ID : 5B4P / pdb\_00005b4p  
Title : Complex structure of human C5a and its binding repebody  
Authors : Kim, H.-S.; Choi, J.M.; Hwang, D.E.  
Deposited on : 2016-04-12  
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

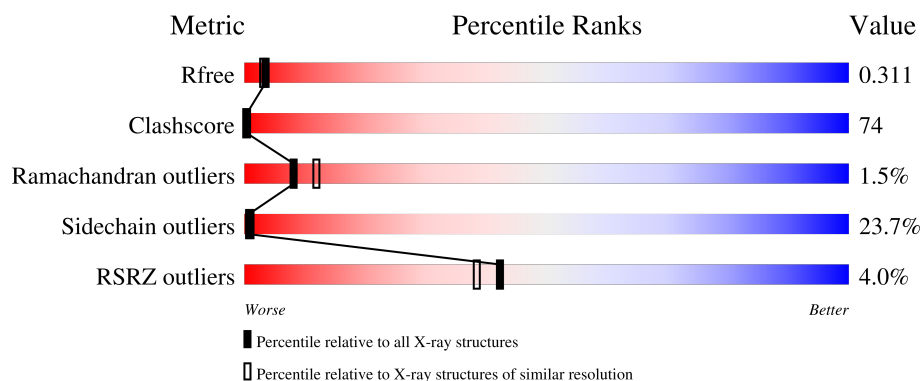
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 4912 (2.40-2.40)                                      |
| Clashscore            | 190562                      | 5391 (2.40-2.40)                                      |
| Ramachandran outliers | 187476                      | 5320 (2.40-2.40)                                      |
| Sidechain outliers    | 187428                      | 5321 (2.40-2.40)                                      |
| RSRZ outliers         | 180081                      | 4916 (2.40-2.40)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                      |
|-----|-------|--------|---------------------------------------------------------------------------------------|
| 1   | A     | 261    | <div> <div>5%</div> <div>28%</div> <div>48%</div> <div>20%</div> <div>..</div> </div> |
| 1   | C     | 261    | <div> <div>3%</div> <div>28%</div> <div>55%</div> <div>16%</div> <div>.</div> </div>  |
| 2   | B     | 75     | <div> <div>%</div> <div>43%</div> <div>40%</div> <div>13%</div> <div>.</div> </div>   |
| 2   | D     | 75     | <div> <div>3%</div> <div>37%</div> <div>44%</div> <div>12%</div> <div>..</div> </div> |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5157 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 repebody.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 254      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1928  | 1227 | 313 | 384 | 4 |         |         |       |
| 1   | C     | 260      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2005  | 1281 | 325 | 394 | 5 |         |         |       |

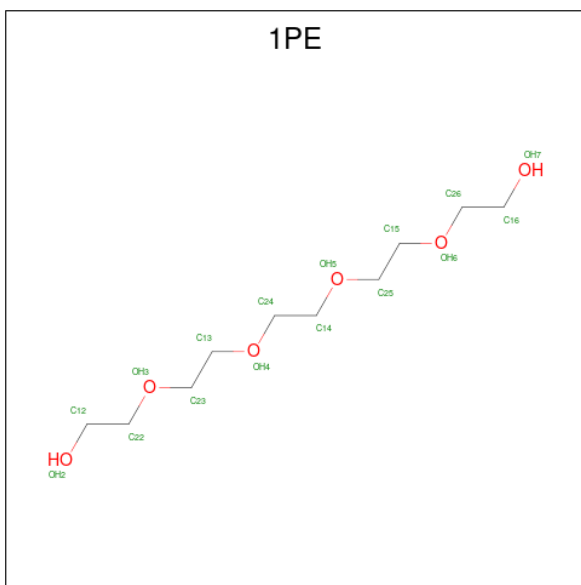
- Molecule 2 is a protein called C5a anaphylatoxin.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | B     | 72       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 540   | 330 | 101 | 101 | 8 |         |         |       |
| 2   | D     | 72       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 543   | 331 | 100 | 104 | 8 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

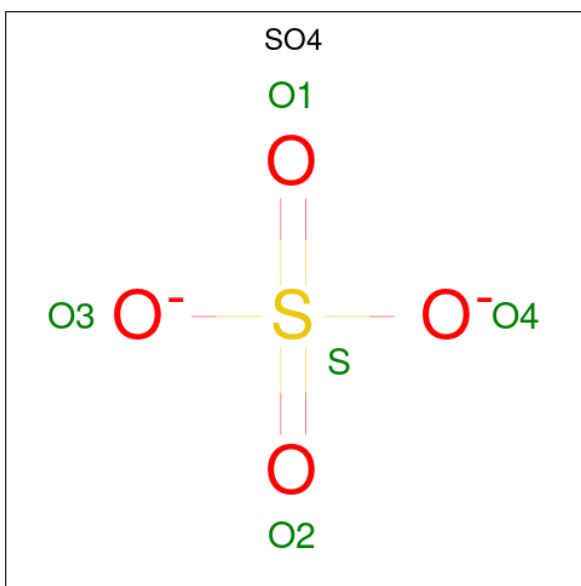
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | 0       | SER      | -      | expression tag | UNP P01031 |
| D     | 0       | SER      | -      | expression tag | UNP P01031 |

- Molecule 3 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 3   | A     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 16    | 10 | 6 |         |         |
| 3   | B     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 16    | 10 | 6 |         |         |

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula:  $\text{O}_4\text{S}$ ).



| Mol | Chain | Residues | Atoms      |        |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|---------|---------|
| 4   | A     | 1        | Total<br>5 | O<br>4 | S<br>1 | 0       | 0       |
| 4   | A     | 1        | Total<br>5 | O<br>4 | S<br>1 | 0       | 0       |

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

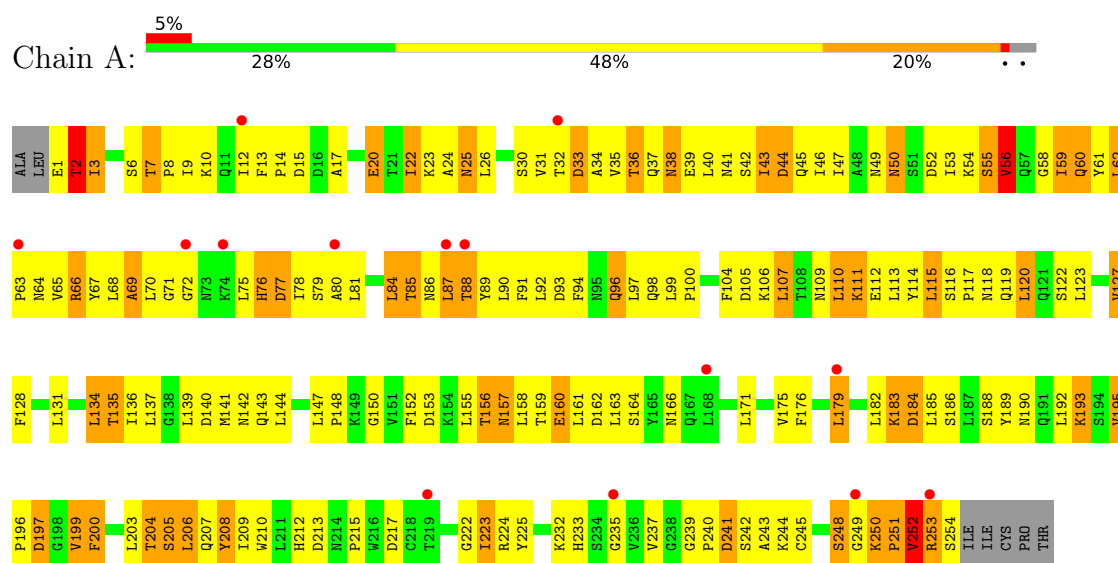
- Molecule 5 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | A     | 28       | Total | O  | 0       | 0       |
|     |       |          | 28    | 28 |         |         |
| 5   | B     | 9        | Total | O  | 0       | 0       |
|     |       |          | 9     | 9  |         |         |
| 5   | C     | 25       | Total | O  | 0       | 0       |
|     |       |          | 25    | 25 |         |         |
| 5   | D     | 7        | Total | O  | 0       | 0       |
|     |       |          | 7     | 7  |         |         |

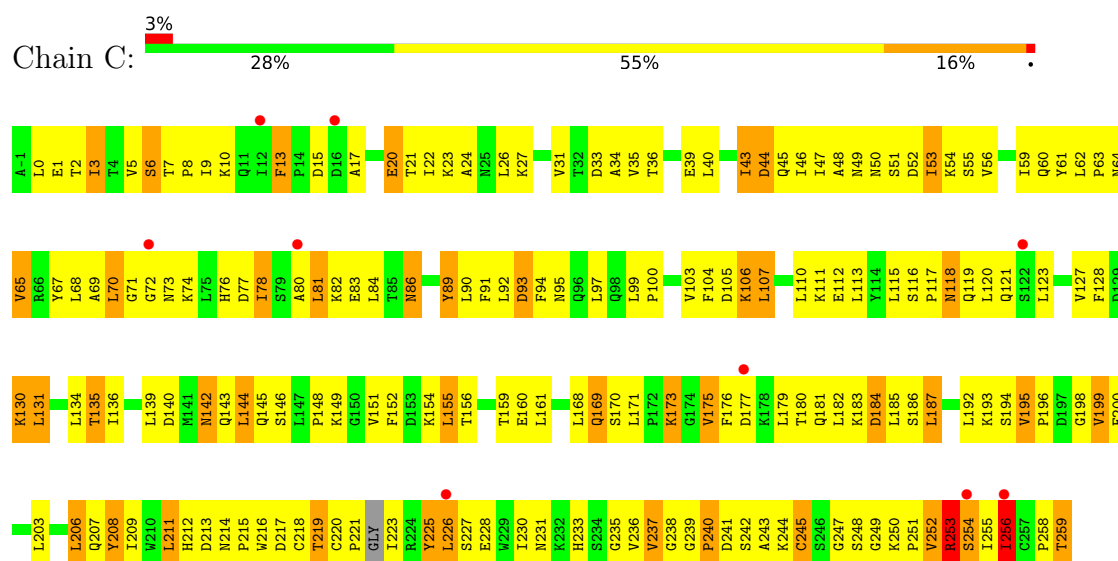
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

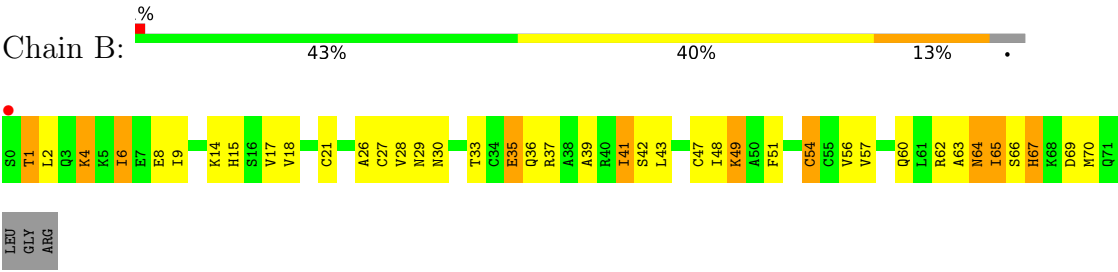
#### • Molecule 1: repebody



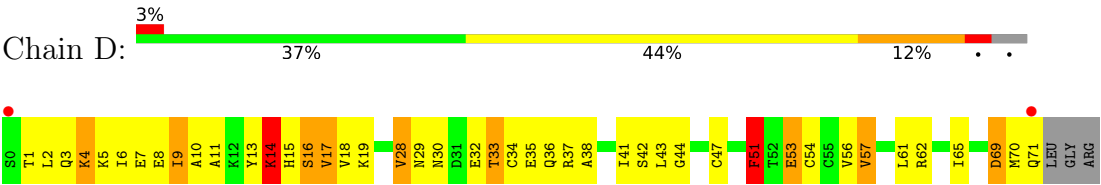
#### • Molecule 1: repebody



#### • Molecule 2: C5a anaphylatoxin



• Molecule 2: C5a anaphylatoxin



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 2 2 21                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 55.84Å 87.55Å 188.39Å<br>90.00° 90.00° 90.00°               | Depositor        |
| Resolution (Å)                                                          | 20.00 – 2.40<br>20.00 – 2.40                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 92.0 (20.00-2.40)<br>92.0 (20.00-2.40)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.88 (at 2.41Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.6.0117                                             | Depositor        |
| R, $R_{free}$                                                           | 0.272 , 0.310<br>0.268 , 0.311                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1846 reflections (4.99%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 41.5                                                        | Xtriage          |
| Anisotropy                                                              | 0.029                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.22 , 29.7                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.93                                                        | EDS              |
| Total number of atoms                                                   | 5157                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 60.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.4408e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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: 1PE, SO4

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     | 0.83         | 0/1966  | 1.13        | 13/2691 (0.5%) |
| 1   | C     | 0.92         | 0/2043  | 1.09        | 7/2786 (0.3%)  |
| 2   | B     | 0.96         | 0/545   | 1.08        | 1/732 (0.1%)   |
| 2   | D     | 0.94         | 0/548   | 1.23        | 4/736 (0.5%)   |
| All | All   | 0.89         | 0/5102  | 1.12        | 25/6945 (0.4%) |

There are no bond length outliers.

