



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:40 AM UTC

PDB ID : 1BXZ / pdb\_00001bxz  
Title : CRYSTAL STRUCTURE OF A THERMOPHILIC ALCOHOL DEHYDROGENASE SUBSTRATE COMPLEX FROM THERMOANAEROBACTER BROCKII  
Authors : Li, C.; Heatwole, J.; Soelaiman, S.; Shoham, M.  
Deposited on : 1998-10-09  
Resolution : 2.99 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

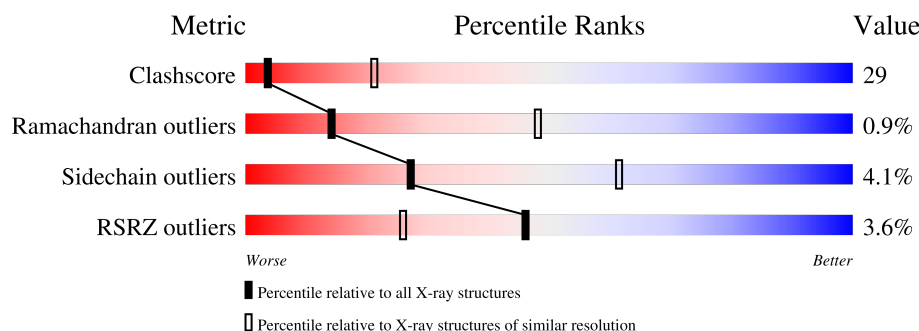
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.99 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 2977 (3.00-3.00)                                      |
| Ramachandran outliers | 187476                      | 2877 (3.00-3.00)                                      |
| Sidechain outliers    | 187428                      | 2880 (3.00-3.00)                                      |
| RSRZ outliers         | 180081                      | 2671 (3.00-3.00)                                      |

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     | 352    | <div> <div>2%</div> <div> <div></div> <div>53%</div> <div>41%</div> <div>6%</div> </div> </div> |
| 1   | B     | 352    | <div> <div>6%</div> <div> <div></div> <div>54%</div> <div>41%</div> <div>5%</div> </div> </div> |
| 1   | C     | 352    | <div> <div>4%</div> <div> <div></div> <div>51%</div> <div>43%</div> <div>6%</div> </div> </div> |
| 1   | D     | 352    | <div> <div>3%</div> <div> <div></div> <div>51%</div> <div>42%</div> <div>7%</div> </div> </div> |

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10852 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 NADP-DEPENDENT ALCOHOL DEHYDROGENASE.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 352      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2643  | 1693 | 455 | 476 | 19 |         |         |       |
| 1   | B     | 352      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2643  | 1693 | 455 | 476 | 19 |         |         |       |
| 1   | C     | 352      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2643  | 1693 | 455 | 476 | 19 |         |         |       |
| 1   | D     | 352      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2643  | 1693 | 455 | 476 | 19 |         |         |       |

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | B     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | C     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | D     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

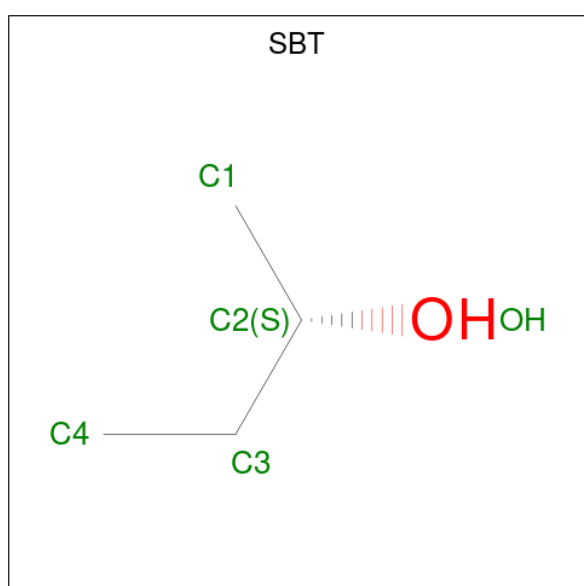
- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | A     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | B     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | C     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | D     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is 2-BUTANOL (CCD ID: SBT) (formula: C<sub>4</sub>H<sub>10</sub>O).



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

- Molecule 6 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 6   | A     | 75       | Total | O  | 0       | 0       |
|     |       |          | 75    | 75 |         |         |

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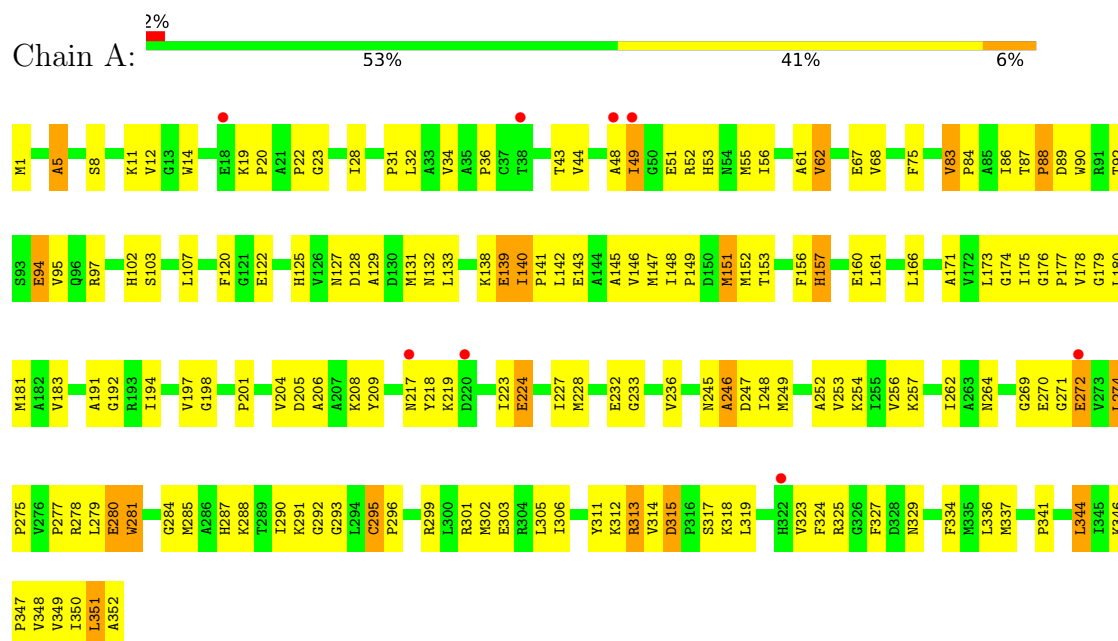
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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 6   | B     | 63       | Total<br>63 | O<br>63 | 0       | 0       |
| 6   | C     | 44       | Total<br>44 | O<br>44 | 0       | 0       |
| 6   | D     | 66       | Total<br>66 | O<br>66 | 0       | 0       |

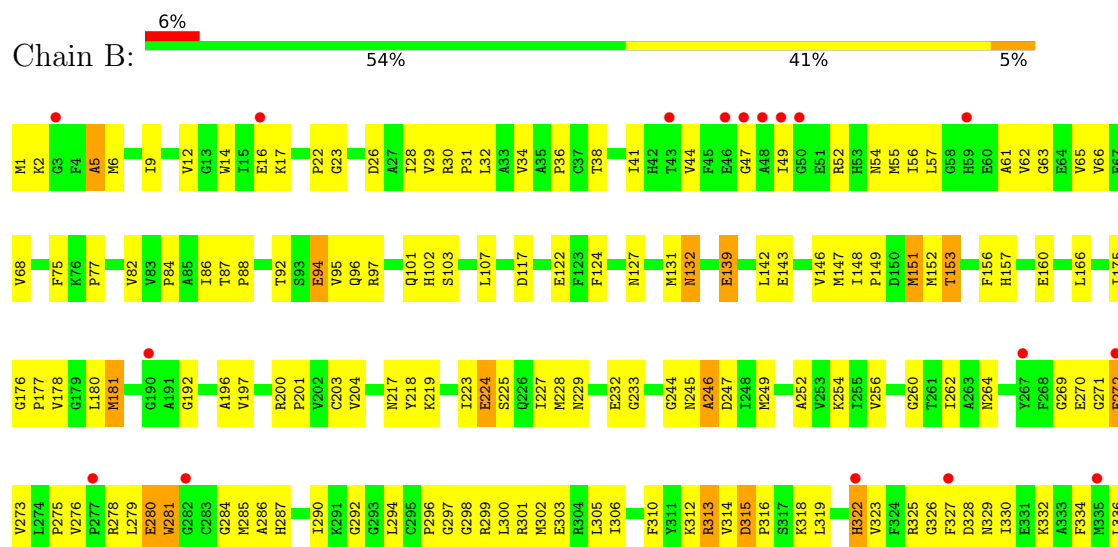
### 3 Residue-property plots

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: NADP-DEPENDENT ALCOHOL DEHYDROGENASE

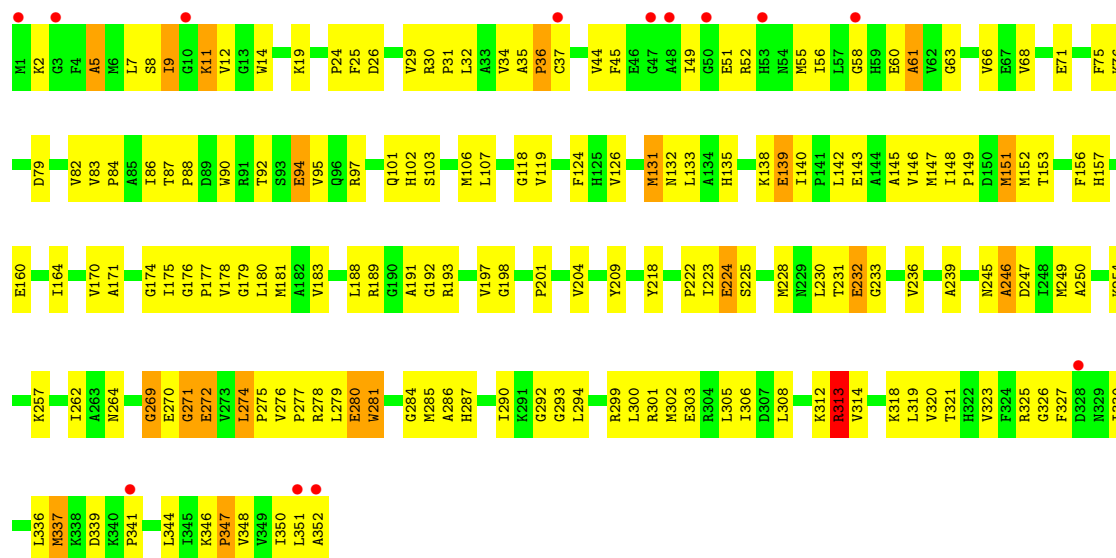


#### • Molecule 1: NADP-DEPENDENT ALCOHOL DEHYDROGENASE

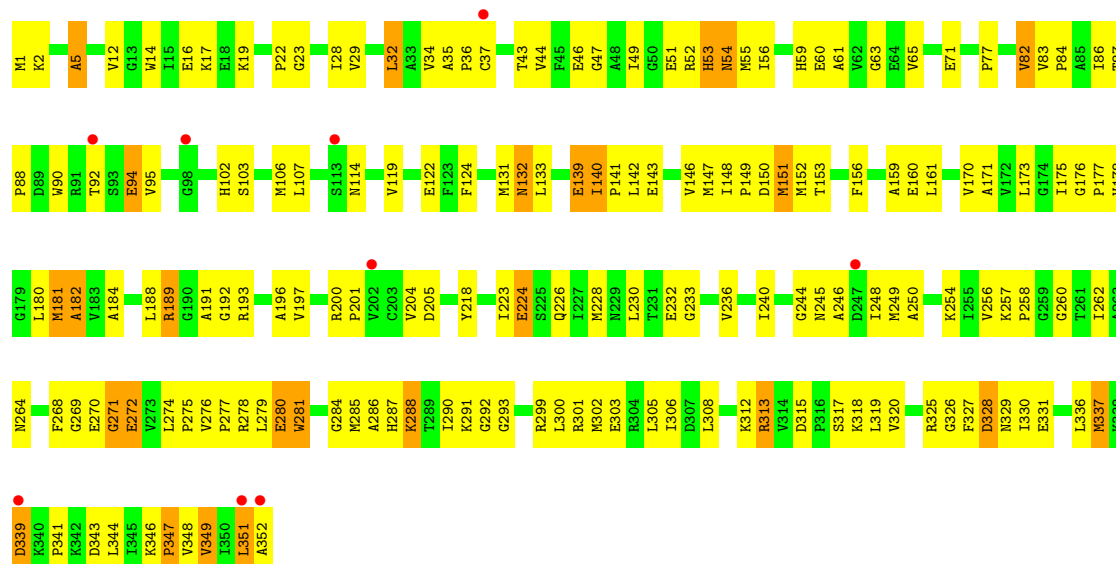




● Molecule 1: NADP-DEPENDENT ALCOHOL DEHYDROGENASE



● Molecule 1: NADP-DEPENDENT ALCOHOL DEHYDROGENASE



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 80.45Å 123.08Å 168.03Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 50.00 – 2.99<br>50.00 – 2.99                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 86.3 (50.00-2.99)<br>83.4 (50.00-2.99)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.08                                                        | Depositor        |
| $R_{sym}$                                                               | 0.08                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 4.81 (at 2.96Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 0.3C                                                    | Depositor        |
| R, $R_{free}$                                                           | 0.214 , 0.264<br>0.234 , (Not available)                    | Depositor<br>DCC |
| $R_{free}$ test set                                                     | No test flags present.                                      | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 46.4                                                        | Xtriage          |
| Anisotropy                                                              | 0.261                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.33 , 55.8                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.90                                                        | EDS              |
| Total number of atoms                                                   | 10852                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 42.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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 [i](#)

