



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:40 PM UTC

PDB ID : 5AVM / pdb\_00005avm  
Title : Crystal structures of 5-aminoimidazole ribonucleotide (AIR) synthetase, PurM, from *Thermus thermophilus*  
Authors : Kanagawa, M.; Baba, S.; Watanabe, Y.; Nakagawa, N.; Ebihara, A.; Sampei, G.; Kawai, G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2015-06-23  
Resolution : 2.20 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

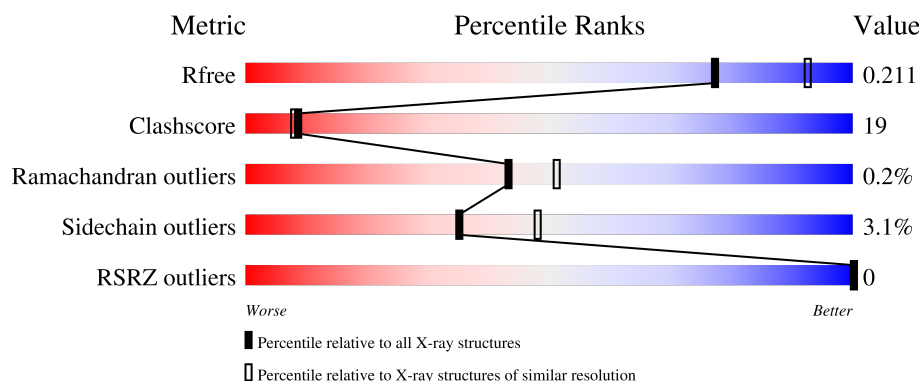
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 6164 (2.20-2.20)                                      |
| Clashscore            | 190562                      | 6851 (2.20-2.20)                                      |
| Ramachandran outliers | 187476                      | 6768 (2.20-2.20)                                      |
| Sidechain outliers    | 187428                      | 6769 (2.20-2.20)                                      |
| RSRZ outliers         | 180081                      | 6166 (2.20-2.20)                                      |

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     | 333    |  |
| 1   | B     | 333    |  |
| 1   | C     | 333    |  |
| 1   | D     | 333    |  |
| 1   | E     | 333    |  |

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| Mol | Chain | Length | Quality of chain                                                                                    |
|-----|-------|--------|-----------------------------------------------------------------------------------------------------|
| 1   | F     | 333    | <br>51% 32% • 15% |
| 1   | G     | 333    | <br>50% 33% • 16% |
| 1   | H     | 333    | <br>51% 32% • 15% |

## 2 Entry composition

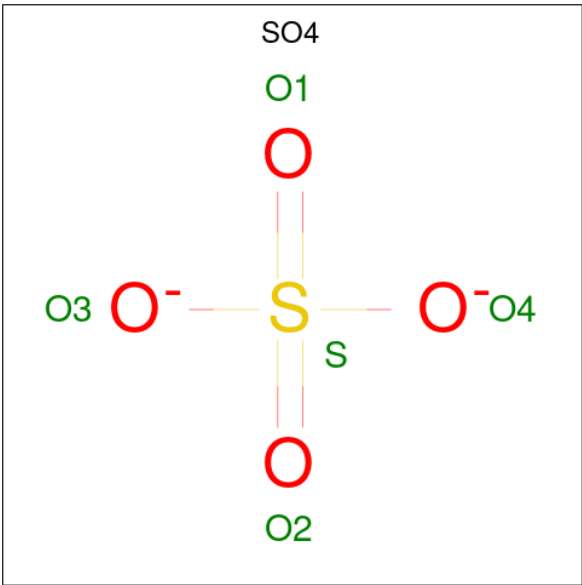
There are 3 unique types of molecules in this entry. The entry contains 18720 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phosphoribosylformylglycinamide cyclo-ligase.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 281      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2100  | 1344 | 363 | 388 | 5 |         |         |       |
| 1   | B     | 283      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2117  | 1355 | 365 | 392 | 5 |         |         |       |
| 1   | C     | 281      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2100  | 1344 | 363 | 388 | 5 |         |         |       |
| 1   | D     | 283      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2117  | 1355 | 365 | 392 | 5 |         |         |       |
| 1   | E     | 281      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2100  | 1344 | 363 | 388 | 5 |         |         |       |
| 1   | F     | 283      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2117  | 1355 | 365 | 392 | 5 |         |         |       |
| 1   | G     | 281      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2100  | 1344 | 363 | 388 | 5 |         |         |       |
| 1   | H     | 283      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2117  | 1355 | 365 | 392 | 5 |         |         |       |

