



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:20 PM UTC

PDB ID : 3JZT / pdb\_00003jzt  
Title : Structure of a cubic crystal form of X (ADRP) domain from FCoV with ADP-ribose  
Authors : Wojdyla, J.A.; Manolaridis, I.; Tucker, P.A.  
Deposited on : 2009-09-24  
Resolution : 3.91 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                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| 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                                                             |

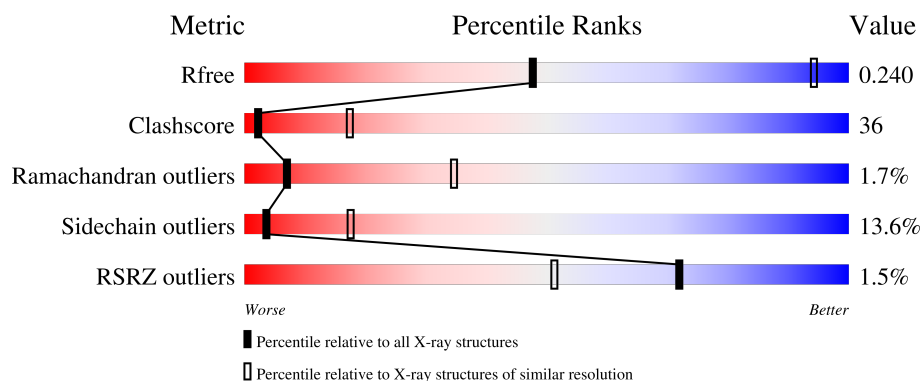
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.91 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                      | 1033 (4.10-3.74)                                      |
| Clashscore            | 190562                      | 1070 (4.10-3.74)                                      |
| Ramachandran outliers | 187476                      | 1017 (4.10-3.74)                                      |
| Sidechain outliers    | 187428                      | 1010 (4.10-3.74)                                      |
| RSRZ outliers         | 180081                      | 1033 (4.10-3.74)                                      |

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     | 168    | <div> <div>39%</div> <div>46%</div> <div>12%</div> <div>.</div> </div>               |
| 1   | B     | 168    | <div> <div>35%</div> <div>48%</div> <div>14%</div> <div>.</div> </div>               |
| 1   | C     | 168    | <div> <div>33%</div> <div>51%</div> <div>15%</div> <div>.</div> </div>               |
| 1   | D     | 168    | <div> <div>2%</div> <div>35%</div> <div>46%</div> <div>18%</div> <div>.</div> </div> |
| 1   | E     | 168    | <div> <div>35%</div> <div>45%</div> <div>16%</div> <div>.</div> </div>               |

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| Mol | Chain | Length | Quality of chain                                                                           |
|-----|-------|--------|--------------------------------------------------------------------------------------------|
| 1   | F     | 168    | <div><div></div><div>2%</div><div>23%</div><div>50%</div><div>21%</div><div>7%</div></div> |
| 1   | G     | 168    | <div><div></div><div>2%</div><div>39%</div><div>48%</div><div>11%</div><div></div></div>   |
| 1   | H     | 168    | <div><div></div><div>2%</div><div>33%</div><div>49%</div><div>14%</div><div></div></div>   |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10495 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.

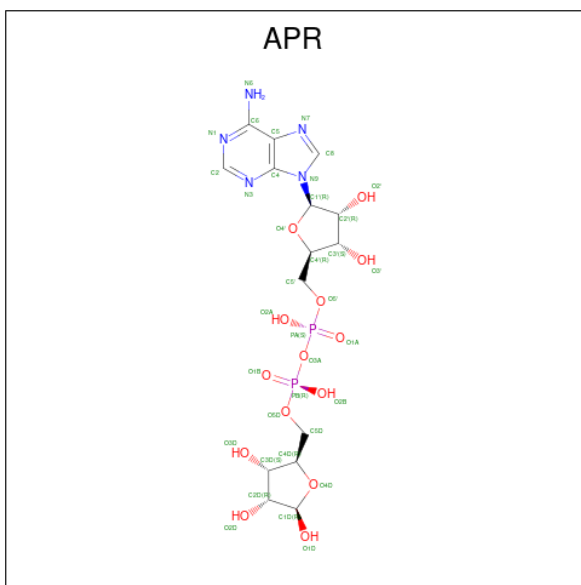
- Molecule 1 is a protein called macro domain of Non-structural protein 3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | A     | 168      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1298  | 834 | 221 | 240 | 3 |         |         |       |
| 1   | B     | 168      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1298  | 834 | 221 | 240 | 3 |         |         |       |
| 1   | C     | 168      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1298  | 834 | 221 | 240 | 3 |         |         |       |
| 1   | D     | 168      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1298  | 834 | 221 | 240 | 3 |         |         |       |
| 1   | E     | 168      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1298  | 834 | 221 | 240 | 3 |         |         |       |
| 1   | F     | 168      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1298  | 834 | 221 | 240 | 3 |         |         |       |
| 1   | G     | 168      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1298  | 834 | 221 | 240 | 3 |         |         |       |
| 1   | H     | 168      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1298  | 834 | 221 | 240 | 3 |         |         |       |

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | G     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 3 is ADENOSINE-5-DIPHOSPHORIBOSE (CCD ID: APR) (formula: C<sub>15</sub>H<sub>23</sub>N<sub>5</sub>O<sub>14</sub>P<sub>2</sub>).



| Mol | Chain | Residues | Atoms       |         |        |         |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|---------|
| 3   | B     | 1        | Total<br>36 | C<br>15 | N<br>5 | O<br>14 | P<br>2 | 0       | 0       |
| 3   | C     | 1        | Total<br>36 | C<br>15 | N<br>5 | O<br>14 | P<br>2 | 0       | 0       |
| 3   | D     | 1        | Total<br>36 | C<br>15 | N<br>5 | O<br>14 | P<br>2 | 0       | 0       |

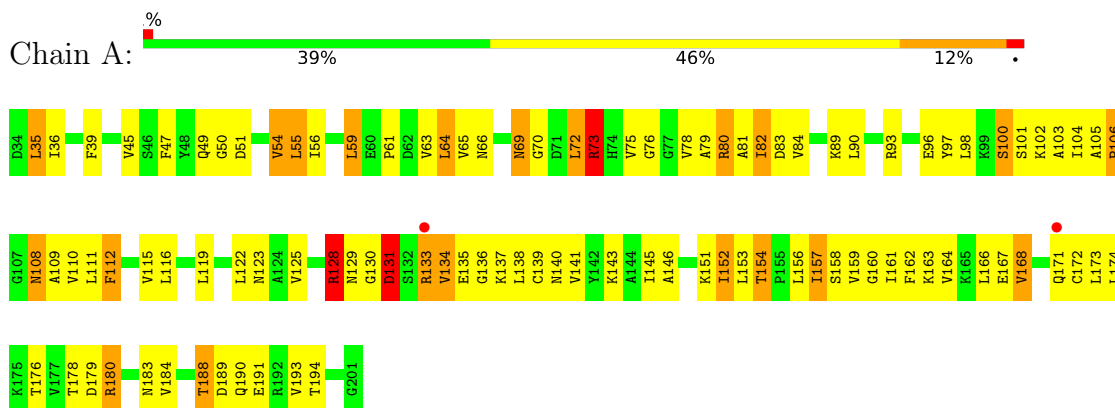
- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 4   | B     | 1        | Total Na<br>1 1 | 0       | 0       |

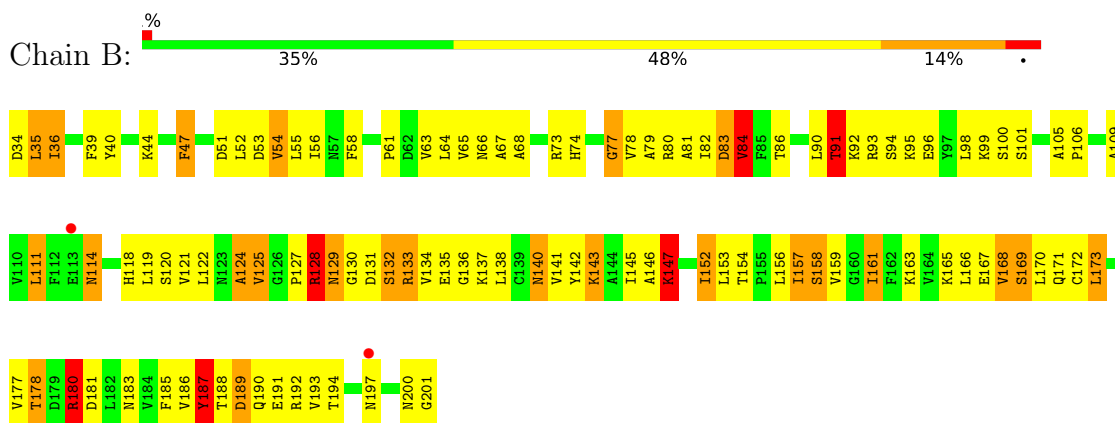
### 3 Residue-property plots

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.

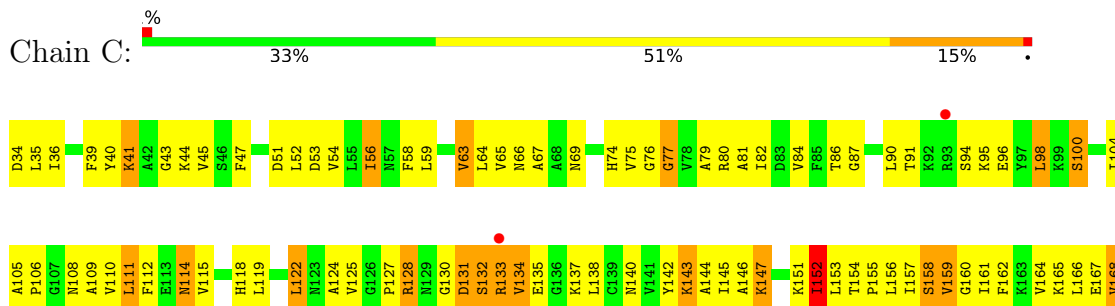
- Molecule 1: macro domain of Non-structural protein 3

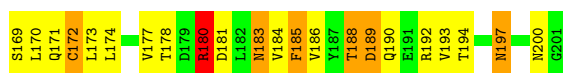


- Molecule 1: macro domain of Non-structural protein 3

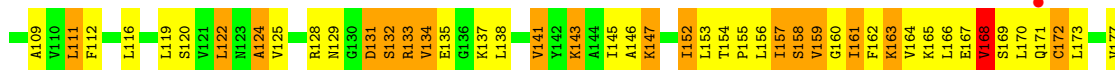
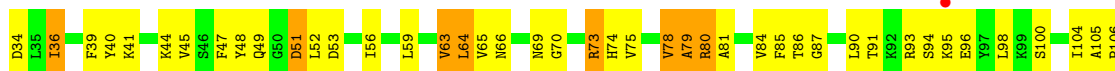


- Molecule 1: macro domain of Non-structural protein 3

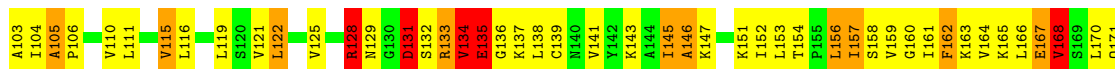




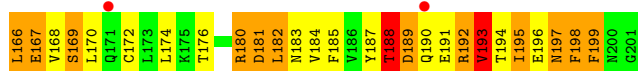
- Molecule 1: macro domain of Non-structural protein 3



- Molecule 1: macro domain of Non-structural protein 3



- Molecule 1: macro domain of Non-structural protein 3

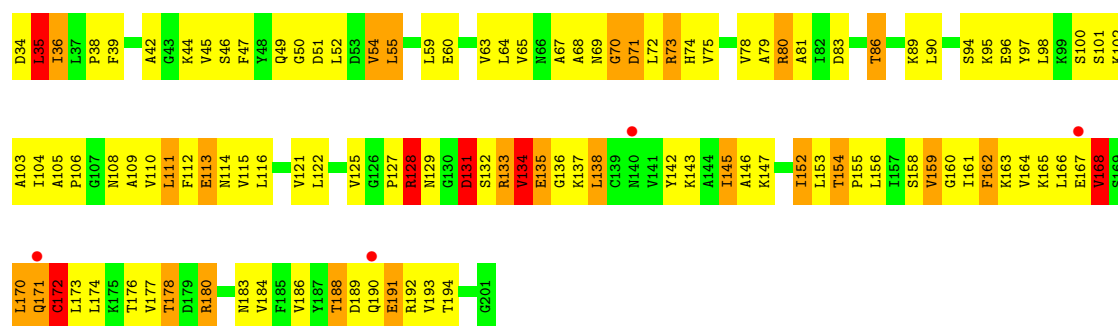


- Molecule 1: macro domain of Non-structural protein 3





- Molecule 1: macro domain of Non-structural protein 3



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 3                                                      | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 220.24Å 220.24Å 220.24Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 19.94 – 3.91<br>19.94 – 3.91                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.8 (19.94-3.91)<br>99.1 (19.94-3.91)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.46                                                        | Depositor        |
| $R_{sym}$                                                               | 0.56                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.10 (at 3.94Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC                                                      | Depositor        |
| R, $R_{free}$                                                           | 0.199 , 0.239<br>0.199 , 0.240                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 465 reflections (1.44%)                                     | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 53.9                                                        | Xtriage          |
| Anisotropy                                                              | 0.000                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 56.8                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$ | Xtriage          |
| Estimated twinning fraction                                             | 0.043 for l,-k,h                                            | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.90                                                        | EDS              |
| Total number of atoms                                                   | 10495                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 31.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CL, NA, APR

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

| Mol | Chain | Bond lengths |                  | Bond angles |                  |
|-----|-------|--------------|------------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5          |
| 1   | A     | 1.74         | 14/1318 (1.1%)   | 1.64        | 22/1782 (1.2%)   |
| 1   | B     | 1.74         | 19/1318 (1.4%)   | 1.57        | 26/1782 (1.5%)   |
| 1   | C     | 1.69         | 19/1318 (1.4%)   | 1.58        | 24/1782 (1.3%)   |
| 1   | D     | 1.73         | 23/1318 (1.7%)   | 1.64        | 25/1782 (1.4%)   |
| 1   | E     | 1.72         | 16/1318 (1.2%)   | 1.67        | 25/1782 (1.4%)   |
| 1   | F     | 1.72         | 19/1318 (1.4%)   | 1.82        | 37/1782 (2.1%)   |
| 1   | G     | 1.66         | 12/1318 (0.9%)   | 1.65        | 24/1782 (1.3%)   |
| 1   | H     | 1.82         | 25/1318 (1.9%)   | 1.66        | 26/1782 (1.5%)   |
| All | All   | 1.73         | 147/10544 (1.4%) | 1.66        | 209/14256 (1.5%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 1   | B     | 0                   | 1                   |
| 1   | F     | 0                   | 2                   |
| 1   | H     | 0                   | 1                   |
| All | All   | 0                   | 5                   |