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

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

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

| Mol | Chain | Bond lengths |                 | Bond angles |                 |
|-----|-------|--------------|-----------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$     | RMSZ        | $\# Z  > 5$     |
| 1   | A     | 0.83         | 7/2701 (0.3%)   | 1.16        | 25/3654 (0.7%)  |
| 1   | B     | 0.72         | 3/2701 (0.1%)   | 1.11        | 8/3654 (0.2%)   |
| 1   | C     | 0.84         | 6/2701 (0.2%)   | 1.14        | 18/3654 (0.5%)  |
| 1   | D     | 0.75         | 7/2701 (0.3%)   | 1.10        | 15/3654 (0.4%)  |
| All | All   | 0.79         | 23/10804 (0.2%) | 1.13        | 66/14616 (0.5%) |

All (23) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 9   | ILE  | CA-CB   | 14.13 | 1.68        | 1.54     |
| 1   | D     | 328 | ASP  | C-O     | 10.28 | 1.36        | 1.24     |
| 1   | A     | 157 | HIS  | ND1-CE1 | 9.88  | 1.42        | 1.32     |
| 1   | A     | 157 | HIS  | CG-ND1  | -8.97 | 1.28        | 1.38     |
| 1   | D     | 54  | ASN  | C-O     | 7.92  | 1.33        | 1.23     |
| 1   | A     | 295 | CYS  | C-O     | -7.81 | 1.14        | 1.23     |
| 1   | C     | 7   | LEU  | C-O     | 7.63  | 1.30        | 1.23     |
| 1   | C     | 269 | GLY  | C-O     | -6.64 | 1.15        | 1.23     |
| 1   | D     | 53  | HIS  | CA-C    | 6.50  | 1.60        | 1.52     |
| 1   | D     | 189 | ARG  | C-N     | 6.40  | 1.41        | 1.33     |
| 1   | A     | 49  | ILE  | N-CA    | 6.26  | 1.54        | 1.46     |
| 1   | A     | 151 | MET  | SD-CE   | -6.03 | 1.64        | 1.79     |
| 1   | B     | 151 | MET  | SD-CE   | -6.02 | 1.64        | 1.79     |
| 1   | A     | 157 | HIS  | CE1-NE2 | -5.98 | 1.26        | 1.32     |
| 1   | A     | 48  | ALA  | CA-C    | 5.85  | 1.60        | 1.52     |
| 1   | C     | 188 | LEU  | C-N     | -5.74 | 1.25        | 1.33     |
| 1   | D     | 151 | MET  | SD-CE   | -5.64 | 1.65        | 1.79     |
| 1   | B     | 181 | MET  | SD-CE   | -5.41 | 1.66        | 1.79     |
| 1   | B     | 244 | GLY  | C-O     | -5.19 | 1.18        | 1.23     |
| 1   | C     | 151 | MET  | SD-CE   | -5.17 | 1.66        | 1.79     |
| 1   | D     | 181 | MET  | SD-CE   | -5.13 | 1.66        | 1.79     |
| 1   | D     | 244 | GLY  | C-O     | -5.05 | 1.18        | 1.23     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | C     | 270 | GLU  | CA-C  | -5.01 | 1.45        | 1.53     |