All (25) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | C     | 238 | GLY  | N-CA-C   | -8.12 | 104.68      | 115.40   |
| 2   | D     | 28  | VAL  | N-CA-C   | 8.06  | 120.19      | 108.58   |
| 1   | A     | 156 | THR  | N-CA-C   | 7.53  | 119.49      | 111.28   |
| 1   | A     | 204 | THR  | N-CA-C   | 7.19  | 118.91      | 111.14   |
| 1   | A     | 204 | THR  | CB-CA-C  | -7.16 | 99.58       | 110.90   |
| 1   | A     | 205 | SER  | N-CA-C   | -7.00 | 105.15      | 113.21   |
| 1   | A     | 2   | THR  | N-CA-C   | 6.88  | 116.94      | 107.73   |
| 1   | A     | 193 | LYS  | N-CA-C   | -6.77 | 105.57      | 114.31   |
| 1   | C     | 78  | ILE  | N-CA-C   | -6.49 | 104.87      | 112.98   |
| 1   | A     | 156 | THR  | CB-CA-C  | -6.27 | 100.38      | 110.79   |
| 2   | D     | 51  | PHE  | N-CA-C   | -6.26 | 104.35      | 112.68   |
| 2   | B     | 54  | CYS  | CA-CB-SG | -6.25 | 100.03      | 114.40   |
| 1   | C     | 235 | GLY  | N-CA-C   | -6.11 | 105.19      | 113.37   |
| 2   | D     | 56  | VAL  | N-CA-C   | 5.97  | 116.09      | 110.30   |
| 2   | D     | 14  | LYS  | N-CA-C   | 5.95  | 117.57      | 111.14   |
| 1   | C     | 13  | PHE  | CA-C-N   | 5.69  | 124.89      | 118.97   |
| 1   | C     | 13  | PHE  | C-N-CA   | 5.69  | 124.89      | 118.97   |
| 1   | A     | 115 | LEU  | N-CA-C   | 5.58  | 118.60      | 110.17   |
| 1   | A     | 76  | HIS  | N-CA-C   | 5.49  | 119.98      | 113.12   |
| 1   | A     | 99  | LEU  | CA-C-N   | -5.28 | 114.19      | 120.11   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 99  | LEU  | C-N-CA | -5.28 | 114.19      | 120.11   |
| 1   | A     | 69  | ALA  | N-CA-C | 5.22  | 117.23      | 107.99   |
| 1   | A     | 105 | ASP  | N-CA-C | 5.12  | 118.31      | 111.75   |
| 1   | C     | 252 | VAL  | CA-C-N | -5.07 | 111.85      | 121.54   |
| 1   | C     | 252 | VAL  | C-N-CA | -5.07 | 111.85      | 121.54   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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     | 1928  | 0        | 1857     | 329     | 0            |
| 1   | C     | 2005  | 0        | 1988     | 296     | 0            |
| 2   | B     | 540   | 0        | 532      | 51      | 0            |
| 2   | D     | 543   | 0        | 532      | 70      | 0            |
| 3   | A     | 16    | 0        | 21       | 2       | 0            |
| 3   | B     | 16    | 0        | 21       | 2       | 0            |
| 4   | A     | 15    | 0        | 0        | 0       | 0            |
| 4   | B     | 5     | 0        | 0        | 0       | 0            |
| 4   | C     | 15    | 0        | 0        | 0       | 0            |
| 4   | D     | 5     | 0        | 0        | 0       | 0            |
| 5   | A     | 28    | 0        | 0        | 3       | 0            |
| 5   | B     | 9     | 0        | 0        | 2       | 0            |
| 5   | C     | 25    | 0        | 0        | 4       | 0            |
| 5   | D     | 7     | 0        | 0        | 2       | 0            |
| All | All   | 5157  | 0        | 4951     | 741     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 74.