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | D     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | D     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | G     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | G     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | G     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

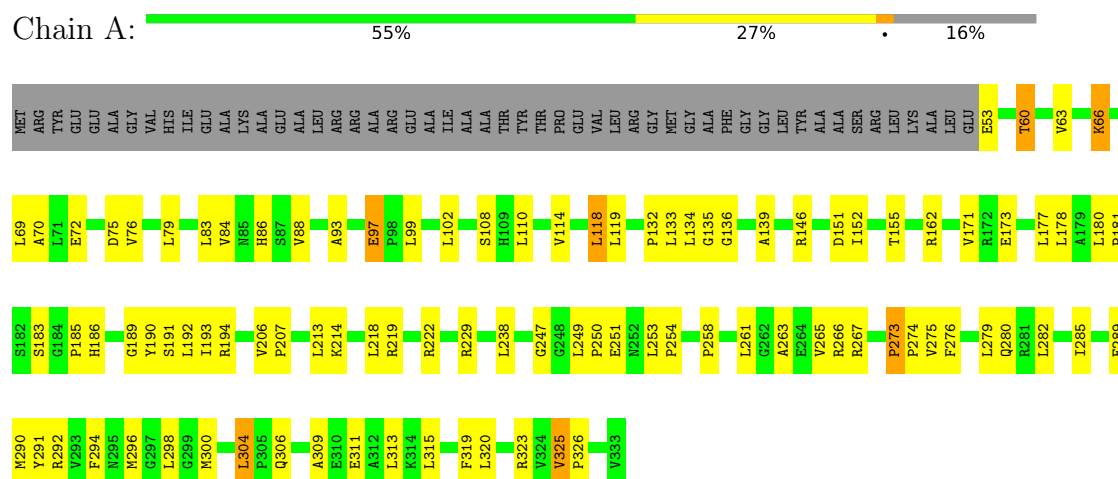
- Molecule 3 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 3   | A     | 203      | Total | O   | 0       | 0       |
|     |       |          | 203   | 203 |         |         |
| 3   | B     | 216      | Total | O   | 0       | 0       |
|     |       |          | 216   | 216 |         |         |
| 3   | C     | 264      | Total | O   | 0       | 0       |
|     |       |          | 264   | 264 |         |         |
| 3   | D     | 252      | Total | O   | 0       | 0       |
|     |       |          | 252   | 252 |         |         |
| 3   | E     | 240      | Total | O   | 0       | 0       |
|     |       |          | 240   | 240 |         |         |
| 3   | F     | 237      | Total | O   | 0       | 0       |
|     |       |          | 237   | 237 |         |         |
| 3   | G     | 202      | Total | O   | 0       | 0       |
|     |       |          | 202   | 202 |         |         |
| 3   | H     | 153      | Total | O   | 0       | 0       |
|     |       |          | 153   | 153 |         |         |