All (147) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | D     | 78  | VAL  | CA-CB  | -9.61 | 1.42        | 1.54     |
| 1   | H     | 138 | LEU  | CG-CD1 | -8.66 | 1.24        | 1.52     |
| 1   | F     | 121 | VAL  | CA-C   | -8.50 | 1.42        | 1.52     |
| 1   | H     | 168 | VAL  | CA-CB  | -8.46 | 1.44        | 1.54     |
| 1   | G     | 81  | ALA  | CA-CB  | -8.23 | 1.40        | 1.53     |
| 1   | C     | 128 | ARG  | CZ-NH1 | -8.16 | 1.21        | 1.32     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | D     | 197 | ASN  | CG-ND2 | -7.86 | 1.16        | 1.33     |
| 1   | B     | 152 | ILE  | CA-CB  | -7.83 | 1.44        | 1.54     |
| 1   | B     | 36  | ILE  | CA-CB  | -7.80 | 1.44        | 1.53     |
| 1   | A     | 115 | VAL  | CA-CB  | -7.70 | 1.43        | 1.54     |
| 1   | A     | 140 | ASN  | CA-C   | -7.63 | 1.42        | 1.52     |
| 1   | C     | 41  | LYS  | CA-C   | -7.55 | 1.43        | 1.52     |
| 1   | D     | 51  | ASP  | CA-C   | -7.37 | 1.43        | 1.52     |
| 1   | A     | 152 | ILE  | CA-CB  | -7.34 | 1.45        | 1.54     |
| 1   | A     | 112 | PHE  | CA-C   | -7.24 | 1.43        | 1.52     |
| 1   | F     | 183 | ASN  | CA-C   | -7.23 | 1.44        | 1.52     |
| 1   | F     | 123 | ASN  | CA-C   | -7.22 | 1.43        | 1.52     |
| 1   | F     | 86  | THR  | CA-CB  | -7.15 | 1.41        | 1.53     |
| 1   | A     | 54  | VAL  | CA-CB  | -7.14 | 1.45        | 1.54     |
| 1   | B     | 125 | VAL  | CA-CB  | 7.13  | 1.62        | 1.53     |
| 1   | F     | 141 | VAL  | CA-CB  | -7.12 | 1.44        | 1.54     |
| 1   | D     | 197 | ASN  | CG-OD1 | -7.01 | 1.10        | 1.23     |
| 1   | F     | 123 | ASN  | CB-CG  | -7.00 | 1.34        | 1.52     |
| 1   | H     | 54  | VAL  | CA-CB  | -7.00 | 1.46        | 1.54     |
| 1   | C     | 45  | VAL  | CA-CB  | -6.89 | 1.45        | 1.54     |
| 1   | B     | 54  | VAL  | CA-CB  | -6.84 | 1.45        | 1.54     |
| 1   | F     | 183 | ASN  | N-CA   | -6.82 | 1.38        | 1.46     |
| 1   | B     | 157 | ILE  | CA-CB  | -6.82 | 1.46        | 1.54     |
| 1   | H     | 145 | ILE  | CA-CB  | -6.81 | 1.46        | 1.54     |
| 1   | E     | 156 | LEU  | CA-C   | -6.72 | 1.44        | 1.52     |
| 1   | D     | 63  | VAL  | CA-CB  | -6.69 | 1.46        | 1.54     |
| 1   | C     | 58  | PHE  | CA-C   | -6.68 | 1.43        | 1.52     |
| 1   | D     | 78  | VAL  | CA-C   | -6.64 | 1.44        | 1.52     |
| 1   | H     | 134 | VAL  | CA-C   | -6.55 | 1.44        | 1.52     |
| 1   | A     | 141 | VAL  | CA-CB  | -6.54 | 1.47        | 1.54     |
| 1   | B     | 186 | VAL  | N-CA   | -6.53 | 1.38        | 1.46     |
| 1   | D     | 45  | VAL  | CA-CB  | -6.47 | 1.46        | 1.54     |
| 1   | H     | 47  | PHE  | CA-C   | -6.47 | 1.44        | 1.52     |
| 1   | D     | 104 | ILE  | CA-CB  | -6.42 | 1.46        | 1.54     |
| 1   | H     | 152 | ILE  | CA-CB  | -6.39 | 1.46        | 1.54     |
| 1   | C     | 183 | ASN  | CA-C   | -6.33 | 1.45        | 1.53     |
| 1   | B     | 180 | ARG  | CA-C   | -6.32 | 1.44        | 1.52     |
| 1   | D     | 79  | ALA  | N-CA   | -6.30 | 1.39        | 1.46     |
| 1   | H     | 193 | VAL  | CA-C   | -6.25 | 1.44        | 1.52     |
| 1   | H     | 121 | VAL  | CA-CB  | -6.22 | 1.47        | 1.54     |
| 1   | F     | 63  | VAL  | CA-CB  | -6.17 | 1.46        | 1.54     |
| 1   | C     | 131 | ASP  | CG-OD2 | -6.16 | 1.13        | 1.25     |
| 1   | D     | 49  | GLN  | CA-C   | -6.16 | 1.45        | 1.52     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | F     | 123 | ASN  | CA-CB  | -6.14 | 1.44        | 1.53     |
| 1   | E     | 134 | VAL  | CA-C   | -6.13 | 1.45        | 1.52     |
| 1   | H     | 184 | VAL  | CA-C   | -6.08 | 1.45        | 1.52     |
| 1   | B     | 86  | THR  | CA-CB  | -6.07 | 1.44        | 1.53     |
| 1   | A     | 47  | PHE  | CA-C   | -6.04 | 1.45        | 1.52     |
| 1   | D     | 183 | ASN  | CG-ND2 | -6.00 | 1.20        | 1.33     |
| 1   | H     | 186 | VAL  | CA-CB  | -6.00 | 1.44        | 1.54     |
| 1   | E     | 105 | ALA  | CA-C   | 5.99  | 1.59        | 1.52     |
| 1   | H     | 191 | GLU  | CA-C   | -5.98 | 1.45        | 1.52     |
| 1   | G     | 82  | ILE  | CA-CB  | -5.97 | 1.47        | 1.54     |
| 1   | F     | 99  | LYS  | CA-C   | 5.94  | 1.60        | 1.52     |
| 1   | G     | 168 | VAL  | CA-CB  | -5.93 | 1.47        | 1.54     |
| 1   | E     | 195 | ILE  | CA-CB  | -5.89 | 1.47        | 1.54     |
| 1   | H     | 134 | VAL  | CB-CG1 | -5.88 | 1.33        | 1.52     |
| 1   | B     | 91  | THR  | CA-CB  | -5.88 | 1.44        | 1.53     |
| 1   | F     | 105 | ALA  | CA-CB  | 5.87  | 1.64        | 1.53     |
| 1   | C     | 186 | VAL  | CA-CB  | -5.87 | 1.46        | 1.55     |
| 1   | A     | 45  | VAL  | CA-CB  | -5.87 | 1.47        | 1.54     |
| 1   | F     | 164 | VAL  | N-CA   | 5.85  | 1.53        | 1.46     |
| 1   | F     | 132 | SER  | CA-C   | 5.83  | 1.60        | 1.52     |
| 1   | F     | 121 | VAL  | CA-CB  | -5.82 | 1.47        | 1.54     |
| 1   | G     | 65  | VAL  | CA-CB  | -5.79 | 1.47        | 1.54     |
| 1   | E     | 135 | GLU  | CB-CG  | -5.79 | 1.35        | 1.52     |
| 1   | C     | 122 | LEU  | CA-C   | -5.79 | 1.45        | 1.53     |
| 1   | H     | 115 | VAL  | CA-CB  | -5.72 | 1.47        | 1.54     |
| 1   | D     | 64  | LEU  | CA-C   | -5.70 | 1.45        | 1.52     |
| 1   | E     | 157 | ILE  | CA-CB  | -5.64 | 1.48        | 1.54     |
| 1   | C     | 63  | VAL  | CA-CB  | -5.63 | 1.47        | 1.54     |
| 1   | C     | 152 | ILE  | CA-CB  | -5.63 | 1.47        | 1.54     |
| 1   | A     | 123 | ASN  | CA-C   | -5.62 | 1.45        | 1.53     |
| 1   | A     | 100 | SER  | CA-C   | -5.61 | 1.44        | 1.52     |
| 1   | H     | 36  | ILE  | CA-C   | 5.61  | 1.59        | 1.52     |
| 1   | C     | 140 | ASN  | N-CA   | -5.58 | 1.39        | 1.46     |
| 1   | E     | 75  | VAL  | CA-CB  | -5.56 | 1.45        | 1.55     |
| 1   | D     | 36  | ILE  | CA-CB  | -5.56 | 1.46        | 1.53     |
| 1   | A     | 64  | LEU  | N-CA   | -5.55 | 1.39        | 1.46     |
| 1   | E     | 156 | LEU  | C-O    | -5.55 | 1.17        | 1.24     |
| 1   | E     | 146 | ALA  | CA-CB  | -5.52 | 1.44        | 1.53     |
| 1   | B     | 58  | PHE  | CA-C   | -5.50 | 1.45        | 1.52     |
| 1   | H     | 75  | VAL  | CA-CB  | -5.50 | 1.45        | 1.55     |
| 1   | A     | 157 | ILE  | CA-CB  | -5.49 | 1.49        | 1.54     |
| 1   | G     | 178 | THR  | CA-CB  | 5.49  | 1.62        | 1.53     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | D     | 157 | ILE  | CA-CB  | -5.48 | 1.48        | 1.54     |
| 1   | E     | 182 | LEU  | N-CA   | -5.48 | 1.39        | 1.45     |
| 1   | C     | 151 | LYS  | CA-C   | -5.42 | 1.46        | 1.52     |
| 1   | E     | 145 | ILE  | CA-CB  | -5.42 | 1.48        | 1.54     |
| 1   | A     | 179 | ASP  | CA-C   | -5.40 | 1.48        | 1.53     |
| 1   | H     | 42  | ALA  | CA-C   | -5.40 | 1.47        | 1.53     |
| 1   | E     | 58  | PHE  | CA-C   | -5.39 | 1.45        | 1.52     |
| 1   | C     | 189 | ASP  | N-CA   | 5.39  | 1.52        | 1.46     |
| 1   | A     | 168 | VAL  | CA-CB  | -5.38 | 1.47        | 1.54     |
| 1   | D     | 152 | ILE  | CA-CB  | -5.35 | 1.47        | 1.54     |
| 1   | G     | 157 | ILE  | CA-CB  | -5.35 | 1.48        | 1.54     |
| 1   | D     | 186 | VAL  | CA-CB  | -5.34 | 1.45        | 1.55     |
| 1   | B     | 140 | ASN  | N-CA   | -5.31 | 1.39        | 1.46     |
| 1   | H     | 113 | GLU  | CA-C   | -5.30 | 1.46        | 1.52     |
| 1   | C     | 144 | ALA  | CA-CB  | -5.30 | 1.44        | 1.53     |
| 1   | D     | 187 | TYR  | CA-C   | 5.30  | 1.59        | 1.52     |
| 1   | B     | 47  | PHE  | CA-C   | -5.29 | 1.46        | 1.52     |
| 1   | B     | 121 | VAL  | CA-CB  | -5.29 | 1.48        | 1.54     |
| 1   | F     | 152 | ILE  | CA-CB  | -5.29 | 1.47        | 1.54     |
| 1   | H     | 172 | CYS  | C-O    | -5.29 | 1.17        | 1.24     |
| 1   | G     | 170 | LEU  | CA-C   | 5.29  | 1.59        | 1.52     |
| 1   | C     | 98  | LEU  | N-CA   | -5.28 | 1.39        | 1.46     |
| 1   | F     | 104 | ILE  | N-CA   | -5.28 | 1.40        | 1.46     |
| 1   | H     | 184 | VAL  | CA-CB  | -5.28 | 1.48        | 1.54     |
| 1   | G     | 188 | THR  | CA-CB  | 5.27  | 1.61        | 1.53     |
| 1   | D     | 179 | ASP  | N-CA   | -5.27 | 1.40        | 1.46     |
| 1   | E     | 121 | VAL  | CA-CB  | -5.26 | 1.48        | 1.54     |
| 1   | H     | 45  | VAL  | CA-CB  | -5.26 | 1.47        | 1.53     |
| 1   | C     | 188 | THR  | N-CA   | 5.26  | 1.52        | 1.45     |
| 1   | E     | 141 | VAL  | N-CA   | -5.25 | 1.40        | 1.46     |
| 1   | F     | 75  | VAL  | CA-CB  | -5.22 | 1.47        | 1.54     |
| 1   | E     | 121 | VAL  | CA-C   | -5.21 | 1.46        | 1.52     |
| 1   | G     | 184 | VAL  | CA-CB  | -5.21 | 1.48        | 1.54     |
| 1   | C     | 128 | ARG  | CZ-NH2 | -5.20 | 1.26        | 1.33     |
| 1   | G     | 156 | LEU  | CA-C   | -5.19 | 1.46        | 1.52     |
| 1   | F     | 102 | LYS  | CG-CD  | 5.18  | 1.68        | 1.52     |
| 1   | B     | 101 | SER  | CA-C   | 5.18  | 1.58        | 1.52     |
| 1   | D     | 122 | LEU  | CA-C   | -5.17 | 1.46        | 1.52     |
| 1   | C     | 174 | LEU  | CA-C   | -5.17 | 1.45        | 1.52     |
| 1   | D     | 141 | VAL  | CA-CB  | -5.16 | 1.48        | 1.54     |
| 1   | G     | 186 | VAL  | CA-C   | -5.14 | 1.46        | 1.52     |
| 1   | B     | 187 | TYR  | CA-C   | 5.14  | 1.59        | 1.52     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 56  | ILE  | CA-C   | -5.13 | 1.45        | 1.52     |
| 1   | E     | 184 | VAL  | CA-CB  | -5.12 | 1.48        | 1.54     |
| 1   | G     | 141 | VAL  | N-CA   | -5.12 | 1.40        | 1.46     |
| 1   | F     | 135 | GLU  | CA-C   | -5.12 | 1.46        | 1.52     |
| 1   | B     | 68  | ALA  | CA-C   | -5.11 | 1.48        | 1.53     |
| 1   | C     | 180 | ARG  | CA-C   | -5.09 | 1.46        | 1.52     |
| 1   | D     | 78  | VAL  | N-CA   | -5.09 | 1.40        | 1.46     |
| 1   | H     | 134 | VAL  | CA-CB  | -5.08 | 1.47        | 1.54     |
| 1   | B     | 124 | ALA  | CA-C   | -5.06 | 1.46        | 1.52     |
| 1   | D     | 163 | LYS  | CA-C   | -5.06 | 1.48        | 1.53     |
| 1   | B     | 197 | ASN  | CG-OD1 | -5.05 | 1.14        | 1.23     |
| 1   | H     | 159 | VAL  | C-O    | 5.05  | 1.30        | 1.24     |
| 1   | D     | 79  | ALA  | CA-CB  | -5.05 | 1.45        | 1.53     |
| 1   | H     | 170 | LEU  | N-CA   | -5.04 | 1.40        | 1.46     |
| 1   | H     | 131 | ASP  | CA-C   | -5.01 | 1.47        | 1.53     |

All (209) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | F     | 78  | VAL  | N-CA-C    | -13.05 | 101.33      | 111.90   |
| 1   | C     | 128 | ARG  | NE-CZ-NH2 | 12.65  | 130.59      | 119.20   |
| 1   | H     | 131 | ASP  | N-CA-C    | -11.02 | 93.20       | 109.63   |
| 1   | E     | 35  | LEU  | N-CA-C    | 10.82  | 127.22      | 111.96   |
| 1   | A     | 35  | LEU  | N-CA-C    | 9.37   | 125.17      | 111.96   |
| 1   | D     | 131 | ASP  | N-CA-C    | -9.23  | 99.06       | 110.41   |
| 1   | H     | 168 | VAL  | CB-CA-C   | -8.90  | 100.36      | 112.02   |
| 1   | F     | 115 | VAL  | N-CA-C    | -8.88  | 102.08      | 110.42   |
| 1   | G     | 70  | GLY  | N-CA-C    | 8.80   | 124.17      | 114.40   |
| 1   | F     | 87  | GLY  | N-CA-C    | -8.77  | 103.07      | 115.43   |
| 1   | B     | 131 | ASP  | N-CA-C    | -8.67  | 99.44       | 110.19   |
| 1   | C     | 131 | ASP  | N-CA-C    | -8.62  | 99.50       | 110.19   |
| 1   | D     | 36  | ILE  | CB-CA-C   | -8.60  | 99.81       | 110.99   |
| 1   | H     | 115 | VAL  | N-CA-C    | -8.52  | 102.12      | 110.72   |
| 1   | F     | 80  | ARG  | N-CA-C    | -8.46  | 101.98      | 111.71   |
| 1   | A     | 134 | VAL  | CB-CA-C   | -8.40  | 97.51       | 111.29   |
| 1   | E     | 70  | GLY  | N-CA-C    | 8.38   | 123.71      | 114.40   |
| 1   | C     | 36  | ILE  | CB-CA-C   | -8.35  | 100.13      | 110.99   |
| 1   | D     | 56  | ILE  | CB-CA-C   | -8.27  | 100.98      | 112.14   |
| 1   | C     | 133 | ARG  | N-CA-C    | -8.12  | 103.33      | 113.23   |
| 1   | B     | 168 | VAL  | CB-CA-C   | -8.10  | 101.38      | 112.24   |
| 1   | C     | 159 | VAL  | N-CA-C    | 8.05   | 118.86      | 110.72   |
| 1   | A     | 54  | VAL  | CB-CA-C   | -8.03  | 101.30      | 112.14   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | F     | 73  | ARG  | N-CA-C     | -7.89 | 98.20       | 109.96   |
| 1   | F     | 82  | ILE  | CB-CA-C    | -7.84 | 101.85      | 111.88   |
| 1   | B     | 185 | PHE  | N-CA-C     | 7.82  | 121.04      | 109.24   |
| 1   | H     | 168 | VAL  | N-CA-C     | 7.76  | 117.82      | 110.53   |
| 1   | D     | 133 | ARG  | N-CA-C     | -7.74 | 103.79      | 113.23   |
| 1   | F     | 37  | LEU  | N-CA-C     | 7.72  | 121.97      | 110.32   |
| 1   | E     | 135 | GLU  | CB-CA-C    | -7.69 | 99.12       | 110.96   |
| 1   | E     | 115 | VAL  | N-CA-C     | -7.68 | 102.96      | 110.72   |
| 1   | G     | 128 | ARG  | N-CA-C     | -7.66 | 100.65      | 110.53   |
| 1   | A     | 131 | ASP  | N-CA-C     | -7.60 | 98.52       | 109.31   |
| 1   | E     | 54  | VAL  | CB-CA-C    | -7.60 | 101.88      | 112.14   |
| 1   | H     | 35  | LEU  | N-CA-C     | 7.58  | 126.95      | 110.80   |
| 1   | F     | 198 | PHE  | N-CA-C     | -7.53 | 102.55      | 112.34   |
| 1   | G     | 131 | ASP  | N-CA-C     | -7.52 | 98.63       | 109.31   |
| 1   | C     | 168 | VAL  | CB-CA-C    | -7.52 | 102.19      | 112.04   |
| 1   | C     | 200 | ASN  | N-CA-C     | 7.48  | 123.33      | 111.81   |
| 1   | B     | 169 | SER  | N-CA-C     | -7.45 | 102.76      | 111.03   |
| 1   | E     | 65  | VAL  | CB-CA-C    | -7.42 | 101.50      | 111.15   |
| 1   | B     | 36  | ILE  | CB-CA-C    | -7.41 | 100.90      | 111.19   |
| 1   | C     | 128 | ARG  | NH1-CZ-NH2 | -7.38 | 109.70      | 119.30   |
| 1   | D     | 147 | LYS  | N-CA-C     | 7.37  | 121.92      | 112.34   |
| 1   | D     | 168 | VAL  | CB-CA-C    | -7.34 | 102.40      | 112.02   |
| 1   | E     | 131 | ASP  | N-CA-C     | -7.31 | 98.93       | 109.31   |
| 1   | B     | 133 | ARG  | N-CA-C     | -7.29 | 103.69      | 112.58   |
| 1   | G     | 80  | ARG  | N-CA-C     | -7.29 | 102.37      | 111.11   |
| 1   | F     | 98  | LEU  | CA-CB-CG   | -7.25 | 90.94       | 116.30   |
| 1   | H     | 134 | VAL  | CB-CA-C    | -7.25 | 99.41       | 111.29   |
| 1   | D     | 200 | ASN  | N-CA-C     | 7.22  | 126.19      | 110.80   |
| 1   | H     | 54  | VAL  | CB-CA-C    | -7.21 | 102.59      | 112.04   |
| 1   | H     | 135 | GLU  | N-CA-C     | 7.20  | 118.82      | 110.97   |
| 1   | D     | 59  | LEU  | N-CA-C     | -7.19 | 104.65      | 113.50   |
| 1   | E     | 35  | LEU  | CA-CB-CG   | -7.19 | 91.13       | 116.30   |
| 1   | G     | 189 | ASP  | N-CA-C     | 7.17  | 118.99      | 111.03   |
| 1   | D     | 159 | VAL  | N-CA-C     | 7.16  | 117.95      | 110.72   |
| 1   | A     | 80  | ARG  | N-CA-C     | -7.14 | 104.45      | 113.01   |
| 1   | B     | 55  | LEU  | N-CA-C     | -7.11 | 102.95      | 111.69   |
| 1   | F     | 169 | SER  | N-CA-C     | -7.09 | 103.48      | 111.14   |
| 1   | H     | 35  | LEU  | CA-CB-CG   | -7.06 | 91.59       | 116.30   |
| 1   | A     | 69  | ASN  | N-CA-C     | -7.03 | 98.58       | 109.76   |
| 1   | E     | 168 | VAL  | CB-CA-C    | -7.03 | 102.83      | 112.04   |
| 1   | F     | 91  | THR  | N-CA-C     | -6.99 | 103.59      | 111.07   |
| 1   | A     | 188 | THR  | CB-CA-C    | -6.99 | 94.96       | 110.19   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | F     | 188 | THR  | CB-CA-C | -6.96 | 95.98       | 110.40   |
| 1   | E     | 80  | ARG  | N-CA-C  | -6.92 | 103.73      | 111.28   |
| 1   | E     | 189 | ASP  | N-CA-C  | 6.90  | 118.69      | 111.03   |
| 1   | E     | 147 | LYS  | N-CA-C  | 6.89  | 121.14      | 112.87   |
| 1   | G     | 168 | VAL  | CB-CA-C | -6.89 | 103.20      | 111.81   |
| 1   | E     | 135 | GLU  | N-CA-C  | 6.89  | 118.48      | 110.97   |
| 1   | D     | 111 | LEU  | N-CA-C  | 6.88  | 119.49      | 108.41   |
| 1   | E     | 128 | ARG  | N-CA-C  | -6.85 | 101.69      | 110.53   |
| 1   | G     | 65  | VAL  | CB-CA-C | -6.84 | 102.25      | 111.15   |
| 1   | F     | 124 | ALA  | CA-C-N  | -6.84 | 113.81      | 122.43   |
| 1   | F     | 124 | ALA  | C-N-CA  | -6.84 | 113.81      | 122.43   |
| 1   | D     | 152 | ILE  | N-CA-C  | 6.82  | 118.42      | 108.53   |
| 1   | H     | 128 | ARG  | N-CA-C  | -6.80 | 100.46      | 110.52   |
| 1   | C     | 111 | LEU  | N-CA-C  | 6.76  | 119.75      | 108.20   |
| 1   | B     | 36  | ILE  | N-CA-C  | 6.74  | 117.34      | 107.37   |
| 1   | A     | 70  | GLY  | N-CA-C  | 6.72  | 122.07      | 114.67   |
| 1   | D     | 178 | THR  | CA-C-N  | -6.68 | 113.34      | 122.95   |
| 1   | D     | 178 | THR  | C-N-CA  | -6.68 | 113.34      | 122.95   |
| 1   | F     | 188 | THR  | N-CA-C  | 6.66  | 119.11      | 110.53   |
| 1   | B     | 118 | HIS  | N-CA-C  | 6.64  | 121.14      | 113.38   |
| 1   | C     | 118 | HIS  | N-CA-C  | 6.63  | 120.95      | 112.86   |
| 1   | F     | 161 | ILE  | N-CA-C  | 6.63  | 119.34      | 111.05   |
| 1   | F     | 140 | ASN  | N-CA-C  | -6.56 | 103.96      | 112.23   |
| 1   | D     | 189 | ASP  | CB-CA-C | -6.55 | 99.91       | 110.79   |
| 1   | E     | 72  | LEU  | N-CA-C  | 6.55  | 123.02      | 113.40   |
| 1   | H     | 193 | VAL  | N-CA-C  | -6.54 | 104.48      | 110.82   |
| 1   | F     | 154 | THR  | CA-C-N  | 6.51  | 127.94      | 120.98   |
| 1   | F     | 154 | THR  | C-N-CA  | 6.51  | 127.94      | 120.98   |
| 1   | F     | 101 | SER  | N-CA-C  | 6.50  | 118.20      | 107.73   |
| 1   | E     | 179 | ASP  | N-CA-C  | 6.47  | 118.61      | 107.28   |
| 1   | G     | 161 | ILE  | CB-CA-C | -6.46 | 102.62      | 112.05   |
| 1   | B     | 96  | GLU  | N-CA-C  | 6.33  | 117.97      | 111.14   |
| 1   | C     | 43  | GLY  | N-CA-C  | -6.31 | 100.23      | 110.95   |
| 1   | C     | 35  | LEU  | N-CA-C  | 6.26  | 117.91      | 111.14   |
| 1   | B     | 114 | ASN  | N-CA-C  | 6.26  | 120.25      | 112.24   |
| 1   | C     | 56  | ILE  | N-CA-C  | -6.25 | 104.42      | 110.42   |
| 1   | D     | 45  | VAL  | CB-CA-C | -6.24 | 103.04      | 111.15   |
| 1   | C     | 178 | THR  | CA-C-N  | -6.24 | 113.72      | 123.13   |
| 1   | C     | 178 | THR  | C-N-CA  | -6.24 | 113.72      | 123.13   |
| 1   | H     | 147 | LYS  | N-CA-C  | 6.22  | 120.33      | 112.87   |
| 1   | G     | 75  | VAL  | N-CA-C  | 6.20  | 118.07      | 109.45   |
| 1   | D     | 73  | ARG  | CA-C-N  | -6.17 | 114.68      | 123.20   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | D     | 73  | ARG  | C-N-CA  | -6.17 | 114.68      | 123.20   |
| 1   | G     | 72  | LEU  | N-CA-C  | 6.17  | 122.47      | 113.40   |
| 1   | B     | 161 | ILE  | N-CA-C  | 6.08  | 121.99      | 109.34   |
| 1   | A     | 154 | THR  | CB-CA-C | -6.08 | 100.64      | 109.45   |
| 1   | G     | 67  | ALA  | CA-C-N  | -6.06 | 113.11      | 122.87   |
| 1   | G     | 67  | ALA  | C-N-CA  | -6.06 | 113.11      | 122.87   |
| 1   | H     | 80  | ARG  | N-CA-C  | -6.03 | 103.88      | 111.11   |
| 1   | A     | 72  | LEU  | N-CA-C  | 6.01  | 122.24      | 113.40   |
| 1   | C     | 132 | SER  | N-CA-C  | 6.01  | 118.10      | 109.14   |
| 1   | G     | 168 | VAL  | N-CA-C  | 6.01  | 116.13      | 110.30   |
| 1   | F     | 104 | ILE  | CB-CA-C | 5.99  | 118.21      | 110.96   |
| 1   | A     | 75  | VAL  | N-CA-C  | 5.99  | 118.39      | 109.17   |
| 1   | E     | 168 | VAL  | N-CA-C  | 5.97  | 116.61      | 110.82   |
| 1   | A     | 55  | LEU  | N-CA-C  | -5.96 | 104.41      | 111.03   |
| 1   | B     | 84  | VAL  | CB-CA-C | -5.94 | 101.55      | 111.29   |
| 1   | A     | 128 | ARG  | N-CA-C  | -5.92 | 102.89      | 110.53   |
| 1   | H     | 65  | VAL  | CB-CA-C | -5.91 | 103.47      | 111.15   |
| 1   | B     | 129 | ASN  | N-CA-C  | 5.90  | 118.27      | 109.59   |
| 1   | B     | 147 | LYS  | N-CA-C  | 5.90  | 120.01      | 112.34   |
| 1   | G     | 171 | GLN  | N-CA-C  | -5.89 | 104.86      | 111.28   |
| 1   | B     | 35  | LEU  | N-CA-C  | 5.86  | 117.36      | 110.97   |
| 1   | F     | 77  | GLY  | CA-C-N  | -5.83 | 117.01      | 122.66   |
| 1   | F     | 77  | GLY  | C-N-CA  | -5.83 | 117.01      | 122.66   |
| 1   | A     | 108 | ASN  | N-CA-C  | 5.82  | 119.04      | 109.72   |
| 1   | D     | 36  | ILE  | N-CA-C  | 5.81  | 116.52      | 107.28   |
| 1   | F     | 35  | LEU  | N-CA-C  | 5.81  | 123.18      | 110.80   |
| 1   | H     | 55  | LEU  | N-CA-C  | -5.81 | 104.58      | 111.03   |
| 1   | F     | 176 | THR  | N-CA-C  | 5.81  | 117.41      | 111.14   |
| 1   | F     | 120 | SER  | CA-C-N  | -5.74 | 114.70      | 122.91   |
| 1   | F     | 120 | SER  | C-N-CA  | -5.74 | 114.70      | 122.91   |
| 1   | C     | 114 | ASN  | N-CA-C  | 5.72  | 119.32      | 111.54   |
| 1   | E     | 69  | ASN  | N-CA-C  | -5.71 | 100.51      | 109.25   |
| 1   | D     | 79  | ALA  | CA-C-N  | -5.70 | 113.04      | 120.44   |
| 1   | D     | 79  | ALA  | C-N-CA  | -5.70 | 113.04      | 120.44   |
| 1   | B     | 152 | ILE  | N-CA-C  | 5.66  | 116.73      | 108.53   |
| 1   | C     | 147 | LYS  | N-CA-C  | 5.64  | 119.26      | 112.38   |
| 1   | C     | 128 | ARG  | N-CA-C  | -5.64 | 102.41      | 110.59   |
| 1   | B     | 131 | ASP  | CA-C-N  | -5.63 | 113.75      | 122.59   |
| 1   | B     | 131 | ASP  | C-N-CA  | -5.63 | 113.75      | 122.59   |
| 1   | G     | 161 | ILE  | N-CA-C  | 5.63  | 118.94      | 111.17   |
| 1   | H     | 188 | THR  | CB-CA-C | -5.62 | 98.16       | 109.68   |
| 1   | H     | 71  | ASP  | N-CA-C  | -5.62 | 106.01      | 112.92   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | E     | 34  | ASP  | CA-C-N   | -5.61 | 113.73      | 122.42   |
| 1   | E     | 34  | ASP  | C-N-CA   | -5.61 | 113.73      | 122.42   |
| 1   | F     | 115 | VAL  | CB-CA-C  | 5.60  | 119.09      | 111.87   |
| 1   | H     | 108 | ASN  | N-CA-C   | 5.58  | 118.66      | 109.85   |
| 1   | F     | 59  | LEU  | N-CA-C   | -5.57 | 106.84      | 113.97   |
| 1   | A     | 65  | VAL  | CB-CA-C  | -5.55 | 103.93      | 111.15   |
| 1   | C     | 185 | PHE  | N-CA-C   | 5.55  | 117.70      | 108.99   |
| 1   | G     | 35  | LEU  | N-CA-C   | 5.54  | 122.60      | 110.80   |
| 1   | D     | 132 | SER  | N-CA-C   | 5.53  | 118.09      | 109.52   |
| 1   | G     | 43  | GLY  | N-CA-C   | -5.53 | 101.73      | 112.02   |
| 1   | F     | 195 | ILE  | CB-CA-C  | -5.52 | 103.16      | 112.16   |
| 1   | A     | 59  | LEU  | N-CA-C   | -5.52 | 106.39      | 113.23   |
| 1   | C     | 45  | VAL  | CB-CA-C  | -5.51 | 103.52      | 111.34   |
| 1   | G     | 115 | VAL  | N-CA-C   | -5.43 | 105.24      | 110.72   |
| 1   | G     | 134 | VAL  | CB-CA-C  | -5.43 | 102.39      | 111.29   |
| 1   | A     | 168 | VAL  | CB-CA-C  | -5.42 | 104.94      | 112.04   |
| 1   | G     | 157 | ILE  | N-CA-C   | 5.42  | 117.44      | 109.63   |
| 1   | B     | 128 | ARG  | N-CA-C   | -5.41 | 102.75      | 110.59   |
| 1   | F     | 72  | LEU  | CB-CA-C  | -5.41 | 101.88      | 110.04   |
| 1   | A     | 152 | ILE  | N-CA-C   | 5.40  | 116.08      | 108.36   |
| 1   | G     | 179 | ASP  | N-CA-C   | 5.39  | 116.37      | 107.20   |
| 1   | B     | 56  | ILE  | CB-CA-C  | -5.39 | 103.81      | 112.16   |
| 1   | D     | 164 | VAL  | N-CA-C   | -5.38 | 100.73      | 108.48   |
| 1   | F     | 114 | ASN  | N-CA-C   | 5.38  | 122.26      | 110.80   |
| 1   | E     | 135 | GLU  | CB-CG-CD | 5.37  | 121.73      | 112.60   |
| 1   | B     | 178 | THR  | CA-C-N   | -5.34 | 115.07      | 123.13   |
| 1   | B     | 178 | THR  | C-N-CA   | -5.34 | 115.07      | 123.13   |
| 1   | F     | 199 | PHE  | N-CA-C   | 5.31  | 119.75      | 113.28   |
| 1   | G     | 81  | ALA  | N-CA-C   | 5.31  | 117.48      | 111.11   |
| 1   | C     | 56  | ILE  | CB-CA-C  | -5.30 | 105.19      | 111.97   |
| 1   | F     | 66  | ASN  | N-CA-C   | 5.29  | 116.94      | 107.80   |
| 1   | E     | 67  | ALA  | CA-C-O   | -5.26 | 115.45      | 120.92   |
| 1   | A     | 82  | ILE  | CB-CA-C  | -5.25 | 104.97      | 112.22   |
| 1   | G     | 54  | VAL  | CB-CA-C  | -5.22 | 105.09      | 112.14   |
| 1   | B     | 101 | SER  | N-CA-C   | 5.20  | 116.19      | 108.60   |
| 1   | D     | 124 | ALA  | N-CA-C   | -5.18 | 101.83      | 110.17   |
| 1   | C     | 164 | VAL  | N-CA-C   | -5.17 | 101.03      | 108.48   |
| 1   | A     | 179 | ASP  | N-CA-C   | 5.16  | 116.32      | 107.28   |
| 1   | A     | 115 | VAL  | N-CA-C   | -5.16 | 104.53      | 111.44   |
| 1   | H     | 70  | GLY  | CA-C-N   | -5.14 | 114.42      | 122.65   |
| 1   | H     | 70  | GLY  | C-N-CA   | -5.14 | 114.42      | 122.65   |
| 1   | H     | 154 | THR  | CA-C-N   | 5.14  | 126.41      | 120.85   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | H     | 154 | THR  | C-N-CA   | 5.14  | 126.41      | 120.85   |
| 1   | A     | 73  | ARG  | N-CA-C   | -5.12 | 102.11      | 110.20   |
| 1   | C     | 111 | LEU  | CA-CB-CG | -5.11 | 98.43       | 116.30   |
| 1   | B     | 189 | ASP  | CB-CA-C  | -5.08 | 102.36      | 110.79   |
| 1   | H     | 36  | ILE  | N-CA-C   | 5.08  | 115.65      | 107.73   |
| 1   | F     | 71  | ASP  | CA-C-N   | -5.08 | 117.49      | 126.32   |
| 1   | F     | 71  | ASP  | C-N-CA   | -5.08 | 117.49      | 126.32   |
| 1   | G     | 188 | THR  | CB-CA-C  | -5.07 | 99.13       | 110.19   |
| 1   | E     | 51  | ASP  | CA-C-N   | -5.07 | 113.74      | 120.63   |
| 1   | E     | 51  | ASP  | C-N-CA   | -5.07 | 113.74      | 120.63   |
| 1   | B     | 111 | LEU  | N-CA-C   | 5.06  | 116.98      | 108.73   |
| 1   | H     | 67  | ALA  | CA-C-N   | -5.06 | 114.87      | 122.81   |
| 1   | H     | 67  | ALA  | C-N-CA   | -5.06 | 114.87      | 122.81   |
| 1   | D     | 185 | PHE  | N-CA-C   | 5.05  | 117.05      | 109.23   |
| 1   | H     | 111 | LEU  | N-CA-C   | 5.03  | 117.44      | 109.24   |
| 1   | F     | 81  | ALA  | N-CA-C   | 5.02  | 117.53      | 111.40   |
| 1   | E     | 188 | THR  | CB-CA-C  | -5.02 | 98.47       | 110.02   |
| 1   | D     | 49  | GLN  | N-CA-C   | -5.02 | 100.86      | 109.24   |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 130 | GLY  | Peptide |
| 1   | B     | 130 | GLY  | Peptide |
| 1   | F     | 101 | SER  | Peptide |
| 1   | F     | 71  | ASP  | Peptide |
| 1   | H     | 71  | ASP  | Peptide |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1298  | 0        | 1338     | 93      | 1            |
| 1   | B     | 1298  | 0        | 1338     | 79      | 0            |
| 1   | C     | 1298  | 0        | 1338     | 95      | 0            |
| 1   | D     | 1298  | 0        | 1338     | 85      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | E     | 1298  | 0        | 1338     | 118     | 0            |
| 1   | F     | 1298  | 0        | 1338     | 138     | 1            |
| 1   | G     | 1298  | 0        | 1338     | 90      | 0            |
| 1   | H     | 1298  | 0        | 1338     | 97      | 0            |
| 2   | A     | 1     | 0        | 0        | 0       | 0            |
| 2   | G     | 1     | 0        | 0        | 0       | 0            |
| 3   | B     | 36    | 0        | 21       | 7       | 0            |
| 3   | C     | 36    | 0        | 21       | 1       | 0            |
| 3   | D     | 36    | 0        | 21       | 1       | 0            |
| 4   | B     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 10495 | 0        | 10767    | 771     | 2            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