All (741) 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) |
|----------------|----------------|--------------------------|-------------------|
| 2:D:14:LYS:HG2 | 2:D:15:HIS:CD2 | 1.37                     | 1.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:36:THR:HG23  | 1:A:39:GLU:CG    | 1.41                     | 1.48              |
| 1:C:17:ALA:CB    | 1:C:53:ILE:HG22  | 1.55                     | 1.36              |
| 1:C:219:THR:C    | 1:C:221:PRO:HD2  | 1.54                     | 1.30              |
| 2:D:1:THR:CG2    | 2:D:4:LYS:HB3    | 1.59                     | 1.29              |
| 1:A:38:ASN:HA    | 1:A:41:ASN:ND2   | 1.52                     | 1.22              |
| 1:A:7:THR:O      | 1:A:34:ALA:HA    | 1.41                     | 1.19              |
| 1:C:226:LEU:HD12 | 1:C:226:LEU:N    | 1.58                     | 1.17              |
| 1:A:223:ILE:HD13 | 1:A:223:ILE:C    | 1.66                     | 1.17              |
| 1:A:85:THR:O     | 1:A:109:ASN:ND2  | 1.78                     | 1.16              |
| 1:A:36:THR:HG23  | 1:A:39:GLU:HG3   | 1.26                     | 1.15              |
| 1:C:219:THR:O    | 1:C:223:ILE:HD11 | 1.46                     | 1.15              |
| 1:C:256:ILE:N    | 1:C:256:ILE:HD12 | 1.61                     | 1.14              |
| 1:A:36:THR:HG23  | 1:A:39:GLU:CD    | 1.72                     | 1.13              |
| 1:C:226:LEU:H    | 1:C:226:LEU:CD1  | 1.57                     | 1.13              |
| 2:D:14:LYS:CG    | 2:D:15:HIS:CD2   | 2.31                     | 1.13              |
| 2:D:4:LYS:HE3    | 2:D:4:LYS:O      | 1.47                     | 1.12              |
| 1:C:17:ALA:HB1   | 1:C:53:ILE:HG22  | 1.13                     | 1.09              |
| 1:C:173:LYS:HD3  | 1:C:173:LYS:N    | 1.67                     | 1.08              |
| 1:A:38:ASN:CA    | 1:A:41:ASN:HD22  | 1.64                     | 1.08              |
| 1:C:253:ARG:O    | 1:C:256:ILE:CD1  | 2.02                     | 1.08              |
| 1:C:220:CYS:N    | 1:C:221:PRO:HD2  | 1.65                     | 1.07              |
| 1:C:256:ILE:HD12 | 1:C:256:ILE:H    | 0.96                     | 1.07              |
| 1:A:38:ASN:HA    | 1:A:41:ASN:HD22  | 0.92                     | 1.07              |
| 1:C:206:LEU:H    | 1:C:206:LEU:CD2  | 1.62                     | 1.07              |
| 1:C:206:LEU:H    | 1:C:206:LEU:HD23 | 0.90                     | 1.06              |
| 1:A:44:ASP:HB3   | 1:A:66:ARG:HD3   | 1.36                     | 1.06              |
| 1:A:9:ILE:HD11   | 1:A:35:VAL:HG11  | 1.30                     | 1.06              |
| 1:A:223:ILE:HD13 | 1:A:224:ARG:N    | 1.68                     | 1.05              |
| 1:A:176:PHE:O    | 1:A:179:LEU:HD12 | 1.55                     | 1.05              |
| 1:C:173:LYS:H    | 1:C:173:LYS:CD   | 1.65                     | 1.05              |
| 1:C:256:ILE:CD1  | 1:C:256:ILE:H    | 1.60                     | 1.05              |
| 2:D:1:THR:HG22   | 2:D:4:LYS:HB3    | 1.30                     | 1.05              |
| 1:A:112:GLU:OE1  | 1:A:114:TYR:OH   | 1.73                     | 1.05              |
| 1:A:196:PRO:O    | 1:A:199:VAL:HG22 | 1.57                     | 1.04              |
| 2:D:1:THR:HG23   | 2:D:4:LYS:HB3    | 1.37                     | 1.04              |
| 1:A:252:VAL:HG13 | 1:A:253:ARG:H    | 1.19                     | 1.03              |
| 1:C:173:LYS:HD3  | 1:C:173:LYS:H    | 0.87                     | 1.03              |
| 1:C:176:PHE:HA   | 1:C:179:LEU:HD13 | 1.37                     | 1.03              |
| 1:A:176:PHE:O    | 1:A:179:LEU:CD1  | 2.08                     | 1.02              |
| 2:B:2:LEU:HD22   | 2:B:6:ILE:HD11   | 1.41                     | 1.02              |
| 1:A:44:ASP:HA    | 1:A:64:ASN:O     | 1.59                     | 1.01              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:253:ARG:O    | 1:C:256:ILE:HD12 | 1.56                     | 1.01              |
| 1:A:36:THR:CG2   | 1:A:39:GLU:CG    | 2.38                     | 1.01              |
| 1:C:240:PRO:HB2  | 1:C:252:VAL:HG21 | 1.38                     | 1.01              |
| 1:C:203:LEU:O    | 1:C:206:LEU:HD21 | 1.60                     | 1.01              |
| 1:A:15:ASP:OD2   | 1:A:55:SER:N     | 1.94                     | 1.00              |
| 1:C:17:ALA:HB3   | 1:C:53:ILE:HG22  | 1.41                     | 1.00              |
| 1:C:206:LEU:HD23 | 1:C:206:LEU:N    | 1.72                     | 1.00              |
| 2:D:53:GLU:O     | 2:D:57:VAL:HG12  | 1.59                     | 1.00              |
| 1:C:258:PRO:O    | 1:C:259:THR:HB   | 1.55                     | 0.99              |
| 1:C:225:TYR:HD1  | 1:C:226:LEU:N    | 1.60                     | 0.99              |
| 1:C:241:ASP:O    | 1:C:244:LYS:NZ   | 1.94                     | 0.99              |
| 1:A:251:PRO:O    | 1:A:252:VAL:HG23 | 1.63                     | 0.99              |
| 2:D:3:GLN:HB3    | 5:D:206:HOH:O    | 1.63                     | 0.98              |
| 1:A:36:THR:CG2   | 1:A:39:GLU:CD    | 2.34                     | 0.98              |
| 1:C:225:TYR:CD1  | 1:C:225:TYR:C    | 2.42                     | 0.97              |
| 1:A:112:GLU:HG2  | 1:A:136:ILE:HB   | 1.46                     | 0.97              |
| 1:A:68:LEU:HD21  | 1:A:70:LEU:HD11  | 1.44                     | 0.97              |
| 2:D:1:THR:CG2    | 2:D:4:LYS:CB     | 2.43                     | 0.96              |
| 1:A:88:THR:HG22  | 1:A:111:LYS:HD2  | 1.48                     | 0.96              |
| 1:A:7:THR:O      | 1:A:34:ALA:CA    | 2.12                     | 0.95              |
| 1:A:72:GLY:HA3   | 1:A:94:PHE:CE1   | 2.01                     | 0.95              |
| 1:C:72:GLY:HA3   | 1:C:94:PHE:CE2   | 1.99                     | 0.95              |
| 2:D:1:THR:HG23   | 2:D:4:LYS:H      | 1.31                     | 0.95              |
| 1:C:198:GLY:N    | 1:C:225:TYR:CE2  | 2.35                     | 0.94              |
| 1:A:206:LEU:C    | 1:A:206:LEU:HD12 | 1.93                     | 0.94              |
| 1:A:44:ASP:CB    | 1:A:66:ARG:HD3   | 1.97                     | 0.93              |
| 1:C:253:ARG:C    | 1:C:256:ILE:HD11 | 1.94                     | 0.93              |
| 1:C:195:VAL:HG13 | 1:C:226:LEU:HD23 | 1.50                     | 0.93              |
| 1:A:65:VAL:HG12  | 1:A:87:LEU:CD1   | 1.99                     | 0.92              |
| 1:C:226:LEU:HD12 | 1:C:226:LEU:H    | 0.76                     | 0.92              |
| 1:A:199:VAL:HG23 | 1:A:200:PHE:CD1  | 2.05                     | 0.91              |
| 1:A:110:LEU:HD12 | 1:A:110:LEU:O    | 1.70                     | 0.91              |
| 2:B:28:VAL:HA    | 5:B:203:HOH:O    | 1.71                     | 0.91              |
| 1:A:84:LEU:O     | 1:A:107:LEU:HD12 | 1.71                     | 0.91              |
| 1:C:240:PRO:CB   | 1:C:252:VAL:HG21 | 2.00                     | 0.90              |
| 1:C:243:ALA:O    | 1:C:244:LYS:HD2  | 1.70                     | 0.90              |
| 2:D:14:LYS:HG2   | 2:D:15:HIS:NE2   | 1.87                     | 0.90              |
| 1:C:17:ALA:HB1   | 1:C:53:ILE:CG2   | 2.01                     | 0.90              |
| 1:C:220:CYS:N    | 1:C:221:PRO:CD   | 2.35                     | 0.89              |
| 1:A:110:LEU:HD12 | 1:A:110:LEU:C    | 1.98                     | 0.89              |
| 1:C:17:ALA:CB    | 1:C:53:ILE:CG2   | 2.49                     | 0.89              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:219:THR:O    | 1:C:223:ILE:CD1  | 2.21                     | 0.89              |
| 1:A:127:VAL:HG22 | 1:A:128:PHE:CD1  | 2.08                     | 0.88              |
| 1:A:200:PHE:HA   | 1:A:203:LEU:CD1  | 2.04                     | 0.88              |
| 2:D:14:LYS:HG2   | 2:D:15:HIS:HD2   | 1.25                     | 0.88              |
| 1:C:254:SER:C    | 1:C:256:ILE:CD1  | 2.47                     | 0.88              |
| 1:A:9:ILE:CD1    | 1:A:35:VAL:HG11  | 2.04                     | 0.87              |
| 1:A:38:ASN:CA    | 1:A:41:ASN:ND2   | 2.30                     | 0.87              |
| 1:A:112:GLU:CG   | 1:A:136:ILE:HB   | 2.04                     | 0.87              |
| 1:A:36:THR:HG23  | 1:A:39:GLU:HG2   | 1.54                     | 0.87              |
| 1:C:82:LYS:O     | 1:C:106:LYS:CB   | 2.22                     | 0.87              |
| 1:A:85:THR:HG22  | 1:A:106:LYS:O    | 1.73                     | 0.86              |
| 1:A:152:PHE:HA   | 1:A:155:LEU:HD12 | 1.57                     | 0.86              |
| 1:A:252:VAL:HG13 | 1:A:253:ARG:N    | 1.84                     | 0.86              |
| 1:A:37:GLN:O     | 1:A:41:ASN:ND2   | 2.09                     | 0.85              |
| 1:C:72:GLY:O     | 1:C:94:PHE:HA    | 1.75                     | 0.85              |
| 1:A:252:VAL:CG1  | 1:A:253:ARG:N    | 2.38                     | 0.85              |
| 2:B:14:LYS:H     | 2:B:14:LYS:HD2   | 1.38                     | 0.85              |
| 2:B:29:ASN:HB3   | 2:B:37:ARG:HD2   | 1.57                     | 0.85              |
| 1:A:7:THR:H      | 1:A:34:ALA:HB1   | 1.41                     | 0.85              |
| 1:C:255:ILE:N    | 1:C:256:ILE:HD12 | 1.91                     | 0.85              |
| 1:C:72:GLY:CA    | 1:C:94:PHE:CE2   | 2.59                     | 0.85              |
| 2:D:28:VAL:HA    | 5:D:202:HOH:O    | 1.75                     | 0.84              |
| 1:A:44:ASP:HB3   | 1:A:66:ARG:CD    | 2.07                     | 0.84              |
| 1:A:223:ILE:C    | 1:A:223:ILE:CD1  | 2.41                     | 0.83              |
| 1:A:200:PHE:HA   | 1:A:203:LEU:HD12 | 1.60                     | 0.83              |
| 1:A:72:GLY:CA    | 1:A:94:PHE:CE1   | 2.62                     | 0.83              |
| 1:A:85:THR:CG2   | 1:A:106:LYS:O    | 2.26                     | 0.83              |
| 2:B:35:GLU:HA    | 2:B:35:GLU:OE1   | 1.77                     | 0.83              |
| 1:A:183:LYS:HA   | 1:A:206:LEU:HA   | 1.59                     | 0.83              |
| 1:A:251:PRO:O    | 1:A:252:VAL:CG2  | 2.27                     | 0.82              |
| 1:A:88:THR:HA    | 1:A:110:LEU:HA   | 1.61                     | 0.82              |
| 1:C:253:ARG:C    | 1:C:256:ILE:CD1  | 2.50                     | 0.82              |
| 1:A:107:LEU:H    | 1:A:107:LEU:HD22 | 1.42                     | 0.82              |
| 1:C:219:THR:HB   | 1:C:221:PRO:CD   | 2.10                     | 0.82              |
| 1:A:200:PHE:CA   | 1:A:203:LEU:HD12 | 2.10                     | 0.82              |
| 2:B:2:LEU:O      | 2:B:6:ILE:HG12   | 1.79                     | 0.82              |
| 1:A:65:VAL:HG12  | 1:A:87:LEU:HD12  | 1.61                     | 0.81              |
| 1:A:111:LYS:HA   | 1:A:134:LEU:HA   | 1.62                     | 0.81              |
| 1:C:225:TYR:CD1  | 1:C:226:LEU:N    | 2.48                     | 0.81              |
| 1:A:22:ILE:HG23  | 1:A:26:LEU:HD12  | 1.62                     | 0.81              |
| 1:A:120:LEU:HD23 | 1:A:122:SER:HB3  | 1.62                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:185:LEU:O    | 1:A:209:ILE:HG13 | 1.80                     | 0.81              |
| 2:B:41:ILE:HG22  | 2:B:48:ILE:HD11  | 1.64                     | 0.80              |
| 1:C:43:ILE:CD1   | 1:C:62:LEU:HD13  | 2.11                     | 0.80              |
| 2:D:1:THR:HG22   | 2:D:4:LYS:CB     | 2.10                     | 0.80              |
| 1:C:152:PHE:HA   | 1:C:155:LEU:HD12 | 1.64                     | 0.80              |
| 2:D:4:LYS:HE3    | 2:D:4:LYS:C      | 2.07                     | 0.79              |
| 2:D:5:LYS:O      | 2:D:9:ILE:CD1    | 2.30                     | 0.79              |
| 1:A:196:PRO:HD2  | 1:A:199:VAL:HG11 | 1.65                     | 0.79              |
| 1:A:20:GLU:OE2   | 1:A:31:VAL:CG2   | 2.30                     | 0.79              |
| 1:A:88:THR:CG2   | 1:A:111:LYS:HD2  | 2.12                     | 0.78              |
| 1:A:96:GLN:OE1   | 1:A:119:GLN:HA   | 1.83                     | 0.78              |
| 1:A:136:ILE:HG12 | 1:A:160:GLU:OE1  | 1.83                     | 0.78              |
| 1:C:230:ILE:HG22 | 1:C:240:PRO:HB3  | 1.65                     | 0.78              |
| 1:C:120:LEU:O    | 1:C:121:GLN:HB2  | 1.82                     | 0.78              |
| 1:A:67:TYR:HD2   | 1:A:89:TYR:HB3   | 1.48                     | 0.78              |
| 1:A:179:LEU:HD12 | 1:A:179:LEU:H    | 1.47                     | 0.78              |
| 2:D:14:LYS:CD    | 2:D:14:LYS:H     | 1.97                     | 0.78              |
| 1:A:253:ARG:O    | 1:A:254:SER:HB2  | 1.81                     | 0.78              |
| 1:C:82:LYS:O     | 1:C:106:LYS:HB3  | 1.84                     | 0.78              |
| 1:A:253:ARG:O    | 1:A:254:SER:CB   | 2.32                     | 0.77              |
| 1:A:20:GLU:OE2   | 1:A:31:VAL:HG21  | 1.84                     | 0.77              |
| 1:A:43:ILE:CD1   | 1:A:62:LEU:HD13  | 2.13                     | 0.77              |
| 1:C:53:ILE:HG12  | 1:C:53:ILE:O     | 1.81                     | 0.77              |
| 1:C:61:TYR:C     | 1:C:62:LEU:HD23  | 2.09                     | 0.77              |
| 1:C:230:ILE:CG2  | 1:C:240:PRO:HB3  | 2.15                     | 0.77              |
| 1:A:90:LEU:HD23  | 1:A:113:LEU:CD1  | 2.14                     | 0.77              |
| 1:A:113:LEU:HD11 | 1:A:115:LEU:HD21 | 1.66                     | 0.77              |
| 1:A:12:ILE:HD12  | 1:A:12:ILE:H     | 1.49                     | 0.77              |
| 1:A:251:PRO:O    | 1:A:252:VAL:CB   | 2.31                     | 0.76              |
| 1:C:198:GLY:HA2  | 1:C:225:TYR:HE2  | 1.50                     | 0.76              |
| 1:C:254:SER:C    | 1:C:256:ILE:HD12 | 2.09                     | 0.76              |
| 1:A:36:THR:HG22  | 1:A:39:GLU:OE1   | 1.86                     | 0.76              |
| 1:C:219:THR:HB   | 1:C:221:PRO:CG   | 2.15                     | 0.76              |
| 1:A:50:ASN:OD1   | 1:A:52:ASP:N     | 2.19                     | 0.76              |
| 1:A:190:ASN:HB3  | 1:A:192:LEU:HD12 | 1.65                     | 0.76              |
| 1:C:195:VAL:CG1  | 1:C:226:LEU:HD23 | 2.15                     | 0.76              |
| 1:C:106:LYS:HB2  | 5:C:401:HOH:O    | 1.84                     | 0.75              |
| 1:C:253:ARG:O    | 1:C:256:ILE:HD11 | 1.85                     | 0.75              |
| 1:A:183:LYS:O    | 1:A:206:LEU:HD13 | 1.86                     | 0.75              |
| 1:C:112:GLU:HG2  | 1:C:136:ILE:HB   | 1.66                     | 0.75              |
| 1:C:254:SER:C    | 1:C:256:ILE:HD13 | 2.12                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:87:LEU:O     | 1:A:110:LEU:HB3  | 1.87                     | 0.75              |
| 1:C:225:TYR:HD1  | 1:C:225:TYR:C    | 1.88                     | 0.75              |
| 1:C:72:GLY:C     | 1:C:94:PHE:CD2   | 2.65                     | 0.74              |
| 1:C:211:LEU:HB3  | 1:C:216:TRP:CZ2  | 2.21                     | 0.74              |
| 2:D:4:LYS:O      | 2:D:4:LYS:CE     | 2.32                     | 0.74              |
| 2:D:29:ASN:HB3   | 2:D:37:ARG:HD2   | 1.68                     | 0.74              |
| 1:A:120:LEU:CD2  | 1:A:122:SER:HB3  | 2.17                     | 0.74              |
| 2:B:67:HIS:C     | 2:B:67:HIS:HD1   | 1.96                     | 0.74              |
| 1:C:256:ILE:N    | 1:C:256:ILE:CD1  | 2.31                     | 0.74              |
| 2:D:5:LYS:O      | 2:D:9:ILE:HD13   | 1.88                     | 0.74              |
| 1:A:7:THR:N      | 1:A:34:ALA:HB1   | 2.03                     | 0.74              |
| 2:D:42:SER:O     | 2:D:43:LEU:HD23  | 1.88                     | 0.73              |
| 1:A:36:THR:CG2   | 1:A:39:GLU:OE1   | 2.36                     | 0.73              |
| 1:C:94:PHE:O     | 1:C:116:SER:HB3  | 1.89                     | 0.73              |
| 1:C:216:TRP:HD1  | 1:C:244:LYS:O    | 1.72                     | 0.73              |
| 1:C:176:PHE:CA   | 1:C:179:LEU:HD13 | 2.17                     | 0.73              |
| 2:D:33:THR:HG23  | 2:D:36:GLN:CD    | 2.13                     | 0.73              |
| 1:A:56:VAL:O     | 1:A:59:ILE:HB    | 1.89                     | 0.73              |
| 1:A:156:THR:OG1  | 1:A:157:ASN:ND2  | 2.20                     | 0.73              |
| 2:B:56:VAL:O     | 2:B:60:GLN:HG3   | 1.89                     | 0.73              |
| 1:A:2:THR:OG1    | 1:A:3:ILE:N      | 2.21                     | 0.73              |
| 1:C:105:ASP:HA   | 1:C:130:LYS:HG2  | 1.71                     | 0.73              |
| 1:C:171:LEU:HB2  | 1:C:196:PRO:HD3  | 1.70                     | 0.72              |
| 1:C:72:GLY:CA    | 1:C:94:PHE:CD2   | 2.72                     | 0.72              |
| 1:A:190:ASN:HB3  | 1:A:192:LEU:CD1  | 2.19                     | 0.72              |
| 1:C:239:GLY:O    | 1:C:242:SER:N    | 2.23                     | 0.72              |
| 1:A:196:PRO:HB2  | 1:A:199:VAL:HG13 | 1.71                     | 0.72              |
| 2:D:1:THR:HG23   | 2:D:4:LYS:CB     | 2.15                     | 0.72              |
| 1:A:25:ASN:C     | 1:A:25:ASN:HD22  | 1.97                     | 0.72              |
| 2:B:14:LYS:HD2   | 2:B:14:LYS:N     | 2.03                     | 0.72              |
| 1:C:207:GLN:C    | 1:C:208:TYR:HD1  | 1.98                     | 0.72              |
| 1:A:36:THR:CG2   | 1:A:39:GLU:HG3   | 2.12                     | 0.71              |
| 1:C:118:ASN:C    | 1:C:118:ASN:OD1  | 2.33                     | 0.71              |
| 1:A:112:GLU:HG2  | 1:A:136:ILE:CB   | 2.20                     | 0.71              |
| 1:A:206:LEU:HD12 | 1:A:207:GLN:N    | 2.05                     | 0.71              |
| 1:C:230:ILE:HG23 | 1:C:236:VAL:HG21 | 1.73                     | 0.71              |
| 1:A:44:ASP:O     | 1:A:66:ARG:N     | 2.24                     | 0.71              |
| 1:A:6:SER:O      | 1:A:7:THR:HG23   | 1.90                     | 0.71              |
| 1:C:78:ILE:O     | 1:C:81:LEU:HG    | 1.91                     | 0.70              |
| 1:C:17:ALA:HB3   | 1:C:53:ILE:CG2   | 2.16                     | 0.70              |
| 2:D:33:THR:HG23  | 2:D:36:GLN:CG    | 2.22                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:210:TRP:NE1  | 1:A:237:VAL:HG11 | 2.05                     | 0.70              |
| 1:C:240:PRO:CB   | 1:C:252:VAL:CG2  | 2.69                     | 0.70              |
| 1:A:13:PHE:HZ    | 1:A:62:LEU:HD21  | 1.57                     | 0.70              |
| 1:C:171:LEU:HD22 | 1:C:192:LEU:HD21 | 1.74                     | 0.70              |
| 2:B:41:ILE:CG2   | 2:B:48:ILE:HD11  | 2.20                     | 0.70              |
| 1:C:43:ILE:HD11  | 1:C:62:LEU:HD13  | 1.73                     | 0.70              |
| 1:C:207:GLN:C    | 1:C:208:TYR:CD1  | 2.70                     | 0.70              |
| 1:A:184:ASP:HA   | 1:A:208:TYR:O    | 1.91                     | 0.70              |
| 1:A:217:ASP:O    | 1:A:223:ILE:HG21 | 1.92                     | 0.70              |
| 1:C:89:TYR:CD1   | 1:C:89:TYR:C     | 2.70                     | 0.70              |
| 1:C:196:PRO:O    | 1:C:199:VAL:HB   | 1.91                     | 0.70              |
| 2:D:35:GLU:HA    | 2:D:35:GLU:OE2   | 1.91                     | 0.70              |
| 1:A:120:LEU:HG   | 1:A:120:LEU:O    | 1.92                     | 0.69              |
| 2:B:14:LYS:H     | 2:B:14:LYS:CD    | 2.06                     | 0.69              |
| 1:C:211:LEU:HB3  | 1:C:216:TRP:HZ2  | 1.57                     | 0.69              |
| 1:A:67:TYR:CD2   | 1:A:89:TYR:HB3   | 2.28                     | 0.68              |
| 1:C:206:LEU:CD2  | 1:C:206:LEU:N    | 2.41                     | 0.68              |
| 1:A:20:GLU:O     | 1:A:23:LYS:HG2   | 1.94                     | 0.68              |
| 1:A:152:PHE:CA   | 1:A:155:LEU:HD12 | 2.24                     | 0.68              |
| 1:A:199:VAL:HG23 | 1:A:200:PHE:CE1  | 2.28                     | 0.68              |
| 1:C:97:LEU:HD21  | 1:C:99:LEU:HD23  | 1.76                     | 0.68              |
| 1:C:226:LEU:N    | 1:C:226:LEU:CD1  | 2.33                     | 0.68              |
| 1:A:159:THR:HG22 | 1:A:160:GLU:HG3  | 1.76                     | 0.68              |
| 1:C:89:TYR:C     | 1:C:89:TYR:HD1   | 2.02                     | 0.68              |
| 2:B:28:VAL:HG12  | 2:B:62:ARG:CZ    | 2.24                     | 0.67              |
| 1:C:83:GLU:OE2   | 1:C:106:LYS:HE2  | 1.95                     | 0.67              |
| 1:A:155:LEU:O    | 1:A:158:LEU:HB2  | 1.94                     | 0.67              |
| 1:C:72:GLY:HA3   | 1:C:94:PHE:HE2   | 1.59                     | 0.67              |
| 1:C:198:GLY:CA   | 1:C:225:TYR:CE2  | 2.76                     | 0.67              |
| 1:A:200:PHE:HA   | 1:A:203:LEU:HD11 | 1.77                     | 0.67              |
| 1:C:195:VAL:HG13 | 1:C:226:LEU:CD2  | 2.23                     | 0.67              |
| 1:C:196:PRO:HG2  | 1:C:199:VAL:CG2  | 2.24                     | 0.66              |
| 2:D:1:THR:HG23   | 2:D:4:LYS:N      | 2.06                     | 0.66              |
| 2:B:15:HIS:HA    | 3:B:101:1PE:H132 | 1.78                     | 0.66              |
| 1:C:90:LEU:HD23  | 1:C:113:LEU:HD11 | 1.77                     | 0.66              |
| 1:C:254:SER:CA   | 1:C:256:ILE:HD13 | 2.26                     | 0.66              |
| 1:C:161:LEU:O    | 1:C:185:LEU:HD12 | 1.94                     | 0.66              |
| 1:A:152:PHE:HA   | 1:A:155:LEU:CD1  | 2.26                     | 0.66              |
| 1:A:183:LYS:O    | 1:A:207:GLN:N    | 2.29                     | 0.66              |
| 1:A:112:GLU:CD   | 1:A:136:ILE:HD12 | 2.21                     | 0.65              |
| 1:C:198:GLY:CA   | 1:C:225:TYR:HE2  | 2.09                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:139:LEU:HA   | 1:A:142:ASN:OD1  | 1.96                     | 0.65              |
| 1:A:203:LEU:O    | 1:A:206:LEU:HB3  | 1.97                     | 0.65              |
| 1:C:116:SER:HB3  | 1:C:117:PRO:HD2  | 1.78                     | 0.65              |
| 2:B:28:VAL:HG12  | 2:B:62:ARG:NH2   | 2.12                     | 0.65              |
| 1:C:239:GLY:O    | 1:C:241:ASP:N    | 2.30                     | 0.65              |
| 1:A:199:VAL:HG23 | 1:A:200:PHE:HD1  | 1.59                     | 0.65              |
| 1:C:48:ALA:O     | 1:C:70:LEU:HA    | 1.96                     | 0.65              |
| 2:B:2:LEU:HD22   | 2:B:6:ILE:CD1    | 2.21                     | 0.65              |
| 1:C:72:GLY:N     | 1:C:94:PHE:CE2   | 2.65                     | 0.65              |
| 1:C:240:PRO:HB3  | 1:C:252:VAL:CG2  | 2.27                     | 0.64              |
| 1:C:44:ASP:HA    | 1:C:65:VAL:HA    | 1.78                     | 0.64              |
| 1:C:43:ILE:HD13  | 1:C:62:LEU:HD13  | 1.79                     | 0.64              |
| 1:A:159:THR:O    | 1:A:182:LEU:HD12 | 1.97                     | 0.64              |
| 1:C:243:ALA:O    | 1:C:251:PRO:HD3  | 1.98                     | 0.64              |
| 1:A:44:ASP:O     | 1:A:65:VAL:HA    | 1.99                     | 0.63              |
| 1:A:249:GLY:C    | 1:A:250:LYS:O    | 2.39                     | 0.63              |
| 1:A:9:ILE:CD1    | 1:A:35:VAL:CG1   | 2.76                     | 0.63              |
| 1:A:111:LYS:HB3  | 1:A:135:THR:HG23 | 1.81                     | 0.63              |
| 1:A:123:LEU:HG   | 1:A:144:LEU:HD21 | 1.81                     | 0.63              |
| 1:C:72:GLY:O     | 1:C:94:PHE:CD2   | 2.51                     | 0.63              |
| 1:A:7:THR:C      | 1:A:34:ALA:HA    | 2.20                     | 0.63              |
| 1:A:33:ASP:OD2   | 1:A:33:ASP:N     | 2.31                     | 0.63              |
| 1:A:72:GLY:HA3   | 1:A:94:PHE:HE1   | 1.57                     | 0.63              |
| 1:C:118:ASN:OD1  | 1:C:120:LEU:N    | 2.32                     | 0.63              |
| 1:C:231:ASN:OD1  | 1:C:252:VAL:HG13 | 1.98                     | 0.63              |
| 1:A:8:PRO:O      | 1:A:12:ILE:HD12  | 1.98                     | 0.63              |
| 2:B:21:CYS:HA    | 5:B:204:HOH:O    | 1.98                     | 0.63              |
| 1:A:98:GLN:O     | 1:A:100:PRO:HD3  | 1.99                     | 0.62              |
| 1:A:8:PRO:O      | 1:A:12:ILE:CD1   | 2.47                     | 0.62              |
| 1:C:199:VAL:N    | 1:C:225:TYR:OH   | 2.32                     | 0.62              |
| 1:A:206:LEU:C    | 1:A:206:LEU:CD1  | 2.65                     | 0.62              |
| 1:A:225:TYR:HD2  | 5:A:418:HOH:O    | 1.80                     | 0.62              |
| 1:A:12:ILE:HG23  | 1:A:61:TYR:HD2   | 1.64                     | 0.62              |
| 1:A:1:GLU:C      | 1:A:2:THR:HG22   | 2.24                     | 0.62              |
| 1:A:65:VAL:HG12  | 1:A:87:LEU:HD11  | 1.81                     | 0.62              |
| 1:A:249:GLY:O    | 1:A:250:LYS:O    | 2.18                     | 0.62              |
| 1:C:127:VAL:HG13 | 1:C:128:PHE:CD2  | 2.34                     | 0.62              |
| 1:A:199:VAL:CG2  | 1:A:200:PHE:CE1  | 2.82                     | 0.62              |
| 1:C:119:GLN:HG2  | 1:C:120:LEU:HD12 | 1.80                     | 0.61              |
| 1:C:219:THR:HB   | 1:C:221:PRO:HD2  | 1.81                     | 0.61              |
| 1:A:171:LEU:O    | 1:A:196:PRO:HG3  | 1.99                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:43:ILE:HD11  | 1:C:62:LEU:CD1   | 2.29                     | 0.61              |
| 2:B:67:HIS:C     | 2:B:67:HIS:ND1   | 2.56                     | 0.61              |
| 1:C:171:LEU:HD22 | 1:C:192:LEU:CD2  | 2.30                     | 0.61              |
| 1:A:137:LEU:CD2  | 1:A:152:PHE:HE1  | 2.13                     | 0.61              |
| 1:A:204:THR:OG1  | 1:A:205:SER:N    | 2.29                     | 0.61              |
| 2:B:63:ALA:CB    | 2:B:65:ILE:HD11  | 2.30                     | 0.61              |
| 1:C:44:ASP:HB3   | 1:C:64:ASN:O     | 2.00                     | 0.61              |
| 1:C:97:LEU:CD2   | 1:C:99:LEU:HD23  | 2.31                     | 0.61              |
| 1:C:196:PRO:HG2  | 1:C:199:VAL:HG23 | 1.81                     | 0.61              |
| 2:D:33:THR:CG2   | 2:D:36:GLN:CD    | 2.72                     | 0.61              |
| 2:B:60:GLN:HB2   | 2:B:70:MET:HE3   | 1.83                     | 0.61              |
| 1:C:252:VAL:O    | 1:C:255:ILE:CB   | 2.49                     | 0.61              |
| 1:A:107:LEU:HD22 | 1:A:107:LEU:N    | 2.14                     | 0.61              |
| 1:A:116:SER:HB3  | 1:A:117:PRO:HD2  | 1.82                     | 0.61              |
| 1:C:20:GLU:HG3   | 1:C:23:LYS:NZ    | 2.16                     | 0.61              |
| 1:A:72:GLY:C     | 1:A:94:PHE:CD1   | 2.78                     | 0.61              |
| 1:A:9:ILE:HD11   | 1:A:35:VAL:CG1   | 2.18                     | 0.61              |
| 1:A:192:LEU:HD12 | 1:A:192:LEU:H    | 1.67                     | 0.60              |
| 1:C:212:HIS:O    | 1:C:213:ASP:HB2  | 1.99                     | 0.60              |
| 1:A:118:ASN:C    | 1:A:118:ASN:OD1  | 2.44                     | 0.60              |
| 2:D:14:LYS:CG    | 2:D:15:HIS:NE2   | 2.58                     | 0.60              |
| 1:C:255:ILE:N    | 1:C:256:ILE:CD1  | 2.59                     | 0.60              |
| 1:A:67:TYR:CE2   | 1:A:89:TYR:CG    | 2.89                     | 0.60              |
| 1:A:159:THR:HG23 | 1:A:183:LYS:HE2  | 1.84                     | 0.60              |
| 1:C:6:SER:HA     | 1:C:35:VAL:O     | 2.01                     | 0.60              |
| 2:D:33:THR:CG2   | 2:D:36:GLN:NE2   | 2.65                     | 0.60              |
| 1:A:183:LYS:O    | 1:A:206:LEU:CD1  | 2.50                     | 0.60              |
| 1:A:244:LYS:HA   | 1:A:249:GLY:O    | 2.02                     | 0.59              |
| 2:B:29:ASN:OD1   | 2:B:30:ASN:N     | 2.35                     | 0.59              |
| 1:A:38:ASN:C     | 1:A:41:ASN:HD22  | 2.10                     | 0.59              |
| 1:C:173:LYS:N    | 1:C:173:LYS:CD   | 2.41                     | 0.59              |
| 1:A:84:LEU:O     | 1:A:107:LEU:CD1  | 2.48                     | 0.59              |
| 1:C:219:THR:HB   | 1:C:221:PRO:HG3  | 1.84                     | 0.59              |
| 1:A:197:ASP:HA   | 1:A:225:TYR:CE2  | 2.37                     | 0.59              |
| 1:A:210:TRP:HE1  | 1:A:237:VAL:HG11 | 1.67                     | 0.59              |
| 1:A:127:VAL:HG22 | 1:A:128:PHE:CE1  | 2.38                     | 0.59              |
| 1:C:175:VAL:HG12 | 1:C:176:PHE:CD2  | 2.38                     | 0.59              |
| 1:A:44:ASP:CA    | 1:A:64:ASN:O     | 2.46                     | 0.59              |
| 2:B:63:ALA:HB3   | 2:B:65:ILE:HD11  | 1.85                     | 0.59              |
| 1:C:22:ILE:HG22  | 1:C:26:LEU:HD12  | 1.84                     | 0.59              |
| 1:A:44:ASP:O     | 1:A:66:ARG:HG2   | 2.03                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:159:THR:CG2  | 1:A:183:LYS:HE2  | 2.33                     | 0.59              |
| 1:A:200:PHE:CD1  | 1:A:200:PHE:N    | 2.71                     | 0.59              |
| 2:D:54:CYS:HA    | 2:D:57:VAL:CG1   | 2.33                     | 0.59              |
| 1:C:90:LEU:HD23  | 1:C:113:LEU:CD1  | 2.33                     | 0.58              |
| 1:C:10:LYS:HE3   | 1:C:31:VAL:CG2   | 2.32                     | 0.58              |
| 1:A:190:ASN:CB   | 1:A:192:LEU:CD1  | 2.80                     | 0.58              |
| 5:A:406:HOH:O    | 2:B:15:HIS:HB3   | 2.03                     | 0.58              |
| 1:C:62:LEU:HD23  | 1:C:62:LEU:N     | 2.15                     | 0.58              |
| 1:C:227:SER:OG   | 1:C:255:ILE:CB   | 2.51                     | 0.58              |
| 2:D:14:LYS:HE2   | 2:D:18:VAL:HG21  | 1.85                     | 0.58              |
| 1:A:66:ARG:HA    | 1:A:87:LEU:HA    | 1.86                     | 0.58              |
| 1:C:10:LYS:HE3   | 1:C:31:VAL:HG21  | 1.86                     | 0.58              |
| 1:A:208:TYR:HB3  | 1:A:237:VAL:HG23 | 1.84                     | 0.58              |
| 1:A:241:ASP:OD1  | 1:A:241:ASP:C    | 2.47                     | 0.58              |
| 1:A:171:LEU:HD12 | 1:A:175:VAL:HG11 | 1.86                     | 0.58              |
| 1:A:251:PRO:O    | 1:A:252:VAL:HB   | 2.03                     | 0.58              |
| 1:C:15:ASP:OD2   | 1:C:55:SER:N     | 2.36                     | 0.57              |
| 1:C:82:LYS:O     | 1:C:106:LYS:HB2  | 2.04                     | 0.57              |
| 1:C:106:LYS:CB   | 5:C:401:HOH:O    | 2.47                     | 0.57              |
| 2:D:14:LYS:H     | 2:D:14:LYS:HD2   | 1.68                     | 0.57              |
| 1:A:67:TYR:CE2   | 1:A:89:TYR:CD1   | 2.92                     | 0.57              |
| 1:C:95:ASN:O     | 1:C:117:PRO:HG2  | 2.05                     | 0.57              |
| 2:D:33:THR:HG23  | 2:D:36:GLN:HG3   | 1.85                     | 0.57              |
| 2:D:29:ASN:CB    | 2:D:37:ARG:HD2   | 2.35                     | 0.57              |
| 1:C:105:ASP:CA   | 1:C:130:LYS:HG2  | 2.34                     | 0.56              |
| 1:A:179:LEU:HD12 | 1:A:179:LEU:N    | 2.17                     | 0.56              |
| 1:A:253:ARG:H    | 1:A:253:ARG:HD2  | 1.71                     | 0.56              |
| 1:C:71:GLY:HA2   | 1:C:93:ASP:O     | 2.05                     | 0.56              |
| 1:C:94:PHE:O     | 1:C:117:PRO:HD2  | 2.05                     | 0.56              |
| 1:C:36:THR:OG1   | 1:C:39:GLU:HG3   | 2.06                     | 0.56              |
| 1:A:110:LEU:C    | 1:A:110:LEU:CD1  | 2.72                     | 0.56              |
| 1:A:200:PHE:CB   | 1:A:203:LEU:HD12 | 2.35                     | 0.56              |
| 1:C:111:LYS:C    | 1:C:134:LEU:HD12 | 2.29                     | 0.56              |
| 1:C:171:LEU:HB2  | 1:C:196:PRO:CD   | 2.35                     | 0.56              |
| 1:A:183:LYS:CA   | 1:A:206:LEU:HA   | 2.35                     | 0.56              |
| 1:A:200:PHE:HB3  | 1:A:203:LEU:HD12 | 1.86                     | 0.56              |
| 1:C:43:ILE:HG12  | 1:C:43:ILE:O     | 2.05                     | 0.56              |
| 1:C:89:TYR:HB2   | 5:C:423:HOH:O    | 2.05                     | 0.56              |
| 2:B:1:THR:HG23   | 2:B:4:LYS:HB2    | 1.87                     | 0.56              |