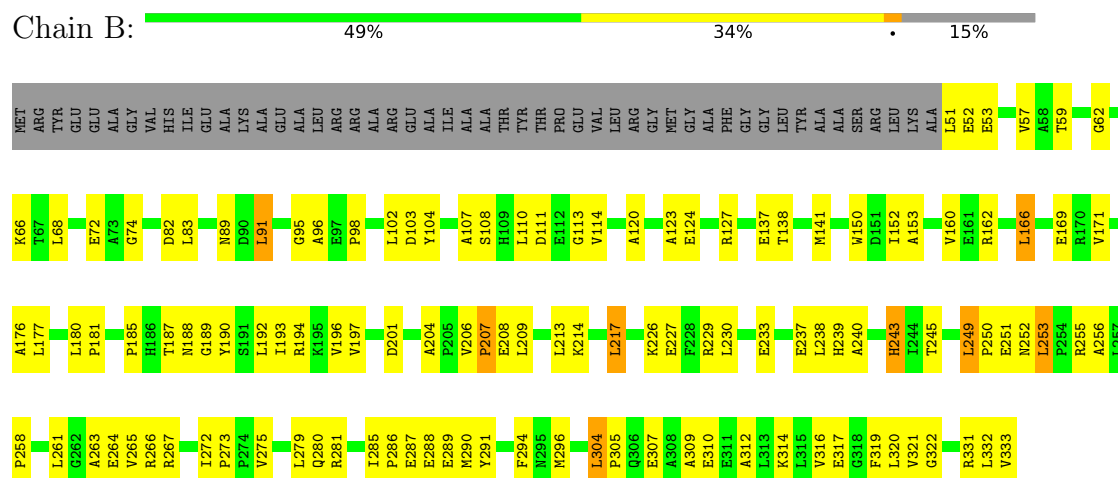
### 3 Residue-property plots [i](#)

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: Phosphoribosylformylglycinamide cyclo-ligase