All (66) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | A     | 351 | LEU  | O-C-N       | -8.93 | 111.21      | 122.82   |
| 1   | D     | 328 | ASP  | O-C-N       | 8.07  | 131.39      | 122.11   |
| 1   | B     | 315 | ASP  | CA-C-N      | 8.02  | 127.66      | 119.56   |
| 1   | B     | 315 | ASP  | C-N-CA      | 8.02  | 127.66      | 119.56   |
| 1   | B     | 281 | TRP  | N-CA-C      | -7.56 | 103.36      | 112.59   |
| 1   | D     | 23  | GLY  | N-CA-C      | -7.16 | 103.30      | 112.10   |
| 1   | A     | 48  | ALA  | CA-C-O      | -6.83 | 112.38      | 120.10   |
| 1   | A     | 23  | GLY  | N-CA-C      | -6.68 | 103.88      | 112.10   |
| 1   | D     | 5   | ALA  | N-CA-C      | 6.62  | 118.19      | 108.86   |
| 1   | A     | 5   | ALA  | N-CA-C      | 6.55  | 118.10      | 108.86   |
| 1   | A     | 352 | ALA  | CB-CA-C     | -6.46 | 100.81      | 110.50   |
| 1   | D     | 54  | ASN  | CA-C-O      | -6.45 | 113.60      | 121.28   |
| 1   | B     | 23  | GLY  | N-CA-C      | -6.45 | 104.43      | 112.23   |
| 1   | B     | 5   | ALA  | N-CA-C      | 6.44  | 117.94      | 108.86   |
| 1   | C     | 9   | ILE  | O-C-N       | -6.27 | 115.98      | 122.63   |
| 1   | B     | 132 | ASN  | N-CA-C      | 6.25  | 120.21      | 112.59   |
| 1   | C     | 281 | TRP  | N-CA-C      | -6.20 | 104.08      | 112.26   |
| 1   | A     | 352 | ALA  | N-CA-C      | 6.19  | 128.33      | 111.00   |
| 1   | A     | 132 | ASN  | N-CA-C      | 6.15  | 121.54      | 113.30   |
| 1   | A     | 32  | LEU  | N-CA-C      | -6.11 | 106.46      | 114.04   |
| 1   | A     | 157 | HIS  | CB-CG-CD2   | -6.09 | 123.28      | 131.20   |
| 1   | D     | 140 | ILE  | CA-C-N      | 6.04  | 125.99      | 119.76   |
| 1   | D     | 140 | ILE  | C-N-CA      | 6.04  | 125.99      | 119.76   |
| 1   | C     | 19  | LYS  | CA-C-N      | 6.00  | 125.96      | 119.78   |
| 1   | C     | 19  | LYS  | C-N-CA      | 6.00  | 125.96      | 119.78   |
| 1   | A     | 281 | TRP  | N-CA-C      | -5.98 | 105.81      | 112.57   |
| 1   | A     | 157 | HIS  | CG-CD2-NE2  | -5.85 | 101.35      | 107.20   |
| 1   | D     | 19  | LYS  | CA-C-N      | 5.85  | 125.86      | 119.89   |
| 1   | D     | 19  | LYS  | C-N-CA      | 5.85  | 125.86      | 119.89   |
| 1   | A     | 157 | HIS  | CE1-NE2-CD2 | 5.79  | 114.79      | 109.00   |
| 1   | C     | 36  | PRO  | CA-C-N      | -5.78 | 113.73      | 122.81   |
| 1   | C     | 36  | PRO  | C-N-CA      | -5.78 | 113.73      | 122.81   |
| 1   | C     | 274 | LEU  | CA-C-N      | 5.77  | 126.67      | 119.98   |
| 1   | C     | 274 | LEU  | C-N-CA      | 5.77  | 126.67      | 119.98   |
| 1   | C     | 5   | ALA  | N-CA-C      | 5.74  | 117.32      | 109.18   |
| 1   | A     | 315 | ASP  | CA-C-N      | 5.72  | 126.47      | 120.12   |
| 1   | A     | 315 | ASP  | C-N-CA      | 5.72  | 126.47      | 120.12   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | D     | 132 | ASN  | N-CA-C | 5.70  | 120.97      | 112.94   |
| 1   | C     | 61  | ALA  | N-CA-C | 5.69  | 117.75      | 108.76   |
| 1   | D     | 281 | TRP  | N-CA-C | -5.69 | 106.24      | 112.72   |
| 1   | A     | 274 | LEU  | CA-C-N | 5.60  | 125.88      | 119.83   |
| 1   | A     | 274 | LEU  | C-N-CA | 5.60  | 125.88      | 119.83   |
| 1   | A     | 90  | TRP  | N-CA-C | 5.56  | 119.81      | 113.19   |
| 1   | D     | 182 | ALA  | N-CA-C | -5.55 | 105.23      | 112.23   |
| 1   | A     | 344 | LEU  | N-CA-C | 5.55  | 118.86      | 109.76   |
| 1   | D     | 90  | TRP  | N-CA-C | 5.52  | 119.49      | 112.87   |
| 1   | A     | 62  | VAL  | N-CA-C | -5.47 | 99.67       | 107.77   |
| 1   | C     | 9   | ILE  | CA-C-O | 5.45  | 127.36      | 121.36   |
| 1   | C     | 11  | LYS  | N-CA-C | 5.43  | 117.25      | 108.34   |
| 1   | A     | 89  | ASP  | N-CA-C | -5.41 | 98.95       | 108.20   |
| 1   | A     | 88  | PRO  | N-CA-C | 5.33  | 118.68      | 111.22   |
| 1   | D     | 32  | LEU  | N-CA-C | -5.30 | 107.48      | 114.31   |
| 1   | C     | 140 | ILE  | N-CA-C | 5.29  | 113.11      | 107.76   |
| 1   | B     | 62  | VAL  | N-CA-C | -5.28 | 100.72      | 108.11   |
| 1   | C     | 90  | TRP  | N-CA-C | 5.25  | 119.31      | 113.01   |
| 1   | A     | 140 | ILE  | CA-C-N | 5.21  | 125.13      | 119.76   |
| 1   | A     | 140 | ILE  | C-N-CA | 5.21  | 125.13      | 119.76   |
| 1   | C     | 269 | GLY  | CA-C-N | -5.21 | 112.52      | 123.20   |
| 1   | C     | 269 | GLY  | C-N-CA | -5.21 | 112.52      | 123.20   |
| 1   | B     | 322 | HIS  | CA-C-O | -5.11 | 115.34      | 121.11   |
| 1   | C     | 313 | ARG  | N-CA-C | -5.08 | 105.44      | 111.69   |
| 1   | A     | 125 | HIS  | N-CA-C | 5.08  | 116.80      | 108.52   |
| 1   | D     | 54  | ASN  | O-C-N  | 5.06  | 129.19      | 122.41   |
| 1   | A     | 83  | VAL  | N-CA-C | 5.04  | 113.48      | 107.73   |
| 1   | D     | 82  | VAL  | N-CA-C | -5.04 | 101.15      | 108.36   |
| 1   | C     | 269 | GLY  | CA-C-O | 5.01  | 129.28      | 120.57   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2643  | 0        | 2690     | 175     | 0            |
| 1   | B     | 2643  | 0        | 2690     | 159     | 0            |
| 1   | C     | 2643  | 0        | 2689     | 176     | 0            |
| 1   | D     | 2643  | 0        | 2689     | 167     | 0            |
| 2   | A     | 1     | 0        | 0        | 0       | 0            |
| 2   | B     | 1     | 0        | 0        | 0       | 0            |
| 2   | C     | 1     | 0        | 0        | 0       | 0            |
| 2   | D     | 1     | 0        | 0        | 0       | 0            |
| 3   | A     | 1     | 0        | 0        | 0       | 0            |
| 3   | B     | 1     | 0        | 0        | 0       | 0            |
| 3   | C     | 1     | 0        | 0        | 0       | 0            |
| 3   | D     | 1     | 0        | 0        | 0       | 0            |
| 4   | A     | 1     | 0        | 0        | 0       | 0            |
| 4   | B     | 1     | 0        | 0        | 0       | 0            |
| 4   | C     | 1     | 0        | 0        | 0       | 0            |
| 4   | D     | 1     | 0        | 0        | 0       | 0            |
| 5   | A     | 5     | 0        | 10       | 0       | 0            |
| 5   | B     | 5     | 0        | 10       | 0       | 0            |
| 5   | C     | 5     | 0        | 10       | 0       | 0            |
| 5   | D     | 5     | 0        | 10       | 0       | 0            |
| 6   | A     | 75    | 0        | 0        | 2       | 0            |
| 6   | B     | 63    | 0        | 0        | 2       | 0            |
| 6   | C     | 44    | 0        | 0        | 1       | 0            |
| 6   | D     | 66    | 0        | 0        | 2       | 0            |
| All | All   | 10852 | 0        | 10798    | 625     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (625) 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:C:254:LYS:HG2  | 1:C:280:GLU:HG3  | 1.33                     | 1.11              |
| 1:C:151:MET:HE2  | 1:C:177:PRO:HB2  | 1.42                     | 1.02              |
| 1:B:153:THR:HG22 | 1:B:301:ARG:HE   | 1.23                     | 1.00              |
| 1:B:147:MET:HE1  | 1:B:346:LYS:HG2  | 1.43                     | 0.97              |
| 1:A:36:PRO:HB2   | 1:A:337:MET:HG3  | 1.46                     | 0.96              |
| 1:B:254:LYS:HG2  | 1:B:280:GLU:HG3  | 1.47                     | 0.96              |
| 1:D:254:LYS:HG2  | 1:D:280:GLU:HG3  | 1.44                     | 0.96              |
| 1:C:36:PRO:HB2   | 1:C:337:MET:HG3  | 1.49                     | 0.95              |
| 1:C:152:MET:HG2  | 1:C:305:LEU:HD13 | 1.49                     | 0.94              |
| 1:C:153:THR:HG22 | 1:C:301:ARG:HE   | 1.32                     | 0.93              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:254:LYS:HG2  | 1:A:280:GLU:HG3  | 1.50                     | 0.92              |
| 1:C:147:MET:HE1  | 1:C:346:LYS:HG2  | 1.52                     | 0.91              |
| 1:A:147:MET:HE1  | 1:A:346:LYS:HG2  | 1.54                     | 0.89              |
| 1:A:151:MET:HE2  | 1:A:177:PRO:HB2  | 1.53                     | 0.89              |
| 1:D:327:PHE:CE1  | 1:D:352:ALA:HB1  | 2.08                     | 0.88              |
| 1:D:147:MET:HE1  | 1:D:346:LYS:HG2  | 1.58                     | 0.86              |
| 1:D:245:ASN:O    | 1:D:248:ILE:HG22 | 1.75                     | 0.86              |
| 1:B:36:PRO:HB2   | 1:B:337:MET:HG3  | 1.56                     | 0.85              |
| 1:B:52:ARG:HH11  | 1:B:55:MET:HE1   | 1.41                     | 0.85              |
| 1:A:94:GLU:HG3   | 1:A:102:HIS:O    | 1.77                     | 0.84              |
| 1:D:153:THR:HG22 | 1:D:301:ARG:HE   | 1.41                     | 0.84              |
| 1:A:337:MET:HA   | 1:A:337:MET:HE2  | 1.59                     | 0.84              |
| 1:B:151:MET:HE2  | 1:B:177:PRO:HB2  | 1.60                     | 0.83              |
| 1:B:92:THR:HG22  | 1:B:95:VAL:HG23  | 1.58                     | 0.83              |
| 1:B:14:TRP:CH2   | 1:B:327:PHE:HB3  | 2.14                     | 0.83              |
| 1:D:36:PRO:HB2   | 1:D:337:MET:HG3  | 1.62                     | 0.82              |
| 1:C:52:ARG:HH11  | 1:C:55:MET:HE1   | 1.47                     | 0.79              |
| 1:C:272:GLU:OE2  | 1:D:279:LEU:HB2  | 1.79                     | 0.79              |
| 1:C:94:GLU:HG3   | 1:C:102:HIS:O    | 1.82                     | 0.79              |
| 1:C:327:PHE:CD1  | 1:C:352:ALA:HB1  | 2.17                     | 0.79              |
| 1:C:278:ARG:HD3  | 1:D:271:GLY:O    | 1.82                     | 0.79              |
| 1:C:299:ARG:O    | 1:C:303:GLU:HG3  | 1.82                     | 0.79              |
| 1:B:181:MET:HA   | 1:B:181:MET:HE2  | 1.65                     | 0.79              |
| 1:A:92:THR:HG22  | 1:A:95:VAL:HG23  | 1.62                     | 0.79              |
| 1:B:228:MET:HE3  | 1:B:233:GLY:HA2  | 1.66                     | 0.78              |
| 1:C:94:GLU:CD    | 1:C:94:GLU:H     | 1.91                     | 0.77              |
| 1:A:148:ILE:HG22 | 1:A:302:MET:HE1  | 1.66                     | 0.77              |
| 1:D:151:MET:HE1  | 1:D:178:VAL:HG23 | 1.66                     | 0.77              |
| 1:C:336:LEU:HG   | 1:C:344:LEU:HD22 | 1.67                     | 0.76              |
| 1:D:151:MET:HE2  | 1:D:177:PRO:HB2  | 1.67                     | 0.76              |
| 1:C:31:PRO:HG2   | 1:C:352:ALA:OXT  | 1.84                     | 0.76              |
| 1:B:31:PRO:O     | 1:B:352:ALA:HB2  | 1.86                     | 0.76              |
| 1:B:152:MET:HG2  | 1:B:305:LEU:HD13 | 1.67                     | 0.76              |
| 1:C:142:LEU:O    | 1:C:146:VAL:HG23 | 1.86                     | 0.75              |
| 1:D:337:MET:HE3  | 1:D:344:LEU:HD21 | 1.66                     | 0.75              |
| 1:D:152:MET:HG2  | 1:D:305:LEU:HD13 | 1.69                     | 0.75              |
| 1:D:176:GLY:O    | 1:D:180:LEU:HG   | 1.87                     | 0.74              |
| 1:D:224:GLU:O    | 1:D:228:MET:HG2  | 1.87                     | 0.74              |
| 1:C:228:MET:HE3  | 1:C:233:GLY:HA2  | 1.68                     | 0.74              |
| 1:B:337:MET:HE3  | 1:B:344:LEU:HD21 | 1.71                     | 0.73              |
| 1:A:337:MET:CE   | 1:A:344:LEU:HD21 | 2.19                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:9:ILE:HG13   | 1:C:51:GLU:OE1   | 1.89                     | 0.73              |
| 1:B:224:GLU:O    | 1:B:228:MET:HG2  | 1.88                     | 0.72              |
| 1:A:279:LEU:HB2  | 1:B:272:GLU:OE2  | 1.88                     | 0.72              |
| 1:C:151:MET:HE2  | 1:C:177:PRO:CB   | 2.17                     | 0.72              |
| 1:A:153:THR:HG22 | 1:A:301:ARG:HE   | 1.54                     | 0.72              |
| 1:B:14:TRP:HH2   | 1:B:327:PHE:HB3  | 1.54                     | 0.72              |
| 1:A:271:GLY:O    | 1:B:278:ARG:HD3  | 1.89                     | 0.72              |
| 1:D:94:GLU:HG3   | 1:D:102:HIS:O    | 1.90                     | 0.72              |
| 1:B:153:THR:HG22 | 1:B:301:ARG:NE   | 2.00                     | 0.71              |
| 1:A:147:MET:HE2  | 1:A:319:LEU:CB   | 2.20                     | 0.71              |
| 1:C:271:GLY:O    | 1:D:278:ARG:HD3  | 1.91                     | 0.71              |
| 1:D:14:TRP:CH2   | 1:D:327:PHE:HB3  | 2.25                     | 0.71              |