| 1:A:13:PHE:CE1   | 1:A:58:GLY:O     | 2.59                     | 0.56              |
| 1:A:37:GLN:C     | 1:A:41:ASN:ND2   | 2.63                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:223:ILE:HD13 | 1:A:224:ARG:CA   | 2.34                     | 0.55              |
| 1:A:59:ILE:HG21  | 1:A:81:LEU:HB3   | 1.87                     | 0.55              |
| 1:A:72:GLY:O     | 1:A:94:PHE:HA    | 2.06                     | 0.55              |
| 1:A:192:LEU:HD12 | 1:A:192:LEU:N    | 2.21                     | 0.55              |
| 1:A:195:VAL:HG21 | 1:A:200:PHE:HE1  | 1.71                     | 0.55              |
| 1:C:6:SER:OG     | 1:C:34:ALA:HB1   | 2.05                     | 0.55              |
| 1:C:62:LEU:O     | 1:C:65:VAL:HG12  | 2.06                     | 0.55              |
| 1:C:93:ASP:OD2   | 2:D:44:GLY:HA3   | 2.06                     | 0.55              |
| 1:C:237:VAL:C    | 1:C:239:GLY:H    | 2.14                     | 0.55              |
| 1:A:116:SER:HB3  | 1:A:117:PRO:CD   | 2.36                     | 0.55              |
| 1:A:239:GLY:O    | 1:A:241:ASP:N    | 2.39                     | 0.55              |
| 1:C:3:ILE:CG2    | 1:C:5:VAL:O      | 2.54                     | 0.55              |
| 2:B:28:VAL:HG23  | 2:B:28:VAL:O     | 2.07                     | 0.55              |
| 1:A:68:LEU:CD2   | 1:A:70:LEU:HD11  | 2.28                     | 0.55              |
| 1:A:72:GLY:CA    | 1:A:94:PHE:CD1   | 2.90                     | 0.55              |
| 1:C:83:GLU:OE2   | 1:C:106:LYS:HG2  | 2.07                     | 0.55              |
| 1:A:36:THR:N     | 1:A:39:GLU:OE1   | 2.30                     | 0.55              |
| 1:C:243:ALA:CB   | 1:C:251:PRO:HG2  | 2.37                     | 0.55              |
| 1:A:7:THR:O      | 1:A:35:VAL:N     | 2.40                     | 0.54              |
| 1:A:37:GLN:C     | 1:A:41:ASN:HD21  | 2.14                     | 0.54              |
| 1:A:212:HIS:O    | 1:A:213:ASP:HB2  | 2.06                     | 0.54              |
| 1:A:243:ALA:O    | 1:A:251:PRO:HD3  | 2.06                     | 0.54              |
| 1:A:47:ILE:HG12  | 1:A:69:ALA:HB3   | 1.90                     | 0.54              |
| 1:A:47:ILE:HD11  | 1:A:67:TYR:HE1   | 1.73                     | 0.54              |
| 1:A:13:PHE:HE1   | 1:A:58:GLY:C     | 2.16                     | 0.54              |
| 1:A:49:ASN:ND2   | 2:B:43:LEU:HD13  | 2.23                     | 0.54              |
| 1:C:220:CYS:O    | 1:C:221:PRO:C    | 2.50                     | 0.54              |
| 1:C:254:SER:HA   | 1:C:256:ILE:HD13 | 1.88                     | 0.54              |
| 2:D:28:VAL:CG1   | 2:D:62:ARG:NH2   | 2.70                     | 0.54              |
| 1:A:208:TYR:HB3  | 1:A:237:VAL:CG2  | 2.38                     | 0.54              |
| 1:C:236:VAL:HG11 | 1:C:240:PRO:HA   | 1.89                     | 0.54              |
| 1:A:23:LYS:HG3   | 1:A:24:ALA:N     | 2.22                     | 0.54              |
| 1:C:221:PRO:HG2  | 1:C:223:ILE:CD1  | 2.37                     | 0.54              |
| 1:C:255:ILE:C    | 1:C:256:ILE:HD12 | 2.31                     | 0.54              |
| 1:A:144:LEU:HD12 | 1:A:166:ASN:OD1  | 2.08                     | 0.54              |
| 1:A:147:LEU:HD23 | 1:A:148:PRO:HD3  | 1.90                     | 0.54              |
| 1:A:183:LYS:HA   | 1:A:205:SER:O    | 2.08                     | 0.54              |
| 1:C:143:GLN:O    | 1:C:144:LEU:C    | 2.49                     | 0.54              |
| 1:C:195:VAL:O    | 1:C:196:PRO:C    | 2.50                     | 0.54              |
| 1:A:88:THR:O     | 1:A:110:LEU:HB2  | 2.08                     | 0.53              |
| 2:B:14:LYS:N     | 2:B:14:LYS:CD    | 2.69                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:254:SER:CA   | 1:C:256:ILE:CD1  | 2.86                     | 0.53              |
| 2:D:10:ALA:C     | 2:D:19:LYS:HZ3   | 2.16                     | 0.53              |
| 2:D:51:PHE:CD1   | 2:D:51:PHE:C     | 2.85                     | 0.53              |
| 1:A:20:GLU:OE2   | 1:A:31:VAL:HG22  | 2.08                     | 0.53              |
| 1:C:140:ASP:N    | 1:C:140:ASP:OD1  | 2.41                     | 0.53              |
| 1:A:7:THR:O      | 1:A:34:ALA:CB    | 2.56                     | 0.53              |
| 1:A:44:ASP:HB2   | 1:A:66:ARG:HD3   | 1.85                     | 0.53              |
| 1:A:204:THR:C    | 1:A:206:LEU:H    | 2.15                     | 0.53              |
| 1:A:208:TYR:HD2  | 1:A:237:VAL:CG2  | 2.21                     | 0.53              |
| 2:B:29:ASN:CB    | 2:B:37:ARG:HD2   | 2.36                     | 0.53              |
| 2:B:33:THR:N     | 2:B:36:GLN:OE1   | 2.34                     | 0.53              |
| 1:C:68:LEU:HD11  | 1:C:70:LEU:HD21  | 1.90                     | 0.53              |
| 1:C:73:ASN:HA    | 1:C:95:ASN:HD22  | 1.74                     | 0.53              |
| 1:C:209:ILE:HG22 | 1:C:236:VAL:HA   | 1.89                     | 0.53              |
| 1:A:136:ILE:HD11 | 3:A:301:1PE:H251 | 1.89                     | 0.53              |
| 1:C:170:SER:N    | 1:C:192:LEU:HD23 | 2.23                     | 0.53              |
| 1:A:12:ILE:HG23  | 1:A:61:TYR:CD2   | 2.42                     | 0.53              |
| 2:B:28:VAL:CG1   | 2:B:62:ARG:CZ    | 2.87                     | 0.53              |
| 1:A:44:ASP:C     | 1:A:65:VAL:HA    | 2.34                     | 0.52              |
| 2:B:60:GLN:O     | 2:B:63:ALA:HB3   | 2.09                     | 0.52              |
| 1:C:255:ILE:CA   | 1:C:256:ILE:HD12 | 2.39                     | 0.52              |
| 1:A:67:TYR:CD2   | 1:A:89:TYR:CG    | 2.97                     | 0.52              |
| 1:C:7:THR:CG2    | 1:C:8:PRO:HD2    | 2.39                     | 0.52              |
| 1:A:157:ASN:N    | 1:A:157:ASN:HD22 | 2.07                     | 0.52              |
| 1:A:1:GLU:HB3    | 1:A:61:TYR:HE1   | 1.74                     | 0.52              |
| 1:C:60:GLN:HB3   | 1:C:80:ALA:O     | 2.10                     | 0.52              |
| 1:A:7:THR:C      | 1:A:34:ALA:CB    | 2.83                     | 0.52              |
| 1:A:66:ARG:HA    | 1:A:86:ASN:O     | 2.09                     | 0.52              |
| 2:B:51:PHE:CD1   | 2:B:51:PHE:C     | 2.87                     | 0.52              |
| 1:A:72:GLY:O     | 1:A:94:PHE:CD1   | 2.62                     | 0.52              |
| 1:A:112:GLU:HG3  | 1:A:136:ILE:HB   | 1.87                     | 0.52              |
| 1:A:193:LYS:HA   | 1:A:215:PRO:O    | 2.09                     | 0.52              |
| 1:C:193:LYS:HA   | 1:C:216:TRP:HA   | 1.91                     | 0.52              |
| 1:C:243:ALA:O    | 1:C:251:PRO:CD   | 2.56                     | 0.52              |
| 1:A:13:PHE:CE1   | 1:A:58:GLY:C     | 2.88                     | 0.52              |
| 1:C:152:PHE:HA   | 1:C:155:LEU:CD1  | 2.37                     | 0.52              |
| 1:A:223:ILE:CD1  | 1:A:224:ARG:N    | 2.58                     | 0.52              |
| 1:A:12:ILE:O     | 1:A:14:PRO:HD3   | 2.10                     | 0.52              |
| 1:A:245:CYS:HB2  | 1:A:248:SER:OG   | 2.09                     | 0.52              |
| 1:C:72:GLY:N     | 1:C:94:PHE:CD2   | 2.77                     | 0.52              |
| 1:C:258:PRO:O    | 1:C:259:THR:CB   | 2.38                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1:GLU:HB3    | 1:A:61:TYR:CE1   | 2.45                     | 0.51              |
| 1:C:128:PHE:HB3  | 1:C:155:LEU:HD21 | 1.92                     | 0.51              |
| 1:A:43:ILE:HD12  | 1:A:62:LEU:HD13  | 1.87                     | 0.51              |
| 1:A:72:GLY:N     | 1:A:94:PHE:CE1   | 2.77                     | 0.51              |
| 1:C:68:LEU:HD23  | 1:C:90:LEU:CD1   | 2.41                     | 0.51              |
| 1:C:118:ASN:OD1  | 1:C:119:GLN:N    | 2.43                     | 0.51              |
| 1:C:171:LEU:CD2  | 1:C:192:LEU:CD2  | 2.89                     | 0.51              |
| 2:D:9:ILE:HD12   | 2:D:9:ILE:N      | 2.24                     | 0.51              |
| 1:A:164:SER:HA   | 1:A:188:SER:O    | 2.11                     | 0.51              |
| 1:C:107:LEU:N    | 1:C:107:LEU:HD13 | 2.25                     | 0.51              |
| 1:C:203:LEU:C    | 1:C:206:LEU:HD21 | 2.33                     | 0.51              |
| 1:A:61:TYR:O     | 1:A:63:PRO:HD3   | 2.11                     | 0.51              |
| 1:A:67:TYR:HD2   | 1:A:89:TYR:CB    | 2.20                     | 0.51              |
| 1:A:152:PHE:HD1  | 1:A:155:LEU:CD1  | 2.24                     | 0.51              |
| 1:C:13:PHE:CE2   | 1:C:22:ILE:HG21  | 2.45                     | 0.51              |
| 1:A:71:GLY:HA2   | 1:A:93:ASP:O     | 2.11                     | 0.51              |
| 1:A:249:GLY:O    | 1:A:250:LYS:C    | 2.54                     | 0.51              |
| 1:A:210:TRP:NE1  | 1:A:237:VAL:CG1  | 2.74                     | 0.51              |
| 1:A:116:SER:C    | 1:A:142:ASN:HD22 | 2.19                     | 0.51              |
| 1:C:185:LEU:O    | 1:C:209:ILE:HA   | 2.10                     | 0.51              |
| 1:C:17:ALA:HB3   | 1:C:53:ILE:CB    | 2.41                     | 0.51              |
| 1:C:112:GLU:N    | 1:C:134:LEU:HD12 | 2.25                     | 0.51              |
| 1:A:60:GLN:HG2   | 1:A:61:TYR:N     | 2.25                     | 0.50              |
| 1:C:199:VAL:HG13 | 1:C:200:PHE:CD1  | 2.47                     | 0.50              |
| 1:C:245:CYS:SG   | 1:C:249:GLY:O    | 2.69                     | 0.50              |
| 1:A:25:ASN:C     | 1:A:25:ASN:ND2   | 2.66                     | 0.50              |
| 2:D:3:GLN:O      | 2:D:7:GLU:HG3    | 2.11                     | 0.50              |
| 2:D:28:VAL:HG12  | 2:D:62:ARG:NH2   | 2.25                     | 0.50              |
| 1:A:59:ILE:HG22  | 1:A:80:ALA:HB1   | 1.93                     | 0.50              |
| 1:C:17:ALA:HB3   | 1:C:53:ILE:CA    | 2.42                     | 0.50              |
| 1:C:179:LEU:HB2  | 1:C:203:LEU:HD21 | 1.93                     | 0.50              |
| 1:A:208:TYR:CD2  | 1:A:237:VAL:HG22 | 2.47                     | 0.50              |
| 1:A:85:THR:HB    | 1:A:109:ASN:HD21 | 1.77                     | 0.50              |
| 1:A:196:PRO:CB   | 1:A:199:VAL:HG13 | 2.42                     | 0.50              |
| 1:C:119:GLN:N    | 1:C:119:GLN:OE1  | 2.32                     | 0.50              |
| 1:C:146:SER:HA   | 1:C:168:LEU:CD2  | 2.42                     | 0.49              |
| 1:A:81:LEU:HB2   | 1:A:84:LEU:HD12  | 1.94                     | 0.49              |
| 1:A:232:LYS:O    | 1:A:233:HIS:CD2  | 2.65                     | 0.49              |
| 2:B:1:THR:O      | 2:B:4:LYS:HB3    | 2.13                     | 0.49              |
| 2:B:41:ILE:CG2   | 2:B:48:ILE:CD1   | 2.89                     | 0.49              |
| 1:C:40:LEU:O     | 1:C:43:ILE:HG23  | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:68:LEU:HB3   | 1:A:90:LEU:HD12  | 1.94                     | 0.49              |
| 1:C:93:ASP:CG    | 2:D:44:GLY:HA3   | 2.37                     | 0.49              |
| 1:C:134:LEU:HD11 | 1:C:136:ILE:O    | 2.12                     | 0.49              |
| 1:C:243:ALA:C    | 1:C:244:LYS:HD2  | 2.36                     | 0.49              |
| 1:A:208:TYR:CD2  | 1:A:237:VAL:CG2  | 2.94                     | 0.49              |
| 1:C:21:THR:O     | 1:C:24:ALA:HB3   | 2.12                     | 0.49              |
| 1:C:104:PHE:CZ   | 1:C:115:LEU:HD21 | 2.48                     | 0.49              |
| 2:B:67:HIS:O     | 2:B:70:MET:HB2   | 2.12                     | 0.49              |
| 2:B:62:ARG:O     | 2:B:64:ASN:OD1   | 2.31                     | 0.49              |
| 1:C:152:PHE:CA   | 1:C:155:LEU:HD12 | 2.38                     | 0.49              |
| 1:C:195:VAL:O    | 1:C:195:VAL:HG22 | 2.13                     | 0.49              |
| 1:A:185:LEU:O    | 1:A:209:ILE:HA   | 2.13                     | 0.49              |
| 1:C:63:PRO:O     | 1:C:86:ASN:HB2   | 2.13                     | 0.49              |
| 1:A:232:LYS:C    | 1:A:233:HIS:CD2  | 2.91                     | 0.49              |
| 1:C:171:LEU:CD2  | 1:C:192:LEU:HD22 | 2.42                     | 0.49              |
| 1:C:121:GLN:O    | 1:C:144:LEU:HA   | 2.13                     | 0.48              |
| 1:A:66:ARG:O     | 1:A:88:THR:N     | 2.46                     | 0.48              |
| 1:A:160:GLU:HA   | 1:A:182:LEU:CD1  | 2.43                     | 0.48              |
| 2:D:70:MET:O     | 2:D:71:GLN:C     | 2.56                     | 0.48              |
| 1:A:77:ASP:C     | 1:A:79:SER:H     | 2.21                     | 0.48              |
| 1:A:142:ASN:HB2  | 1:A:144:LEU:CD1  | 2.43                     | 0.48              |
| 2:D:14:LYS:CD    | 2:D:14:LYS:N     | 2.72                     | 0.48              |
| 1:A:25:ASN:ND2   | 1:A:25:ASN:O     | 2.46                     | 0.48              |
| 1:A:43:ILE:HD11  | 1:A:62:LEU:HD13  | 1.95                     | 0.48              |
| 1:A:46:ILE:HB    | 1:A:68:LEU:CD1   | 2.43                     | 0.48              |
| 1:C:180:THR:OG1  | 1:C:181:GLN:N    | 2.47                     | 0.48              |
| 2:D:13:TYR:O     | 2:D:19:LYS:HE2   | 2.14                     | 0.48              |
| 1:C:183:LYS:O    | 1:C:206:LEU:HA   | 2.12                     | 0.48              |
| 1:A:115:LEU:C    | 1:A:142:ASN:HD21 | 2.21                     | 0.48              |
| 1:A:209:ILE:HG12 | 1:A:210:TRP:N    | 2.28                     | 0.48              |
| 2:D:14:LYS:H     | 2:D:14:LYS:HD3   | 1.74                     | 0.48              |
| 1:A:13:PHE:CZ    | 1:A:62:LEU:HD21  | 2.43                     | 0.48              |
| 1:A:59:ILE:HD13  | 1:A:59:ILE:HA    | 1.72                     | 0.48              |
| 1:A:65:VAL:CG1   | 1:A:87:LEU:CD1   | 2.83                     | 0.48              |
| 1:A:89:TYR:CD1   | 1:A:89:TYR:C     | 2.92                     | 0.48              |
| 1:A:112:GLU:HG2  | 1:A:136:ILE:CG2  | 2.44                     | 0.48              |
| 1:A:139:LEU:CA   | 1:A:142:ASN:OD1  | 2.61                     | 0.48              |
| 1:A:123:LEU:HG   | 1:A:144:LEU:CD2  | 2.43                     | 0.48              |
| 1:A:127:VAL:CG2  | 1:A:128:PHE:CE1  | 2.97                     | 0.48              |
| 1:C:20:GLU:HG3   | 1:C:23:LYS:HZ2   | 1.77                     | 0.48              |
| 1:A:85:THR:HG23  | 1:A:106:LYS:O    | 2.12                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:200:PHE:HD1  | 1:A:200:PHE:H    | 1.61                     | 0.47              |
| 1:C:183:LYS:C    | 1:C:184:ASP:OD1  | 2.56                     | 0.47              |
| 1:C:7:THR:HG22   | 1:C:8:PRO:HD2    | 1.94                     | 0.47              |
| 1:C:106:LYS:N    | 5:C:401:HOH:O    | 2.34                     | 0.47              |
| 1:A:10:LYS:HD3   | 1:A:31:VAL:CG1   | 2.44                     | 0.47              |
| 1:A:59:ILE:HG22  | 1:A:80:ALA:CB    | 2.45                     | 0.47              |
| 1:A:139:LEU:C    | 1:A:142:ASN:OD1  | 2.57                     | 0.47              |
| 1:C:107:LEU:N    | 1:C:107:LEU:CD1  | 2.76                     | 0.47              |
| 2:D:2:LEU:HD13   | 2:D:2:LEU:C      | 2.40                     | 0.47              |
| 1:A:128:PHE:HA   | 1:A:131:LEU:HD12 | 1.96                     | 0.47              |
| 2:B:6:ILE:HG12   | 2:B:6:ILE:H      | 1.51                     | 0.47              |
| 1:C:106:LYS:HA   | 1:C:106:LYS:HD3  | 1.58                     | 0.47              |
| 1:C:207:GLN:O    | 1:C:208:TYR:CD1  | 2.67                     | 0.47              |
| 1:C:239:GLY:C    | 1:C:241:ASP:N    | 2.72                     | 0.47              |
| 1:A:15:ASP:OD2   | 1:A:55:SER:CA    | 2.63                     | 0.47              |
| 1:C:89:TYR:OH    | 2:D:15:HIS:ND1   | 2.48                     | 0.47              |
| 1:C:104:PHE:HZ   | 1:C:115:LEU:HD21 | 1.79                     | 0.47              |
| 1:C:184:ASP:OD1  | 1:C:184:ASP:N    | 2.46                     | 0.47              |
| 2:D:32:GLU:OE1   | 2:D:37:ARG:HA    | 2.14                     | 0.47              |
| 1:C:8:PRO:HA     | 1:C:33:ASP:O     | 2.14                     | 0.47              |
| 1:C:50:ASN:OD1   | 1:C:52:ASP:HB2   | 2.14                     | 0.47              |
| 1:C:54:LYS:O     | 1:C:76:HIS:N     | 2.33                     | 0.47              |
| 1:A:43:ILE:HD11  | 1:A:65:VAL:CG2   | 2.45                     | 0.47              |
| 1:A:46:ILE:HB    | 1:A:68:LEU:HD12  | 1.97                     | 0.47              |
| 1:A:199:VAL:CG2  | 1:A:200:PHE:CD1  | 2.90                     | 0.47              |
| 2:B:15:HIS:HB2   | 2:B:18:VAL:HG23  | 1.97                     | 0.47              |
| 1:C:219:THR:O    | 1:C:223:ILE:CG1  | 2.63                     | 0.47              |
| 1:C:183:LYS:HG2  | 1:C:207:GLN:NE2  | 2.30                     | 0.47              |
| 1:C:195:VAL:HG23 | 1:C:199:VAL:HG11 | 1.97                     | 0.47              |
| 1:C:219:THR:CB   | 1:C:221:PRO:HD2  | 2.45                     | 0.47              |
| 1:A:9:ILE:HG12   | 1:A:35:VAL:HG13  | 1.96                     | 0.46              |
| 2:B:41:ILE:HG21  | 2:B:48:ILE:CD1   | 2.45                     | 0.46              |
| 1:A:175:VAL:HG13 | 1:A:176:PHE:CG   | 2.50                     | 0.46              |
| 1:A:59:ILE:HG22  | 1:A:80:ALA:C     | 2.39                     | 0.46              |
| 1:A:60:GLN:HB3   | 1:A:80:ALA:O     | 2.15                     | 0.46              |
| 2:B:49:LYS:HB2   | 2:B:49:LYS:HE2   | 1.37                     | 0.46              |
| 1:C:219:THR:CA   | 1:C:221:PRO:HD2  | 2.40                     | 0.46              |
| 2:D:14:LYS:NZ    | 2:D:18:VAL:HG11  | 2.31                     | 0.46              |
| 1:A:104:PHE:CE2  | 1:A:115:LEU:HD11 | 2.50                     | 0.46              |
| 1:C:23:LYS:O     | 1:C:27:LYS:N     | 2.48                     | 0.46              |
| 1:C:81:LEU:C     | 1:C:83:GLU:H     | 2.23                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:43:LEU:HD12  | 2:D:47:CYS:SG    | 2.56                     | 0.46              |
| 1:A:116:SER:CA   | 1:A:142:ASN:HD22 | 2.28                     | 0.46              |
| 1:A:13:PHE:HE1   | 1:A:58:GLY:O     | 1.97                     | 0.46              |
| 1:C:247:GLY:O    | 1:C:248:SER:OG   | 2.30                     | 0.46              |
| 2:D:38:ALA:O     | 2:D:41:ILE:HB    | 2.16                     | 0.46              |
| 1:C:195:VAL:CG2  | 1:C:199:VAL:HG11 | 2.46                     | 0.46              |
| 1:A:17:ALA:HB3   | 1:A:53:ILE:HA    | 1.98                     | 0.46              |
| 1:A:17:ALA:HB1   | 1:A:53:ILE:HG13  | 1.98                     | 0.46              |
| 1:A:116:SER:CA   | 1:A:142:ASN:ND2  | 2.79                     | 0.46              |
| 2:D:4:LYS:HE3    | 2:D:4:LYS:CA     | 2.46                     | 0.46              |
| 2:D:14:LYS:CD    | 2:D:15:HIS:HD2   | 2.29                     | 0.46              |
| 1:A:1:GLU:C      | 1:A:2:THR:CG2    | 2.88                     | 0.46              |
| 3:B:101:1PE:H262 | 2:D:16:SER:HB3   | 1.98                     | 0.46              |
| 1:C:139:LEU:HD23 | 1:C:139:LEU:HA   | 1.83                     | 0.46              |
| 1:C:175:VAL:CG1  | 1:C:176:PHE:CD2  | 2.99                     | 0.46              |
| 2:B:26:ALA:O     | 2:B:27:CYS:C     | 2.58                     | 0.45              |
| 2:D:29:ASN:HB2   | 2:D:37:ARG:NH1   | 2.31                     | 0.45              |
| 2:D:11:ALA:HA    | 2:D:19:LYS:NZ    | 2.31                     | 0.45              |
| 1:C:69:ALA:CB    | 1:C:91:PHE:HB3   | 2.47                     | 0.45              |
| 2:D:11:ALA:HA    | 2:D:19:LYS:HZ1   | 1.81                     | 0.45              |
| 1:A:158:LEU:HD21 | 1:A:161:LEU:HB2  | 1.98                     | 0.45              |
| 1:A:186:SER:HB2  | 1:A:210:TRP:CE3  | 2.51                     | 0.45              |
| 3:A:301:1PE:H161 | 2:B:14:LYS:HE2   | 1.98                     | 0.45              |
| 1:C:123:LEU:O    | 1:C:148:PRO:CG   | 2.64                     | 0.45              |
| 1:C:50:ASN:OD1   | 1:C:52:ASP:N     | 2.50                     | 0.45              |
| 1:A:30:SER:OG    | 1:A:31:VAL:N     | 2.44                     | 0.45              |
| 1:A:157:ASN:HD22 | 1:A:157:ASN:H    | 1.65                     | 0.45              |
| 1:A:161:LEU:C    | 1:A:161:LEU:HD12 | 2.42                     | 0.45              |
| 1:C:56:VAL:HG23  | 1:C:80:ALA:HB3   | 1.98                     | 0.45              |
| 1:A:8:PRO:HA     | 1:A:34:ALA:HA    | 1.98                     | 0.45              |
| 1:A:104:PHE:HA   | 1:A:107:LEU:CD2  | 2.47                     | 0.45              |
| 1:A:128:PHE:O    | 1:A:131:LEU:HB2  | 2.16                     | 0.45              |
| 1:A:137:LEU:CD2  | 1:A:152:PHE:CE1  | 2.98                     | 0.45              |
| 1:C:218:CYS:HB2  | 1:C:245:CYS:HB3  | 1.32                     | 0.45              |
| 2:D:33:THR:O     | 2:D:34:CYS:C     | 2.58                     | 0.45              |
| 2:B:2:LEU:CD2    | 2:B:6:ILE:HD11   | 2.31                     | 0.45              |
| 1:C:49:ASN:HB2   | 2:D:17:VAL:CG1   | 2.47                     | 0.45              |
| 1:C:219:THR:O    | 1:C:221:PRO:HD2  | 2.06                     | 0.45              |
| 2:D:2:LEU:CD1    | 2:D:6:ILE:HD11   | 2.46                     | 0.45              |
| 1:A:54:LYS:O     | 1:A:76:HIS:HB2   | 2.16                     | 0.45              |
| 1:A:62:LEU:H     | 1:A:62:LEU:HG    | 1.59                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:72:GLY:C     | 1:C:94:PHE:HD2   | 2.20                     | 0.45              |
| 1:C:119:GLN:H    | 1:C:119:GLN:CD   | 2.21                     | 0.45              |
| 1:A:92:LEU:O     | 1:A:116:SER:OG   | 2.34                     | 0.44              |
| 1:A:140:ASP:N    | 1:A:140:ASP:OD1  | 2.50                     | 0.44              |
| 1:C:220:CYS:O    | 1:C:221:PRO:O    | 2.35                     | 0.44              |
| 1:C:27:LYS:HE3   | 1:C:27:LYS:HB2   | 1.92                     | 0.44              |
| 1:C:225:TYR:HD1  | 1:C:226:LEU:CA   | 2.28                     | 0.44              |
| 1:A:36:THR:HG22  | 1:A:39:GLU:CD    | 2.26                     | 0.44              |
| 1:A:159:THR:C    | 1:A:160:GLU:HG3  | 2.40                     | 0.44              |
| 2:B:66:SER:O     | 2:B:69:ASP:N     | 2.51                     | 0.44              |
| 1:C:110:LEU:HD13 | 1:C:113:LEU:HD13 | 1.98                     | 0.44              |
| 1:A:197:ASP:HA   | 1:A:225:TYR:CD2  | 2.52                     | 0.44              |
| 1:A:208:TYR:HD2  | 1:A:237:VAL:HG22 | 1.81                     | 0.44              |
| 1:C:159:THR:HG23 | 1:C:183:LYS:HD3  | 1.99                     | 0.44              |
| 1:C:175:VAL:CG1  | 1:C:176:PHE:N    | 2.80                     | 0.44              |
| 1:A:107:LEU:H    | 1:A:107:LEU:CD2  | 2.23                     | 0.44              |
| 1:C:104:PHE:HB3  | 1:C:131:LEU:HD21 | 2.00                     | 0.44              |
| 1:A:85:THR:HB    | 1:A:109:ASN:ND2  | 2.31                     | 0.44              |
| 1:A:175:VAL:HG13 | 1:A:176:PHE:N    | 2.32                     | 0.44              |
| 1:C:142:ASN:HB3  | 1:C:144:LEU:HG   | 2.00                     | 0.44              |
| 1:A:89:TYR:CE1   | 1:A:91:PHE:HB2   | 2.53                     | 0.44              |
| 1:A:147:LEU:HA   | 1:A:148:PRO:HD3  | 1.63                     | 0.44              |
| 1:C:84:LEU:HD23  | 1:C:84:LEU:HA    | 1.65                     | 0.44              |
| 1:C:169:GLN:C    | 1:C:192:LEU:HD23 | 2.42                     | 0.44              |
| 2:D:65:ILE:CG2   | 2:D:69:ASP:HB2   | 2.48                     | 0.44              |
| 1:A:3:ILE:HD13   | 1:A:7:THR:OG1    | 2.18                     | 0.44              |
| 1:C:61:TYR:O     | 1:C:62:LEU:HD23  | 2.17                     | 0.44              |
| 2:D:33:THR:HG21  | 2:D:36:GLN:NE2   | 2.32                     | 0.44              |
| 1:C:8:PRO:HA     | 1:C:34:ALA:HA    | 1.98                     | 0.43              |
| 1:C:97:LEU:CD2   | 1:C:99:LEU:CD2   | 2.96                     | 0.43              |
| 1:C:192:LEU:O    | 1:C:215:PRO:HD2  | 2.18                     | 0.43              |
| 1:C:69:ALA:HA    | 1:C:91:PHE:O     | 2.18                     | 0.43              |
| 1:C:111:LYS:HA   | 1:C:134:LEU:HA   | 1.99                     | 0.43              |
| 1:A:67:TYR:CD2   | 1:A:89:TYR:CB    | 2.97                     | 0.43              |
| 1:A:75:LEU:CD2   | 1:A:78:ILE:HG22  | 2.48                     | 0.43              |
| 1:C:10:LYS:HE3   | 1:C:31:VAL:HG22  | 2.01                     | 0.43              |
| 2:D:61:LEU:HD23  | 2:D:70:MET:HE1   | 2.01                     | 0.43              |
| 1:A:22:ILE:HG23  | 1:A:26:LEU:CD1   | 2.42                     | 0.43              |
| 2:B:63:ALA:O     | 2:B:64:ASN:CB    | 2.67                     | 0.43              |
| 1:C:44:ASP:CA    | 1:C:65:VAL:HA    | 2.47                     | 0.43              |
| 1:C:154:LYS:HD2  | 1:C:154:LYS:HA   | 1.72                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:9:ILE:HD13   | 2:B:57:VAL:HG21  | 1.99                     | 0.43              |
| 1:C:176:PHE:O    | 1:C:177:ASP:C    | 2.60                     | 0.43              |
| 1:C:240:PRO:C    | 1:C:242:SER:H    | 2.26                     | 0.43              |
| 1:C:244:LYS:HA   | 1:C:251:PRO:HD3  | 2.00                     | 0.43              |
| 1:C:250:LYS:HA   | 1:C:251:PRO:HD3  | 1.83                     | 0.43              |
| 1:A:9:ILE:HB     | 1:A:31:VAL:O     | 2.18                     | 0.43              |
| 2:B:66:SER:O     | 2:B:67:HIS:C     | 2.61                     | 0.43              |
| 2:D:61:LEU:CD2   | 2:D:70:MET:HE1   | 2.48                     | 0.43              |
| 1:A:182:LEU:HD12 | 1:A:183:LYS:N    | 2.34                     | 0.43              |
| 1:C:208:TYR:CD1  | 1:C:208:TYR:N    | 2.84                     | 0.43              |
| 2:D:10:ALA:O     | 2:D:11:ALA:C     | 2.60                     | 0.43              |
| 1:A:6:SER:OG     | 1:A:34:ALA:HB1   | 2.19                     | 0.43              |
| 1:A:112:GLU:CG   | 1:A:136:ILE:CB   | 2.87                     | 0.43              |
| 1:A:161:LEU:HD11 | 1:A:163:LEU:HD21 | 2.01                     | 0.43              |
| 1:C:151:VAL:HG13 | 1:C:152:PHE:CG   | 2.54                     | 0.43              |
| 2:D:6:ILE:HA     | 2:D:9:ILE:HD13   | 2.00                     | 0.43              |
| 1:A:40:LEU:O     | 1:A:43:ILE:HG23  | 2.18                     | 0.43              |
| 1:A:189:TYR:CE1  | 1:A:213:ASP:OD1  | 2.72                     | 0.43              |
| 1:C:92:LEU:HD12  | 1:C:115:LEU:HD23 | 2.01                     | 0.43              |
| 1:C:243:ALA:HB3  | 1:C:251:PRO:HG2  | 2.00                     | 0.43              |
| 1:A:196:PRO:HD2  | 1:A:199:VAL:CG1  | 2.43                     | 0.42              |
| 1:A:159:THR:O    | 1:A:182:LEU:CD1  | 2.65                     | 0.42              |
| 1:C:82:LYS:O     | 1:C:106:LYS:CG   | 2.65                     | 0.42              |
| 1:A:116:SER:HA   | 1:A:142:ASN:ND2  | 2.33                     | 0.42              |
| 1:C:67:TYR:HA    | 1:C:89:TYR:O     | 2.19                     | 0.42              |
| 1:A:150:GLY:HA2  | 1:A:153:ASP:CG   | 2.45                     | 0.42              |
| 1:C:78:ILE:HD13  | 1:C:97:LEU:HD21  | 2.01                     | 0.42              |
| 1:C:116:SER:CB   | 1:C:117:PRO:HD2  | 2.47                     | 0.42              |
| 1:C:198:GLY:HA2  | 1:C:225:TYR:CE2  | 2.37                     | 0.42              |
| 1:C:123:LEU:O    | 1:C:148:PRO:HG3  | 2.19                     | 0.42              |
| 1:A:49:ASN:N     | 5:A:402:HOH:O    | 2.39                     | 0.42              |
| 1:A:88:THR:CA    | 1:A:110:LEU:HA   | 2.42                     | 0.42              |
| 1:C:97:LEU:HD22  | 1:C:99:LEU:HG    | 2.00                     | 0.42              |
| 1:A:12:ILE:H     | 1:A:12:ILE:CD1   | 2.26                     | 0.42              |
| 1:C:62:LEU:O     | 1:C:65:VAL:CG1   | 2.68                     | 0.42              |
| 1:C:130:LYS:N    | 1:C:130:LYS:HD2  | 2.34                     | 0.42              |
| 1:C:135:THR:OG1  | 1:C:136:ILE:HG13 | 2.20                     | 0.42              |
| 2:B:63:ALA:HB3   | 2:B:65:ILE:CD1   | 2.49                     | 0.42              |
| 1:C:154:LYS:O    | 1:C:156:THR:N    | 2.53                     | 0.42              |
| 1:A:12:ILE:HD12  | 1:A:12:ILE:N     | 2.24                     | 0.42              |
| 1:A:161:LEU:HD12 | 1:A:162:ASP:N    | 2.35                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:20:GLU:HG3   | 1:A:23:LYS:HE2   | 2.02                     | 0.41              |
| 1:A:157:ASN:ND2  | 1:A:157:ASN:N    | 2.68                     | 0.41              |
| 1:C:151:VAL:HG13 | 1:C:152:PHE:CD2  | 2.55                     | 0.41              |
| 1:A:199:VAL:HG21 | 1:A:200:PHE:CE1  | 2.55                     | 0.41              |
| 1:C:26:LEU:HD21  | 1:C:43:ILE:CG2   | 2.51                     | 0.41              |
| 1:C:113:LEU:HD12 | 1:C:113:LEU:HA   | 1.91                     | 0.41              |
| 1:A:12:ILE:C     | 1:A:14:PRO:HD3   | 2.46                     | 0.41              |
| 1:A:50:ASN:CG    | 1:A:52:ASP:H     | 2.27                     | 0.41              |
| 1:A:140:ASP:O    | 1:A:141:MET:HB2  | 2.20                     | 0.41              |
| 1:A:161:LEU:O    | 1:A:185:LEU:HD12 | 2.20                     | 0.41              |
| 1:C:20:GLU:HG3   | 1:C:23:LYS:HZ3   | 1.82                     | 0.41              |
| 1:C:243:ALA:HB1  | 1:C:251:PRO:HG2  | 2.02                     | 0.41              |
| 2:D:5:LYS:O      | 2:D:9:ILE:HD12   | 2.13                     | 0.41              |
| 1:C:183:LYS:HE3  | 1:C:207:GLN:HE22 | 1.85                     | 0.41              |
| 2:B:39:ALA:C     | 2:B:41:ILE:H     | 2.27                     | 0.41              |
| 1:C:72:GLY:O     | 1:C:94:PHE:CA    | 2.57                     | 0.41              |
| 1:C:159:THR:C    | 1:C:182:LEU:HD12 | 2.44                     | 0.41              |
| 1:C:226:LEU:O    | 1:C:230:ILE:HG13 | 2.20                     | 0.41              |
| 2:D:2:LEU:HD13   | 2:D:2:LEU:O      | 2.20                     | 0.41              |
| 2:B:63:ALA:CB    | 2:B:65:ILE:CD1   | 2.97                     | 0.41              |
| 1:C:225:TYR:N    | 1:C:226:LEU:HD12 | 2.36                     | 0.41              |
| 1:A:90:LEU:HD23  | 1:A:113:LEU:HD12 | 2.00                     | 0.41              |
| 1:C:83:GLU:OE2   | 1:C:106:LYS:CG   | 2.69                     | 0.41              |
| 1:C:151:VAL:CG1  | 1:C:152:PHE:CD2  | 3.03                     | 0.41              |
| 1:C:46:ILE:HG22  | 1:C:47:ILE:N     | 2.35                     | 0.41              |
| 1:C:127:VAL:HG13 | 1:C:128:PHE:CG   | 2.56                     | 0.41              |
| 1:A:6:SER:OG     | 1:A:34:ALA:CB    | 2.69                     | 0.41              |
| 1:A:43:ILE:HD11  | 1:A:65:VAL:HG22  | 2.02                     | 0.41              |
| 1:C:73:ASN:HA    | 1:C:95:ASN:ND2   | 2.35                     | 0.41              |
| 1:C:119:GLN:HE21 | 1:C:120:LEU:HD13 | 1.86                     | 0.41              |
| 2:D:10:ALA:O     | 2:D:13:TYR:N     | 2.53                     | 0.41              |
| 1:C:146:SER:HA   | 1:C:168:LEU:HD23 | 2.03                     | 0.41              |
| 1:A:179:LEU:HD22 | 1:A:182:LEU:HD22 | 2.03                     | 0.40              |
| 2:B:54:CYS:O     | 2:B:57:VAL:CG2   | 2.69                     | 0.40              |
| 1:C:73:ASN:O     | 1:C:95:ASN:HB2   | 2.21                     | 0.40              |
| 1:C:86:ASN:HD22  | 1:C:86:ASN:HA    | 1.64                     | 0.40              |
| 1:C:186:SER:O    | 1:C:187:LEU:HD23 | 2.21                     | 0.40              |
| 1:C:216:TRP:CD1  | 1:C:244:LYS:O    | 2.63                     | 0.40              |
| 1:A:209:ILE:N    | 1:A:235:GLY:O    | 2.54                     | 0.40              |
| 1:C:176:PHE:CE1  | 1:C:185:LEU:HD21 | 2.56                     | 0.40              |
| 1:A:242:SER:OG   | 1:A:243:ALA:N    | 2.55                     | 0.40              |