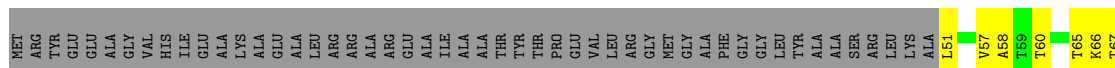


#### • Molecule 1: Phosphoribosylformylglycinamide cyclo-ligase

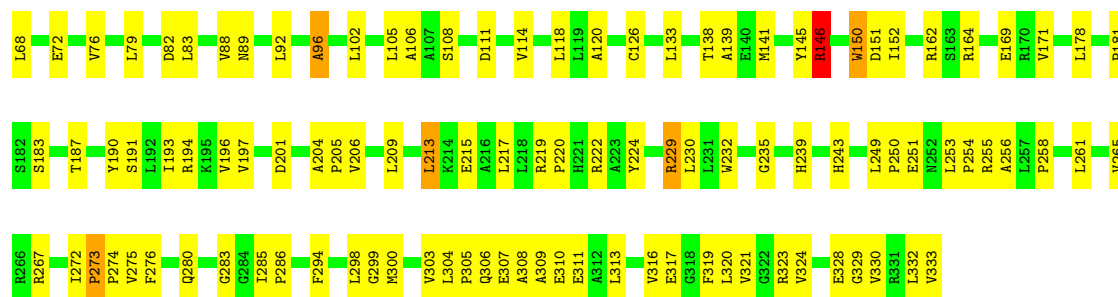


#### • Molecule 1: Phosphoribosylformylglycinamide cyclo-ligase

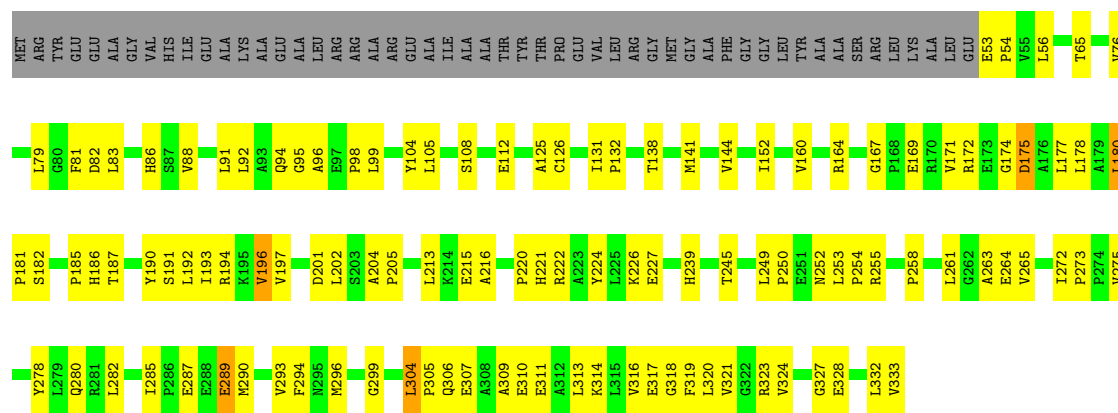




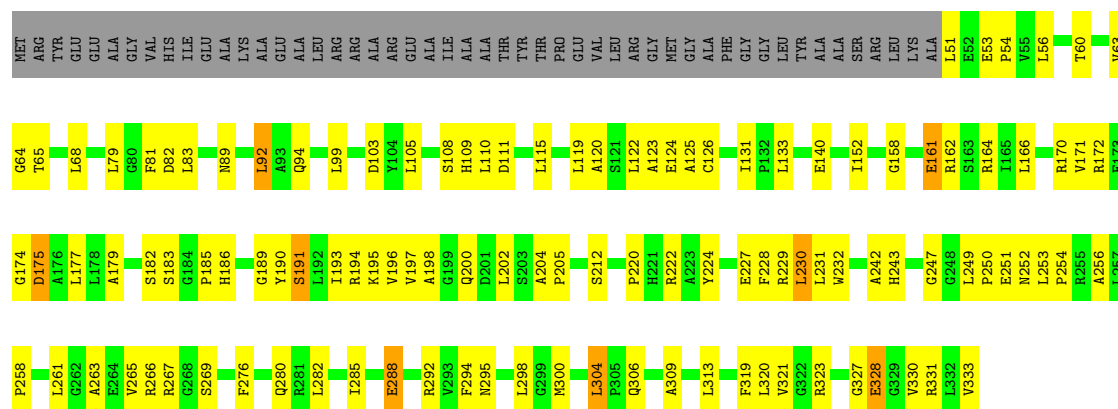




- Molecule 1: Phosphoribosylformylglycinamide cyclo-ligase



- Molecule 1: Phosphoribosylformylglycinamidine cyclo-ligase



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 2                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 142.33Å 142.63Å 218.62Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 50.00 – 2.20<br>50.00 – 2.20                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 96.6 (50.00-2.20)<br>97.4 (50.00-2.20)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.09                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 4.34 (at 2.20Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.3                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.163 , 0.215<br>0.161 , 0.211                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 21116 reflections (9.41%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 29.2                                                        | Xtriage          |
| Anisotropy                                                              | 0.045                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.36 , 34.4                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$ | Xtriage          |
| Estimated twinning fraction                                             | 0.396 for k,h,-l                                            | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.96                                                        | EDS              |
| Total number of atoms                                                   | 18720                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 30.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.83 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.4672e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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

| Mol | Chain | Bond lengths |             | Bond angles |                 |
|-----|-------|--------------|-------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$ | RMSZ        | # $ Z  > 5$     |
| 1   | A     | 0.44         | 0/2146      | 0.96        | 10/2923 (0.3%)  |
| 1   | B     | 0.42         | 0/2163      | 0.98        | 7/2946 (0.2%)   |
| 1   | C     | 0.45         | 0/2146      | 0.98        | 7/2923 (0.2%)   |
| 1   | D     | 0.46         | 0/2163      | 1.00        | 9/2946 (0.3%)   |
| 1   | E     | 0.44         | 0/2146      | 0.94        | 5/2923 (0.2%)   |
| 1   | F     | 0.43         | 0/2163      | 0.94        | 8/2946 (0.3%)   |
| 1   | G     | 0.44         | 0/2146      | 1.03        | 12/2923 (0.4%)  |
| 1   | H     | 0.41         | 0/2163      | 0.97        | 7/2946 (0.2%)   |
| All | All   | 0.44         | 0/17236     | 0.97        | 65/23476 (0.3%) |

There are no bond length outliers.