All (771) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:35:LEU:HD23  | 1:H:36:ILE:CD1   | 1.58                     | 1.30              |
| 1:H:35:LEU:HD23  | 1:H:36:ILE:HD13  | 1.18                     | 1.15              |
| 1:H:35:LEU:CD2   | 1:H:36:ILE:CD1   | 2.27                     | 1.12              |
| 1:F:34:ASP:OD2   | 1:F:35:LEU:N     | 1.86                     | 1.08              |
| 1:D:177:VAL:HG12 | 1:D:177:VAL:O    | 1.55                     | 1.05              |
| 1:H:35:LEU:CD2   | 1:H:36:ILE:HD13  | 1.85                     | 1.02              |
| 1:A:188:THR:HG22 | 1:A:189:ASP:N    | 1.70                     | 1.00              |
| 1:F:180:ARG:HG2  | 1:F:180:ARG:HH11 | 1.27                     | 0.99              |
| 1:E:180:ARG:HG2  | 1:E:180:ARG:HH11 | 1.27                     | 0.99              |
| 1:E:180:ARG:HH11 | 1:E:180:ARG:CG   | 1.74                     | 0.98              |
| 1:D:180:ARG:HH11 | 1:D:180:ARG:CG   | 1.78                     | 0.97              |
| 1:H:35:LEU:CD2   | 1:H:36:ILE:HD11  | 1.93                     | 0.97              |
| 1:A:180:ARG:HG2  | 1:A:180:ARG:HH11 | 1.25                     | 0.96              |
| 1:G:180:ARG:CG   | 1:G:180:ARG:HH11 | 1.77                     | 0.96              |
| 1:A:69:ASN:OD1   | 1:A:69:ASN:O     | 1.83                     | 0.96              |
| 1:C:190:GLN:HB2  | 1:E:198:PHE:O    | 1.66                     | 0.96              |
| 1:G:69:ASN:O     | 1:G:69:ASN:OD1   | 1.83                     | 0.95              |
| 1:A:180:ARG:HH11 | 1:A:180:ARG:CG   | 1.80                     | 0.94              |
| 1:E:73:ARG:HH21  | 1:E:73:ARG:HG3   | 1.30                     | 0.93              |
| 1:C:177:VAL:HG12 | 1:C:177:VAL:O    | 1.69                     | 0.92              |
| 1:H:180:ARG:HG2  | 1:H:180:ARG:HH11 | 1.36                     | 0.91              |
| 1:G:180:ARG:HH11 | 1:G:180:ARG:HG2  | 1.34                     | 0.90              |
| 1:F:69:ASN:OD1   | 1:F:69:ASN:N     | 2.02                     | 0.90              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:73:ARG:HH21  | 1:A:73:ARG:HG3   | 1.37                     | 0.90              |
| 1:B:180:ARG:CG   | 1:B:180:ARG:HH11 | 1.84                     | 0.89              |
| 1:C:194:THR:HG23 | 1:E:171:GLN:NE2  | 1.86                     | 0.88              |
| 1:D:143:LYS:O    | 1:D:146:ALA:HB3  | 1.74                     | 0.88              |
| 1:C:197:ASN:HB3  | 1:E:175:LYS:NZ   | 1.88                     | 0.87              |
| 1:F:100:SER:O    | 1:F:101:SER:OG   | 1.92                     | 0.86              |
| 1:F:35:LEU:HG    | 1:F:36:ILE:N     | 1.91                     | 0.85              |
| 1:G:73:ARG:HH21  | 1:G:73:ARG:HG3   | 1.40                     | 0.85              |
| 1:H:180:ARG:HH11 | 1:H:180:ARG:CG   | 1.90                     | 0.85              |
| 1:F:51:ASP:O     | 1:F:55:LEU:HG    | 1.77                     | 0.84              |
| 1:D:180:ARG:HH11 | 1:D:180:ARG:HG2  | 1.41                     | 0.84              |
| 1:C:143:LYS:O    | 1:C:146:ALA:HB3  | 1.78                     | 0.84              |
| 1:H:35:LEU:HG    | 1:H:35:LEU:O     | 1.67                     | 0.84              |
| 1:B:180:ARG:HH11 | 1:B:180:ARG:HG2  | 1.41                     | 0.83              |
| 1:A:129:ASN:HB2  | 1:A:163:LYS:O    | 1.78                     | 0.82              |
| 1:A:154:THR:HG23 | 1:A:154:THR:O    | 1.80                     | 0.81              |
| 1:F:159:VAL:HG12 | 1:F:160:GLY:N    | 1.94                     | 0.81              |
| 1:F:159:VAL:HG12 | 1:F:160:GLY:H    | 1.45                     | 0.80              |
| 1:A:188:THR:CG2  | 1:A:189:ASP:N    | 2.41                     | 0.80              |
| 1:F:128:ARG:HH11 | 1:F:128:ARG:HB2  | 1.44                     | 0.80              |
| 1:F:188:THR:HG22 | 1:F:189:ASP:N    | 1.95                     | 0.80              |
| 1:C:180:ARG:HH11 | 1:C:180:ARG:CG   | 1.93                     | 0.80              |
| 1:F:53:ASP:HB2   | 1:G:75:VAL:HG12  | 1.64                     | 0.80              |
| 1:D:132:SER:O    | 1:D:137:LYS:HE3  | 1.82                     | 0.79              |
| 1:D:80:ARG:HB3   | 1:D:80:ARG:CZ    | 2.13                     | 0.79              |
| 1:G:152:ILE:O    | 1:G:183:ASN:HB2  | 1.83                     | 0.79              |
| 1:D:73:ARG:HH21  | 1:D:73:ARG:HG3   | 1.47                     | 0.79              |
| 1:B:143:LYS:O    | 1:B:146:ALA:HB3  | 1.82                     | 0.79              |
| 1:E:106:PRO:HA   | 1:E:125:VAL:HG12 | 1.65                     | 0.79              |
| 1:F:180:ARG:HH11 | 1:F:180:ARG:CG   | 1.95                     | 0.78              |
| 1:E:73:ARG:HH21  | 1:E:73:ARG:CG    | 1.97                     | 0.78              |
| 1:A:111:LEU:HD13 | 1:A:122:LEU:HD12 | 1.64                     | 0.78              |
| 1:C:180:ARG:HH11 | 1:C:180:ARG:HG2  | 1.47                     | 0.78              |
| 1:C:194:THR:HG23 | 1:E:171:GLN:HE21 | 1.45                     | 0.77              |
| 1:F:56:ILE:HD12  | 1:F:85:PHE:CD2   | 2.20                     | 0.77              |
| 1:E:188:THR:HG22 | 1:E:189:ASP:N    | 1.99                     | 0.77              |
| 1:H:158:SER:HB3  | 1:H:164:VAL:HG21 | 1.66                     | 0.76              |
| 1:D:94:SER:O     | 1:D:95:LYS:C     | 2.26                     | 0.76              |
| 1:E:69:ASN:OD1   | 1:E:69:ASN:O     | 2.02                     | 0.76              |
| 1:H:73:ARG:HH21  | 1:H:73:ARG:HG3   | 1.50                     | 0.76              |
| 1:F:76:GLY:O     | 1:F:80:ARG:HB3   | 1.85                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:111:LEU:HD23 | 1:G:113:GLU:HG2  | 1.66                     | 0.76              |
| 1:C:165:LYS:HB3  | 1:C:168:VAL:HG23 | 1.66                     | 0.75              |
| 1:A:158:SER:O    | 1:A:164:VAL:HG23 | 1.87                     | 0.75              |
| 1:G:106:PRO:HA   | 1:G:125:VAL:HG12 | 1.67                     | 0.75              |
| 1:A:78:VAL:O     | 1:A:81:ALA:HB3   | 1.86                     | 0.75              |
| 1:B:73:ARG:HH21  | 1:B:73:ARG:HG3   | 1.51                     | 0.75              |
| 1:D:44:LYS:HD2   | 1:D:181:ASP:OD1  | 1.86                     | 0.75              |
| 1:E:129:ASN:HB2  | 1:E:163:LYS:O    | 1.87                     | 0.75              |
| 1:H:159:VAL:HG12 | 1:H:160:GLY:N    | 2.01                     | 0.74              |
| 1:H:158:SER:O    | 1:H:164:VAL:HG23 | 1.87                     | 0.74              |
| 1:F:69:ASN:C     | 1:F:71:ASP:H     | 1.93                     | 0.74              |
| 1:E:73:ARG:HG3   | 1:E:73:ARG:NH2   | 2.01                     | 0.74              |
| 1:H:134:VAL:HG23 | 1:H:135:GLU:N    | 2.03                     | 0.74              |
| 1:A:158:SER:HB3  | 1:A:164:VAL:HG21 | 1.69                     | 0.74              |
| 1:G:128:ARG:HB3  | 1:G:131:ASP:OD2  | 1.88                     | 0.73              |
| 1:B:165:LYS:HB3  | 1:B:168:VAL:HG23 | 1.70                     | 0.73              |
| 1:A:35:LEU:HG    | 1:A:35:LEU:O     | 1.82                     | 0.73              |
| 1:E:159:VAL:HG12 | 1:E:160:GLY:N    | 2.03                     | 0.73              |
| 1:E:188:THR:HG22 | 1:E:190:GLN:N    | 2.04                     | 0.73              |
| 1:F:34:ASP:CG    | 1:F:35:LEU:H     | 1.96                     | 0.73              |
| 1:F:82:ILE:HG22  | 1:F:83:ASP:N     | 2.04                     | 0.73              |
| 1:C:189:ASP:O    | 1:C:193:VAL:HG23 | 1.89                     | 0.73              |
| 1:D:177:VAL:O    | 1:D:177:VAL:CG1  | 2.29                     | 0.73              |
| 1:E:35:LEU:O     | 1:E:35:LEU:HG    | 1.64                     | 0.72              |
| 1:C:132:SER:O    | 1:C:137:LYS:HE3  | 1.90                     | 0.72              |
| 1:E:171:GLN:OE1  | 1:E:171:GLN:HA   | 1.88                     | 0.72              |
| 1:A:106:PRO:HA   | 1:A:125:VAL:HG12 | 1.72                     | 0.72              |
| 1:F:110:VAL:HG12 | 1:F:111:LEU:N    | 2.05                     | 0.71              |
| 1:F:104:ILE:HG22 | 1:F:125:VAL:CG2  | 2.21                     | 0.71              |
| 1:C:188:THR:HB   | 1:C:190:GLN:HB3  | 1.73                     | 0.71              |
| 1:E:75:VAL:HG12  | 1:G:53:ASP:HB2   | 1.70                     | 0.71              |
| 1:F:159:VAL:CG1  | 1:F:160:GLY:H    | 2.03                     | 0.71              |
| 1:F:188:THR:HG22 | 1:F:189:ASP:H    | 1.54                     | 0.70              |
| 1:G:129:ASN:HB2  | 1:G:163:LYS:O    | 1.90                     | 0.70              |
| 1:F:155:PRO:HD3  | 1:F:185:PHE:CE2  | 2.26                     | 0.70              |
| 1:F:188:THR:HB   | 1:F:191:GLU:H    | 1.57                     | 0.70              |
| 1:G:154:THR:HG23 | 1:G:154:THR:O    | 1.90                     | 0.70              |
| 1:F:52:LEU:O     | 1:F:56:ILE:HG13  | 1.92                     | 0.70              |
| 1:H:68:ALA:O     | 1:H:125:VAL:HG22 | 1.90                     | 0.70              |
| 1:D:106:PRO:HA   | 1:D:125:VAL:HG12 | 1.73                     | 0.70              |
| 1:E:158:SER:HB3  | 1:E:164:VAL:HG21 | 1.74                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:39:PHE:CE2   | 1:F:192:ARG:HG3  | 2.26                     | 0.70              |
| 1:B:189:ASP:O    | 1:B:193:VAL:HG23 | 1.92                     | 0.69              |
| 1:B:138:LEU:HD11 | 1:B:158:SER:HB2  | 1.72                     | 0.69              |
| 1:H:154:THR:O    | 1:H:154:THR:HG23 | 1.92                     | 0.69              |
| 1:F:110:VAL:CG1  | 1:F:111:LEU:N    | 2.55                     | 0.69              |
| 1:B:36:ILE:HG22  | 1:B:36:ILE:O     | 1.92                     | 0.69              |
| 1:D:133:ARG:O    | 1:D:135:GLU:N    | 2.26                     | 0.69              |
| 1:F:94:SER:O     | 1:F:95:LYS:C     | 2.34                     | 0.69              |
| 1:F:45:VAL:HG13  | 1:F:182:LEU:HD23 | 1.74                     | 0.69              |
| 1:B:54:VAL:O     | 1:B:54:VAL:HG12  | 1.92                     | 0.69              |
| 1:E:152:ILE:O    | 1:E:183:ASN:HB2  | 1.92                     | 0.69              |
| 1:F:104:ILE:CG2  | 1:F:125:VAL:CG2  | 2.71                     | 0.69              |
| 1:D:133:ARG:C    | 1:D:135:GLU:N    | 2.47                     | 0.69              |
| 1:E:111:LEU:CD1  | 1:E:122:LEU:HD12 | 2.22                     | 0.69              |
| 1:F:97:TYR:HD2   | 1:F:98:LEU:HG    | 1.56                     | 0.68              |
| 1:A:73:ARG:HH21  | 1:A:73:ARG:CG    | 2.05                     | 0.68              |
| 1:B:127:PRO:HD2  | 1:B:138:LEU:CD1  | 2.23                     | 0.68              |
| 1:F:34:ASP:CG    | 1:F:35:LEU:N     | 2.51                     | 0.68              |
| 1:A:152:ILE:O    | 1:A:183:ASN:HB2  | 1.94                     | 0.68              |
| 1:A:188:THR:HG22 | 1:A:189:ASP:H    | 1.53                     | 0.68              |
| 1:H:129:ASN:HB2  | 1:H:163:LYS:O    | 1.93                     | 0.68              |
| 1:A:76:GLY:HA2   | 1:A:80:ARG:HH12  | 1.59                     | 0.68              |
| 1:F:104:ILE:HG22 | 1:F:125:VAL:HG21 | 1.75                     | 0.68              |
| 1:H:159:VAL:CG1  | 1:H:160:GLY:N    | 2.57                     | 0.68              |
| 1:G:188:THR:HG22 | 1:G:189:ASP:N    | 2.09                     | 0.68              |
| 1:A:83:ASP:OD2   | 1:A:90:LEU:HB3   | 1.94                     | 0.67              |
| 1:F:180:ARG:HG2  | 1:F:180:ARG:NH1  | 2.03                     | 0.67              |
| 1:G:111:LEU:HG   | 1:G:112:PHE:N    | 2.09                     | 0.67              |
| 1:C:188:THR:HG22 | 1:E:200:ASN:O    | 1.94                     | 0.67              |
| 1:H:100:SER:O    | 1:H:101:SER:OG   | 2.11                     | 0.67              |
| 1:H:134:VAL:HG23 | 1:H:135:GLU:H    | 1.59                     | 0.67              |
| 1:C:138:LEU:HD11 | 1:C:158:SER:HB2  | 1.75                     | 0.67              |
| 1:E:111:LEU:HD13 | 1:E:122:LEU:HD12 | 1.75                     | 0.67              |
| 1:C:44:LYS:HD2   | 1:C:181:ASP:OD1  | 1.94                     | 0.66              |
| 1:D:165:LYS:HB3  | 1:D:168:VAL:HG23 | 1.75                     | 0.66              |
| 1:H:35:LEU:HD21  | 1:H:36:ILE:CD1   | 2.24                     | 0.66              |
| 1:C:133:ARG:C    | 1:C:135:GLU:N    | 2.53                     | 0.66              |
| 1:C:190:GLN:CB   | 1:E:198:PHE:O    | 2.42                     | 0.66              |
| 1:C:197:ASN:HB3  | 1:E:175:LYS:HZ1  | 1.60                     | 0.66              |
| 1:F:56:ILE:HG21  | 1:F:85:PHE:HE2   | 1.60                     | 0.66              |
| 1:H:159:VAL:CG1  | 1:H:160:GLY:H    | 2.09                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:165:LYS:HB3  | 1:C:168:VAL:CG2  | 2.26                     | 0.66              |
| 1:C:177:VAL:O    | 1:C:177:VAL:CG1  | 2.43                     | 0.66              |
| 1:F:106:PRO:HA   | 1:F:125:VAL:HG12 | 1.78                     | 0.65              |
| 1:A:80:ARG:O     | 1:A:80:ARG:HG2   | 1.95                     | 0.65              |
| 1:A:105:ALA:O    | 1:A:106:PRO:C    | 2.40                     | 0.65              |
| 1:D:133:ARG:O    | 1:D:134:VAL:C    | 2.36                     | 0.65              |
| 1:E:159:VAL:CG1  | 1:E:160:GLY:N    | 2.60                     | 0.65              |
| 1:F:188:THR:HB   | 1:F:191:GLU:HB2  | 1.79                     | 0.65              |
| 1:F:94:SER:C     | 1:F:96:GLU:N     | 2.48                     | 0.65              |
| 1:C:133:ARG:O    | 1:C:135:GLU:N    | 2.30                     | 0.64              |
| 1:H:35:LEU:HD23  | 1:H:36:ILE:HD11  | 1.58                     | 0.64              |
| 1:H:73:ARG:HH21  | 1:H:73:ARG:CG    | 2.09                     | 0.64              |
| 1:F:71:ASP:O     | 1:F:72:LEU:HB2   | 1.96                     | 0.64              |
| 1:A:76:GLY:HA2   | 1:A:80:ARG:NH1   | 2.13                     | 0.64              |
| 1:F:52:LEU:HG    | 1:F:56:ILE:HD11  | 1.80                     | 0.64              |
| 1:H:102:LYS:HG2  | 1:H:103:ALA:N    | 2.12                     | 0.63              |
| 1:F:94:SER:O     | 1:F:96:GLU:N     | 2.31                     | 0.63              |
| 1:H:133:ARG:C    | 1:H:135:GLU:N    | 2.52                     | 0.63              |
| 1:C:133:ARG:O    | 1:C:134:VAL:C    | 2.41                     | 0.63              |
| 1:C:64:LEU:HB2   | 1:C:119:LEU:HD11 | 1.79                     | 0.63              |
| 1:C:197:ASN:OD1  | 1:E:171:GLN:HG3  | 1.97                     | 0.63              |
| 1:E:83:ASP:OD2   | 1:E:90:LEU:HB3   | 1.98                     | 0.63              |
| 1:G:105:ALA:O    | 1:G:106:PRO:C    | 2.40                     | 0.63              |
| 1:H:152:ILE:O    | 1:H:183:ASN:HB2  | 1.98                     | 0.63              |
| 1:C:188:THR:HG22 | 1:E:200:ASN:C    | 2.23                     | 0.63              |
| 1:D:36:ILE:HG22  | 1:D:36:ILE:O     | 1.97                     | 0.63              |
| 1:B:111:LEU:HD12 | 1:B:122:LEU:HA   | 1.80                     | 0.62              |
| 1:D:180:ARG:CG   | 1:D:180:ARG:NH1  | 2.49                     | 0.62              |
| 1:G:133:ARG:C    | 1:G:135:GLU:N    | 2.54                     | 0.62              |
| 1:A:133:ARG:HG2  | 1:A:136:GLY:H    | 1.65                     | 0.62              |
| 1:D:109:ALA:HB2  | 1:D:124:ALA:HA   | 1.82                     | 0.62              |
| 1:F:40:TYR:CD2   | 1:F:41:LYS:N     | 2.67                     | 0.62              |
| 1:B:127:PRO:HD2  | 1:B:138:LEU:HD12 | 1.80                     | 0.62              |
| 1:D:94:SER:O     | 1:D:96:GLU:N     | 2.33                     | 0.62              |
| 1:D:173:LEU:HD23 | 1:D:173:LEU:C    | 2.25                     | 0.62              |
| 1:E:128:ARG:HB3  | 1:E:131:ASP:OD2  | 2.00                     | 0.62              |
| 1:E:188:THR:CG2  | 1:E:189:ASP:N    | 2.62                     | 0.62              |
| 1:D:189:ASP:O    | 1:D:193:VAL:HG23 | 2.00                     | 0.62              |
| 1:E:75:VAL:CG1   | 1:G:53:ASP:HB2   | 2.28                     | 0.62              |
| 1:E:159:VAL:CG1  | 1:E:160:GLY:H    | 2.13                     | 0.62              |
| 1:E:188:THR:HG22 | 1:E:190:GLN:H    | 1.65                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:173:LEU:HD23 | 1:B:173:LEU:C    | 2.23                     | 0.62              |
| 1:F:53:ASP:HB2   | 1:G:75:VAL:CG1   | 2.30                     | 0.61              |
| 1:G:55:LEU:O     | 1:G:56:ILE:C     | 2.40                     | 0.61              |
| 1:A:133:ARG:C    | 1:A:135:GLU:N    | 2.56                     | 0.61              |
| 1:B:177:VAL:HG12 | 1:B:177:VAL:O    | 2.00                     | 0.61              |