| 1:D:156:PHE:O    | 1:D:160:GLU:HG3  | 1.90                     | 0.71              |
| 1:D:228:MET:HE3  | 1:D:233:GLY:HA2  | 1.73                     | 0.71              |
| 1:A:337:MET:HE3  | 1:A:344:LEU:HD21 | 1.71                     | 0.71              |
| 1:C:337:MET:HE2  | 1:C:337:MET:HA   | 1.71                     | 0.71              |
| 1:A:94:GLU:CD    | 1:A:94:GLU:H     | 1.98                     | 0.71              |
| 1:A:5:ALA:HB2    | 1:A:56:ILE:HA    | 1.73                     | 0.70              |
| 1:B:30:ARG:HB2   | 1:B:66:VAL:HG11  | 1.72                     | 0.70              |
| 1:A:142:LEU:O    | 1:A:146:VAL:HG23 | 1.92                     | 0.69              |
| 1:C:5:ALA:HB2    | 1:C:56:ILE:HA    | 1.74                     | 0.69              |
| 1:A:49:ILE:HG21  | 1:A:52:ARG:HH12  | 1.57                     | 0.69              |
| 1:D:197:VAL:HG11 | 1:D:223:ILE:HD13 | 1.73                     | 0.69              |
| 1:C:106:MET:HE2  | 1:D:258:PRO:HG3  | 1.73                     | 0.68              |
| 1:D:337:MET:HA   | 1:D:337:MET:HE2  | 1.75                     | 0.68              |
| 1:B:337:MET:HE2  | 1:B:337:MET:HA   | 1.75                     | 0.68              |
| 1:C:102:HIS:NE2  | 1:D:286:ALA:HA   | 2.09                     | 0.68              |
| 1:C:249:MET:HE2  | 1:C:276:VAL:HG22 | 1.76                     | 0.68              |
| 1:C:250:ALA:O    | 1:C:254:LYS:HG3  | 1.94                     | 0.68              |
| 1:D:249:MET:HE1  | 1:D:290:ILE:HD13 | 1.76                     | 0.67              |
| 1:A:318:LYS:N    | 1:A:318:LYS:HD2  | 2.09                     | 0.67              |
| 1:B:336:LEU:HG   | 1:B:344:LEU:HD22 | 1.76                     | 0.67              |
| 1:C:279:LEU:HB2  | 1:D:272:GLU:OE2  | 1.95                     | 0.67              |
| 1:D:94:GLU:CD    | 1:D:94:GLU:H     | 2.02                     | 0.67              |
| 1:A:151:MET:HE2  | 1:A:177:PRO:CB   | 2.24                     | 0.67              |
| 1:C:37:CYS:HB2   | 1:C:60:GLU:OE2   | 1.94                     | 0.67              |
| 1:A:302:MET:O    | 1:A:306:ILE:HG13 | 1.95                     | 0.67              |
| 1:A:86:ILE:HG22  | 1:A:88:PRO:HD3   | 1.78                     | 0.66              |
| 1:A:228:MET:HE3  | 1:A:233:GLY:HA2  | 1.77                     | 0.66              |
| 1:B:101:GLN:HB3  | 1:B:294:LEU:HD23 | 1.77                     | 0.66              |
| 1:B:52:ARG:NH1   | 1:B:55:MET:HE1   | 2.09                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:52:ARG:HH11  | 1:D:55:MET:HE1   | 1.60                     | 0.66              |
| 1:A:131:MET:HE2  | 1:A:131:MET:HA   | 1.77                     | 0.66              |
| 1:A:272:GLU:OE2  | 1:B:279:LEU:HB2  | 1.95                     | 0.66              |
| 1:B:197:VAL:HG11 | 1:B:223:ILE:HD13 | 1.77                     | 0.65              |
| 1:B:312:LYS:HD2  | 1:B:312:LYS:N    | 2.12                     | 0.65              |
| 1:B:142:LEU:O    | 1:B:146:VAL:HG23 | 1.96                     | 0.65              |
| 1:C:179:GLY:O    | 1:C:183:VAL:HG23 | 1.96                     | 0.65              |
| 1:B:156:PHE:O    | 1:B:160:GLU:HG3  | 1.97                     | 0.65              |
| 1:D:5:ALA:HB2    | 1:D:56:ILE:HA    | 1.79                     | 0.65              |
| 1:D:14:TRP:HH2   | 1:D:327:PHE:HB3  | 1.60                     | 0.65              |
| 1:D:156:PHE:CE1  | 1:D:181:MET:HE3  | 2.30                     | 0.65              |
| 1:C:176:GLY:O    | 1:C:180:LEU:HG   | 1.97                     | 0.65              |
| 1:C:86:ILE:CG2   | 1:C:88:PRO:HD3   | 2.27                     | 0.65              |
| 1:A:166:LEU:HD21 | 1:C:189:ARG:HD3  | 1.79                     | 0.64              |
| 1:C:30:ARG:HB2   | 1:C:66:VAL:HG11  | 1.78                     | 0.64              |
| 1:A:156:PHE:O    | 1:A:160:GLU:HG3  | 1.97                     | 0.64              |
| 1:C:293:GLY:HA2  | 1:D:285:MET:HA   | 1.78                     | 0.64              |
| 1:C:151:MET:HE1  | 1:C:178:VAL:HG23 | 1.80                     | 0.64              |
| 1:D:302:MET:O    | 1:D:306:ILE:HG13 | 1.97                     | 0.64              |
| 1:C:12:VAL:HG13  | 1:C:44:VAL:HG11  | 1.79                     | 0.64              |
| 1:B:318:LYS:HD2  | 1:B:318:LYS:N    | 2.12                     | 0.63              |
| 1:C:153:THR:HG22 | 1:C:301:ARG:NE   | 2.10                     | 0.63              |
| 1:B:131:MET:HA   | 1:B:131:MET:HE2  | 1.80                     | 0.63              |
| 1:A:152:MET:HE3  | 1:A:314:VAL:HG21 | 1.81                     | 0.63              |
| 1:A:278:ARG:HH21 | 1:B:269:GLY:HA2  | 1.63                     | 0.63              |
| 1:B:148:ILE:HG22 | 1:B:302:MET:HE1  | 1.81                     | 0.63              |
| 1:B:94:GLU:HG3   | 1:B:102:HIS:O    | 1.99                     | 0.63              |
| 1:A:148:ILE:HG22 | 1:A:302:MET:CE   | 2.28                     | 0.62              |
| 1:A:153:THR:HG22 | 1:A:301:ARG:NE   | 2.13                     | 0.62              |
| 1:D:82:VAL:HG12  | 1:D:302:MET:HE2  | 1.81                     | 0.62              |
| 1:C:281:TRP:CZ3  | 1:C:284:GLY:HA2  | 2.34                     | 0.62              |
| 1:B:176:GLY:O    | 1:B:180:LEU:HG   | 1.98                     | 0.62              |
| 1:C:148:ILE:HG22 | 1:C:302:MET:HE1  | 1.81                     | 0.62              |
| 1:B:5:ALA:HB2    | 1:B:56:ILE:HA    | 1.82                     | 0.62              |
| 1:D:142:LEU:O    | 1:D:146:VAL:HG23 | 2.00                     | 0.62              |
| 1:D:236:VAL:O    | 1:D:257:LYS:HG3  | 2.00                     | 0.62              |
| 1:A:344:LEU:HD11 | 1:A:347:PRO:HD3  | 1.81                     | 0.62              |
| 1:B:152:MET:HE3  | 1:B:314:VAL:HG21 | 1.82                     | 0.62              |
| 1:C:126:VAL:HG11 | 1:C:133:LEU:HD21 | 1.81                     | 0.62              |
| 1:C:2:LYS:HE2    | 1:C:14:TRP:CE3   | 2.34                     | 0.62              |
| 1:A:151:MET:HE1  | 1:A:178:VAL:HG23 | 1.82                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:166:LEU:HD21 | 1:D:189:ARG:HD3  | 1.82                     | 0.61              |
| 1:A:102:HIS:HE1  | 1:B:287:HIS:CD2  | 2.18                     | 0.61              |
| 1:B:92:THR:CG2   | 1:B:95:VAL:HG23  | 2.29                     | 0.61              |
| 1:D:299:ARG:O    | 1:D:303:GLU:HG3  | 2.00                     | 0.61              |
| 1:A:256:VAL:O    | 1:A:288:LYS:HE2  | 2.00                     | 0.61              |
| 1:C:143:GLU:H    | 1:C:143:GLU:CD   | 2.07                     | 0.61              |
| 1:C:171:ALA:HB2  | 1:C:236:VAL:HG11 | 1.81                     | 0.61              |
| 1:D:281:TRP:CE3  | 1:D:284:GLY:HA2  | 2.35                     | 0.61              |
| 1:C:31:PRO:CG    | 1:C:352:ALA:OXT  | 2.48                     | 0.61              |
| 1:C:36:PRO:HD2   | 1:C:347:PRO:HG2  | 1.82                     | 0.61              |
| 1:D:351:LEU:C    | 1:D:351:LEU:HD13 | 2.25                     | 0.61              |
| 1:A:299:ARG:O    | 1:A:303:GLU:HG3  | 2.00                     | 0.61              |
| 1:A:179:GLY:O    | 1:A:183:VAL:HG23 | 2.00                     | 0.61              |
| 1:D:147:MET:HE2  | 1:D:319:LEU:CB   | 2.30                     | 0.61              |
| 1:C:318:LYS:N    | 1:C:318:LYS:HD2  | 2.14                     | 0.61              |
| 1:D:318:LYS:HD2  | 1:D:318:LYS:N    | 2.16                     | 0.61              |
| 1:A:92:THR:HG21  | 1:A:103:SER:OG   | 2.01                     | 0.60              |
| 1:B:12:VAL:CG1   | 1:B:44:VAL:HG11  | 2.31                     | 0.60              |
| 1:B:313:ARG:HD3  | 1:D:191:ALA:O    | 2.01                     | 0.60              |
| 1:A:52:ARG:HD2   | 1:A:55:MET:CE    | 2.31                     | 0.60              |
| 1:A:278:ARG:NH2  | 1:B:269:GLY:HA2  | 2.15                     | 0.60              |
| 1:A:147:MET:HE2  | 1:A:319:LEU:HB3  | 1.82                     | 0.60              |
| 1:A:52:ARG:HH11  | 1:A:55:MET:HE1   | 1.66                     | 0.60              |
| 1:B:30:ARG:HB2   | 1:B:66:VAL:CG1   | 2.32                     | 0.60              |
| 1:A:236:VAL:O    | 1:A:257:LYS:HG3  | 2.02                     | 0.60              |
| 1:A:256:VAL:HG21 | 1:A:262:ILE:HG12 | 1.83                     | 0.60              |
| 1:A:249:MET:HE1  | 1:A:290:ILE:HD13 | 1.84                     | 0.60              |
| 1:D:336:LEU:HG   | 1:D:344:LEU:HD22 | 1.83                     | 0.60              |
| 1:A:12:VAL:HG13  | 1:A:44:VAL:HG11  | 1.83                     | 0.59              |
| 1:B:2:LYS:H      | 1:B:122:GLU:CD   | 2.10                     | 0.59              |
| 1:B:322:HIS:ND1  | 1:B:344:LEU:HD13 | 2.16                     | 0.59              |
| 1:D:84:PRO:HD3   | 1:D:302:MET:HG3  | 1.84                     | 0.59              |
| 1:A:166:LEU:CD2  | 1:C:189:ARG:HH11 | 2.16                     | 0.59              |
| 1:D:92:THR:HG22  | 1:D:95:VAL:HG23  | 1.83                     | 0.59              |
| 1:D:151:MET:HE2  | 1:D:177:PRO:CB   | 2.32                     | 0.59              |
| 1:A:92:THR:HG22  | 1:A:95:VAL:CG2   | 2.30                     | 0.59              |
| 1:A:281:TRP:CE3  | 1:A:284:GLY:HA2  | 2.37                     | 0.59              |
| 1:B:86:ILE:HG22  | 1:B:88:PRO:HD3   | 1.84                     | 0.59              |
| 1:A:92:THR:CG2   | 1:A:95:VAL:HG23  | 2.31                     | 0.59              |
| 1:A:171:ALA:HB2  | 1:A:236:VAL:HG11 | 1.85                     | 0.59              |
| 1:A:147:MET:HE2  | 1:A:319:LEU:HB2  | 1.85                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:325:ARG:HG3  | 1:A:325:ARG:HH11 | 1.66                     | 0.59              |
| 1:D:131:MET:HE2  | 1:D:131:MET:HA   | 1.85                     | 0.59              |
| 1:B:264:ASN:O    | 1:B:292:GLY:HA2  | 2.03                     | 0.58              |
| 1:C:337:MET:HA   | 1:C:337:MET:CE   | 2.33                     | 0.58              |
| 1:D:2:LYS:HE2    | 1:D:14:TRP:CE3   | 2.37                     | 0.58              |
| 1:A:8:SER:OG     | 1:A:11:LYS:HD2   | 2.04                     | 0.58              |
| 1:A:94:GLU:HG2   | 1:A:103:SER:HA   | 1.85                     | 0.58              |
| 1:D:148:ILE:HG22 | 1:D:302:MET:HE1  | 1.85                     | 0.58              |
| 1:C:281:TRP:CE3  | 1:C:284:GLY:HA2  | 2.39                     | 0.58              |
| 1:D:246:ALA:O    | 1:D:275:PRO:HD2  | 2.04                     | 0.58              |
| 1:D:5:ALA:CB     | 1:D:56:ILE:HA    | 2.34                     | 0.58              |
| 1:D:193:ARG:NH2  | 1:D:230:LEU:HB3  | 2.19                     | 0.57              |
| 1:A:245:ASN:HD21 | 1:A:270:GLU:CG   | 2.17                     | 0.57              |
| 1:B:82:VAL:HG12  | 1:B:302:MET:HE2  | 1.86                     | 0.57              |
| 1:C:157:HIS:CE1  | 1:D:287:HIS:HE2  | 2.21                     | 0.57              |
| 1:D:147:MET:HE2  | 1:D:319:LEU:HB3  | 1.86                     | 0.57              |
| 1:D:173:LEU:HD13 | 1:D:248:ILE:HD11 | 1.85                     | 0.57              |
| 1:A:191:ALA:O    | 1:C:313:ARG:HD3  | 2.04                     | 0.57              |
| 1:A:253:VAL:HA   | 1:A:262:ILE:HD11 | 1.87                     | 0.57              |
| 1:B:56:ILE:HB    | 1:B:117:ASP:HB3  | 1.87                     | 0.57              |
| 1:D:264:ASN:ND2  | 1:D:268:PHE:HE1  | 2.03                     | 0.56              |
| 1:D:249:MET:HE2  | 1:D:276:VAL:HG22 | 1.87                     | 0.56              |
| 1:B:262:ILE:HD12 | 1:B:262:ILE:N    | 2.20                     | 0.56              |
| 1:C:34:VAL:HG12  | 1:C:61:ALA:HB2   | 1.87                     | 0.56              |
| 1:D:43:THR:HG23  | 1:D:49:ILE:HG12  | 1.88                     | 0.56              |
| 1:A:52:ARG:HH11  | 1:A:52:ARG:HG3   | 1.70                     | 0.56              |
| 1:A:278:ARG:HD3  | 1:B:271:GLY:O    | 2.04                     | 0.56              |
| 1:C:49:ILE:HD12  | 1:C:52:ARG:HH12  | 1.71                     | 0.56              |
| 1:D:36:PRO:HD2   | 1:D:347:PRO:HG2  | 1.88                     | 0.56              |
| 1:A:102:HIS:NE2  | 1:B:286:ALA:HA   | 2.20                     | 0.56              |
| 1:C:82:VAL:HG12  | 1:C:302:MET:HE2  | 1.87                     | 0.56              |