All (65) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | C     | 66  | LYS  | N-CA-C | -8.65 | 101.77      | 111.71   |
| 1   | B     | 252 | ASN  | N-CA-C | 8.13  | 120.22      | 111.36   |
| 1   | D     | 252 | ASN  | N-CA-C | 7.98  | 122.28      | 112.23   |
| 1   | C     | 133 | LEU  | N-CA-C | -7.81 | 98.02       | 109.11   |
| 1   | G     | 252 | ASN  | N-CA-C | 7.46  | 120.50      | 111.40   |
| 1   | D     | 108 | SER  | N-CA-C | -7.40 | 103.15      | 111.14   |
| 1   | A     | 191 | SER  | N-CA-C | -7.25 | 103.31      | 111.14   |
| 1   | C     | 285 | ILE  | N-CA-C | 7.06  | 114.70      | 108.63   |
| 1   | H     | 108 | SER  | N-CA-C | -6.98 | 103.10      | 111.69   |
| 1   | C     | 293 | VAL  | N-CA-C | 6.93  | 117.52      | 111.56   |
| 1   | A     | 108 | SER  | N-CA-C | -6.88 | 103.78      | 111.28   |
| 1   | G     | 95  | GLY  | N-CA-C | -6.79 | 105.85      | 115.43   |
| 1   | A     | 66  | LYS  | N-CA-C | -6.77 | 103.93      | 111.71   |
| 1   | H     | 103 | ASP  | N-CA-C | 6.77  | 119.44      | 109.69   |
| 1   | H     | 230 | LEU  | N-CA-C | -6.76 | 105.59      | 114.31   |
| 1   | B     | 108 | SER  | N-CA-C | -6.66 | 104.02      | 111.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 103 | ASP  | N-CA-C | 6.49  | 119.58      | 109.52   |
| 1   | F     | 191 | SER  | N-CA-C | -6.37 | 104.43      | 111.82   |
| 1   | C     | 108 | SER  | N-CA-C | -6.27 | 104.44      | 111.28   |
| 1   | D     | 112 | GLU  | N-CA-C | 6.03  | 117.85      | 111.28   |
| 1   | A     | 133 | LEU  | N-CA-C | -5.97 | 98.16       | 108.56   |
| 1   | A     | 273 | PRO  | CA-C-N | 5.93  | 127.26      | 119.84   |
| 1   | A     | 273 | PRO  | C-N-CA | 5.93  | 127.26      | 119.84   |
| 1   | D     | 96  | ALA  | N-CA-C | 5.90  | 119.29      | 110.14   |
| 1   | G     | 191 | SER  | N-CA-C | -5.88 | 105.94      | 113.23   |
| 1   | C     | 210 | GLY  | N-CA-C | -5.79 | 107.26      | 115.30   |
| 1   | F     | 108 | SER  | N-CA-C | -5.68 | 105.17      | 111.36   |
| 1   | A     | 146 | ARG  | N-CA-C | -5.66 | 102.52      | 110.50   |
| 1   | E     | 252 | ASN  | N-CA-C | 5.66  | 120.32      | 113.41   |
| 1   | E     | 180 | LEU  | N-CA-C | -5.66 | 101.42      | 109.62   |
| 1   | G     | 196 | VAL  | N-CA-C | 5.63  | 115.76      | 110.30   |
| 1   | D     | 180 | LEU  | N-CA-C | -5.56 | 100.59      | 109.04   |
| 1   | G     | 289 | GLU  | N-CA-C | -5.56 | 105.62      | 112.90   |
| 1   | F     | 329 | GLY  | N-CA-C | 5.55  | 119.70      | 111.76   |
| 1   | B     | 243 | HIS  | N-CA-C | -5.52 | 100.18      | 108.96   |
| 1   | E     | 108 | SER  | N-CA-C | -5.50 | 105.20      | 111.14   |
| 1   | G     | 245 | THR  | CA-C-O | 5.45  | 121.10      | 117.94   |
| 1   | H     | 161 | GLU  | N-CA-C | -5.44 | 101.80      | 109.96   |
| 1   | D     | 191 | SER  | N-CA-C | -5.41 | 105.30      | 111.14   |
| 1   | B     | 192 | LEU  | N-CA-C | -5.39 | 105.32      | 111.14   |
| 1   | G     | 245 | THR  | N-CA-C | 5.38  | 113.19      | 108.78   |
| 1   | C     | 252 | ASN  | N-CA-C | 5.37  | 119.93      | 112.90   |
| 1   | B     | 180 | LEU  | N-CA-C | -5.33 | 101.90      | 109.62   |
| 1   | G     | 220 | PRO  | N-CA-C | 5.31  | 119.53      | 111.15   |
| 1   | G     | 108 | SER  | N-CA-C | -5.30 | 105.58      | 111.36   |
| 1   | H     | 191 | SER  | N-CA-C | -5.30 | 105.62      | 111.71   |
| 1   | D     | 180 | LEU  | CA-C-N | 5.28  | 125.20      | 119.76   |
| 1   | D     | 180 | LEU  | C-N-CA | 5.28  | 125.20      | 119.76   |
| 1   | E     | 196 | VAL  | N-CA-C | 5.25  | 116.03      | 110.72   |
| 1   | A     | 180 | LEU  | N-CA-C | -5.25 | 102.01      | 109.62   |
| 1   | D     | 181 | PRO  | N-CA-C | 5.23  | 119.31      | 111.14   |
| 1   | F     | 219 | ARG  | CA-C-N | 5.21  | 125.21      | 119.90   |
| 1   | F     | 219 | ARG  | C-N-CA | 5.21  | 125.21      | 119.90   |
| 1   | F     | 181 | PRO  | N-CA-C | 5.18  | 119.23      | 111.14   |
| 1   | F     | 96  | ALA  | N-CA-C | 5.18  | 118.50      | 110.17   |
| 1   | F     | 146 | ARG  | N-CA-C | -5.17 | 102.64      | 110.28   |
| 1   | B     | 181 | PRO  | N-CA-C | 5.14  | 118.94      | 111.03   |
| 1   | E     | 146 | ARG  | N-CA-C | -5.11 | 102.92      | 110.48   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 181 | PRO  | N-CA-C  | 5.10  | 118.88      | 111.03   |
| 1   | A     | 60  | THR  | N-CA-C  | -5.09 | 101.98      | 110.17   |
| 1   | H     | 252 | ASN  | N-CA-C  | 5.09  | 119.37      | 112.04   |
| 1   | H     | 174 | GLY  | N-CA-C  | -5.04 | 108.65      | 115.36   |
| 1   | G     | 245 | THR  | CB-CA-C | -5.03 | 109.83      | 117.07   |
| 1   | G     | 167 | GLY  | CA-C-N  | 5.01  | 125.04      | 119.32   |
| 1   | G     | 167 | GLY  | C-N-CA  | 5.01  | 125.04      | 119.32   |