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| Atom-1           | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|----------------|--------------------------|-------------------|
| 1:C:171:LEU:HD13 | 1:C:171:LEU:HA | 1.95                     | 0.40              |
| 1:C:100:PRO:HD2  | 1:C:103:VAL:HB | 2.02                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1   | A     | 252/261 (97%) | 224 (89%) | 22 (9%)  | 6 (2%)   | 4           | 5   |
| 1   | C     | 256/261 (98%) | 226 (88%) | 26 (10%) | 4 (2%)   | 7           | 11  |
| 2   | B     | 70/75 (93%)   | 62 (89%)  | 8 (11%)  | 0        | 100         | 100 |
| 2   | D     | 70/75 (93%)   | 63 (90%)  | 7 (10%)  | 0        | 100         | 100 |
| All | All   | 648/672 (96%) | 575 (89%) | 63 (10%) | 10 (2%)  | 8           | 12  |

All (10) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 252 | VAL  |
| 1   | C     | 254 | SER  |
| 1   | A     | 240 | PRO  |
| 1   | C     | 253 | ARG  |
| 1   | C     | 240 | PRO  |
| 1   | C     | 256 | ILE  |
| 1   | A     | 222 | GLY  |
| 1   | A     | 250 | LYS  |
| 1   | A     | 56  | VAL  |
| 1   | A     | 251 | 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     | 215/237 (91%) | 163 (76%) | 52 (24%)  | 1           | 1 |
| 1   | C     | 229/237 (97%) | 173 (76%) | 56 (24%)  | 1           | 1 |
| 2   | B     | 58/64 (91%)   | 45 (78%)  | 13 (22%)  | 1           | 1 |
| 2   | D     | 59/64 (92%)   | 47 (80%)  | 12 (20%)  | 1           | 1 |
| All | All   | 561/602 (93%) | 428 (76%) | 133 (24%) | 1           | 1 |