| 1:C:131:MET:HE2  | 1:C:131:MET:HA   | 1.88                     | 0.56              |
| 1:C:92:THR:HG22  | 1:C:95:VAL:HG23  | 1.87                     | 0.56              |
| 1:B:94:GLU:H     | 1:B:94:GLU:CD    | 2.13                     | 0.56              |
| 1:A:201:PRO:HA   | 1:A:204:VAL:HG22 | 1.88                     | 0.56              |
| 1:B:84:PRO:HD3   | 1:B:302:MET:HG3  | 1.87                     | 0.56              |
| 1:B:151:MET:HE1  | 1:B:178:VAL:HG23 | 1.87                     | 0.56              |
| 1:B:249:MET:HE1  | 1:B:290:ILE:HD13 | 1.87                     | 0.55              |
| 1:D:312:LYS:HD2  | 1:D:312:LYS:N    | 2.21                     | 0.55              |
| 1:A:5:ALA:CB     | 1:A:56:ILE:HA    | 2.36                     | 0.55              |
| 1:B:2:LYS:O      | 1:B:122:GLU:HG3  | 2.07                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:52:ARG:NH1   | 1:C:55:MET:HE1   | 2.19                     | 0.55              |
| 1:B:36:PRO:HD2   | 1:B:347:PRO:HG2  | 1.88                     | 0.55              |
| 1:B:254:LYS:CG   | 1:B:280:GLU:HG3  | 2.29                     | 0.55              |
| 1:B:272:GLU:HG2  | 6:B:435:HOH:O    | 2.06                     | 0.55              |
| 1:D:143:GLU:CD   | 1:D:143:GLU:H    | 2.15                     | 0.55              |
| 1:A:14:TRP:CH2   | 1:A:327:PHE:HB3  | 2.41                     | 0.55              |
| 1:A:296:PRO:HG2  | 1:A:301:ARG:NE   | 2.20                     | 0.55              |
| 1:C:14:TRP:CH2   | 1:C:327:PHE:HB3  | 2.41                     | 0.55              |
| 1:C:308:LEU:O    | 1:C:313:ARG:HB2  | 2.06                     | 0.55              |
| 1:A:22:PRO:HG3   | 1:A:67:GLU:HG2   | 1.89                     | 0.55              |
| 1:A:94:GLU:CG    | 1:A:103:SER:HA   | 2.36                     | 0.55              |
| 1:B:12:VAL:HG13  | 1:B:44:VAL:HG11  | 1.87                     | 0.55              |
| 1:A:311:TYR:CE2  | 1:C:193:ARG:HB2  | 2.41                     | 0.55              |
| 1:D:264:ASN:HD21 | 1:D:268:PHE:HE1  | 1.53                     | 0.55              |
| 1:D:86:ILE:HG22  | 1:D:88:PRO:HD3   | 1.89                     | 0.55              |
| 1:A:312:LYS:HD2  | 1:A:312:LYS:N    | 2.22                     | 0.55              |
| 1:C:224:GLU:O    | 1:C:228:MET:HG2  | 2.07                     | 0.55              |
| 1:C:82:VAL:CG1   | 1:C:302:MET:HE2  | 2.36                     | 0.54              |
| 1:A:84:PRO:HD3   | 1:A:302:MET:HG3  | 1.88                     | 0.54              |
| 1:A:139:GLU:H    | 1:A:139:GLU:CD   | 2.15                     | 0.54              |
| 1:C:86:ILE:HG22  | 1:C:88:PRO:HD3   | 1.88                     | 0.54              |
| 1:C:236:VAL:O    | 1:C:257:LYS:HG3  | 2.06                     | 0.54              |
| 1:A:224:GLU:O    | 1:A:228:MET:HG2  | 2.07                     | 0.54              |
| 1:C:143:GLU:OE2  | 1:C:350:ILE:HD11 | 2.08                     | 0.54              |
| 1:C:11:LYS:HA    | 6:C:624:HOH:O    | 2.07                     | 0.54              |
| 1:A:49:ILE:HG22  | 1:A:52:ARG:NH2   | 2.22                     | 0.54              |
| 1:A:252:ALA:O    | 1:A:256:VAL:HG23 | 2.07                     | 0.54              |
| 1:A:161:LEU:O    | 1:A:291:LYS:HD2  | 2.08                     | 0.54              |
| 1:B:44:VAL:HG21  | 1:B:57:LEU:HD11  | 1.90                     | 0.54              |
| 1:D:250:ALA:O    | 1:D:254:LYS:HG3  | 2.06                     | 0.54              |
| 1:C:138:LYS:HD3  | 1:C:139:GLU:OE2  | 2.07                     | 0.54              |
| 1:C:325:ARG:HH11 | 1:C:325:ARG:HG3  | 1.72                     | 0.54              |
| 1:C:52:ARG:HH11  | 1:C:52:ARG:HG3   | 1.73                     | 0.53              |
| 1:C:287:HIS:CE1  | 1:D:293:GLY:HA3  | 2.43                     | 0.53              |
| 1:C:126:VAL:HG11 | 1:C:133:LEU:CD2  | 2.37                     | 0.53              |
| 1:B:84:PRO:HB3   | 1:B:302:MET:SD   | 2.48                     | 0.53              |
| 1:B:139:GLU:HG3  | 1:B:310:PHE:HE1  | 1.73                     | 0.53              |
| 1:D:49:ILE:HD12  | 1:D:52:ARG:HH12  | 1.74                     | 0.53              |
| 1:A:22:PRO:HD3   | 1:A:28:ILE:CG1   | 2.39                     | 0.53              |
| 1:B:139:GLU:HG3  | 1:B:310:PHE:CE1  | 2.43                     | 0.53              |
| 1:C:197:VAL:HG11 | 1:C:223:ILE:HD13 | 1.90                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:94:GLU:CG    | 1:C:103:SER:HA   | 2.39                     | 0.53              |
| 1:C:264:ASN:O    | 1:C:292:GLY:HA2  | 2.09                     | 0.53              |
| 1:A:138:LYS:HD3  | 1:A:139:GLU:OE2  | 2.09                     | 0.53              |
| 1:C:148:ILE:HG22 | 1:C:302:MET:CE   | 2.38                     | 0.53              |
| 1:D:175:ILE:HG21 | 1:D:196:ALA:HB1  | 1.91                     | 0.53              |
| 1:A:245:ASN:O    | 1:A:248:ILE:HG22 | 2.09                     | 0.52              |
| 1:B:302:MET:O    | 1:B:306:ILE:HG13 | 2.09                     | 0.52              |
| 1:B:97:ARG:HG2   | 1:C:300:LEU:HD21 | 1.91                     | 0.52              |
| 1:B:151:MET:HE2  | 1:B:177:PRO:CB   | 2.36                     | 0.52              |
| 1:C:147:MET:CE   | 1:C:346:LYS:HG2  | 2.33                     | 0.52              |
| 1:C:68:VAL:HG11  | 1:C:75:PHE:O     | 2.10                     | 0.52              |
| 1:C:58:GLY:C     | 1:C:119:VAL:HG22 | 2.33                     | 0.52              |
| 1:A:52:ARG:HD2   | 1:A:55:MET:HE3   | 1.91                     | 0.52              |
| 1:A:166:LEU:HD23 | 1:C:189:ARG:HH11 | 1.75                     | 0.52              |
| 1:A:293:GLY:HA3  | 1:B:287:HIS:CD2  | 2.45                     | 0.52              |
| 1:C:5:ALA:CB     | 1:C:56:ILE:HA    | 2.38                     | 0.52              |
| 1:A:192:GLY:O    | 1:C:313:ARG:NH1  | 2.41                     | 0.51              |
| 1:A:277:PRO:HB2  | 1:A:280:GLU:HG2  | 1.92                     | 0.51              |
| 1:B:38:THR:O     | 1:B:41:ILE:HB    | 2.08                     | 0.51              |
| 1:D:182:ALA:HB1  | 1:D:240:ILE:HG21 | 1.92                     | 0.51              |
| 1:B:299:ARG:O    | 1:B:303:GLU:HG3  | 2.09                     | 0.51              |
| 1:C:86:ILE:HG23  | 1:C:88:PRO:HD3   | 1.93                     | 0.51              |
| 1:C:201:PRO:HA   | 1:C:204:VAL:HG22 | 1.90                     | 0.51              |
| 1:D:92:THR:HG21  | 1:D:103:SER:OG   | 2.10                     | 0.51              |
| 1:A:153:THR:CG2  | 1:A:301:ARG:HE   | 2.22                     | 0.51              |
| 1:B:1:MET:HB3    | 1:B:17:LYS:O     | 2.11                     | 0.51              |
| 1:D:52:ARG:NH1   | 1:D:55:MET:HE1   | 2.25                     | 0.51              |
| 1:B:143:GLU:CD   | 1:B:143:GLU:H    | 2.18                     | 0.51              |
| 1:C:339:ASP:O    | 1:C:341:PRO:HD3  | 2.10                     | 0.51              |
| 1:A:175:ILE:HG12 | 1:A:198:GLY:HA3  | 1.91                     | 0.51              |
| 1:A:313:ARG:HD3  | 1:C:191:ALA:O    | 2.11                     | 0.51              |
| 1:B:148:ILE:HG22 | 1:B:302:MET:CE   | 2.40                     | 0.51              |
| 1:C:164:ILE:HD13 | 1:C:170:VAL:HG21 | 1.93                     | 0.51              |
| 1:C:249:MET:CE   | 1:C:276:VAL:HG22 | 2.40                     | 0.51              |
| 1:C:336:LEU:HD11 | 1:C:341:PRO:HG2  | 1.93                     | 0.51              |
| 1:D:61:ALA:HB2   | 1:D:119:VAL:HG21 | 1.93                     | 0.51              |
| 1:D:320:VAL:HA   | 1:D:346:LYS:O    | 2.11                     | 0.51              |
| 1:C:92:THR:HG21  | 1:C:103:SER:HA   | 1.92                     | 0.50              |
| 1:C:156:PHE:O    | 1:C:160:GLU:HG3  | 2.11                     | 0.50              |
| 1:A:208:LYS:HD2  | 6:A:456:HOH:O    | 2.09                     | 0.50              |
| 1:B:1:MET:O      | 1:B:16:GLU:HA    | 2.10                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:287:HIS:ND1  | 1:D:102:HIS:HE1  | 2.09                     | 0.50              |
| 1:D:256:VAL:O    | 1:D:288:LYS:HE2  | 2.11                     | 0.50              |
| 1:D:279:LEU:HB3  | 1:D:280:GLU:OE2  | 2.12                     | 0.50              |
| 1:A:51:GLU:HG3   | 1:A:53:HIS:CE1   | 2.47                     | 0.50              |
| 1:B:139:GLU:CG   | 1:B:310:PHE:HE1  | 2.24                     | 0.50              |
| 1:B:225:SER:O    | 1:B:229:ASN:ND2  | 2.45                     | 0.50              |
| 1:C:30:ARG:HB2   | 1:C:66:VAL:CG1   | 2.41                     | 0.50              |
| 1:C:344:LEU:HD11 | 1:C:347:PRO:HD3  | 1.92                     | 0.50              |
| 1:D:264:ASN:O    | 1:D:292:GLY:HA2  | 2.11                     | 0.50              |
| 1:A:152:MET:HG2  | 1:A:305:LEU:HD13 | 1.94                     | 0.50              |
| 1:A:269:GLY:HA2  | 1:B:278:ARG:HH21 | 1.76                     | 0.50              |
| 1:B:151:MET:HE1  | 1:B:177:PRO:HG2  | 1.92                     | 0.50              |
| 1:C:201:PRO:O    | 1:C:204:VAL:HG22 | 2.12                     | 0.50              |
| 1:C:218:TYR:CD1  | 1:C:218:TYR:C    | 2.89                     | 0.50              |
| 1:D:12:VAL:HG13  | 1:D:44:VAL:HG11  | 1.93                     | 0.50              |
| 1:D:201:PRO:HA   | 1:D:204:VAL:HG22 | 1.93                     | 0.50              |
| 1:A:102:HIS:CD2  | 1:A:107:LEU:H    | 2.29                     | 0.50              |
| 1:A:129:ALA:HB1  | 1:A:133:LEU:HD12 | 1.92                     | 0.50              |
| 1:A:223:ILE:O    | 1:A:227:ILE:HD13 | 2.11                     | 0.50              |
| 1:B:26:ASP:OD1   | 1:B:127:ASN:HA   | 2.12                     | 0.50              |
| 1:B:29:VAL:HB    | 1:B:124:PHE:CE1  | 2.47                     | 0.50              |
| 1:D:337:MET:HA   | 1:D:337:MET:CE   | 2.41                     | 0.50              |
| 1:A:176:GLY:O    | 1:A:180:LEU:HG   | 2.12                     | 0.50              |
| 1:A:181:MET:SD   | 1:A:319:LEU:HD11 | 2.51                     | 0.50              |
| 1:C:156:PHE:CE1  | 1:C:181:MET:HE3  | 2.47                     | 0.50              |
| 1:A:5:ALA:HB1    | 1:A:55:MET:O     | 2.12                     | 0.50              |
| 1:B:175:ILE:HG13 | 1:B:203:CYS:HB3  | 1.93                     | 0.49              |
| 1:C:285:MET:HE2  | 6:D:501:HOH:O    | 2.11                     | 0.49              |
| 1:D:59:HIS:HE1   | 1:D:150:ASP:OD2  | 1.94                     | 0.49              |
| 1:A:49:ILE:HG22  | 1:A:52:ARG:HH22  | 1.75                     | 0.49              |
| 1:D:184:ALA:O    | 1:D:188:LEU:HG   | 2.13                     | 0.49              |
| 1:A:173:LEU:HB3  | 1:A:248:ILE:HD11 | 1.93                     | 0.49              |
| 1:B:323:VAL:HA   | 1:B:348:VAL:O    | 2.12                     | 0.49              |
| 1:B:329:ASN:ND2  | 1:B:332:LYS:HE2  | 2.28                     | 0.49              |
| 1:B:337:MET:HA   | 1:B:337:MET:CE   | 2.43                     | 0.49              |
| 1:C:24:PRO:HG2   | 1:C:25:PHE:CD1   | 2.47                     | 0.49              |
| 1:C:302:MET:O    | 1:C:306:ILE:HG13 | 2.12                     | 0.49              |
| 1:A:87:THR:HG22  | 1:A:127:ASN:OD1  | 2.12                     | 0.49              |
| 1:B:192:GLY:O    | 1:D:313:ARG:NH1  | 2.39                     | 0.49              |
| 1:B:256:VAL:CG1  | 1:B:260:GLY:HA3  | 2.43                     | 0.49              |
| 1:C:34:VAL:HG12  | 1:C:61:ALA:CB    | 2.42                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:308:LEU:O    | 1:D:313:ARG:HB2  | 2.12                     | 0.49              |
| 1:A:337:MET:HA   | 1:A:337:MET:CE   | 2.36                     | 0.49              |
| 1:D:92:THR:HG21  | 1:D:103:SER:HA   | 1.95                     | 0.49              |
| 1:B:298:GLY:O    | 1:B:302:MET:HG2  | 2.13                     | 0.49              |
| 1:D:280:GLU:H    | 1:D:280:GLU:CD   | 2.19                     | 0.49              |
| 1:A:246:ALA:HB1  | 1:A:275:PRO:HD3  | 1.94                     | 0.48              |
| 1:A:318:LYS:N    | 1:A:318:LYS:CD   | 2.76                     | 0.48              |
| 1:A:152:MET:HG3  | 1:A:181:MET:CE   | 2.43                     | 0.48              |