| 1:G:35:LEU:O     | 1:G:35:LEU:HG    | 1.95                     | 0.61              |
| 1:A:173:LEU:C    | 1:A:173:LEU:HD23 | 2.24                     | 0.61              |
| 1:F:80:ARG:CG    | 1:F:81:ALA:N     | 2.58                     | 0.61              |
| 1:H:83:ASP:OD2   | 1:H:90:LEU:HB3   | 1.99                     | 0.61              |
| 1:H:188:THR:HG22 | 1:H:189:ASP:N    | 2.16                     | 0.61              |
| 1:A:154:THR:O    | 1:A:154:THR:CG2  | 2.49                     | 0.61              |
| 1:C:111:LEU:HD12 | 1:C:122:LEU:HA   | 1.82                     | 0.61              |
| 1:A:180:ARG:CG   | 1:A:180:ARG:NH1  | 2.50                     | 0.61              |
| 1:B:73:ARG:HG3   | 1:B:73:ARG:NH2   | 2.15                     | 0.61              |
| 1:B:105:ALA:O    | 1:B:106:PRO:C    | 2.43                     | 0.61              |
| 1:E:102:LYS:HG2  | 1:E:103:ALA:N    | 2.11                     | 0.61              |
| 1:F:159:VAL:CG1  | 1:F:160:GLY:N    | 2.59                     | 0.61              |
| 1:F:197:ASN:C    | 1:F:199:PHE:N    | 2.55                     | 0.61              |
| 1:H:166:LEU:O    | 1:H:167:GLU:C    | 2.42                     | 0.60              |
| 1:A:100:SER:O    | 1:A:101:SER:OG   | 2.20                     | 0.60              |
| 1:F:44:LYS:HB3   | 1:F:181:ASP:HB3  | 1.83                     | 0.60              |
| 1:E:180:ARG:CG   | 1:E:180:ARG:NH1  | 2.46                     | 0.60              |
| 1:F:53:ASP:OD1   | 1:F:53:ASP:N     | 2.34                     | 0.60              |
| 1:H:73:ARG:HG3   | 1:H:73:ARG:NH2   | 2.16                     | 0.60              |
| 1:H:167:GLU:OE2  | 1:H:167:GLU:N    | 2.32                     | 0.60              |
| 1:H:106:PRO:HA   | 1:H:125:VAL:HG12 | 1.83                     | 0.60              |
| 1:G:145:ILE:O    | 1:G:146:ALA:C    | 2.44                     | 0.60              |
| 1:C:127:PRO:HD2  | 1:C:138:LEU:CD1  | 2.32                     | 0.60              |
| 1:F:69:ASN:O     | 1:F:71:ASP:N     | 2.34                     | 0.59              |
| 1:C:153:LEU:HD12 | 1:C:183:ASN:O    | 2.01                     | 0.59              |
| 1:F:97:TYR:CD2   | 1:F:98:LEU:HG    | 2.37                     | 0.59              |
| 1:H:190:GLN:O    | 1:H:194:THR:OG1  | 2.19                     | 0.59              |
| 1:B:106:PRO:HA   | 1:B:125:VAL:HG12 | 1.83                     | 0.59              |
| 1:D:73:ARG:HG3   | 1:D:73:ARG:NH2   | 2.13                     | 0.59              |
| 1:D:143:LYS:O    | 1:D:146:ALA:CB   | 2.48                     | 0.59              |
| 1:F:155:PRO:HD3  | 1:F:185:PHE:HE2  | 1.66                     | 0.59              |
| 1:F:138:LEU:HD11 | 1:F:158:SER:HB2  | 1.85                     | 0.59              |
| 1:F:193:VAL:HG12 | 1:F:194:THR:N    | 2.16                     | 0.59              |
| 1:D:94:SER:C     | 1:D:96:GLU:N     | 2.60                     | 0.59              |
| 1:E:105:ALA:O    | 1:E:106:PRO:C    | 2.45                     | 0.59              |
| 1:D:65:VAL:CG2   | 1:D:154:THR:HB   | 2.32                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:91:THR:O     | 1:F:94:SER:N     | 2.32                     | 0.58              |
| 1:B:39:PHE:O     | 1:B:40:TYR:HB2   | 2.03                     | 0.58              |
| 1:G:159:VAL:HG12 | 1:G:160:GLY:N    | 2.18                     | 0.58              |
| 1:E:100:SER:O    | 1:E:101:SER:OG   | 2.20                     | 0.58              |
| 1:E:188:THR:HG21 | 1:E:190:GLN:HB2  | 1.86                     | 0.58              |
| 1:F:82:ILE:CG2   | 1:F:90:LEU:HD22  | 2.33                     | 0.58              |
| 1:C:143:LYS:O    | 1:C:146:ALA:CB   | 2.51                     | 0.58              |
| 1:C:154:THR:OG1  | 1:C:155:PRO:HD2  | 2.04                     | 0.58              |
| 1:D:79:ALA:O     | 1:D:80:ARG:C     | 2.41                     | 0.58              |
| 1:D:109:ALA:CB   | 1:D:124:ALA:HA   | 2.34                     | 0.58              |
| 1:B:189:ASP:HB2  | 1:E:40:TYR:CE1   | 2.38                     | 0.58              |
| 1:E:173:LEU:C    | 1:E:173:LEU:HD23 | 2.28                     | 0.58              |
| 1:H:35:LEU:HD23  | 1:H:36:ILE:CG1   | 2.28                     | 0.58              |
| 1:A:73:ARG:HG3   | 1:A:73:ARG:NH2   | 2.08                     | 0.58              |
| 1:A:159:VAL:HG12 | 1:A:160:GLY:N    | 2.16                     | 0.58              |
| 1:F:110:VAL:CG1  | 1:F:111:LEU:H    | 2.17                     | 0.58              |
| 1:H:111:LEU:HD12 | 1:H:122:LEU:HA   | 1.85                     | 0.58              |
| 1:C:127:PRO:HD2  | 1:C:138:LEU:HD12 | 1.85                     | 0.58              |
| 1:E:171:GLN:OE1  | 1:E:171:GLN:CA   | 2.52                     | 0.58              |
| 1:F:69:ASN:C     | 1:F:71:ASP:N     | 2.55                     | 0.58              |
| 1:C:39:PHE:O     | 1:C:40:TYR:HB2   | 2.04                     | 0.57              |
| 1:D:165:LYS:HB3  | 1:D:168:VAL:CG2  | 2.34                     | 0.57              |
| 1:D:145:ILE:O    | 1:D:146:ALA:C    | 2.46                     | 0.57              |
| 1:G:100:SER:O    | 1:G:101:SER:OG   | 2.21                     | 0.57              |
| 1:A:111:LEU:HD12 | 1:A:122:LEU:HA   | 1.87                     | 0.57              |
| 1:B:94:SER:O     | 1:B:95:LYS:C     | 2.46                     | 0.57              |
| 1:B:132:SER:O    | 1:B:137:LYS:HE3  | 2.04                     | 0.57              |
| 1:F:40:TYR:CD2   | 1:F:40:TYR:C     | 2.82                     | 0.57              |
| 1:E:166:LEU:O    | 1:E:167:GLU:C    | 2.45                     | 0.57              |
| 1:E:190:GLN:O    | 1:E:194:THR:OG1  | 2.22                     | 0.57              |
| 1:D:75:VAL:O     | 3:D:477:APR:HR'1 | 2.05                     | 0.56              |
| 1:G:68:ALA:O     | 1:G:125:VAL:HG22 | 2.05                     | 0.56              |
| 1:H:128:ARG:HB3  | 1:H:131:ASP:OD2  | 2.04                     | 0.56              |
| 1:H:173:LEU:C    | 1:H:173:LEU:HD23 | 2.31                     | 0.56              |
| 1:A:66:ASN:HB2   | 1:A:82:ILE:HD12  | 1.87                     | 0.56              |
| 1:G:49:GLN:HG2   | 1:G:50:GLY:N     | 2.20                     | 0.56              |
| 1:D:47:PHE:N     | 1:D:47:PHE:CD2   | 2.73                     | 0.56              |
| 1:D:180:ARG:HH11 | 1:D:180:ARG:HG3  | 1.65                     | 0.56              |
| 1:D:191:GLU:O    | 1:D:192:ARG:C    | 2.49                     | 0.56              |
| 1:G:159:VAL:CG1  | 1:G:160:GLY:N    | 2.68                     | 0.56              |
| 1:C:74:HIS:CE1   | 1:C:90:LEU:HD21  | 2.41                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:180:ARG:HG2  | 1:G:180:ARG:NH1  | 2.15                     | 0.56              |
| 1:H:133:ARG:HG2  | 1:H:136:GLY:H    | 1.70                     | 0.56              |
| 1:F:80:ARG:HG3   | 1:F:81:ALA:N     | 2.01                     | 0.56              |
| 1:H:94:SER:O     | 1:H:95:LYS:C     | 2.48                     | 0.56              |
| 1:B:128:ARG:HH11 | 1:B:128:ARG:HB2  | 1.70                     | 0.56              |
| 1:B:129:ASN:HB2  | 1:B:163:LYS:O    | 2.06                     | 0.56              |
| 1:F:39:PHE:CZ    | 1:F:192:ARG:HG3  | 2.41                     | 0.56              |
| 1:C:173:LEU:C    | 1:C:173:LEU:HD23 | 2.31                     | 0.56              |
| 1:C:184:VAL:HG12 | 1:C:185:PHE:N    | 2.20                     | 0.56              |
| 1:F:104:ILE:HG21 | 1:F:125:VAL:HG23 | 1.88                     | 0.56              |
| 1:F:155:PRO:CD   | 1:F:185:PHE:CE2  | 2.89                     | 0.56              |
| 1:H:158:SER:HB3  | 1:H:164:VAL:CG2  | 2.33                     | 0.56              |
| 1:E:154:THR:HG23 | 1:E:154:THR:O    | 2.05                     | 0.56              |
| 1:C:197:ASN:HB3  | 1:E:175:LYS:HZ2  | 1.70                     | 0.55              |
| 1:F:56:ILE:HD12  | 1:F:85:PHE:CE2   | 2.40                     | 0.55              |
| 1:C:133:ARG:C    | 1:C:135:GLU:H    | 2.14                     | 0.55              |
| 1:E:158:SER:O    | 1:E:164:VAL:HG23 | 2.06                     | 0.55              |
| 1:G:69:ASN:O     | 1:G:69:ASN:CG    | 2.50                     | 0.55              |
| 1:A:128:ARG:HB3  | 1:A:131:ASP:OD2  | 2.06                     | 0.55              |
| 1:D:133:ARG:C    | 1:D:135:GLU:H    | 2.12                     | 0.55              |
| 1:E:80:ARG:HH21  | 1:G:53:ASP:CG    | 2.14                     | 0.55              |
| 1:G:180:ARG:CG   | 1:G:180:ARG:NH1  | 2.50                     | 0.55              |
| 1:A:159:VAL:CG1  | 1:A:160:GLY:N    | 2.69                     | 0.55              |
| 1:A:176:THR:C    | 1:A:178:THR:H    | 2.14                     | 0.55              |
| 1:D:190:GLN:HA   | 1:E:193:VAL:HG11 | 1.87                     | 0.55              |
| 1:E:180:ARG:HG2  | 1:E:180:ARG:NH1  | 2.08                     | 0.55              |
| 1:B:65:VAL:HG12  | 1:B:66:ASN:N     | 2.22                     | 0.55              |
| 1:H:170:LEU:O    | 1:H:171:GLN:C    | 2.50                     | 0.55              |
| 1:E:111:LEU:HD12 | 1:E:122:LEU:HA   | 1.88                     | 0.55              |
| 1:E:133:ARG:C    | 1:E:135:GLU:N    | 2.56                     | 0.55              |
| 1:G:80:ARG:HH11  | 1:G:80:ARG:HB3   | 1.72                     | 0.55              |
| 1:C:74:HIS:CD2   | 1:C:90:LEU:HD23  | 2.42                     | 0.54              |
| 1:D:188:THR:HB   | 1:D:190:GLN:HB3  | 1.87                     | 0.54              |
| 1:A:49:GLN:HG2   | 1:A:50:GLY:N     | 2.22                     | 0.54              |
| 1:D:65:VAL:HG21  | 1:D:154:THR:HB   | 1.89                     | 0.54              |
| 1:F:170:LEU:HD23 | 1:F:198:PHE:CD1  | 2.42                     | 0.54              |
| 1:G:80:ARG:HB3   | 1:G:80:ARG:NH1   | 2.23                     | 0.54              |
| 1:A:102:LYS:HG2  | 1:A:103:ALA:N    | 2.15                     | 0.54              |
| 1:D:111:LEU:HD12 | 1:D:122:LEU:HA   | 1.90                     | 0.54              |
| 1:E:172:CYS:O    | 1:E:173:LEU:C    | 2.49                     | 0.54              |
| 1:F:40:TYR:HE2   | 1:F:42:ALA:HB2   | 1.73                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:133:ARG:HG2  | 1:G:136:GLY:H    | 1.72                     | 0.54              |
| 1:H:49:GLN:HG2   | 1:H:50:GLY:N     | 2.23                     | 0.54              |
| 1:F:180:ARG:CG   | 1:F:180:ARG:NH1  | 2.64                     | 0.54              |
| 1:B:169:SER:O    | 1:B:170:LEU:C    | 2.50                     | 0.53              |
| 1:G:83:ASP:OD2   | 1:G:90:LEU:HB3   | 2.08                     | 0.53              |
| 1:D:138:LEU:CD2  | 1:D:169:SER:HA   | 2.38                     | 0.53              |
| 1:D:138:LEU:HD21 | 1:D:169:SER:HA   | 1.91                     | 0.53              |
| 1:F:154:THR:HG23 | 1:F:154:THR:O    | 2.08                     | 0.53              |
| 1:G:136:GLY:O    | 1:G:137:LYS:C    | 2.50                     | 0.53              |
| 1:H:105:ALA:O    | 1:H:106:PRO:C    | 2.49                     | 0.53              |
| 1:B:44:LYS:HD2   | 1:B:181:ASP:OD1  | 2.09                     | 0.53              |
| 1:E:159:VAL:HG12 | 1:E:160:GLY:H    | 1.70                     | 0.53              |
| 1:C:145:ILE:O    | 1:C:146:ALA:C    | 2.52                     | 0.53              |
| 1:G:73:ARG:HH21  | 1:G:73:ARG:CG    | 2.16                     | 0.53              |
| 1:H:159:VAL:HG12 | 1:H:160:GLY:H    | 1.69                     | 0.53              |
| 1:C:52:LEU:O     | 1:C:53:ASP:C     | 2.52                     | 0.53              |
| 1:H:128:ARG:NH1  | 1:H:162:PHE:HE1  | 2.06                     | 0.53              |
| 1:B:157:ILE:O    | 1:B:158:SER:HB2  | 2.07                     | 0.53              |
| 1:B:167:GLU:OE1  | 1:B:194:THR:HG22 | 2.09                     | 0.53              |
| 1:F:104:ILE:HG22 | 1:F:125:VAL:CB   | 2.39                     | 0.53              |
| 1:G:176:THR:C    | 1:G:178:THR:H    | 2.17                     | 0.53              |
| 1:C:65:VAL:HG21  | 1:C:154:THR:HB   | 1.91                     | 0.53              |
| 1:G:143:LYS:O    | 1:G:146:ALA:HB3  | 2.09                     | 0.53              |
| 1:H:172:CYS:O    | 1:H:173:LEU:C    | 2.50                     | 0.53              |
| 1:H:127:PRO:HD2  | 1:H:138:LEU:HD12 | 1.91                     | 0.53              |
| 1:C:157:ILE:O    | 1:C:158:SER:HB2  | 2.08                     | 0.53              |
| 1:C:47:PHE:N     | 1:C:47:PHE:CD2   | 2.75                     | 0.52              |
| 1:C:81:ALA:O     | 1:C:84:VAL:HB    | 2.09                     | 0.52              |
| 1:C:188:THR:CB   | 1:C:190:GLN:HB3  | 2.38                     | 0.52              |
| 1:F:35:LEU:O     | 1:F:37:LEU:HG    | 2.10                     | 0.52              |
| 1:G:69:ASN:OD1   | 1:G:69:ASN:C     | 2.47                     | 0.52              |
| 1:A:116:LEU:HB2  | 1:A:119:LEU:HB3  | 1.91                     | 0.52              |
| 1:F:104:ILE:HG22 | 1:F:125:VAL:HB   | 1.91                     | 0.52              |
| 1:F:155:PRO:HB3  | 1:F:185:PHE:CZ   | 2.45                     | 0.52              |
| 1:F:71:ASP:O     | 1:F:72:LEU:CB    | 2.58                     | 0.52              |
| 1:G:173:LEU:HD23 | 1:G:173:LEU:C    | 2.35                     | 0.52              |
| 1:A:188:THR:HG22 | 1:A:190:GLN:N    | 2.24                     | 0.52              |
| 1:D:39:PHE:O     | 1:D:40:TYR:HB2   | 2.07                     | 0.52              |
| 1:B:133:ARG:C    | 1:B:135:GLU:N    | 2.66                     | 0.52              |
| 1:F:135:GLU:O    | 1:F:136:GLY:C    | 2.52                     | 0.52              |
| 1:D:100:SER:O    | 1:D:100:SER:OG   | 2.28                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:35:LEU:HD23  | 1:E:36:ILE:HD11  | 1.90                     | 0.52              |
| 1:F:39:PHE:CG    | 1:F:192:ARG:HD2  | 2.45                     | 0.52              |
| 1:F:158:SER:HA   | 1:F:162:PHE:CD2  | 2.44                     | 0.52              |
| 1:B:143:LYS:O    | 1:B:147:LYS:HE3  | 2.10                     | 0.52              |
| 1:D:116:LEU:HB2  | 1:D:119:LEU:HB3  | 1.92                     | 0.52              |
| 1:D:200:ASN:O    | 1:G:190:GLN:OE1  | 2.28                     | 0.52              |
| 1:H:44:LYS:HB2   | 1:H:180:ARG:O    | 2.10                     | 0.52              |
| 1:B:133:ARG:O    | 1:B:134:VAL:C    | 2.52                     | 0.51              |
| 1:C:52:LEU:HD13  | 1:C:185:PHE:CE1  | 2.45                     | 0.51              |
| 1:F:181:ASP:OD1  | 1:F:181:ASP:N    | 2.43                     | 0.51              |
| 1:G:190:GLN:O    | 1:G:194:THR:OG1  | 2.22                     | 0.51              |
| 1:H:154:THR:O    | 1:H:154:THR:CG2  | 2.57                     | 0.51              |
| 1:C:53:ASP:OD1   | 1:C:53:ASP:N     | 2.44                     | 0.51              |
| 1:E:51:ASP:O     | 1:E:55:LEU:HG    | 2.10                     | 0.51              |
| 1:B:54:VAL:HG22  | 1:C:75:VAL:HB    | 1.93                     | 0.51              |
| 1:F:94:SER:C     | 1:F:96:GLU:H     | 2.17                     | 0.51              |
| 1:B:77:GLY:HA2   | 3:B:477:APR:N7   | 2.25                     | 0.51              |
| 1:C:167:GLU:OE1  | 1:C:194:THR:HG22 | 2.11                     | 0.51              |
| 1:B:93:ARG:HA    | 1:B:93:ARG:NE    | 2.26                     | 0.51              |
| 1:E:52:LEU:O     | 1:E:53:ASP:C     | 2.54                     | 0.51              |
| 1:G:165:LYS:HB2  | 1:G:168:VAL:HG23 | 1.93                     | 0.51              |
| 1:A:190:GLN:O    | 1:A:194:THR:OG1  | 2.27                     | 0.51              |
| 1:C:106:PRO:HA   | 1:C:125:VAL:HG12 | 1.93                     | 0.51              |
| 1:A:153:LEU:HD12 | 1:A:183:ASN:O    | 2.11                     | 0.50              |
| 1:F:38:PRO:HD3   | 1:F:48:TYR:CZ    | 2.47                     | 0.50              |
| 1:F:197:ASN:C    | 1:F:199:PHE:H    | 2.19                     | 0.50              |
| 1:A:66:ASN:HB2   | 1:A:82:ILE:CD1   | 2.41                     | 0.50              |
| 1:G:51:ASP:O     | 1:G:55:LEU:HG    | 2.11                     | 0.50              |
| 1:G:104:ILE:CD1  | 1:G:110:VAL:HB   | 2.41                     | 0.50              |
| 1:A:136:GLY:O    | 1:A:137:LYS:C    | 2.55                     | 0.50              |
| 1:B:189:ASP:HB2  | 1:E:40:TYR:HE1   | 1.75                     | 0.50              |
| 1:H:170:LEU:C    | 1:H:170:LEU:HD12 | 2.37                     | 0.50              |
| 1:H:180:ARG:CG   | 1:H:180:ARG:NH1  | 2.60                     | 0.50              |
| 1:A:39:PHE:CD2   | 1:A:39:PHE:C     | 2.90                     | 0.50              |