All (133) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 2   | THR  |
| 1   | A     | 3   | ILE  |
| 1   | A     | 7   | THR  |
| 1   | A     | 20  | GLU  |
| 1   | A     | 22  | ILE  |
| 1   | A     | 25  | ASN  |
| 1   | A     | 32  | THR  |
| 1   | A     | 33  | ASP  |
| 1   | A     | 36  | THR  |
| 1   | A     | 38  | ASN  |
| 1   | A     | 42  | SER  |
| 1   | A     | 43  | ILE  |
| 1   | A     | 44  | ASP  |
| 1   | A     | 45  | GLN  |
| 1   | A     | 50  | ASN  |
| 1   | A     | 55  | SER  |
| 1   | A     | 56  | VAL  |
| 1   | A     | 59  | ILE  |
| 1   | A     | 60  | GLN  |
| 1   | A     | 62  | LEU  |
| 1   | A     | 66  | ARG  |
| 1   | A     | 77  | ASP  |
| 1   | A     | 84  | LEU  |
| 1   | A     | 85  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 87  | LEU  |
| 1   | A     | 88  | THR  |
| 1   | A     | 96  | GLN  |
| 1   | A     | 97  | LEU  |
| 1   | A     | 107 | LEU  |
| 1   | A     | 110 | LEU  |
| 1   | A     | 111 | LYS  |
| 1   | A     | 120 | LEU  |
| 1   | A     | 127 | VAL  |
| 1   | A     | 134 | LEU  |
| 1   | A     | 135 | THR  |
| 1   | A     | 143 | GLN  |
| 1   | A     | 157 | ASN  |
| 1   | A     | 160 | GLU  |
| 1   | A     | 179 | LEU  |
| 1   | A     | 183 | LYS  |
| 1   | A     | 184 | ASP  |
| 1   | A     | 195 | VAL  |
| 1   | A     | 197 | ASP  |
| 1   | A     | 199 | VAL  |
| 1   | A     | 200 | PHE  |
| 1   | A     | 206 | LEU  |
| 1   | A     | 208 | TYR  |
| 1   | A     | 223 | ILE  |
| 1   | A     | 241 | ASP  |
| 1   | A     | 248 | SER  |
| 1   | A     | 252 | VAL  |
| 1   | A     | 253 | ARG  |
| 2   | B     | 1   | THR  |
| 2   | B     | 4   | LYS  |
| 2   | B     | 6   | ILE  |
| 2   | B     | 8   | GLU  |
| 2   | B     | 17  | VAL  |
| 2   | B     | 35  | GLU  |
| 2   | B     | 41  | ILE  |
| 2   | B     | 42  | SER  |
| 2   | B     | 47  | CYS  |
| 2   | B     | 49  | LYS  |
| 2   | B     | 64  | ASN  |
| 2   | B     | 65  | ILE  |
| 2   | B     | 67  | HIS  |
| 1   | C     | 0   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 1   | GLU  |
| 1   | C     | 2   | THR  |
| 1   | C     | 3   | ILE  |
| 1   | C     | 6   | SER  |
| 1   | C     | 9   | ILE  |
| 1   | C     | 20  | GLU  |
| 1   | C     | 43  | ILE  |
| 1   | C     | 44  | ASP  |
| 1   | C     | 45  | GLN  |
| 1   | C     | 51  | SER  |
| 1   | C     | 53  | ILE  |
| 1   | C     | 59  | ILE  |
| 1   | C     | 65  | VAL  |
| 1   | C     | 70  | LEU  |
| 1   | C     | 74  | LYS  |
| 1   | C     | 77  | ASP  |
| 1   | C     | 81  | LEU  |
| 1   | C     | 86  | ASN  |
| 1   | C     | 89  | TYR  |
| 1   | C     | 93  | ASP  |
| 1   | C     | 106 | LYS  |
| 1   | C     | 107 | LEU  |
| 1   | C     | 118 | ASN  |
| 1   | C     | 130 | LYS  |
| 1   | C     | 131 | LEU  |
| 1   | C     | 135 | THR  |
| 1   | C     | 142 | ASN  |
| 1   | C     | 144 | LEU  |
| 1   | C     | 145 | GLN  |
| 1   | C     | 149 | LYS  |
| 1   | C     | 155 | LEU  |
| 1   | C     | 160 | GLU  |
| 1   | C     | 169 | GLN  |
| 1   | C     | 173 | LYS  |
| 1   | C     | 175 | VAL  |
| 1   | C     | 184 | ASP  |
| 1   | C     | 187 | LEU  |
| 1   | C     | 194 | SER  |
| 1   | C     | 195 | VAL  |
| 1   | C     | 199 | VAL  |
| 1   | C     | 206 | LEU  |
| 1   | C     | 208 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 211 | LEU  |
| 1   | C     | 214 | ASN  |
| 1   | C     | 217 | ASP  |
| 1   | C     | 219 | THR  |
| 1   | C     | 225 | TYR  |
| 1   | C     | 226 | LEU  |
| 1   | C     | 228 | GLU  |
| 1   | C     | 233 | HIS  |
| 1   | C     | 237 | VAL  |
| 1   | C     | 245 | CYS  |
| 1   | C     | 253 | ARG  |
| 1   | C     | 256 | ILE  |
| 1   | C     | 259 | THR  |
| 2   | D     | 4   | LYS  |
| 2   | D     | 8   | GLU  |
| 2   | D     | 9   | ILE  |
| 2   | D     | 14  | LYS  |
| 2   | D     | 16  | SER  |
| 2   | D     | 17  | VAL  |
| 2   | D     | 30  | ASN  |
| 2   | D     | 33  | THR  |
| 2   | D     | 51  | PHE  |
| 2   | D     | 53  | GLU  |
| 2   | D     | 57  | VAL  |
| 2   | D     | 69  | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 25  | ASN  |
| 1   | A     | 37  | GLN  |
| 1   | A     | 41  | ASN  |
| 1   | A     | 64  | ASN  |
| 1   | A     | 109 | ASN  |
| 1   | A     | 142 | ASN  |
| 1   | A     | 143 | GLN  |
| 1   | A     | 157 | ASN  |
| 1   | A     | 167 | GLN  |
| 1   | A     | 231 | ASN  |
| 1   | A     | 233 | HIS  |
| 1   | C     | 64  | ASN  |
| 1   | C     | 86  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 95  | ASN  |
| 1   | C     | 145 | GLN  |
| 1   | C     | 207 | GLN  |
| 2   | D     | 36  | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