| 1:C:92:THR:CG2   | 1:C:94:GLU:HG2   | 2.43                     | 0.48              |
| 1:C:157:HIS:HE1  | 1:D:287:HIS:HE2  | 1.61                     | 0.48              |
| 1:C:8:SER:HB3    | 1:C:11:LYS:HD2   | 1.95                     | 0.48              |
| 1:D:339:ASP:OD1  | 1:D:339:ASP:N    | 2.45                     | 0.48              |
| 1:A:157:HIS:CE1  | 1:B:287:HIS:HE1  | 2.31                     | 0.48              |
| 1:C:174:GLY:O    | 1:C:179:GLY:HA3  | 2.13                     | 0.48              |
| 1:C:323:VAL:HA   | 1:C:348:VAL:O    | 2.13                     | 0.48              |
| 1:A:87:THR:HG22  | 1:A:87:THR:O     | 2.13                     | 0.48              |
| 1:C:147:MET:HE2  | 1:C:319:LEU:CB   | 2.44                     | 0.48              |
| 1:D:173:LEU:HD23 | 1:D:197:VAL:HG21 | 1.96                     | 0.48              |
| 1:D:256:VAL:CG1  | 1:D:260:GLY:HA3  | 2.43                     | 0.48              |
| 1:D:325:ARG:HG3  | 1:D:325:ARG:HH11 | 1.79                     | 0.48              |
| 1:A:201:PRO:O    | 1:A:204:VAL:HG22 | 2.14                     | 0.48              |
| 1:A:277:PRO:O    | 1:A:281:TRP:HB2  | 2.14                     | 0.48              |
| 1:C:147:MET:HE2  | 1:C:319:LEU:HB3  | 1.96                     | 0.48              |
| 1:D:171:ALA:HB2  | 1:D:236:VAL:HG11 | 1.95                     | 0.48              |
| 1:B:34:VAL:HG12  | 1:B:61:ALA:CB    | 2.44                     | 0.48              |
| 1:D:159:ALA:HA   | 1:D:240:ILE:HD11 | 1.96                     | 0.48              |
| 1:D:312:LYS:NZ   | 6:D:419:HOH:O    | 2.46                     | 0.47              |
| 1:A:31:PRO:HG2   | 1:A:351:LEU:HD23 | 1.96                     | 0.47              |
| 1:B:16:GLU:HG2   | 6:B:463:HOH:O    | 2.14                     | 0.47              |
| 1:C:171:ALA:O    | 1:C:239:ALA:HA   | 2.14                     | 0.47              |
| 1:B:92:THR:HG22  | 1:B:95:VAL:CG2   | 2.37                     | 0.47              |
| 1:C:139:GLU:H    | 1:C:139:GLU:CD   | 2.22                     | 0.47              |
| 1:C:341:PRO:HD2  | 1:C:344:LEU:HB3  | 1.95                     | 0.47              |
| 1:D:32:LEU:HG    | 1:D:63:GLY:HA2   | 1.96                     | 0.47              |
| 1:D:327:PHE:CZ   | 1:D:352:ALA:HB1  | 2.49                     | 0.47              |
| 1:A:293:GLY:HA2  | 1:B:285:MET:HA   | 1.96                     | 0.47              |
| 1:B:252:ALA:O    | 1:B:256:VAL:HG23 | 2.15                     | 0.47              |
| 1:C:94:GLU:HG3   | 1:C:103:SER:HA   | 1.95                     | 0.47              |
| 1:B:325:ARG:HG3  | 1:B:325:ARG:HH11 | 1.80                     | 0.47              |
| 1:B:341:PRO:HD2  | 1:B:344:LEU:HB3  | 1.97                     | 0.47              |
| 1:C:312:LYS:HD2  | 1:C:312:LYS:N    | 2.29                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:1:MET:HG3    | 1:A:122:GLU:HB2  | 1.96                     | 0.47              |
| 1:A:254:LYS:CG   | 1:A:280:GLU:HG3  | 2.32                     | 0.47              |
| 1:A:323:VAL:HA   | 1:A:348:VAL:O    | 2.14                     | 0.47              |
| 1:B:218:TYR:CD1  | 1:B:218:TYR:C    | 2.92                     | 0.47              |
| 1:C:5:ALA:HB1    | 1:C:55:MET:C     | 2.40                     | 0.47              |
| 1:C:14:TRP:HH2   | 1:C:327:PHE:HB3  | 1.80                     | 0.47              |
| 1:C:271:GLY:C    | 1:D:278:ARG:HD3  | 2.40                     | 0.47              |
| 1:C:277:PRO:O    | 1:C:281:TRP:HB2  | 2.14                     | 0.47              |
| 1:D:82:VAL:CG1   | 1:D:302:MET:HE2  | 2.45                     | 0.47              |
| 1:D:83:VAL:HG22  | 1:D:133:LEU:CD2  | 2.44                     | 0.47              |
| 1:A:175:ILE:CD1  | 1:A:198:GLY:HA3  | 2.45                     | 0.47              |
| 1:C:76:LYS:HG2   | 1:C:79:ASP:OD2   | 2.15                     | 0.47              |
| 1:C:175:ILE:CD1  | 1:C:198:GLY:HA3  | 2.44                     | 0.47              |
| 1:A:86:ILE:CG2   | 1:A:88:PRO:HD3   | 2.44                     | 0.47              |
| 1:C:152:MET:HG3  | 1:C:181:MET:CE   | 2.45                     | 0.47              |
| 1:D:17:LYS:NZ    | 1:D:54:ASN:O     | 2.46                     | 0.47              |
| 1:A:287:HIS:CD2  | 1:B:102:HIS:HE2  | 2.32                     | 0.46              |
| 1:A:313:ARG:NH1  | 1:C:192:GLY:O    | 2.47                     | 0.46              |
| 1:C:87:THR:HG23  | 1:C:132:ASN:CB   | 2.45                     | 0.46              |
| 1:A:334:PHE:O    | 1:A:337:MET:HB2  | 2.16                     | 0.46              |
| 1:B:92:THR:CG2   | 1:B:94:GLU:HG2   | 2.45                     | 0.46              |
| 1:B:284:GLY:C    | 1:B:285:MET:HG3  | 2.40                     | 0.46              |
| 1:B:341:PRO:HD2  | 1:B:344:LEU:CB   | 2.46                     | 0.46              |
| 1:B:350:ILE:HG22 | 1:B:351:LEU:N    | 2.30                     | 0.46              |
| 1:D:151:MET:HE2  | 1:D:177:PRO:CG   | 2.45                     | 0.46              |
| 1:A:197:VAL:HG11 | 1:A:223:ILE:HD13 | 1.96                     | 0.46              |
| 1:A:20:PRO:HB2   | 1:A:28:ILE:HD12  | 1.98                     | 0.46              |
| 1:B:246:ALA:HB1  | 1:B:275:PRO:HD3  | 1.98                     | 0.46              |
| 1:A:325:ARG:HG3  | 1:A:325:ARG:NH1  | 2.31                     | 0.46              |
| 1:D:51:GLU:HG3   | 1:D:53:HIS:CE1   | 2.49                     | 0.46              |
| 1:B:223:ILE:O    | 1:B:227:ILE:HD13 | 2.15                     | 0.46              |
| 1:D:106:MET:O    | 1:D:107:LEU:HB2  | 2.16                     | 0.46              |
| 1:B:65:VAL:O     | 1:B:77:PRO:HA    | 2.16                     | 0.46              |
| 1:C:86:ILE:HD11  | 1:C:294:LEU:HD11 | 1.97                     | 0.46              |
| 1:A:22:PRO:HD3   | 1:A:28:ILE:HG13  | 1.97                     | 0.46              |
| 1:D:281:TRP:CZ3  | 1:D:284:GLY:HA2  | 2.50                     | 0.46              |
| 1:A:102:HIS:HE1  | 1:B:287:HIS:HD2  | 1.62                     | 0.46              |
| 1:A:324:PHE:HB3  | 1:A:329:ASN:OD1  | 2.16                     | 0.46              |
| 1:B:157:HIS:HA   | 1:B:160:GLU:OE1  | 2.16                     | 0.46              |
| 1:B:313:ARG:NH1  | 1:D:192:GLY:O    | 2.48                     | 0.46              |
| 1:C:224:GLU:H    | 1:C:224:GLU:CD   | 2.24                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:327:PHE:O    | 1:D:328:ASP:C    | 2.58                     | 0.46              |
| 1:A:51:GLU:CG    | 1:A:53:HIS:CE1   | 2.99                     | 0.45              |
| 1:B:201:PRO:O    | 1:B:204:VAL:HG22 | 2.16                     | 0.45              |
| 1:C:321:THR:OG1  | 1:C:344:LEU:HD12 | 2.17                     | 0.45              |
| 1:B:151:MET:SD   | 1:B:346:LYS:HE3  | 2.56                     | 0.45              |
| 1:C:327:PHE:O    | 1:C:330:ILE:HG13 | 2.17                     | 0.45              |
| 1:D:35:ALA:HA    | 1:D:36:PRO:HD3   | 1.80                     | 0.45              |
| 1:A:51:GLU:CG    | 1:A:53:HIS:HE1   | 2.29                     | 0.45              |
| 1:C:45:PHE:CD1   | 1:C:45:PHE:N     | 2.83                     | 0.45              |
| 1:C:106:MET:HG2  | 1:C:107:LEU:HG   | 1.99                     | 0.45              |
| 1:D:200:ARG:HA   | 1:D:201:PRO:HD2  | 1.85                     | 0.45              |
| 1:A:92:THR:HG21  | 1:A:103:SER:HA   | 1.98                     | 0.45              |
| 1:B:22:PRO:HD3   | 1:B:28:ILE:CG1   | 2.47                     | 0.45              |
| 1:D:351:LEU:O    | 1:D:352:ALA:HB3  | 2.16                     | 0.45              |
| 1:B:344:LEU:HD11 | 1:B:347:PRO:HD3  | 1.98                     | 0.45              |
| 1:D:161:LEU:O    | 1:D:291:LYS:HD2  | 2.17                     | 0.45              |
| 1:C:318:LYS:N    | 1:C:318:LYS:CD   | 2.78                     | 0.45              |
| 1:A:275:PRO:HA   | 1:B:273:VAL:HG13 | 1.99                     | 0.45              |
| 1:C:193:ARG:NH2  | 1:C:230:LEU:HB3  | 2.31                     | 0.45              |
| 1:D:2:LYS:HG2    | 1:D:14:TRP:CE3   | 2.52                     | 0.45              |
| 1:D:151:MET:CE   | 1:D:178:VAL:HG23 | 2.40                     | 0.45              |
| 1:A:151:MET:HE2  | 1:A:177:PRO:CG   | 2.47                     | 0.45              |
| 1:A:245:ASN:HD21 | 1:A:270:GLU:HG3  | 1.82                     | 0.45              |
| 1:B:5:ALA:CB     | 1:B:56:ILE:HA    | 2.45                     | 0.45              |
| 1:B:86:ILE:CG2   | 1:B:88:PRO:HD3   | 2.46                     | 0.45              |
| 1:C:12:VAL:CG1   | 1:C:44:VAL:HG11  | 2.47                     | 0.45              |
| 1:D:92:THR:HG22  | 1:D:95:VAL:CG2   | 2.46                     | 0.45              |
| 1:A:278:ARG:HG2  | 1:B:272:GLU:HA   | 1.99                     | 0.45              |
| 1:A:295:CYS:HA   | 1:A:296:PRO:HD3  | 1.83                     | 0.45              |
| 1:B:87:THR:HG23  | 1:B:132:ASN:CB   | 2.47                     | 0.45              |
| 1:B:200:ARG:HB2  | 1:B:203:CYS:SG   | 2.56                     | 0.45              |
| 1:B:245:ASN:O    | 1:B:246:ALA:C    | 2.60                     | 0.45              |
| 1:C:209:TYR:CE2  | 1:C:318:LYS:HG2  | 2.52                     | 0.45              |
| 1:C:101:GLN:HG2  | 1:C:294:LEU:O    | 2.17                     | 0.44              |
| 1:C:269:GLY:HA2  | 1:D:278:ARG:HH21 | 1.82                     | 0.44              |
| 1:D:94:GLU:CG    | 1:D:103:SER:HA   | 2.47                     | 0.44              |
| 1:B:32:LEU:HG    | 1:B:63:GLY:HA2   | 1.98                     | 0.44              |
| 1:B:49:ILE:HD12  | 1:B:52:ARG:HH12  | 1.82                     | 0.44              |
| 1:C:293:GLY:CA   | 1:D:285:MET:HA   | 2.46                     | 0.44              |
| 1:D:65:VAL:O     | 1:D:77:PRO:HA    | 2.17                     | 0.44              |
| 1:D:87:THR:HG23  | 1:D:132:ASN:CB   | 2.47                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:43:THR:CG2   | 1:A:49:ILE:HD12  | 2.48                     | 0.44              |
| 1:A:191:ALA:HB3  | 1:A:194:ILE:HD11 | 2.00                     | 0.44              |
| 1:C:102:HIS:CD2  | 1:D:258:PRO:HB3  | 2.53                     | 0.44              |
| 1:D:151:MET:SD   | 1:D:346:LYS:HE3  | 2.57                     | 0.44              |
| 1:D:245:ASN:HD21 | 1:D:270:GLU:HG3  | 1.82                     | 0.44              |
| 1:A:5:ALA:HB1    | 1:A:55:MET:C     | 2.42                     | 0.44              |
| 1:A:92:THR:CG2   | 1:A:103:SER:OG   | 2.64                     | 0.44              |
| 1:A:224:GLU:OE1  | 1:A:224:GLU:N    | 2.36                     | 0.44              |
| 1:C:249:MET:HE1  | 1:C:290:ILE:HD13 | 1.99                     | 0.44              |
| 1:D:339:ASP:O    | 1:D:341:PRO:HD3  | 2.16                     | 0.44              |
| 1:A:177:PRO:HG2  | 6:A:427:HOH:O    | 2.18                     | 0.44              |
| 1:A:272:GLU:HA   | 1:B:278:ARG:HG2  | 2.00                     | 0.44              |
| 1:A:351:LEU:HD12 | 1:A:351:LEU:HA   | 1.82                     | 0.44              |
| 1:C:92:THR:HG22  | 1:C:95:VAL:CG2   | 2.47                     | 0.44              |
| 1:D:32:LEU:O     | 1:D:351:LEU:N    | 2.50                     | 0.44              |
| 1:D:34:VAL:CG2   | 1:D:349:VAL:HG13 | 2.48                     | 0.44              |
| 1:D:318:LYS:N    | 1:D:318:LYS:CD   | 2.80                     | 0.44              |
| 1:A:336:LEU:HG   | 1:A:344:LEU:HD22 | 1.99                     | 0.44              |
| 1:B:92:THR:HG21  | 1:B:103:SER:OG   | 2.18                     | 0.44              |
| 1:C:246:ALA:HB1  | 1:C:275:PRO:HD3  | 2.00                     | 0.44              |
| 1:D:29:VAL:HB    | 1:D:124:PHE:CE1  | 2.53                     | 0.44              |
| 1:B:1:MET:HG3    | 1:B:122:GLU:HB2  | 1.99                     | 0.44              |
| 1:B:270:GLU:OE1  | 1:B:270:GLU:HA   | 2.18                     | 0.44              |
| 1:C:278:ARG:HH21 | 1:D:269:GLY:HA2  | 1.82                     | 0.44              |
| 1:D:245:ASN:HD21 | 1:D:270:GLU:CG   | 2.31                     | 0.44              |
| 1:B:92:THR:HG23  | 1:B:94:GLU:HG2   | 1.99                     | 0.44              |
| 1:B:96:GLN:HE21  | 1:C:131:MET:CE   | 2.31                     | 0.44              |