| 1:F:88:GLY:O     | 1:F:92:LYS:HG2   | 2.12                     | 0.50              |
| 1:H:136:GLY:O    | 1:H:137:LYS:C    | 2.54                     | 0.50              |
| 1:C:52:LEU:O     | 1:C:54:VAL:N     | 2.45                     | 0.50              |
| 1:F:96:GLU:HA    | 1:F:99:LYS:HE3   | 1.93                     | 0.50              |
| 1:A:79:ALA:C     | 1:A:81:ALA:N     | 2.69                     | 0.50              |
| 1:D:160:GLY:O    | 1:D:161:ILE:C    | 2.55                     | 0.50              |
| 1:A:111:LEU:CD1  | 1:A:122:LEU:HD12 | 2.38                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:109:ALA:CB   | 1:B:124:ALA:HA   | 2.42                     | 0.49              |
| 1:C:63:VAL:HB    | 1:C:152:ILE:HG23 | 1.94                     | 0.49              |
| 1:F:104:ILE:HG21 | 1:F:125:VAL:CG2  | 2.41                     | 0.49              |
| 1:B:109:ALA:HB2  | 1:B:124:ALA:HA   | 1.93                     | 0.49              |
| 1:C:76:GLY:O     | 1:C:77:GLY:C     | 2.52                     | 0.49              |
| 1:C:109:ALA:HB2  | 1:C:124:ALA:HA   | 1.93                     | 0.49              |
| 1:E:153:LEU:HD12 | 1:E:183:ASN:O    | 2.12                     | 0.49              |
| 1:D:105:ALA:O    | 1:D:106:PRO:C    | 2.55                     | 0.49              |
| 1:F:128:ARG:HB2  | 1:F:128:ARG:NH1  | 2.20                     | 0.49              |
| 1:A:145:ILE:O    | 1:A:146:ALA:C    | 2.54                     | 0.49              |
| 1:A:158:SER:HB3  | 1:A:164:VAL:CG2  | 2.41                     | 0.49              |
| 1:B:111:LEU:HD12 | 1:B:122:LEU:CA   | 2.42                     | 0.49              |
| 1:E:111:LEU:HD12 | 1:E:122:LEU:HD12 | 1.94                     | 0.49              |
| 1:G:188:THR:CG2  | 1:G:189:ASP:N    | 2.76                     | 0.49              |
| 1:H:39:PHE:CE2   | 1:H:192:ARG:HG2  | 2.48                     | 0.49              |
| 1:A:76:GLY:CA    | 1:A:80:ARG:NH1   | 2.76                     | 0.49              |
| 1:F:192:ARG:O    | 1:F:195:ILE:HB   | 2.12                     | 0.49              |
| 1:G:73:ARG:HG3   | 1:G:73:ARG:NH2   | 2.13                     | 0.49              |
| 1:B:138:LEU:CD2  | 1:B:169:SER:HA   | 2.42                     | 0.49              |
| 1:B:188:THR:HB   | 1:B:190:GLN:HB3  | 1.95                     | 0.49              |
| 1:H:176:THR:C    | 1:H:178:THR:H    | 2.20                     | 0.49              |
| 1:B:138:LEU:HD23 | 1:B:169:SER:HA   | 1.95                     | 0.48              |
| 1:B:191:GLU:OE1  | 3:B:477:APR:O3'  | 2.25                     | 0.48              |
| 1:D:154:THR:OG1  | 1:D:155:PRO:HD2  | 2.13                     | 0.48              |
| 1:G:112:PHE:N    | 1:G:112:PHE:CD1  | 2.79                     | 0.48              |
| 1:H:134:VAL:CG2  | 1:H:135:GLU:N    | 2.73                     | 0.48              |
| 1:A:79:ALA:C     | 1:A:81:ALA:H     | 2.20                     | 0.48              |
| 1:B:143:LYS:O    | 1:B:146:ALA:CB   | 2.58                     | 0.48              |
| 1:C:86:THR:O     | 1:C:87:GLY:C     | 2.54                     | 0.48              |
| 1:D:129:ASN:HB2  | 1:D:163:LYS:O    | 2.13                     | 0.48              |
| 1:F:174:LEU:HA   | 1:F:174:LEU:HD23 | 1.28                     | 0.48              |
| 1:B:180:ARG:CG   | 1:B:180:ARG:NH1  | 2.56                     | 0.48              |
| 1:E:133:ARG:HG2  | 1:E:136:GLY:H    | 1.78                     | 0.48              |
| 1:E:158:SER:HB3  | 1:E:164:VAL:CG2  | 2.41                     | 0.48              |
| 1:F:35:LEU:HG    | 1:F:36:ILE:HG13  | 1.94                     | 0.48              |
| 1:G:104:ILE:HD11 | 1:G:110:VAL:HB   | 1.96                     | 0.48              |
| 1:H:133:ARG:O    | 1:H:134:VAL:C    | 2.55                     | 0.48              |
| 1:B:65:VAL:HG21  | 1:B:154:THR:HB   | 1.95                     | 0.48              |
| 1:B:153:LEU:HD12 | 1:B:183:ASN:O    | 2.13                     | 0.48              |
| 1:C:160:GLY:O    | 1:C:162:PHE:N    | 2.47                     | 0.48              |
| 1:C:197:ASN:OD1  | 1:E:171:GLN:CG   | 2.61                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:128:ARG:NH1  | 1:H:162:PHE:CE1  | 2.82                     | 0.48              |
| 1:G:38:PRO:HB3   | 1:G:46:SER:HB3   | 1.95                     | 0.48              |
| 1:H:35:LEU:HD21  | 1:H:36:ILE:HD11  | 1.86                     | 0.48              |
| 1:A:69:ASN:O     | 1:A:69:ASN:CG    | 2.56                     | 0.48              |
| 1:C:80:ARG:HE    | 1:C:84:VAL:HG23  | 1.77                     | 0.48              |
| 1:C:138:LEU:CD2  | 1:C:169:SER:HA   | 2.44                     | 0.48              |
| 1:F:157:ILE:HG22 | 1:F:158:SER:N    | 2.27                     | 0.48              |
| 1:C:180:ARG:CG   | 1:C:180:ARG:NH1  | 2.63                     | 0.48              |
| 1:A:188:THR:HB   | 1:A:191:GLU:H    | 1.79                     | 0.47              |
| 1:B:127:PRO:HD2  | 1:B:138:LEU:HD13 | 1.94                     | 0.47              |
| 1:E:100:SER:C    | 1:E:101:SER:HG   | 2.20                     | 0.47              |
| 1:H:145:ILE:O    | 1:H:146:ALA:C    | 2.57                     | 0.47              |
| 1:C:52:LEU:C     | 1:C:54:VAL:N     | 2.71                     | 0.47              |
| 1:D:52:LEU:O     | 1:D:53:ASP:C     | 2.57                     | 0.47              |
| 1:D:157:ILE:CG2  | 1:D:158:SER:N    | 2.75                     | 0.47              |
| 1:F:104:ILE:CG2  | 1:F:125:VAL:HG21 | 2.38                     | 0.47              |
| 1:G:159:VAL:CG1  | 1:G:160:GLY:H    | 2.27                     | 0.47              |
| 1:B:77:GLY:CA    | 3:B:477:APR:N7   | 2.77                     | 0.47              |
| 1:C:105:ALA:O    | 1:C:108:ASN:N    | 2.48                     | 0.47              |
| 1:D:112:PHE:N    | 1:D:112:PHE:CD1  | 2.80                     | 0.47              |
| 1:E:80:ARG:NH2   | 1:G:53:ASP:OD1   | 2.41                     | 0.47              |
| 1:F:138:LEU:CD2  | 1:F:169:SER:HA   | 2.44                     | 0.47              |
| 1:F:155:PRO:N    | 1:F:185:PHE:CE2  | 2.82                     | 0.47              |
| 1:G:154:THR:O    | 1:G:184:VAL:HA   | 2.14                     | 0.47              |
| 1:G:154:THR:O    | 1:G:154:THR:CG2  | 2.58                     | 0.47              |
| 1:C:114:ASN:O    | 1:C:115:VAL:C    | 2.55                     | 0.47              |
| 1:H:59:LEU:O     | 1:H:60:GLU:C     | 2.57                     | 0.47              |
| 1:A:166:LEU:C    | 1:A:166:LEU:HD23 | 2.39                     | 0.47              |
| 1:A:176:THR:O    | 1:A:178:THR:HG23 | 2.15                     | 0.47              |
| 1:E:94:SER:O     | 1:E:95:LYS:C     | 2.56                     | 0.47              |
| 1:E:104:ILE:HD11 | 1:E:110:VAL:HB   | 1.96                     | 0.47              |
| 1:F:39:PHE:O     | 1:F:40:TYR:HB2   | 2.15                     | 0.47              |
| 1:F:59:LEU:HD23  | 1:F:59:LEU:HA    | 1.61                     | 0.47              |
| 1:G:136:GLY:O    | 1:G:139:CYS:N    | 2.48                     | 0.47              |
| 1:H:79:ALA:O     | 1:H:80:ARG:C     | 2.55                     | 0.47              |
| 1:C:65:VAL:CG2   | 1:C:154:THR:HB   | 2.45                     | 0.47              |
| 1:E:55:LEU:O     | 1:E:56:ILE:C     | 2.58                     | 0.47              |
| 1:F:104:ILE:CG2  | 1:F:125:VAL:HB   | 2.45                     | 0.47              |
| 1:F:129:ASN:HB2  | 1:F:163:LYS:O    | 2.15                     | 0.47              |
| 1:G:111:LEU:CD2  | 1:G:113:GLU:HG2  | 2.42                     | 0.47              |
| 1:G:191:GLU:O    | 1:G:192:ARG:C    | 2.55                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:169:SER:O    | 1:D:170:LEU:C    | 2.58                     | 0.47              |
| 1:E:78:VAL:O     | 1:E:81:ALA:HB3   | 2.15                     | 0.47              |
| 1:F:70:GLY:O     | 1:F:103:ALA:HB1  | 2.15                     | 0.47              |
| 1:H:78:VAL:O     | 1:H:81:ALA:HB3   | 2.14                     | 0.47              |
| 1:D:98:LEU:HD23  | 1:D:98:LEU:HA    | 1.67                     | 0.47              |
| 1:F:93:ARG:NH2   | 1:F:96:GLU:OE2   | 2.37                     | 0.47              |
| 1:G:78:VAL:O     | 1:G:81:ALA:HB3   | 2.15                     | 0.47              |
| 1:B:66:ASN:HB2   | 1:B:82:ILE:HD13  | 1.97                     | 0.47              |
| 1:C:94:SER:O     | 1:C:95:LYS:C     | 2.57                     | 0.47              |
| 1:C:142:TYR:CZ   | 1:C:173:LEU:HB2  | 2.50                     | 0.47              |
| 1:C:184:VAL:CG1  | 1:C:185:PHE:N    | 2.78                     | 0.47              |
| 1:E:176:THR:C    | 1:E:178:THR:H    | 2.22                     | 0.47              |
| 1:E:180:ARG:HH11 | 1:E:180:ARG:HG3  | 1.72                     | 0.47              |
| 1:F:40:TYR:HD2   | 1:F:41:LYS:N     | 2.11                     | 0.47              |
| 1:H:109:ALA:HB1  | 1:H:122:LEU:HD21 | 1.97                     | 0.47              |
| 1:D:195:ILE:O    | 1:D:198:PHE:HB3  | 2.15                     | 0.46              |
| 1:F:40:TYR:CE2   | 1:F:42:ALA:HB2   | 2.50                     | 0.46              |
| 1:F:157:ILE:O    | 1:F:158:SER:HB2  | 2.15                     | 0.46              |
| 1:G:133:ARG:C    | 1:G:135:GLU:H    | 2.20                     | 0.46              |
| 1:B:65:VAL:CG2   | 1:B:154:THR:HB   | 2.45                     | 0.46              |
| 1:G:140:ASN:O    | 1:G:141:VAL:C    | 2.57                     | 0.46              |
| 1:G:158:SER:HB2  | 1:G:164:VAL:HG21 | 1.97                     | 0.46              |
| 1:F:74:HIS:HB3   | 1:F:79:ALA:HB1   | 1.96                     | 0.46              |
| 1:H:36:ILE:HD13  | 1:H:36:ILE:N     | 2.28                     | 0.46              |
| 1:H:38:PRO:HB3   | 1:H:46:SER:HB3   | 1.97                     | 0.46              |
| 1:B:74:HIS:CD2   | 1:B:90:LEU:HD23  | 2.50                     | 0.46              |
| 1:D:81:ALA:O     | 1:D:84:VAL:HB    | 2.15                     | 0.46              |
| 1:F:166:LEU:O    | 1:F:167:GLU:C    | 2.58                     | 0.46              |
| 1:E:35:LEU:HD23  | 1:E:36:ILE:CD1   | 2.46                     | 0.46              |
| 1:E:106:PRO:HA   | 1:E:125:VAL:CG1  | 2.41                     | 0.46              |
| 1:F:82:ILE:HG22  | 1:F:90:LEU:HD22  | 1.96                     | 0.46              |
| 1:F:91:THR:O     | 1:F:92:LYS:C     | 2.59                     | 0.46              |
| 1:G:39:PHE:CD2   | 1:G:39:PHE:C     | 2.93                     | 0.46              |
| 1:G:180:ARG:HH11 | 1:G:180:ARG:HG3  | 1.68                     | 0.46              |
| 1:B:114:ASN:H    | 1:B:120:SER:HG   | 1.63                     | 0.46              |
| 1:C:188:THR:CG2  | 1:E:200:ASN:O    | 2.63                     | 0.46              |
| 1:H:100:SER:C    | 1:H:101:SER:OG   | 2.58                     | 0.46              |
| 1:B:35:LEU:HA    | 1:B:35:LEU:HD12  | 1.69                     | 0.46              |
| 1:B:170:LEU:HD12 | 1:B:170:LEU:HA   | 1.65                     | 0.46              |
| 1:A:55:LEU:O     | 1:A:56:ILE:C     | 2.58                     | 0.46              |
| 1:F:68:ALA:O     | 1:F:125:VAL:HG22 | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:195:ILE:O    | 1:F:199:PHE:HD1  | 1.99                     | 0.46              |
| 1:G:98:LEU:HD23  | 1:G:98:LEU:HA    | 1.44                     | 0.46              |
| 1:A:188:THR:CG2  | 1:A:189:ASP:H    | 2.17                     | 0.46              |
| 1:D:86:THR:O     | 1:D:87:GLY:C     | 2.59                     | 0.46              |
| 1:E:49:GLN:HG2   | 1:E:50:GLY:N     | 2.30                     | 0.46              |
| 1:E:115:VAL:O    | 1:E:116:LEU:HD23 | 2.15                     | 0.46              |
| 1:A:193:VAL:O    | 1:A:194:THR:C    | 2.55                     | 0.46              |
| 1:D:180:ARG:NH1  | 1:D:180:ARG:HG3  | 2.26                     | 0.46              |
| 1:H:74:HIS:HB3   | 1:H:79:ALA:HB1   | 1.97                     | 0.46              |
| 1:C:143:LYS:HB2  | 1:C:143:LYS:NZ   | 2.31                     | 0.45              |
| 1:G:53:ASP:OD1   | 1:G:53:ASP:N     | 2.50                     | 0.45              |
| 1:A:157:ILE:HD13 | 1:A:157:ILE:HA   | 1.74                     | 0.45              |
| 1:F:196:GLU:O    | 1:F:199:PHE:HB2  | 2.16                     | 0.45              |
| 1:H:104:ILE:HD11 | 1:H:110:VAL:HB   | 1.97                     | 0.45              |
| 1:B:98:LEU:HD23  | 1:B:98:LEU:HA    | 1.68                     | 0.45              |
| 1:B:191:GLU:O    | 1:B:194:THR:N    | 2.48                     | 0.45              |
| 1:D:170:LEU:HD12 | 1:D:170:LEU:HA   | 1.47                     | 0.45              |
| 1:F:188:THR:CG2  | 1:F:189:ASP:N    | 2.64                     | 0.45              |
| 1:H:165:LYS:HB2  | 1:H:168:VAL:HG23 | 1.98                     | 0.45              |
| 1:H:180:ARG:HG2  | 1:H:180:ARG:NH1  | 2.17                     | 0.45              |
| 1:C:197:ASN:HB3  | 1:E:175:LYS:CE   | 2.47                     | 0.45              |
| 1:D:157:ILE:HG22 | 1:D:158:SER:N    | 2.29                     | 0.45              |
| 1:H:51:ASP:O     | 1:H:55:LEU:HG    | 2.15                     | 0.45              |
| 1:E:100:SER:C    | 1:E:101:SER:OG   | 2.59                     | 0.45              |
| 1:G:188:THR:HB   | 1:G:191:GLU:H    | 1.81                     | 0.45              |
| 1:E:181:ASP:OD2  | 1:E:181:ASP:N    | 2.50                     | 0.45              |
| 1:A:69:ASN:OD1   | 1:A:69:ASN:C     | 2.47                     | 0.45              |
| 1:D:131:ASP:O    | 1:D:134:VAL:CG2  | 2.65                     | 0.45              |
| 1:H:156:LEU:HA   | 1:H:156:LEU:HD23 | 1.64                     | 0.45              |
| 1:A:35:LEU:HD23  | 1:A:36:ILE:HD11  | 1.99                     | 0.45              |
| 1:A:156:LEU:HA   | 1:A:156:LEU:HD23 | 1.56                     | 0.45              |
| 1:B:166:LEU:C    | 1:B:166:LEU:HD23 | 2.42                     | 0.45              |
| 1:F:55:LEU:C     | 1:F:57:ASN:N     | 2.72                     | 0.45              |
| 1:F:106:PRO:HA   | 1:F:125:VAL:CG1  | 2.47                     | 0.45              |
| 1:F:119:LEU:HA   | 1:F:119:LEU:HD12 | 1.30                     | 0.45              |
| 1:G:115:VAL:HG21 | 1:G:121:VAL:HB   | 1.99                     | 0.45              |
| 1:H:59:LEU:HD23  | 1:H:59:LEU:HA    | 1.46                     | 0.45              |
| 1:A:154:THR:O    | 1:A:184:VAL:HA   | 2.17                     | 0.45              |
| 1:C:76:GLY:N     | 1:C:80:ARG:HB2   | 2.32                     | 0.45              |
| 1:B:100:SER:O    | 1:B:100:SER:OG   | 2.34                     | 0.44              |
| 1:E:136:GLY:O    | 1:E:137:LYS:C    | 2.59                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:92:LYS:O     | 1:F:96:GLU:HB2   | 2.16                     | 0.44              |
| 1:F:156:LEU:HD23 | 1:F:156:LEU:HA   | 1.84                     | 0.44              |
| 1:G:36:ILE:HD12  | 1:G:36:ILE:HG23  | 1.64                     | 0.44              |
| 1:G:61:PRO:HA    | 1:G:151:LYS:HB3  | 1.99                     | 0.44              |
| 1:A:143:LYS:O    | 1:A:146:ALA:HB3  | 2.17                     | 0.44              |
| 1:A:145:ILE:HG21 | 1:A:145:ILE:HD13 | 1.76                     | 0.44              |
| 1:B:39:PHE:CE1   | 1:B:192:ARG:HG3  | 2.51                     | 0.44              |
| 1:D:74:HIS:NE2   | 1:D:90:LEU:HD21  | 2.32                     | 0.44              |
| 1:D:160:GLY:O    | 1:D:162:PHE:N    | 2.51                     | 0.44              |
| 1:H:89:LYS:O     | 1:H:90:LEU:C     | 2.59                     | 0.44              |
| 1:A:54:VAL:O     | 1:A:54:VAL:HG12  | 2.16                     | 0.44              |
| 1:A:89:LYS:HD3   | 1:A:93:ARG:HH12  | 1.83                     | 0.44              |
| 1:C:66:ASN:HB2   | 1:C:82:ILE:HD13  | 1.99                     | 0.44              |
| 1:D:74:HIS:CE1   | 1:D:90:LEU:HD21  | 2.53                     | 0.44              |
| 1:G:113:GLU:HA   | 1:G:120:SER:OG   | 2.17                     | 0.44              |
| 1:C:65:VAL:HG11  | 1:C:145:ILE:HD11 | 2.00                     | 0.44              |
| 1:E:102:LYS:HG2  | 1:E:103:ALA:O    | 2.17                     | 0.44              |
| 1:F:127:PRO:HD2  | 1:F:138:LEU:CD1  | 2.48                     | 0.44              |
| 1:B:74:HIS:NE2   | 1:B:90:LEU:HD21  | 2.33                     | 0.44              |
| 1:F:40:TYR:C     | 1:F:40:TYR:HD2   | 2.24                     | 0.44              |
| 1:F:89:LYS:HD3   | 1:F:93:ARG:NH1   | 2.32                     | 0.44              |
| 1:G:188:THR:HG22 | 1:G:190:GLN:N    | 2.33                     | 0.44              |