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     | 2100  | 0        | 2126     | 79      | 0            |
| 1   | B     | 2117  | 0        | 2143     | 93      | 0            |
| 1   | C     | 2100  | 0        | 2126     | 60      | 0            |
| 1   | D     | 2117  | 0        | 2143     | 86      | 0            |
| 1   | E     | 2100  | 0        | 2126     | 52      | 0            |
| 1   | F     | 2117  | 0        | 2143     | 103     | 0            |
| 1   | G     | 2100  | 0        | 2126     | 107     | 0            |
| 1   | H     | 2117  | 0        | 2143     | 90      | 0            |
| 2   | A     | 15    | 0        | 0        | 0       | 0            |
| 2   | B     | 10    | 0        | 0        | 0       | 0            |
| 2   | C     | 10    | 0        | 0        | 0       | 0            |
| 2   | D     | 10    | 0        | 0        | 0       | 0            |
| 2   | E     | 10    | 0        | 0        | 0       | 0            |
| 2   | F     | 5     | 0        | 0        | 0       | 0            |
| 2   | G     | 15    | 0        | 0        | 0       | 0            |
| 2   | H     | 10    | 0        | 0        | 0       | 0            |
| 3   | A     | 203   | 0        | 0        | 7       | 0            |
| 3   | B     | 216   | 0        | 0        | 12      | 0            |
| 3   | C     | 264   | 0        | 0        | 5       | 0            |
| 3   | D     | 252   | 0        | 0        | 12      | 0            |
| 3   | E     | 240   | 0        | 0        | 5       | 0            |
| 3   | F     | 237   | 0        | 0        | 20      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | G     | 202   | 0        | 0        | 15      | 0            |
| 3   | H     | 153   | 0        | 0        | 13      | 0            |
| All | All   | 18720 | 0        | 17076    | 639     | 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 19.