10 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 | $\# Z  > 2$ |
| 4   | SO4  | C     | 302 | -    | 4,4,4        | 0.55 | 0           | 6,6,6       | 0.18 | 0           |
| 4   | SO4  | A     | 302 | -    | 4,4,4        | 0.44 | 0           | 6,6,6       | 0.14 | 0           |
| 4   | SO4  | B     | 102 | -    | 4,4,4        | 0.50 | 0           | 6,6,6       | 0.10 | 0           |
| 4   | SO4  | D     | 101 | -    | 4,4,4        | 0.46 | 0           | 6,6,6       | 0.16 | 0           |
| 3   | 1PE  | B     | 101 | -    | 15,15,15     | 0.90 | 0           | 14,14,14    | 1.28 | 1 (7%)      |
| 4   | SO4  | A     | 303 | -    | 4,4,4        | 0.50 | 0           | 6,6,6       | 0.13 | 0           |
| 4   | SO4  | A     | 304 | -    | 4,4,4        | 0.42 | 0           | 6,6,6       | 0.24 | 0           |
| 4   | SO4  | C     | 303 | -    | 4,4,4        | 0.47 | 0           | 6,6,6       | 0.21 | 0           |
| 4   | SO4  | C     | 301 | -    | 4,4,4        | 0.45 | 0           | 6,6,6       | 0.13 | 0           |
| 3   | 1PE  | A     | 301 | -    | 15,15,15     | 0.84 | 0           | 14,14,14    | 1.11 | 1 (7%)      |