| 1:B:67:ALA:HB1   | 3:B:477:APR:O1B  | 2.17                     | 0.44              |
| 1:C:69:ASN:OD1   | 1:C:69:ASN:N     | 2.51                     | 0.44              |
| 1:C:130:GLY:C    | 1:C:131:ASP:O    | 2.55                     | 0.44              |
| 1:E:98:LEU:HA    | 1:E:98:LEU:HD23  | 1.38                     | 0.44              |
| 1:A:166:LEU:O    | 1:A:167:GLU:C    | 2.61                     | 0.44              |
| 1:C:105:ALA:O    | 1:C:106:PRO:C    | 2.61                     | 0.44              |
| 1:E:156:LEU:HD23 | 1:E:156:LEU:HA   | 1.70                     | 0.44              |
| 1:G:193:VAL:O    | 1:G:196:GLU:N    | 2.51                     | 0.44              |
| 1:H:70:GLY:HA2   | 1:H:125:VAL:HG21 | 1.99                     | 0.44              |
| 1:A:59:LEU:HD23  | 1:A:59:LEU:HA    | 1.60                     | 0.44              |
| 1:B:47:PHE:N     | 1:B:47:PHE:CD2   | 2.86                     | 0.44              |
| 1:B:65:VAL:HG12  | 1:B:66:ASN:H     | 1.81                     | 0.44              |
| 1:C:166:LEU:HD23 | 1:C:166:LEU:C    | 2.43                     | 0.44              |
| 1:E:133:ARG:O    | 1:E:134:VAL:C    | 2.55                     | 0.44              |
| 1:A:174:LEU:HD23 | 1:A:174:LEU:HA   | 1.75                     | 0.44              |
| 1:E:180:ARG:NH1  | 1:E:180:ARG:HG3  | 2.32                     | 0.44              |
| 1:F:64:LEU:HD13  | 1:F:153:LEU:HB3  | 2.00                     | 0.44              |
| 1:C:74:HIS:NE2   | 1:C:90:LEU:HD21  | 2.33                     | 0.43              |
| 1:C:190:GLN:HA   | 1:E:198:PHE:CE1  | 2.53                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:63:VAL:HA    | 1:D:120:SER:O    | 2.18                     | 0.43              |
| 1:F:50:GLY:O     | 1:F:187:TYR:HD1  | 2.01                     | 0.43              |
| 1:F:127:PRO:HD2  | 1:F:138:LEU:HD12 | 2.00                     | 0.43              |
| 1:G:89:LYS:O     | 1:G:90:LEU:C     | 2.60                     | 0.43              |
| 1:G:110:VAL:CG1  | 1:G:111:LEU:N    | 2.80                     | 0.43              |
| 1:G:174:LEU:HD23 | 1:G:174:LEU:HA   | 1.62                     | 0.43              |
| 1:G:188:THR:HG22 | 1:G:190:GLN:H    | 1.83                     | 0.43              |
| 1:B:141:VAL:O    | 1:B:145:ILE:HG13 | 2.18                     | 0.43              |
| 1:A:173:LEU:C    | 1:A:173:LEU:CD2  | 2.90                     | 0.43              |
| 1:C:94:SER:C     | 1:C:96:GLU:N     | 2.76                     | 0.43              |
| 1:A:110:VAL:CG1  | 1:A:111:LEU:N    | 2.78                     | 0.43              |
| 1:B:200:ASN:HB3  | 1:B:201:GLY:H    | 1.54                     | 0.43              |
| 1:D:74:HIS:CD2   | 1:D:90:LEU:HD23  | 2.53                     | 0.43              |
| 1:G:179:ASP:O    | 1:G:180:ARG:HB2  | 2.18                     | 0.43              |
| 1:H:98:LEU:HA    | 1:H:98:LEU:HD23  | 1.24                     | 0.43              |
| 1:B:166:LEU:HD23 | 1:B:166:LEU:O    | 2.19                     | 0.43              |
| 1:E:86:THR:HG22  | 1:E:116:LEU:HG   | 2.01                     | 0.43              |
| 1:E:170:LEU:HD12 | 1:E:170:LEU:C    | 2.42                     | 0.43              |
| 1:H:188:THR:HB   | 1:H:191:GLU:H    | 1.83                     | 0.43              |
| 1:A:104:ILE:CD1  | 1:A:110:VAL:HB   | 2.48                     | 0.43              |
| 1:D:131:ASP:O    | 1:D:134:VAL:HG23 | 2.19                     | 0.43              |
| 1:F:86:THR:HB    | 1:F:89:LYS:HB2   | 2.01                     | 0.43              |
| 1:G:112:PHE:N    | 1:G:112:PHE:HD1  | 2.17                     | 0.43              |
| 1:G:158:SER:HB2  | 1:G:164:VAL:CG2  | 2.49                     | 0.43              |
| 1:H:102:LYS:HB3  | 1:H:102:LYS:HE2  | 1.75                     | 0.43              |
| 1:H:112:PHE:CD1  | 1:H:112:PHE:N    | 2.83                     | 0.43              |
| 1:B:91:THR:O     | 1:B:92:LYS:C     | 2.60                     | 0.43              |
| 1:C:54:VAL:HG12  | 1:C:54:VAL:O     | 2.19                     | 0.43              |
| 1:D:156:LEU:CD1  | 1:D:166:LEU:HD21 | 2.49                     | 0.43              |
| 1:D:167:GLU:OE1  | 1:D:194:THR:HG22 | 2.18                     | 0.43              |
| 1:E:154:THR:O    | 1:E:184:VAL:HA   | 2.19                     | 0.43              |
| 1:F:132:SER:O    | 1:F:133:ARG:C    | 2.62                     | 0.43              |
| 1:H:142:TYR:O    | 1:H:145:ILE:HB   | 2.19                     | 0.43              |
| 1:A:80:ARG:O     | 1:A:84:VAL:HG23  | 2.18                     | 0.43              |
| 1:E:97:TYR:CD2   | 1:E:97:TYR:C     | 2.95                     | 0.43              |
| 1:E:157:ILE:O    | 1:E:158:SER:HB2  | 2.19                     | 0.43              |
| 1:F:154:THR:O    | 1:F:184:VAL:HA   | 2.19                     | 0.43              |
| 1:H:86:THR:HG22  | 1:H:116:LEU:HG   | 2.01                     | 0.43              |
| 1:H:153:LEU:HD12 | 1:H:153:LEU:HA   | 1.70                     | 0.43              |
| 1:A:55:LEU:HD23  | 1:A:55:LEU:HA    | 1.70                     | 0.43              |
| 1:A:122:LEU:C    | 1:A:122:LEU:HD23 | 2.43                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:165:LYS:O    | 1:C:168:VAL:HG23 | 2.19                     | 0.43              |
| 1:E:165:LYS:HB2  | 1:E:168:VAL:HG23 | 2.01                     | 0.43              |
| 1:A:188:THR:HG22 | 1:A:189:ASP:CA   | 2.45                     | 0.43              |
| 1:B:83:ASP:HB3   | 1:B:84:VAL:H     | 1.72                     | 0.43              |
| 1:E:54:VAL:O     | 1:E:58:PHE:HD2   | 2.02                     | 0.43              |
| 1:F:157:ILE:O    | 1:F:158:SER:CB   | 2.66                     | 0.43              |
| 1:G:167:GLU:OE2  | 1:G:167:GLU:N    | 2.50                     | 0.43              |
| 1:H:170:LEU:O    | 1:H:170:LEU:HD12 | 2.18                     | 0.43              |
| 1:A:133:ARG:C    | 1:A:135:GLU:H    | 2.25                     | 0.42              |
| 1:E:104:ILE:CD1  | 1:E:110:VAL:HB   | 2.49                     | 0.42              |
| 1:F:76:GLY:O     | 1:F:80:ARG:CZ    | 2.67                     | 0.42              |
| 1:F:127:PRO:O    | 1:F:158:SER:OG   | 2.37                     | 0.42              |
| 1:F:188:THR:CG2  | 1:F:189:ASP:H    | 2.26                     | 0.42              |
| 1:G:79:ALA:O     | 1:G:80:ARG:C     | 2.62                     | 0.42              |
| 1:G:158:SER:O    | 1:G:164:VAL:HG23 | 2.19                     | 0.42              |
| 1:H:113:GLU:O    | 1:H:114:ASN:C    | 2.62                     | 0.42              |
| 1:B:191:GLU:O    | 1:B:192:ARG:C    | 2.62                     | 0.42              |
| 1:E:97:TYR:O     | 1:E:101:SER:HB2  | 2.19                     | 0.42              |
| 1:F:100:SER:C    | 1:F:101:SER:HG   | 2.10                     | 0.42              |
| 1:E:35:LEU:O     | 1:E:35:LEU:CG    | 2.50                     | 0.42              |
| 1:E:153:LEU:HD12 | 1:E:153:LEU:HA   | 1.59                     | 0.42              |
| 1:H:64:LEU:HA    | 1:H:64:LEU:HD12  | 1.70                     | 0.42              |
| 1:H:143:LYS:O    | 1:H:146:ALA:HB3  | 2.20                     | 0.42              |
| 1:A:100:SER:C    | 1:A:101:SER:OG   | 2.62                     | 0.42              |
| 1:A:158:SER:O    | 1:A:164:VAL:CG2  | 2.61                     | 0.42              |
| 1:C:98:LEU:HA    | 1:C:98:LEU:HD23  | 1.68                     | 0.42              |
| 1:C:171:GLN:HB3  | 1:C:172:CYS:H    | 1.65                     | 0.42              |
| 1:D:200:ASN:HB3  | 1:D:201:GLY:H    | 1.52                     | 0.42              |
| 1:E:69:ASN:O     | 1:E:69:ASN:CG    | 2.62                     | 0.42              |
| 1:A:98:LEU:HA    | 1:A:98:LEU:HD23  | 1.50                     | 0.42              |
| 1:B:64:LEU:HB2   | 1:B:119:LEU:HD11 | 2.02                     | 0.42              |
| 1:F:154:THR:HG21 | 1:F:182:LEU:HD11 | 2.00                     | 0.42              |
| 1:G:153:LEU:HA   | 1:G:153:LEU:HD12 | 1.67                     | 0.42              |
| 1:G:165:LYS:O    | 1:G:166:LEU:C    | 2.62                     | 0.42              |
| 1:A:51:ASP:O     | 1:A:55:LEU:HG    | 2.19                     | 0.42              |
| 1:A:112:PHE:N    | 1:A:112:PHE:CD1  | 2.87                     | 0.42              |
| 1:E:174:LEU:HD23 | 1:E:174:LEU:HA   | 1.62                     | 0.42              |
| 1:H:154:THR:OG1  | 1:H:155:PRO:HD2  | 2.19                     | 0.42              |
| 1:H:174:LEU:HD23 | 1:H:174:LEU:HA   | 1.63                     | 0.42              |
| 1:B:156:LEU:HD23 | 1:B:156:LEU:HA   | 1.88                     | 0.42              |
| 3:B:477:APR:HO'3 | 3:B:477:APR:HO'2 | 1.57                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:104:ILE:HD11 | 1:C:110:VAL:CG2  | 2.50                     | 0.42              |
| 1:D:65:VAL:HG12  | 1:D:66:ASN:N     | 2.35                     | 0.42              |
| 1:D:69:ASN:HB2   | 1:D:70:GLY:H     | 1.74                     | 0.42              |
| 1:G:59:LEU:HD23  | 1:G:59:LEU:HA    | 1.58                     | 0.42              |
| 1:H:96:GLU:O     | 1:H:97:TYR:C     | 2.62                     | 0.42              |
| 1:D:85:PHE:C     | 1:D:87:GLY:H     | 2.27                     | 0.42              |
| 1:D:132:SER:O    | 1:D:133:ARG:CB   | 2.68                     | 0.42              |
| 1:E:38:PRO:HB3   | 1:E:46:SER:HB3   | 2.00                     | 0.42              |
| 1:E:111:LEU:HD12 | 1:E:111:LEU:HA   | 1.80                     | 0.42              |
| 1:F:110:VAL:HG13 | 1:F:111:LEU:H    | 1.83                     | 0.42              |
| 1:G:173:LEU:C    | 1:G:173:LEU:CD2  | 2.93                     | 0.42              |
| 1:D:80:ARG:HB3   | 1:D:80:ARG:NH1   | 2.35                     | 0.42              |
| 1:E:59:LEU:HA    | 1:E:59:LEU:HD23  | 1.59                     | 0.42              |
| 1:A:176:THR:C    | 1:A:178:THR:N    | 2.77                     | 0.41              |
| 1:A:189:ASP:O    | 1:A:190:GLN:C    | 2.63                     | 0.41              |
| 1:E:145:ILE:O    | 1:E:146:ALA:C    | 2.59                     | 0.41              |
| 1:G:100:SER:C    | 1:G:101:SER:OG   | 2.62                     | 0.41              |
| 1:A:188:THR:HG22 | 1:A:190:GLN:H    | 1.85                     | 0.41              |
| 1:A:188:THR:HG21 | 1:A:190:GLN:HB2  | 2.01                     | 0.41              |
| 1:C:67:ALA:HB1   | 3:C:477:APR:O1B  | 2.20                     | 0.41              |
| 1:C:170:LEU:HA   | 1:C:170:LEU:HD12 | 1.56                     | 0.41              |
| 1:E:110:VAL:CG1  | 1:E:111:LEU:N    | 2.84                     | 0.41              |
| 1:H:52:LEU:HD12  | 1:H:52:LEU:HA    | 1.83                     | 0.41              |
| 1:A:96:GLU:O     | 1:A:97:TYR:C     | 2.61                     | 0.41              |
| 1:A:105:ALA:O    | 1:A:108:ASN:N    | 2.51                     | 0.41              |
| 1:C:105:ALA:O    | 1:C:108:ASN:HB2  | 2.21                     | 0.41              |
| 1:D:64:LEU:HB2   | 1:D:119:LEU:HD11 | 2.00                     | 0.41              |
| 1:D:153:LEU:HD12 | 1:D:183:ASN:O    | 2.20                     | 0.41              |
| 1:E:61:PRO:HA    | 1:E:151:LYS:HB3  | 2.01                     | 0.41              |
| 1:G:55:LEU:HA    | 1:G:55:LEU:HD23  | 1.79                     | 0.41              |
| 1:B:136:GLY:O    | 1:B:140:ASN:HB2  | 2.19                     | 0.41              |
| 1:D:154:THR:C    | 1:D:185:PHE:CE2  | 2.98                     | 0.41              |
| 1:B:52:LEU:O     | 1:B:53:ASP:C     | 2.61                     | 0.41              |
| 1:B:80:ARG:O     | 1:B:81:ALA:C     | 2.64                     | 0.41              |
| 1:E:143:LYS:O    | 1:E:146:ALA:HB3  | 2.20                     | 0.41              |
| 1:E:173:LEU:C    | 1:E:173:LEU:CD2  | 2.92                     | 0.41              |
| 1:A:64:LEU:HA    | 1:A:64:LEU:HD12  | 1.68                     | 0.41              |
| 1:B:191:GLU:OE1  | 3:B:477:APR:O2'  | 2.26                     | 0.41              |
| 1:C:192:ARG:HH11 | 1:C:192:ARG:HD3  | 1.73                     | 0.41              |
| 1:F:189:ASP:C    | 1:F:191:GLU:N    | 2.78                     | 0.41              |
| 1:H:54:VAL:H     | 1:H:54:VAL:HG23  | 1.58                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:168:VAL:O    | 1:E:172:CYS:HB2  | 2.20                     | 0.41              |
| 1:F:52:LEU:CG    | 1:F:56:ILE:HD11  | 2.47                     | 0.41              |
| 1:H:159:VAL:HG13 | 1:H:160:GLY:H    | 1.84                     | 0.41              |
| 1:A:131:ASP:OD2  | 1:A:131:ASP:N    | 2.52                     | 0.41              |
| 1:B:78:VAL:O     | 1:B:79:ALA:C     | 2.62                     | 0.41              |
| 1:F:82:ILE:HG21  | 1:F:90:LEU:HD22  | 2.01                     | 0.41              |
| 1:C:156:LEU:HD23 | 1:C:156:LEU:HA   | 1.87                     | 0.41              |
| 1:C:157:ILE:HD13 | 1:C:157:ILE:HA   | 1.72                     | 0.41              |
| 1:D:78:VAL:O     | 1:D:79:ALA:C     | 2.58                     | 0.41              |
| 1:D:173:LEU:C    | 1:D:173:LEU:CD2  | 2.93                     | 0.41              |
| 1:F:170:LEU:HD11 | 1:F:174:LEU:HG   | 2.03                     | 0.41              |
| 1:H:112:PHE:N    | 1:H:112:PHE:HD1  | 2.19                     | 0.41              |
| 1:A:153:LEU:HD12 | 1:A:153:LEU:HA   | 1.65                     | 0.41              |
| 1:B:187:TYR:HB2  | 3:B:477:APR:C4   | 2.51                     | 0.41              |
| 1:E:40:TYR:HE2   | 1:E:42:ALA:HB2   | 1.86                     | 0.41              |
| 1:E:55:LEU:HA    | 1:E:55:LEU:HD23  | 1.79                     | 0.41              |
| 1:E:73:ARG:CG    | 1:E:73:ARG:NH2   | 2.66                     | 0.41              |
| 1:E:188:THR:HB   | 1:E:191:GLU:H    | 1.86                     | 0.41              |
| 1:H:69:ASN:OD1   | 1:H:73:ARG:O     | 2.39                     | 0.41              |
| 1:A:61:PRO:HA    | 1:A:151:LYS:HB3  | 2.02                     | 0.40              |
| 1:A:109:ALA:HB1  | 1:A:122:LEU:HD21 | 2.03                     | 0.40              |
| 1:B:133:ARG:O    | 1:B:137:LYS:HG3  | 2.21                     | 0.40              |
| 1:E:116:LEU:HB2  | 1:E:119:LEU:HB3  | 2.03                     | 0.40              |
| 1:F:105:ALA:HB3  | 1:F:108:ASN:HB2  | 2.03                     | 0.40              |
| 1:F:158:SER:HA   | 1:F:162:PHE:HD2  | 1.86                     | 0.40              |
| 1:G:153:LEU:HD12 | 1:G:183:ASN:O    | 2.21                     | 0.40              |
| 1:B:142:TYR:CE1  | 1:B:173:LEU:HB2  | 2.56                     | 0.40              |
| 1:E:188:THR:HG22 | 1:E:189:ASP:CA   | 2.50                     | 0.40              |
| 1:F:89:LYS:HZ3   | 1:F:89:LYS:HG3   | 1.54                     | 0.40              |
| 1:F:111:LEU:HA   | 1:F:111:LEU:HD12 | 1.78                     | 0.40              |
| 1:H:97:TYR:C     | 1:H:97:TYR:CD2   | 2.99                     | 0.40              |
| 1:H:173:LEU:HD23 | 1:H:173:LEU:O    | 2.21                     | 0.40              |
| 1:C:56:ILE:HD13  | 1:C:56:ILE:HG21  | 1.86                     | 0.40              |
| 1:C:111:LEU:HG   | 1:C:112:PHE:N    | 2.32                     | 0.40              |
| 1:D:93:ARG:NE    | 1:D:93:ARG:HA    | 2.36                     | 0.40              |
| 1:D:137:LYS:O    | 1:D:141:VAL:HG23 | 2.21                     | 0.40              |
| 1:D:171:GLN:HB3  | 1:D:172:CYS:H    | 1.72                     | 0.40              |
| 1:E:162:PHE:HD1  | 1:E:162:PHE:HA   | 1.81                     | 0.40              |
| 1:F:38:PRO:HD3   | 1:F:48:TYR:CE1   | 2.57                     | 0.40              |
| 1:G:97:TYR:O     | 1:G:101:SER:HB2  | 2.22                     | 0.40              |
| 1:H:116:LEU:HA   | 1:H:116:LEU:HD23 | 1.73                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:79:ALA:O     | 1:C:80:ARG:C     | 2.63                     | 0.40              |
| 1:D:189:ASP:O    | 1:D:190:GLN:C    | 2.65                     | 0.40              |
| 1:E:166:LEU:HD23 | 1:E:166:LEU:C    | 2.46                     | 0.40              |
| 1:F:192:ARG:HA   | 1:F:195:ILE:HD12 | 2.04                     | 0.40              |
| 1:C:100:SER:O    | 1:C:100:SER:OG   | 2.39                     | 0.40              |
| 1:D:48:TYR:CD2   | 1:D:48:TYR:N     | 2.89                     | 0.40              |
| 1:D:155:PRO:N    | 1:D:185:PHE:CE2  | 2.90                     | 0.40              |
| 1:E:36:ILE:HA    | 1:E:36:ILE:HD13  | 1.75                     | 0.40              |
| 1:E:53:ASP:OD1   | 1:E:53:ASP:N     | 2.55                     | 0.40              |
| 1:F:60:GLU:N     | 1:F:61:PRO:CD    | 2.85                     | 0.40              |