| 1:B:175:ILE:HG21 | 1:B:196:ALA:HB1  | 1.99                     | 0.44              |
| 1:C:31:PRO:CB    | 1:C:352:ALA:OXT  | 2.66                     | 0.44              |
| 1:B:41:ILE:HD13  | 1:B:334:PHE:CE1  | 2.52                     | 0.44              |
| 1:B:281:TRP:CE3  | 1:B:284:GLY:HA2  | 2.53                     | 0.44              |
| 1:C:94:GLU:HG2   | 1:C:103:SER:HA   | 2.00                     | 0.44              |
| 1:C:145:ALA:O    | 1:C:149:PRO:HD3  | 2.18                     | 0.44              |
| 1:A:264:ASN:O    | 1:A:292:GLY:HA2  | 2.18                     | 0.43              |
| 1:B:296:PRO:HG2  | 1:B:301:ARG:NE   | 2.33                     | 0.43              |
| 1:D:43:THR:HG23  | 1:D:49:ILE:CG1   | 2.48                     | 0.43              |
| 1:A:87:THR:CG2   | 1:A:127:ASN:OD1  | 2.66                     | 0.43              |
| 1:A:315:ASP:OD2  | 1:A:317:SER:HB2  | 2.18                     | 0.43              |
| 1:A:323:VAL:HG22 | 1:A:348:VAL:HG22 | 2.00                     | 0.43              |
| 1:C:82:VAL:HG12  | 1:C:149:PRO:HG3  | 2.00                     | 0.43              |
| 1:C:87:THR:HG23  | 1:C:132:ASN:CG   | 2.43                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:6:MET:HE3    | 1:B:9:ILE:HA     | 2.00                     | 0.43              |
| 1:C:94:GLU:CD    | 1:C:94:GLU:N     | 2.69                     | 0.43              |
| 1:A:151:MET:SD   | 1:A:346:LYS:HE3  | 2.58                     | 0.43              |
| 1:B:2:LYS:HE2    | 1:B:14:TRP:CE3   | 2.53                     | 0.43              |
| 1:C:9:ILE:CG1    | 1:C:51:GLU:OE1   | 2.63                     | 0.43              |
| 1:D:284:GLY:C    | 1:D:285:MET:HG3  | 2.43                     | 0.43              |
| 1:D:329:ASN:C    | 1:D:331:GLU:N    | 2.75                     | 0.43              |
| 1:C:92:THR:HG21  | 1:C:94:GLU:HG2   | 2.00                     | 0.43              |
| 1:C:152:MET:HE3  | 1:C:314:VAL:HG21 | 2.00                     | 0.43              |
| 1:C:92:THR:HG23  | 1:C:95:VAL:H     | 1.83                     | 0.43              |
| 1:D:148:ILE:HG22 | 1:D:302:MET:CE   | 2.47                     | 0.43              |
| 1:D:181:MET:SD   | 1:D:319:LEU:HD11 | 2.58                     | 0.43              |
| 1:D:218:TYR:CD1  | 1:D:218:TYR:C    | 2.97                     | 0.43              |
| 1:C:36:PRO:CD    | 1:C:347:PRO:HG2  | 2.48                     | 0.43              |
| 1:D:52:ARG:NH1   | 1:D:114:ASN:O    | 2.52                     | 0.43              |
| 1:D:146:VAL:HG12 | 1:D:146:VAL:O    | 2.18                     | 0.43              |
| 1:D:351:LEU:C    | 1:D:351:LEU:CD1  | 2.91                     | 0.43              |
| 1:B:313:ARG:O    | 1:B:314:VAL:HG13 | 2.18                     | 0.43              |
| 1:C:31:PRO:HB2   | 1:C:352:ALA:OXT  | 2.19                     | 0.43              |
| 1:A:92:THR:HG21  | 1:A:103:SER:CB   | 2.49                     | 0.43              |
| 1:B:300:LEU:HD21 | 1:C:97:ARG:HG2   | 2.00                     | 0.43              |
| 1:C:222:PRO:HB2  | 1:C:225:SER:OG   | 2.18                     | 0.43              |
| 1:C:245:ASN:O    | 1:C:247:ASP:N    | 2.51                     | 0.43              |
| 1:A:19:LYS:HA    | 1:A:20:PRO:HD3   | 1.89                     | 0.43              |
| 1:A:52:ARG:NH1   | 1:A:55:MET:HE1   | 2.32                     | 0.43              |
| 1:A:218:TYR:C    | 1:A:218:TYR:CD1  | 2.96                     | 0.43              |
| 1:B:148:ILE:N    | 1:B:149:PRO:CD   | 2.82                     | 0.43              |
| 1:B:315:ASP:HA   | 1:B:316:PRO:HD3  | 1.73                     | 0.43              |
| 1:D:139:GLU:CD   | 1:D:139:GLU:H    | 2.27                     | 0.43              |
| 1:A:62:VAL:HG23  | 1:A:146:VAL:HG22 | 2.01                     | 0.42              |
| 1:A:128:ASP:CG   | 1:A:131:MET:HB2  | 2.44                     | 0.42              |
| 1:A:245:ASN:O    | 1:A:246:ALA:C    | 2.62                     | 0.42              |
| 1:A:68:VAL:HG11  | 1:A:75:PHE:O     | 2.20                     | 0.42              |
| 1:C:231:THR:O    | 1:C:232:GLU:C    | 2.61                     | 0.42              |
| 1:C:147:MET:CE   | 1:C:151:MET:HG3  | 2.49                     | 0.42              |
| 1:C:245:ASN:O    | 1:C:246:ALA:C    | 2.62                     | 0.42              |
| 1:D:122:GLU:HA   | 1:D:327:PHE:CZ   | 2.55                     | 0.42              |
| 1:A:34:VAL:HB    | 1:A:120:PHE:HE1  | 1.84                     | 0.42              |
| 1:B:147:MET:HE2  | 1:B:319:LEU:CB   | 2.49                     | 0.42              |
| 1:C:75:PHE:CE1   | 1:C:135:HIS:CE1  | 3.07                     | 0.42              |
| 1:D:327:PHE:O    | 1:D:330:ILE:N    | 2.45                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:83:VAL:HG22  | 1:C:133:LEU:CD2  | 2.50                     | 0.42              |
| 1:A:217:ASN:OD1  | 1:A:219:LYS:HB2  | 2.19                     | 0.42              |
| 1:C:147:MET:HE3  | 1:C:151:MET:HG3  | 2.01                     | 0.42              |
| 1:C:254:LYS:HE2  | 1:C:280:GLU:CD   | 2.44                     | 0.42              |
| 1:D:153:THR:HG22 | 1:D:301:ARG:NE   | 2.21                     | 0.42              |
| 1:D:274:LEU:HA   | 1:D:275:PRO:HD3  | 1.89                     | 0.42              |
| 1:D:341:PRO:C    | 1:D:343:ASP:H    | 2.27                     | 0.42              |
| 1:B:249:MET:HE2  | 1:B:276:VAL:HG22 | 2.01                     | 0.42              |
| 1:A:145:ALA:O    | 1:A:149:PRO:HD3  | 2.20                     | 0.42              |
| 1:A:152:MET:HG3  | 1:A:181:MET:HE2  | 2.01                     | 0.42              |
| 1:D:329:ASN:HD22 | 1:D:329:ASN:HA   | 1.65                     | 0.42              |
| 1:A:140:ILE:HA   | 1:A:141:PRO:HD3  | 1.86                     | 0.42              |
| 1:A:341:PRO:HD2  | 1:A:344:LEU:CB   | 2.50                     | 0.42              |
| 1:B:152:MET:CG   | 1:B:305:LEU:HD13 | 2.46                     | 0.42              |
| 1:D:94:GLU:HG3   | 1:D:103:SER:HA   | 2.02                     | 0.42              |
| 1:D:277:PRO:O    | 1:D:281:TRP:HB2  | 2.20                     | 0.42              |
| 1:D:312:LYS:HD2  | 1:D:312:LYS:H    | 1.85                     | 0.42              |
| 1:A:97:ARG:HG2   | 1:D:300:LEU:HD21 | 2.00                     | 0.42              |
| 1:D:12:VAL:CG1   | 1:D:44:VAL:HG11  | 2.50                     | 0.42              |
| 1:D:337:MET:HE3  | 1:D:344:LEU:CD2  | 2.43                     | 0.42              |
| 1:A:83:VAL:HA    | 1:A:84:PRO:HD2   | 1.95                     | 0.41              |
| 1:A:274:LEU:HA   | 1:A:275:PRO:HD3  | 1.88                     | 0.41              |
| 1:B:82:VAL:CG1   | 1:B:302:MET:HE2  | 2.49                     | 0.41              |
| 1:B:330:ILE:HG12 | 1:B:349:VAL:HG11 | 2.02                     | 0.41              |
| 1:C:249:MET:HB3  | 1:C:275:PRO:O    | 2.20                     | 0.41              |
| 1:A:143:GLU:OE2  | 1:A:350:ILE:HD11 | 2.20                     | 0.41              |
| 1:D:147:MET:HE2  | 1:D:319:LEU:HB2  | 2.02                     | 0.41              |
| 1:B:200:ARG:HD3  | 1:B:203:CYS:SG   | 2.61                     | 0.41              |
| 1:A:12:VAL:CG1   | 1:A:44:VAL:HG11  | 2.47                     | 0.41              |
| 1:A:34:VAL:HG12  | 1:A:61:ALA:HB2   | 2.02                     | 0.41              |
| 1:A:157:HIS:O    | 1:A:161:LEU:HG   | 2.19                     | 0.41              |
| 1:A:285:MET:HB2  | 1:B:107:LEU:HD21 | 2.02                     | 0.41              |
| 1:B:318:LYS:N    | 1:B:318:LYS:CD   | 2.80                     | 0.41              |
| 1:A:138:LYS:HE2  | 1:A:139:GLU:OE1  | 2.20                     | 0.41              |
| 1:B:52:ARG:HH11  | 1:B:52:ARG:HG3   | 1.85                     | 0.41              |
| 1:B:217:ASN:OD1  | 1:B:219:LYS:HB2  | 2.20                     | 0.41              |
| 1:D:37:CYS:HB2   | 1:D:60:GLU:OE2   | 2.20                     | 0.41              |
| 1:D:92:THR:CG2   | 1:D:103:SER:OG   | 2.68                     | 0.41              |
| 1:A:206:ALA:O    | 1:A:209:TYR:HB3  | 2.20                     | 0.41              |
| 1:C:262:ILE:N    | 1:C:262:ILE:HD12 | 2.36                     | 0.41              |
| 1:B:28:ILE:O     | 1:B:66:VAL:HG22  | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:68:VAL:HG11  | 1:B:75:PHE:O     | 2.19                     | 0.41              |
| 1:B:245:ASN:HD21 | 1:B:270:GLU:HB2  | 1.86                     | 0.41              |
| 1:C:32:LEU:HG    | 1:C:63:GLY:HA2   | 2.02                     | 0.41              |
| 1:C:286:ALA:HA   | 1:D:102:HIS:NE2  | 2.35                     | 0.41              |
| 1:A:174:GLY:O    | 1:A:179:GLY:HA3  | 2.21                     | 0.41              |
| 1:B:254:LYS:HG2  | 1:B:280:GLU:CG   | 2.34                     | 0.41              |
| 1:C:151:MET:HE2  | 1:C:177:PRO:CG   | 2.51                     | 0.41              |
| 1:C:246:ALA:O    | 1:C:275:PRO:HD2  | 2.21                     | 0.41              |
| 1:C:327:PHE:CG   | 1:C:352:ALA:HB1  | 2.55                     | 0.41              |
| 1:D:22:PRO:HD3   | 1:D:28:ILE:CG1   | 2.50                     | 0.41              |
| 1:D:140:ILE:HA   | 1:D:141:PRO:HD3  | 1.79                     | 0.41              |
| 1:B:34:VAL:HG12  | 1:B:61:ALA:HB2   | 2.02                     | 0.41              |
| 1:D:92:THR:HG21  | 1:D:103:SER:CA   | 2.51                     | 0.41              |
| 1:B:227:ILE:HD12 | 1:B:227:ILE:N    | 2.36                     | 0.41              |
| 1:B:245:ASN:O    | 1:B:247:ASP:N    | 2.54                     | 0.41              |
| 1:D:1:MET:O      | 1:D:16:GLU:HA    | 2.20                     | 0.41              |
| 1:D:204:VAL:HG23 | 1:D:205:ASP:N    | 2.36                     | 0.41              |
| 1:D:262:ILE:N    | 1:D:262:ILE:HD12 | 2.36                     | 0.41              |
| 1:A:245:ASN:O    | 1:A:247:ASP:N    | 2.54                     | 0.40              |
| 1:C:29:VAL:HB    | 1:C:124:PHE:CE1  | 2.56                     | 0.40              |
| 1:C:320:VAL:HG22 | 1:C:348:VAL:HG11 | 2.03                     | 0.40              |
| 1:D:87:THR:HG23  | 1:D:132:ASN:CG   | 2.46                     | 0.40              |
| 1:D:92:THR:CG2   | 1:D:94:GLU:HG2   | 2.51                     | 0.40              |
| 1:D:315:ASP:OD2  | 1:D:317:SER:HB2  | 2.21                     | 0.40              |
| 1:A:253:VAL:HA   | 1:A:262:ILE:CD1  | 2.51                     | 0.40              |
| 1:A:293:GLY:CA   | 1:B:287:HIS:CD2  | 3.04                     | 0.40              |
| 1:C:35:ALA:HA    | 1:C:36:PRO:HD3   | 1.87                     | 0.40              |
| 1:C:151:MET:SD   | 1:C:346:LYS:HE3  | 2.61                     | 0.40              |
| 1:D:46:GLU:O     | 1:D:47:GLY:C     | 2.64                     | 0.40              |
| 1:C:84:PRO:HD3   | 1:C:302:MET:HG3  | 2.03                     | 0.40              |
| 1:D:226:GLN:O    | 1:D:230:LEU:HG   | 2.21                     | 0.40              |
| 1:A:49:ILE:HG22  | 1:A:49:ILE:O     | 2.22                     | 0.40              |
| 1:A:204:VAL:HG23 | 1:A:205:ASP:N    | 2.36                     | 0.40              |
| 1:B:17:LYS:NZ    | 1:B:54:ASN:O     | 2.49                     | 0.40              |
| 1:D:170:VAL:HG12 | 1:D:171:ALA:N    | 2.36                     | 0.40              |
| 1:D:173:LEU:HD13 | 1:D:248:ILE:CD1  | 2.50                     | 0.40              |
| 1:B:86:ILE:HB    | 1:B:297:GLY:HA3  | 2.02                     | 0.40              |
| 1:B:175:ILE:HG13 | 1:B:175:ILE:O    | 2.21                     | 0.40              |
| 1:B:327:PHE:O    | 1:B:328:ASP:C    | 2.63                     | 0.40              |
| 1:C:274:LEU:HA   | 1:C:275:PRO:HD3  | 1.83                     | 0.40              |
| 1:D:173:LEU:HB3  | 1:D:248:ILE:HD11 | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | A     | 350/352 (99%)   | 318 (91%)  | 31 (9%)   | 1 (0%)   | 36          | 70 |
| 1   | B     | 350/352 (99%)   | 316 (90%)  | 31 (9%)   | 3 (1%)   | 14          | 48 |
| 1   | C     | 350/352 (99%)   | 308 (88%)  | 37 (11%)  | 5 (1%)   | 9           | 36 |
| 1   | D     | 350/352 (99%)   | 311 (89%)  | 35 (10%)  | 4 (1%)   | 11          | 43 |
| All | All   | 1400/1408 (99%) | 1253 (90%) | 134 (10%) | 13 (1%)  | 14          | 48 |