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 |
|-----|------|-------|-----|------|---------|------------|-------|
| 3   | 1PE  | A     | 301 | -    | -       | 8/13/13/13 | -     |
| 3   | 1PE  | B     | 101 | -    | -       | 6/13/13/13 | -     |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3   | B     | 101 | 1PE  | C23-OH3-C22 | 3.02 | 126.48      | 113.26   |
| 3   | A     | 301 | 1PE  | C23-OH3-C22 | 2.40 | 123.76      | 113.26   |

There are no chirality outliers.

All (14) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | B     | 101 | 1PE  | C12-C22-OH3-C23 |
| 3   | B     | 101 | 1PE  | OH4-C13-C23-OH3 |
| 3   | A     | 301 | 1PE  | OH5-C14-C24-OH4 |
| 3   | B     | 101 | 1PE  | OH5-C14-C24-OH4 |
| 3   | A     | 301 | 1PE  | OH2-C12-C22-OH3 |
| 3   | A     | 301 | 1PE  | OH6-C15-C25-OH5 |
| 3   | A     | 301 | 1PE  | OH4-C13-C23-OH3 |
| 3   | B     | 101 | 1PE  | C15-C25-OH5-C14 |
| 3   | A     | 301 | 1PE  | OH7-C16-C26-OH6 |
| 3   | B     | 101 | 1PE  | C23-C13-OH4-C24 |
| 3   | A     | 301 | 1PE  | C23-C13-OH4-C24 |
| 3   | A     | 301 | 1PE  | C14-C24-OH4-C13 |
| 3   | B     | 101 | 1PE  | C16-C26-OH6-C15 |
| 3   | A     | 301 | 1PE  | C24-C14-OH5-C25 |

There are no ring outliers.

2 monomers are involved in 4 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | B     | 101 | 1PE  | 2       | 0            |
| 3   | A     | 301 | 1PE  | 2       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|---------------|-----------------------|-------|
| 1   | A     | 254/261 (97%) | 0.46   | 14 (5%) 30 27 | 30, 65, 97, 135       | 0     |
| 1   | C     | 260/261 (99%) | 0.24   | 9 (3%) 47 43  | 26, 55, 90, 121       | 0     |
| 2   | B     | 72/75 (96%)   | 0.14   | 1 (1%) 73 69  | 31, 49, 95, 118       | 0     |
| 2   | D     | 72/75 (96%)   | 0.05   | 2 (2%) 55 51  | 30, 50, 102, 128      | 0     |
| All | All   | 658/672 (97%) | 0.29   | 26 (3%) 42 38 | 26, 57, 95, 135       | 0     |

All (26) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 87  | LEU  | 8.1  |
| 1   | A     | 63  | PRO  | 3.5  |
| 1   | C     | 254 | SER  | 3.2  |
| 1   | A     | 179 | LEU  | 3.2  |
| 1   | A     | 253 | ARG  | 2.8  |
| 1   | A     | 235 | GLY  | 2.7  |
| 1   | A     | 32  | THR  | 2.7  |
| 2   | B     | 0   | SER  | 2.6  |
| 1   | C     | 122 | SER  | 2.6  |
| 1   | A     | 12  | ILE  | 2.6  |
| 1   | C     | 72  | GLY  | 2.5  |
| 1   | C     | 80  | ALA  | 2.5  |
| 1   | A     | 72  | GLY  | 2.4  |
| 1   | A     | 88  | THR  | 2.3  |
| 1   | C     | 256 | ILE  | 2.3  |
| 2   | D     | 71  | GLN  | 2.3  |
| 2   | D     | 0   | SER  | 2.3  |
| 1   | C     | 16  | ASP  | 2.2  |
| 1   | C     | 226 | LEU  | 2.2  |
| 1   | C     | 12  | ILE  | 2.2  |
| 1   | A     | 74  | LYS  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 219 | THR  | 2.1  |
| 1   | A     | 168 | LEU  | 2.1  |
| 1   | A     | 249 | GLY  | 2.0  |
| 1   | C     | 177 | ASP  | 2.0  |
| 1   | A     | 80  | ALA  | 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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 4   | SO4  | B     | 102 | 5/5   | 0.63 | 0.10 | 123,131,132,135            | 0     |
| 4   | SO4  | C     | 301 | 5/5   | 0.63 | 0.17 | 155,161,164,168            | 0     |
| 4   | SO4  | C     | 302 | 5/5   | 0.63 | 0.13 | 161,167,168,169            | 0     |
| 4   | SO4  | D     | 101 | 5/5   | 0.64 | 0.09 | 132,132,135,136            | 0     |
| 4   | SO4  | C     | 303 | 5/5   | 0.72 | 0.09 | 108,109,118,130            | 0     |
| 4   | SO4  | A     | 303 | 5/5   | 0.75 | 0.08 | 127,129,134,144            | 0     |
| 3   | 1PE  | B     | 101 | 16/16 | 0.79 | 0.14 | 73,80,86,89                | 0     |
| 4   | SO4  | A     | 302 | 5/5   | 0.79 | 0.13 | 162,162,171,172            | 0     |
| 4   | SO4  | A     | 304 | 5/5   | 0.83 | 0.09 | 108,118,121,122            | 0     |
| 3   | 1PE  | A     | 301 | 16/16 | 0.83 | 0.12 | 57,75,101,103              | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.