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

| Atom-1         | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------------|--------------------------|-------------------|
| 1:F:100:SER:OG | 1:F:118:HIS:O[8_544]  | 2.08                     | 0.12              |
| 1:A:35:LEU:O   | 1:A:163:LYS:NZ[6_445] | 2.11                     | 0.09              |

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 1   | A     | 166/168 (99%) | 138 (83%) | 26 (16%) | 2 (1%)   | 10          | 41 |
| 1   | B     | 166/168 (99%) | 130 (78%) | 30 (18%) | 6 (4%)   | 2           | 23 |
| 1   | C     | 166/168 (99%) | 130 (78%) | 33 (20%) | 3 (2%)   | 6           | 34 |
| 1   | D     | 166/168 (99%) | 127 (76%) | 37 (22%) | 2 (1%)   | 10          | 41 |
| 1   | E     | 166/168 (99%) | 139 (84%) | 26 (16%) | 1 (1%)   | 21          | 56 |
| 1   | F     | 166/168 (99%) | 132 (80%) | 30 (18%) | 4 (2%)   | 4           | 29 |
| 1   | G     | 166/168 (99%) | 137 (82%) | 28 (17%) | 1 (1%)   | 21          | 56 |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | H     | 166/168 (99%)   | 138 (83%)  | 25 (15%)  | 3 (2%)   | 6           | 34 |
| All | All   | 1328/1344 (99%) | 1071 (81%) | 235 (18%) | 22 (2%)  | 7           | 35 |

All (22) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 161 | ILE  |
| 1   | D     | 161 | ILE  |
| 1   | C     | 134 | VAL  |
| 1   | D     | 134 | VAL  |
| 1   | G     | 134 | VAL  |
| 1   | F     | 95  | LYS  |
| 1   | H     | 178 | THR  |
| 1   | B     | 83  | ASP  |
| 1   | B     | 161 | ILE  |
| 1   | B     | 171 | GLN  |
| 1   | B     | 84  | VAL  |
| 1   | B     | 77  | GLY  |
| 1   | C     | 77  | GLY  |
| 1   | E     | 177 | VAL  |
| 1   | F     | 134 | VAL  |
| 1   | H     | 134 | VAL  |
| 1   | H     | 177 | VAL  |
| 1   | F     | 106 | PRO  |
| 1   | A     | 134 | VAL  |
| 1   | F     | 193 | VAL  |
| 1   | B     | 61  | PRO  |
| 1   | A     | 106 | 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     | 143/143 (100%) | 129 (90%) | 14 (10%) | 7           | 27 |
| 1   | B     | 143/143 (100%) | 126 (88%) | 17 (12%) | 5           | 21 |

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| Mol | Chain | Analysed         | Rotameric | Outliers  | Percentiles |    |
|-----|-------|------------------|-----------|-----------|-------------|----|
| 1   | C     | 143/143 (100%)   | 128 (90%) | 15 (10%)  | 6           | 24 |
| 1   | D     | 143/143 (100%)   | 129 (90%) | 14 (10%)  | 7           | 27 |
| 1   | E     | 143/143 (100%)   | 119 (83%) | 24 (17%)  | 2           | 13 |
| 1   | F     | 143/143 (100%)   | 107 (75%) | 36 (25%)  | 0           | 4  |
| 1   | G     | 143/143 (100%)   | 124 (87%) | 19 (13%)  | 4           | 18 |
| 1   | H     | 143/143 (100%)   | 126 (88%) | 17 (12%)  | 5           | 21 |
| All | All   | 1144/1144 (100%) | 988 (86%) | 156 (14%) | 3           | 17 |

All (156) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 63  | VAL  |
| 1   | A     | 72  | LEU  |
| 1   | A     | 73  | ARG  |
| 1   | A     | 128 | ARG  |
| 1   | A     | 131 | ASP  |
| 1   | A     | 133 | ARG  |
| 1   | A     | 138 | LEU  |
| 1   | A     | 139 | CYS  |
| 1   | A     | 161 | ILE  |
| 1   | A     | 162 | PHE  |
| 1   | A     | 168 | VAL  |
| 1   | A     | 171 | GLN  |
| 1   | A     | 172 | CYS  |
| 1   | A     | 180 | ARG  |
| 1   | B     | 34  | ASP  |
| 1   | B     | 51  | ASP  |
| 1   | B     | 63  | VAL  |
| 1   | B     | 91  | THR  |
| 1   | B     | 99  | LYS  |
| 1   | B     | 128 | ARG  |
| 1   | B     | 132 | SER  |
| 1   | B     | 143 | LYS  |
| 1   | B     | 147 | LYS  |
| 1   | B     | 152 | ILE  |
| 1   | B     | 158 | SER  |
| 1   | B     | 159 | VAL  |
| 1   | B     | 172 | CYS  |
| 1   | B     | 173 | LEU  |
| 1   | B     | 178 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 180 | ARG  |
| 1   | B     | 187 | TYR  |
| 1   | C     | 34  | ASP  |
| 1   | C     | 41  | LYS  |
| 1   | C     | 51  | ASP  |
| 1   | C     | 59  | LEU  |
| 1   | C     | 91  | THR  |
| 1   | C     | 100 | SER  |
| 1   | C     | 128 | ARG  |
| 1   | C     | 143 | LYS  |
| 1   | C     | 147 | LYS  |
| 1   | C     | 152 | ILE  |
| 1   | C     | 158 | SER  |
| 1   | C     | 159 | VAL  |
| 1   | C     | 172 | CYS  |
| 1   | C     | 180 | ARG  |
| 1   | C     | 197 | ASN  |
| 1   | D     | 34  | ASP  |
| 1   | D     | 41  | LYS  |
| 1   | D     | 51  | ASP  |
| 1   | D     | 80  | ARG  |
| 1   | D     | 91  | THR  |
| 1   | D     | 128 | ARG  |
| 1   | D     | 143 | LYS  |
| 1   | D     | 147 | LYS  |
| 1   | D     | 152 | ILE  |
| 1   | D     | 158 | SER  |
| 1   | D     | 159 | VAL  |
| 1   | D     | 168 | VAL  |
| 1   | D     | 172 | CYS  |
| 1   | D     | 180 | ARG  |
| 1   | E     | 34  | ASP  |
| 1   | E     | 63  | VAL  |
| 1   | E     | 72  | LEU  |
| 1   | E     | 73  | ARG  |
| 1   | E     | 80  | ARG  |
| 1   | E     | 86  | THR  |
| 1   | E     | 122 | LEU  |
| 1   | E     | 128 | ARG  |
| 1   | E     | 131 | ASP  |
| 1   | E     | 132 | SER  |
| 1   | E     | 133 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 134 | VAL  |
| 1   | E     | 135 | GLU  |
| 1   | E     | 138 | LEU  |
| 1   | E     | 139 | CYS  |
| 1   | E     | 161 | ILE  |
| 1   | E     | 162 | PHE  |
| 1   | E     | 167 | GLU  |
| 1   | E     | 168 | VAL  |
| 1   | E     | 172 | CYS  |
| 1   | E     | 180 | ARG  |
| 1   | E     | 190 | GLN  |
| 1   | E     | 197 | ASN  |
| 1   | E     | 200 | ASN  |
| 1   | F     | 40  | TYR  |
| 1   | F     | 45  | VAL  |
| 1   | F     | 46  | SER  |
| 1   | F     | 49  | GLN  |
| 1   | F     | 53  | ASP  |
| 1   | F     | 56  | ILE  |
| 1   | F     | 63  | VAL  |
| 1   | F     | 69  | ASN  |
| 1   | F     | 73  | ARG  |
| 1   | F     | 80  | ARG  |
| 1   | F     | 82  | ILE  |
| 1   | F     | 89  | LYS  |
| 1   | F     | 91  | THR  |
| 1   | F     | 98  | LEU  |
| 1   | F     | 99  | LYS  |
| 1   | F     | 104 | ILE  |
| 1   | F     | 128 | ARG  |
| 1   | F     | 135 | GLU  |
| 1   | F     | 137 | LYS  |
| 1   | F     | 139 | CYS  |
| 1   | F     | 140 | ASN  |
| 1   | F     | 152 | ILE  |
| 1   | F     | 158 | SER  |
| 1   | F     | 166 | LEU  |
| 1   | F     | 167 | GLU  |
| 1   | F     | 168 | VAL  |
| 1   | F     | 172 | CYS  |
| 1   | F     | 180 | ARG  |
| 1   | F     | 181 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 182 | LEU  |
| 1   | F     | 188 | THR  |
| 1   | F     | 189 | ASP  |
| 1   | F     | 190 | GLN  |
| 1   | F     | 192 | ARG  |
| 1   | F     | 193 | VAL  |
| 1   | F     | 197 | ASN  |
| 1   | G     | 34  | ASP  |
| 1   | G     | 63  | VAL  |
| 1   | G     | 72  | LEU  |
| 1   | G     | 73  | ARG  |
| 1   | G     | 122 | LEU  |
| 1   | G     | 128 | ARG  |
| 1   | G     | 131 | ASP  |
| 1   | G     | 132 | SER  |
| 1   | G     | 133 | ARG  |
| 1   | G     | 134 | VAL  |
| 1   | G     | 138 | LEU  |
| 1   | G     | 158 | SER  |
| 1   | G     | 161 | ILE  |
| 1   | G     | 162 | PHE  |
| 1   | G     | 168 | VAL  |
| 1   | G     | 172 | CYS  |
| 1   | G     | 180 | ARG  |
| 1   | G     | 190 | GLN  |
| 1   | G     | 197 | ASN  |
| 1   | H     | 34  | ASP  |
| 1   | H     | 35  | LEU  |
| 1   | H     | 63  | VAL  |
| 1   | H     | 72  | LEU  |
| 1   | H     | 73  | ARG  |
| 1   | H     | 86  | THR  |
| 1   | H     | 128 | ARG  |
| 1   | H     | 131 | ASP  |
| 1   | H     | 132 | SER  |
| 1   | H     | 133 | ARG  |
| 1   | H     | 134 | VAL  |
| 1   | H     | 161 | ILE  |
| 1   | H     | 162 | PHE  |
| 1   | H     | 168 | VAL  |
| 1   | H     | 171 | GLN  |
| 1   | H     | 172 | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 180 | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 108 | ASN  |
| 1   | D     | 66  | ASN  |
| 1   | D     | 123 | ASN  |
| 1   | F     | 49  | GLN  |
| 1   | F     | 108 | ASN  |
| 1   | H     | 66  | ASN  |
| 1   | H     | 114 | ASN  |
| 1   | H     | 123 | ASN  |

### 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](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | APR  | D     | 477 | -    | 39,39,39     | 1.75 | 6 (15%)  | 56,60,60    | 2.08 | 13 (23%) |
| 3   | APR  | C     | 477 | -    | 39,39,39     | 1.45 | 5 (12%)  | 56,60,60    | 2.20 | 16 (28%) |
| 3   | APR  | B     | 477 | -    | 39,39,39     | 2.16 | 11 (28%) | 56,60,60    | 2.17 | 17 (30%) |

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   | APR  | D     | 477 | -    | -       | 7/22/54/54 | 0/4/4/4 |
| 3   | APR  | C     | 477 | -    | -       | 8/22/54/54 | 0/4/4/4 |
| 3   | APR  | B     | 477 | -    | -       | 6/22/54/54 | 0/4/4/4 |

All (22) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | B     | 477 | APR  | C5-C4   | 6.26  | 1.50        | 1.39     |
| 3   | B     | 477 | APR  | PA-O3A  | 6.10  | 1.66        | 1.59     |
| 3   | D     | 477 | APR  | PB-O3A  | 5.54  | 1.65        | 1.59     |
| 3   | D     | 477 | APR  | PA-O3A  | 4.94  | 1.64        | 1.59     |
| 3   | C     | 477 | APR  | C5-N7   | -4.88 | 1.30        | 1.39     |
| 3   | B     | 477 | APR  | PB-O3A  | 4.20  | 1.64        | 1.59     |
| 3   | D     | 477 | APR  | C5-N7   | -4.08 | 1.31        | 1.39     |
| 3   | D     | 477 | APR  | C5-C4   | 3.99  | 1.46        | 1.39     |
| 3   | B     | 477 | APR  | C4-N3   | 3.79  | 1.41        | 1.34     |
| 3   | B     | 477 | APR  | C8-N7   | 3.57  | 1.38        | 1.31     |
| 3   | C     | 477 | APR  | C5-C4   | 3.23  | 1.44        | 1.39     |
| 3   | B     | 477 | APR  | C5-C6   | 2.81  | 1.48        | 1.41     |
| 3   | D     | 477 | APR  | C8-N7   | 2.74  | 1.36        | 1.31     |
| 3   | C     | 477 | APR  | PA-O3A  | 2.67  | 1.62        | 1.59     |
| 3   | B     | 477 | APR  | C1'-N9  | 2.65  | 1.53        | 1.46     |
| 3   | C     | 477 | APR  | C8-N9   | -2.59 | 1.33        | 1.37     |
| 3   | B     | 477 | APR  | O1D-C1D | 2.30  | 1.46        | 1.39     |
| 3   | D     | 477 | APR  | O1D-C1D | 2.28  | 1.46        | 1.39     |
| 3   | B     | 477 | APR  | C2-N3   | 2.21  | 1.37        | 1.33     |
| 3   | B     | 477 | APR  | C2-N1   | 2.18  | 1.37        | 1.33     |
| 3   | B     | 477 | APR  | C1D-C2D | 2.14  | 1.55        | 1.52     |
| 3   | C     | 477 | APR  | C5D-C4D | 2.09  | 1.57        | 1.51     |