All (13) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 246 | ALA  |
| 1   | B     | 246 | ALA  |
| 1   | C     | 246 | ALA  |
| 1   | D     | 351 | LEU  |
| 1   | C     | 271 | GLY  |
| 1   | C     | 351 | LEU  |
| 1   | D     | 288 | LYS  |
| 1   | B     | 326 | GLY  |
| 1   | B     | 47  | GLY  |
| 1   | C     | 326 | GLY  |
| 1   | C     | 118 | GLY  |
| 1   | D     | 326 | GLY  |
| 1   | D     | 271 | GLY  |

### 5.3.2 Protein sidechains [i](#)

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     | 274/274 (100%)   | 266 (97%)  | 8 (3%)   | 37          | 70 |
| 1   | B     | 274/274 (100%)   | 263 (96%)  | 11 (4%)  | 28          | 62 |
| 1   | C     | 274/274 (100%)   | 262 (96%)  | 12 (4%)  | 25          | 60 |
| 1   | D     | 274/274 (100%)   | 260 (95%)  | 14 (5%)  | 21          | 55 |
| All | All   | 1096/1096 (100%) | 1051 (96%) | 45 (4%)  | 27          | 61 |

All (45) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 94  | GLU  |
| 1   | A     | 139 | GLU  |
| 1   | A     | 224 | GLU  |
| 1   | A     | 232 | GLU  |
| 1   | A     | 272 | GLU  |
| 1   | A     | 280 | GLU  |
| 1   | A     | 313 | ARG  |
| 1   | A     | 349 | VAL  |
| 1   | B     | 94  | GLU  |
| 1   | B     | 139 | GLU  |
| 1   | B     | 153 | THR  |
| 1   | B     | 224 | GLU  |
| 1   | B     | 232 | GLU  |
| 1   | B     | 272 | GLU  |
| 1   | B     | 280 | GLU  |
| 1   | B     | 313 | ARG  |
| 1   | B     | 337 | MET  |
| 1   | B     | 347 | PRO  |
| 1   | B     | 351 | LEU  |
| 1   | C     | 26  | ASP  |
| 1   | C     | 71  | GLU  |
| 1   | C     | 94  | GLU  |
| 1   | C     | 131 | MET  |
| 1   | C     | 139 | GLU  |
| 1   | C     | 224 | GLU  |
| 1   | C     | 232 | GLU  |
| 1   | C     | 272 | GLU  |
| 1   | C     | 280 | GLU  |
| 1   | C     | 313 | ARG  |
| 1   | C     | 337 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 347 | PRO  |
| 1   | D     | 71  | GLU  |
| 1   | D     | 94  | GLU  |
| 1   | D     | 139 | GLU  |
| 1   | D     | 149 | PRO  |
| 1   | D     | 224 | GLU  |
| 1   | D     | 232 | GLU  |
| 1   | D     | 272 | GLU  |
| 1   | D     | 280 | GLU  |
| 1   | D     | 313 | ARG  |
| 1   | D     | 337 | MET  |
| 1   | D     | 339 | ASP  |
| 1   | D     | 347 | PRO  |
| 1   | D     | 348 | VAL  |
| 1   | D     | 349 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 53  | HIS  |
| 1   | A     | 102 | HIS  |
| 1   | A     | 135 | HIS  |
| 1   | A     | 287 | HIS  |
| 1   | B     | 96  | GLN  |
| 1   | B     | 229 | ASN  |
| 1   | B     | 287 | HIS  |
| 1   | B     | 329 | ASN  |
| 1   | C     | 53  | HIS  |
| 1   | C     | 135 | HIS  |
| 1   | C     | 157 | HIS  |
| 1   | D     | 53  | HIS  |
| 1   | D     | 59  | HIS  |
| 1   | D     | 96  | GLN  |
| 1   | D     | 102 | HIS  |
| 1   | D     | 135 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 5   | SBT  | D     | 353 | -    | 4,4,4        | 1.09 | 0           | 4,4,4       | 0.21 | 0           |
| 5   | SBT  | C     | 353 | -    | 4,4,4        | 1.34 | 0           | 4,4,4       | 1.18 | 1 (25%)     |
| 5   | SBT  | A     | 353 | -    | 4,4,4        | 0.77 | 0           | 4,4,4       | 0.27 | 0           |
| 5   | SBT  | B     | 353 | -    | 4,4,4        | 0.85 | 0           | 4,4,4       | 0.88 | 0           |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 5   | SBT  | D     | 353 | -    | -       | 0/2/2/2  | -     |
| 5   | SBT  | C     | 353 | -    | -       | 0/2/2/2  | -     |
| 5   | SBT  | A     | 353 | -    | -       | 0/2/2/2  | -     |
| 5   | SBT  | B     | 353 | -    | -       | 0/2/2/2  | -     |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 5   | C     | 353 | SBT  | OH-C2-C1 | 2.07 | 118.38      | 109.45   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|------------------|--------|---------------|-----------------------|-------|
| 1   | A     | 352/352 (100%)   | 0.30   | 8 (2%) 61 38  | 15, 39, 61, 70        | 0     |
| 1   | B     | 352/352 (100%)   | 0.42   | 21 (5%) 27 14 | 17, 40, 63, 78        | 0     |
| 1   | C     | 352/352 (100%)   | 0.37   | 13 (3%) 45 25 | 19, 42, 65, 78        | 0     |
| 1   | D     | 352/352 (100%)   | 0.31   | 9 (2%) 57 34  | 20, 40, 63, 72        | 0     |
| All | All   | 1408/1408 (100%) | 0.35   | 51 (3%) 46 26 | 15, 40, 63, 78        | 0     |

All (51) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 352 | ALA  | 6.7  |
| 1   | B     | 48  | ALA  | 4.4  |
| 1   | B     | 352 | ALA  | 3.9  |
| 1   | C     | 1   | MET  | 3.9  |
| 1   | A     | 49  | ILE  | 3.8  |
| 1   | B     | 272 | GLU  | 3.4  |
| 1   | C     | 53  | HIS  | 3.3  |
| 1   | C     | 50  | GLY  | 3.2  |
| 1   | B     | 47  | GLY  | 3.2  |
| 1   | C     | 58  | GLY  | 3.2  |
| 1   | C     | 47  | GLY  | 3.1  |
| 1   | A     | 272 | GLU  | 3.1  |
| 1   | C     | 10  | GLY  | 3.0  |
| 1   | A     | 38  | THR  | 3.0  |
| 1   | B     | 46  | GLU  | 3.0  |
| 1   | C     | 37  | CYS  | 2.9  |
| 1   | A     | 48  | ALA  | 2.8  |
| 1   | B     | 49  | ILE  | 2.7  |
| 1   | D     | 247 | ASP  | 2.7  |
| 1   | B     | 190 | GLY  | 2.7  |
| 1   | B     | 16  | GLU  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 352 | ALA  | 2.6  |
| 1   | C     | 328 | ASP  | 2.6  |
| 1   | B     | 282 | GLY  | 2.6  |
| 1   | D     | 37  | CYS  | 2.5  |
| 1   | C     | 48  | ALA  | 2.5  |
| 1   | A     | 217 | ASN  | 2.5  |
| 1   | B     | 3   | GLY  | 2.5  |
| 1   | B     | 267 | TYR  | 2.4  |
| 1   | D     | 202 | VAL  | 2.3  |
| 1   | B     | 322 | HIS  | 2.3  |
| 1   | B     | 351 | LEU  | 2.3  |
| 1   | D     | 113 | SER  | 2.3  |
| 1   | D     | 351 | LEU  | 2.3  |
| 1   | B     | 50  | GLY  | 2.3  |
| 1   | C     | 351 | LEU  | 2.2  |
| 1   | B     | 342 | LYS  | 2.2  |
| 1   | B     | 43  | THR  | 2.2  |
| 1   | D     | 339 | ASP  | 2.2  |
| 1   | B     | 277 | PRO  | 2.2  |
| 1   | B     | 339 | ASP  | 2.2  |
| 1   | C     | 341 | PRO  | 2.2  |
| 1   | A     | 220 | ASP  | 2.1  |
| 1   | C     | 3   | GLY  | 2.1  |
| 1   | D     | 92  | THR  | 2.1  |
| 1   | A     | 18  | GLU  | 2.1  |
| 1   | B     | 335 | MET  | 2.0  |
| 1   | A     | 322 | HIS  | 2.0  |
| 1   | B     | 59  | HIS  | 2.0  |
| 1   | B     | 327 | PHE  | 2.0  |
| 1   | D     | 98  | GLY  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 4   | MG   | C     | 356 | 1/1   | 0.80 | 0.23 | 34,34,34,34                | 0     |
| 2   | ZN   | B     | 354 | 1/1   | 0.82 | 0.35 | 27,27,27,27                | 0     |
| 4   | MG   | D     | 356 | 1/1   | 0.87 | 0.22 | 33,33,33,33                | 0     |
| 2   | ZN   | A     | 354 | 1/1   | 0.88 | 0.29 | 26,26,26,26                | 0     |
| 4   | MG   | B     | 356 | 1/1   | 0.88 | 0.24 | 35,35,35,35                | 0     |
| 4   | MG   | A     | 356 | 1/1   | 0.89 | 0.14 | 19,19,19,19                | 0     |
| 5   | SBT  | C     | 353 | 5/5   | 0.89 | 0.14 | 44,44,48,49                | 0     |
| 5   | SBT  | B     | 353 | 5/5   | 0.90 | 0.12 | 25,29,33,35                | 0     |
| 5   | SBT  | D     | 353 | 5/5   | 0.90 | 0.13 | 41,42,44,46                | 0     |
| 2   | ZN   | C     | 354 | 1/1   | 0.91 | 0.30 | 26,26,26,26                | 0     |
| 3   | CL   | D     | 355 | 1/1   | 0.92 | 0.22 | 45,45,45,45                | 0     |
| 5   | SBT  | A     | 353 | 5/5   | 0.93 | 0.13 | 36,37,38,39                | 0     |
| 2   | ZN   | D     | 354 | 1/1   | 0.93 | 0.33 | 28,28,28,28                | 0     |
| 3   | CL   | C     | 355 | 1/1   | 0.96 | 0.14 | 29,29,29,29                | 0     |
| 3   | CL   | A     | 355 | 1/1   | 0.97 | 0.19 | 27,27,27,27                | 0     |
| 3   | CL   | B     | 355 | 1/1   | 0.97 | 0.17 | 25,25,25,25                | 0     |

## 6.5 Other polymers

There are no such residues in this entry.