All (46) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | B     | 477 | APR  | C5-C4-N3    | -8.13 | 115.53      | 126.72   |
| 3   | C     | 477 | APR  | C5-C4-N3    | -7.75 | 116.04      | 126.72   |
| 3   | D     | 477 | APR  | C5-C4-N3    | -7.39 | 116.55      | 126.72   |
| 3   | B     | 477 | APR  | N3-C4-N9    | 6.65  | 138.48      | 127.17   |
| 3   | D     | 477 | APR  | N3-C4-N9    | 6.41  | 138.07      | 127.17   |
| 3   | C     | 477 | APR  | N3-C4-N9    | 6.22  | 137.74      | 127.17   |
| 3   | C     | 477 | APR  | C2-N3-C4    | 4.10  | 121.84      | 111.83   |
| 3   | C     | 477 | APR  | N6-C6-N1    | 4.05  | 127.39      | 118.38   |
| 3   | D     | 477 | APR  | C2-N3-C4    | 3.91  | 121.39      | 111.83   |
| 3   | C     | 477 | APR  | O4'-C1'-C2' | -3.89 | 98.29       | 106.62   |
| 3   | B     | 477 | APR  | C2-N3-C4    | 3.81  | 121.13      | 111.83   |
| 3   | D     | 477 | APR  | O3'-C3'-C4' | -3.78 | 100.22      | 111.08   |
| 3   | C     | 477 | APR  | C3'-C2'-C1' | 3.70  | 108.47      | 101.46   |
| 3   | D     | 477 | APR  | N6-C6-N1    | 3.66  | 126.53      | 118.38   |
| 3   | C     | 477 | APR  | C4'-O4'-C1' | 3.63  | 117.47      | 109.47   |
| 3   | B     | 477 | APR  | C4-C5-N7    | -3.61 | 106.45      | 110.58   |
| 3   | D     | 477 | APR  | C5-C6-N6    | -3.60 | 114.37      | 123.29   |
| 3   | D     | 477 | APR  | C1D-C2D-C3D | 3.43  | 106.50      | 102.29   |
| 3   | D     | 477 | APR  | N3-C2-N1    | -3.39 | 123.45      | 128.58   |
| 3   | B     | 477 | APR  | C5-N7-C8    | 3.17  | 108.43      | 103.45   |
| 3   | C     | 477 | APR  | C6-C5-C4    | 3.09  | 121.40      | 117.18   |
| 3   | D     | 477 | APR  | O3D-C3D-C2D | -3.09 | 101.92      | 111.82   |
| 3   | B     | 477 | APR  | O2A-PA-O1A  | 3.01  | 126.47      | 112.44   |
| 3   | C     | 477 | APR  | C5-C6-N6    | -2.93 | 116.03      | 123.29   |
| 3   | B     | 477 | APR  | C2D-C3D-C4D | 2.90  | 108.20      | 102.61   |
| 3   | C     | 477 | APR  | N3-C2-N1    | -2.84 | 124.28      | 128.58   |
| 3   | B     | 477 | APR  | N3-C2-N1    | -2.74 | 124.44      | 128.58   |
| 3   | B     | 477 | APR  | C4'-O4'-C1' | 2.71  | 115.44      | 109.47   |
| 3   | C     | 477 | APR  | O2A-PA-O1A  | 2.62  | 124.63      | 112.44   |
| 3   | C     | 477 | APR  | O3'-C3'-C4' | -2.60 | 103.61      | 111.08   |
| 3   | B     | 477 | APR  | O2'-C2'-C3' | -2.46 | 103.92      | 111.82   |
| 3   | B     | 477 | APR  | O3D-C3D-C2D | -2.39 | 104.16      | 111.82   |
| 3   | B     | 477 | APR  | C3'-C2'-C1' | 2.37  | 105.95      | 101.46   |
| 3   | D     | 477 | APR  | O2A-PA-O1A  | 2.32  | 123.25      | 112.44   |
| 3   | D     | 477 | APR  | O2D-C2D-C3D | -2.32 | 104.39      | 111.82   |
| 3   | B     | 477 | APR  | O4D-C1D-C2D | 2.29  | 107.85      | 104.67   |
| 3   | B     | 477 | APR  | C2'-C1'-N9  | 2.27  | 118.93      | 113.30   |
| 3   | B     | 477 | APR  | N6-C6-N1    | 2.26  | 123.41      | 118.38   |
| 3   | D     | 477 | APR  | O2B-PB-O3A  | 2.22  | 113.28      | 107.27   |
| 3   | C     | 477 | APR  | O3D-C3D-C4D | -2.19 | 104.78      | 111.08   |
| 3   | C     | 477 | APR  | C4-C5-N7    | -2.19 | 108.08      | 110.58   |
| 3   | B     | 477 | APR  | C5-C6-N6    | -2.16 | 117.94      | 123.29   |
| 3   | B     | 477 | APR  | O4'-C1'-C2' | -2.03 | 102.28      | 106.62   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 3   | C     | 477 | APR  | C5-N7-C8  | 2.03  | 106.64      | 103.45   |
| 3   | D     | 477 | APR  | C1'-N9-C8 | -2.00 | 122.65      | 127.09   |
| 3   | C     | 477 | APR  | C1'-N9-C8 | -2.00 | 122.65      | 127.09   |

There are no chirality outliers.

All (21) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | B     | 477 | APR  | C5'-O5'-PA-O1A  |
| 3   | B     | 477 | APR  | C5'-O5'-PA-O3A  |
| 3   | C     | 477 | APR  | C3D-C4D-C5D-O5D |
| 3   | C     | 477 | APR  | O4D-C4D-C5D-O5D |
| 3   | B     | 477 | APR  | PA-O3A-PB-O5D   |
| 3   | C     | 477 | APR  | PA-O3A-PB-O5D   |
| 3   | D     | 477 | APR  | C3D-C4D-C5D-O5D |
| 3   | B     | 477 | APR  | C2'-C1'-N9-C8   |
| 3   | C     | 477 | APR  | C2'-C1'-N9-C8   |
| 3   | D     | 477 | APR  | C2'-C1'-N9-C8   |
| 3   | D     | 477 | APR  | PA-O3A-PB-O1B   |
| 3   | C     | 477 | APR  | C3'-C4'-C5'-O5' |
| 3   | C     | 477 | APR  | O4'-C4'-C5'-O5' |
| 3   | D     | 477 | APR  | C5'-O5'-PA-O1A  |
| 3   | C     | 477 | APR  | C2'-C1'-N9-C4   |
| 3   | D     | 477 | APR  | C2'-C1'-N9-C4   |
| 3   | D     | 477 | APR  | PA-O3A-PB-O5D   |
| 3   | D     | 477 | APR  | O4'-C1'-N9-C8   |
| 3   | B     | 477 | APR  | O4'-C1'-N9-C8   |
| 3   | B     | 477 | APR  | PA-O3A-PB-O1B   |
| 3   | C     | 477 | APR  | PA-O3A-PB-O1B   |

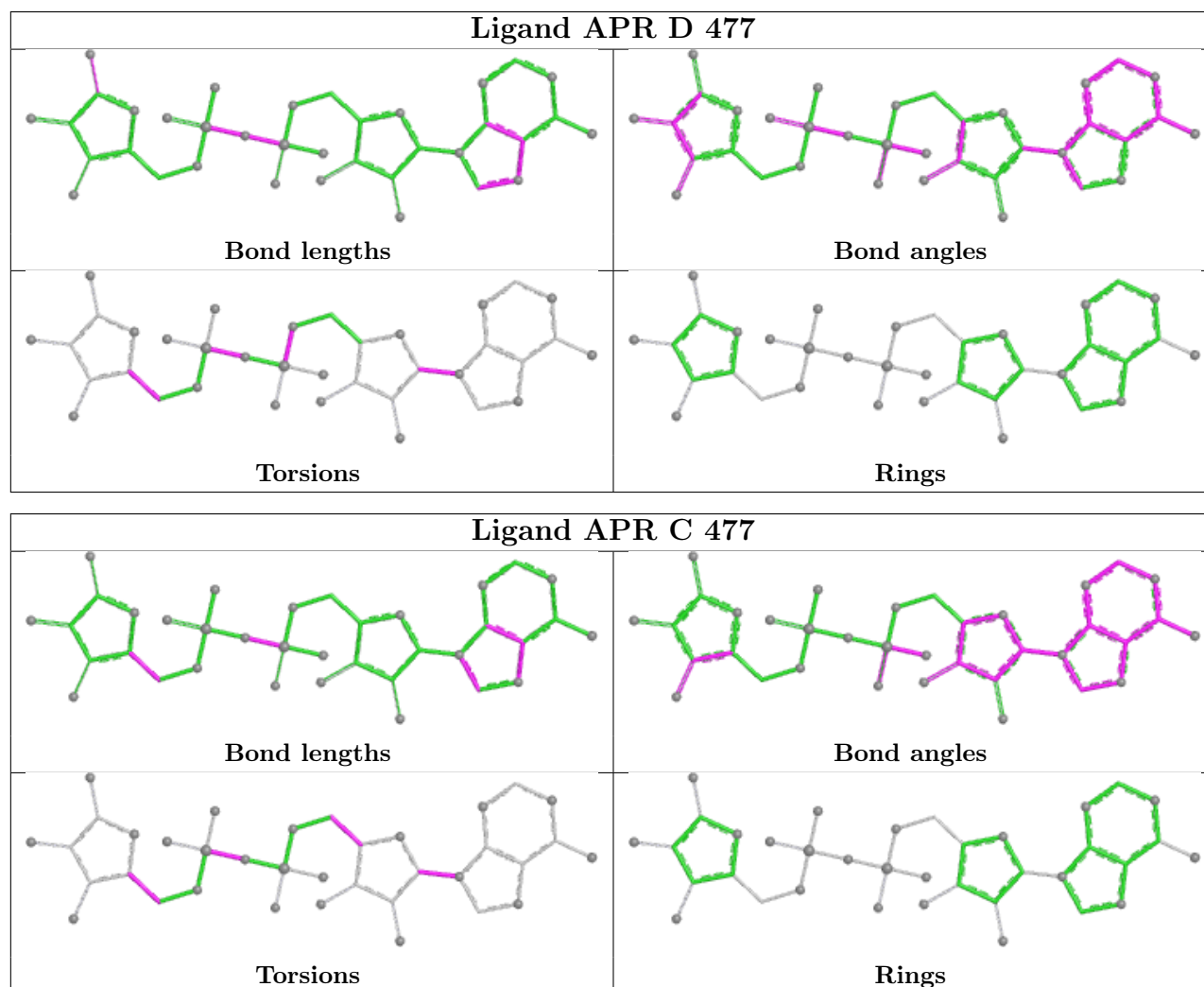
There are no ring outliers.

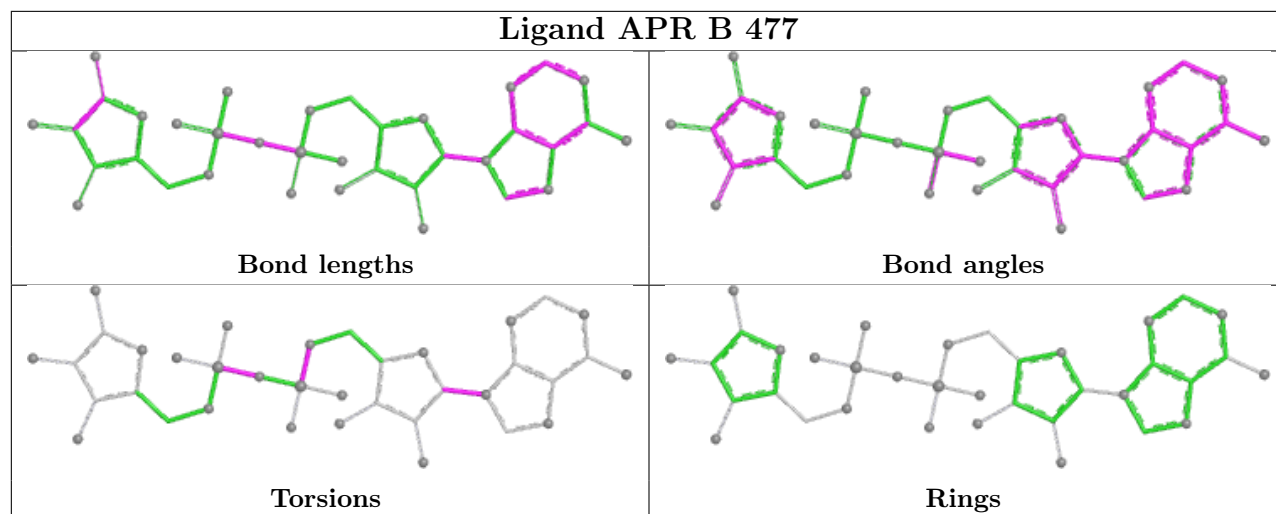
3 monomers are involved in 9 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | D     | 477 | APR  | 1       | 0            |
| 3   | C     | 477 | APR  | 1       | 0            |
| 3   | B     | 477 | APR  | 7       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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     | 168/168 (100%)   | -0.50  | 2 (1%)    | 76 56 | 6, 26, 43, 49         | 8 (4%)  |
| 1   | B     | 168/168 (100%)   | -0.38  | 2 (1%)    | 76 56 | 17, 32, 50, 58        | 5 (2%)  |
| 1   | C     | 168/168 (100%)   | -0.40  | 2 (1%)    | 76 56 | 17, 31, 50, 58        | 4 (2%)  |
| 1   | D     | 168/168 (100%)   | -0.42  | 3 (1%)    | 67 48 | 14, 31, 51, 58        | 6 (3%)  |
| 1   | E     | 168/168 (100%)   | -0.43  | 1 (0%)    | 85 70 | 7, 26, 44, 53         | 5 (2%)  |
| 1   | F     | 168/168 (100%)   | -0.50  | 3 (1%)    | 67 48 | 7, 31, 59, 65         | 6 (3%)  |
| 1   | G     | 168/168 (100%)   | -0.41  | 3 (1%)    | 67 48 | 8, 26, 44, 56         | 6 (3%)  |
| 1   | H     | 168/168 (100%)   | -0.45  | 4 (2%)    | 59 42 | 9, 26, 44, 52         | 7 (4%)  |
| All | All   | 1344/1344 (100%) | -0.44  | 20 (1%)   | 72 51 | 6, 29, 48, 65         | 47 (3%) |

All (20) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 95  | LYS  | 5.1  |
| 1   | H     | 171 | GLN  | 4.5  |
| 1   | B     | 197 | ASN  | 4.0  |
| 1   | F     | 171 | GLN  | 3.9  |
| 1   | F     | 95  | LYS  | 3.7  |
| 1   | F     | 190 | GLN  | 3.2  |
| 1   | D     | 171 | GLN  | 3.1  |
| 1   | H     | 140 | ASN  | 2.9  |
| 1   | A     | 171 | GLN  | 2.9  |
| 1   | G     | 171 | GLN  | 2.8  |
| 1   | C     | 93  | ARG  | 2.8  |
| 1   | E     | 190 | GLN  | 2.7  |
| 1   | G     | 190 | GLN  | 2.7  |
| 1   | A     | 133 | ARG  | 2.7  |
| 1   | H     | 167 | GLU  | 2.7  |
| 1   | G     | 95  | LYS  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 197 | ASN  | 2.3  |
| 1   | H     | 190 | GLN  | 2.2  |
| 1   | C     | 133 | ARG  | 2.2  |
| 1   | B     | 113 | GLU  | 2.1  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

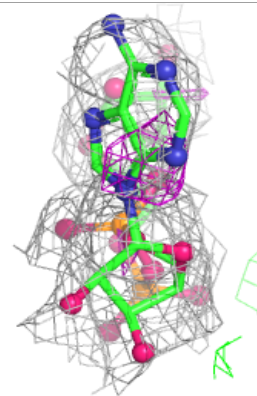
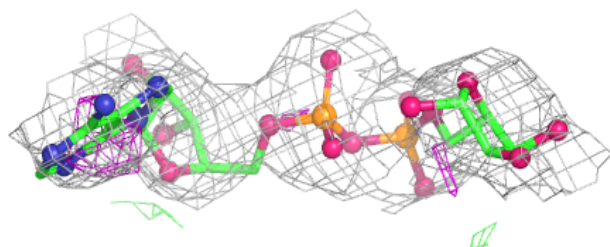
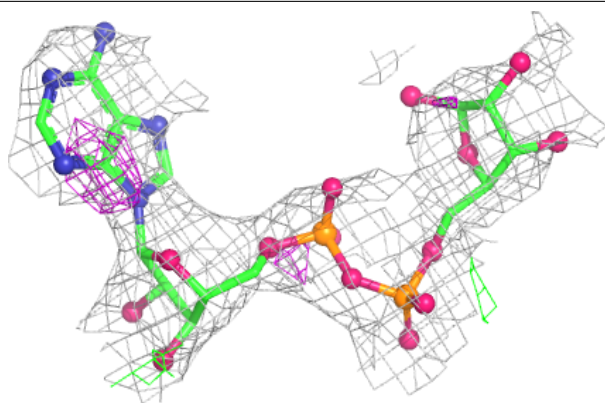
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 4   | NA   | B     | 3   | 1/1   | 0.88 | 0.11 | 16,16,16,16                 | 0     |
| 3   | APR  | B     | 477 | 36/36 | 0.94 | 0.12 | 55,59,64,64                 | 0     |
| 2   | CL   | A     | 1   | 1/1   | 0.94 | 0.04 | 52,52,52,52                 | 0     |
| 3   | APR  | C     | 477 | 36/36 | 0.96 | 0.10 | 55,59,63,64                 | 0     |
| 3   | APR  | D     | 477 | 36/36 | 0.96 | 0.09 | 55,59,63,64                 | 0     |
| 2   | CL   | G     | 2   | 1/1   | 0.96 | 0.08 | 41,41,41,41                 | 0     |

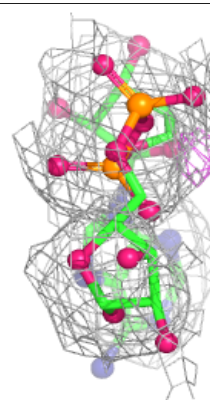
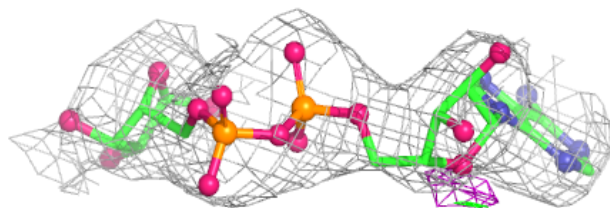
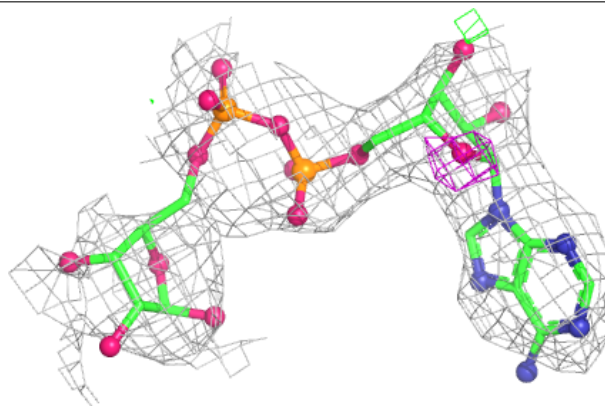
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

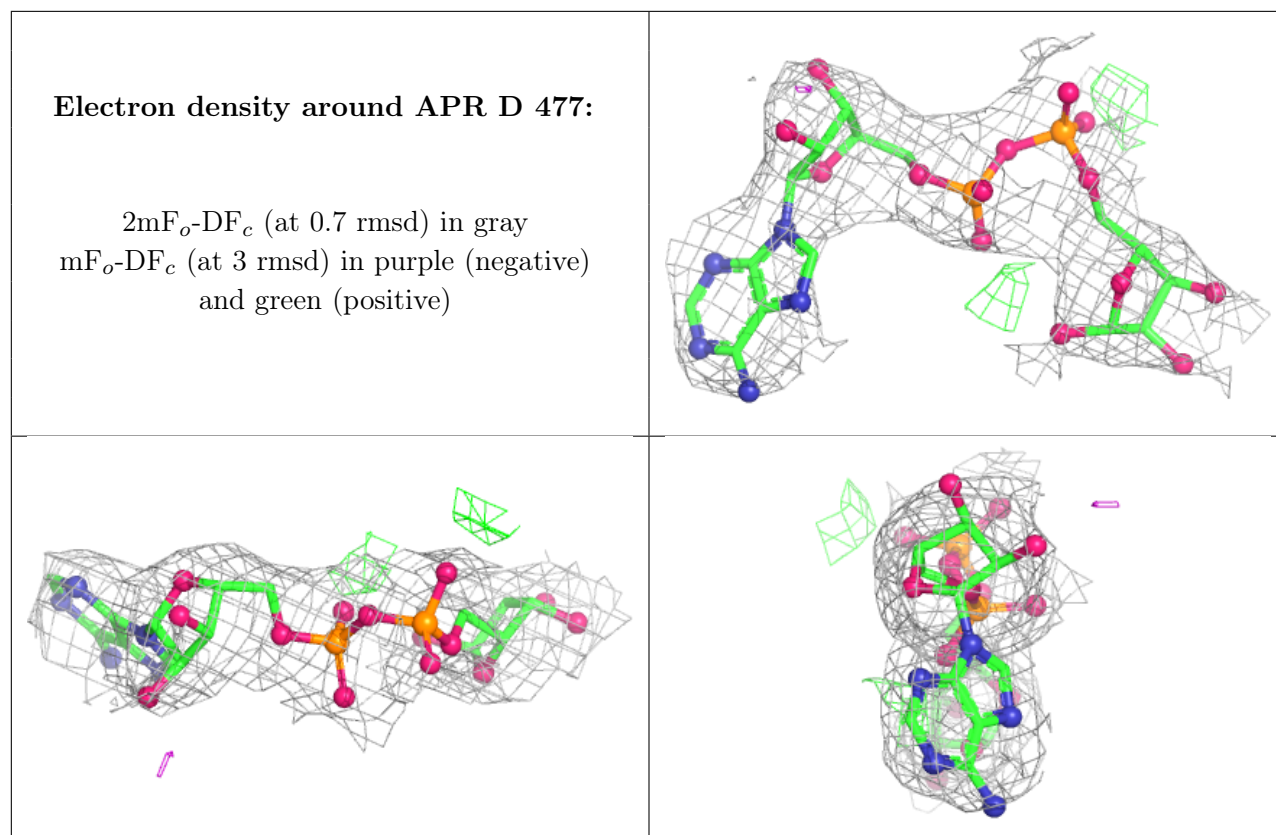
**Electron density around APR B 477:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around APR C 477:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.