All (639) 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:G:285:ILE:HB   | 1:G:290:MET:HE1  | 1.46                     | 0.94              |
| 1:B:294:PHE:HB2  | 1:B:296:MET:HE3  | 1.51                     | 0.90              |
| 1:G:294:PHE:HB2  | 1:G:296:MET:HE3  | 1.52                     | 0.89              |
| 1:F:265:VAL:HG13 | 1:F:321:VAL:HG12 | 1.60                     | 0.84              |
| 1:A:83:LEU:HD22  | 1:A:152:ILE:HG22 | 1.61                     | 0.82              |
| 1:D:191:SER:O    | 1:D:195:LYS:HG2  | 1.80                     | 0.81              |
| 1:B:296:MET:HE2  | 1:B:296:MET:HA   | 1.62                     | 0.80              |
| 1:A:183:SER:HB2  | 1:A:219:ARG:HD2  | 1.63                     | 0.80              |
| 1:A:304:LEU:HD13 | 1:A:309:ALA:HB2  | 1.63                     | 0.80              |
| 1:D:281:ARG:HD2  | 3:D:507:HOH:O    | 1.83                     | 0.79              |
| 1:F:72:GLU:CD    | 1:F:194:ARG:HH21 | 1.92                     | 0.78              |
| 1:B:258:PRO:HG2  | 1:B:261:LEU:HD12 | 1.66                     | 0.78              |
| 1:B:249:LEU:HD21 | 1:B:253:LEU:HD12 | 1.65                     | 0.78              |
| 1:G:112:GLU:HG3  | 3:G:625:HOH:O    | 1.83                     | 0.78              |
| 1:G:202:LEU:HD23 | 1:G:213:LEU:HD23 | 1.66                     | 0.77              |
| 1:F:169:GLU:CG   | 1:G:172:ARG:HH21 | 1.98                     | 0.77              |
| 1:H:313:LEU:HD11 | 1:H:320:LEU:HG   | 1.67                     | 0.76              |
| 1:D:267:ARG:HG3  | 1:D:333:VAL:O    | 1.85                     | 0.76              |
| 1:F:169:GLU:HG3  | 1:G:172:ARG:HH21 | 1.51                     | 0.76              |
| 1:F:267:ARG:HD3  | 1:F:332:LEU:HD23 | 1.68                     | 0.76              |
| 1:H:331:ARG:HH11 | 1:H:333:VAL:HG12 | 1.51                     | 0.75              |
| 1:G:141:MET:HE2  | 1:G:144:VAL:HG21 | 1.69                     | 0.75              |
| 1:H:190:TYR:O    | 1:H:194:ARG:HG3  | 1.87                     | 0.75              |
| 1:B:59:THR:HG22  | 1:B:91:LEU:HD13  | 1.68                     | 0.74              |
| 1:G:171:VAL:HB   | 1:G:258:PRO:HD3  | 1.70                     | 0.74              |
| 1:D:60:THR:HG22  | 1:D:155:THR:OG1  | 1.89                     | 0.73              |
| 1:D:216:ALA:HA   | 1:D:219:ARG:HH12 | 1.54                     | 0.73              |
| 1:B:238:LEU:HD13 | 1:B:304:LEU:HD23 | 1.71                     | 0.72              |
| 1:F:230:LEU:HD12 | 1:F:316:VAL:HG12 | 1.71                     | 0.72              |
| 1:G:320:LEU:HD13 | 3:G:587:HOH:O    | 1.90                     | 0.71              |
| 1:H:319:PHE:O    | 1:H:321:VAL:HG13 | 1.90                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:69:LEU:HD13  | 1:A:194:ARG:HG2  | 1.72                     | 0.71              |
| 1:A:258:PRO:HG2  | 1:A:261:LEU:HD12 | 1.72                     | 0.71              |
| 1:C:311:GLU:O    | 1:C:315:LEU:HD13 | 1.91                     | 0.70              |
| 1:E:309:ALA:HB1  | 1:E:320:LEU:HD21 | 1.73                     | 0.70              |
| 1:D:313:LEU:HD11 | 1:D:320:LEU:HG   | 1.74                     | 0.70              |
| 1:D:141:MET:HE2  | 1:D:144:VAL:HG21 | 1.73                     | 0.70              |
| 1:G:193:ILE:O    | 1:G:197:VAL:HG22 | 1.91                     | 0.70              |
| 1:B:227:GLU:HG3  | 1:B:316:VAL:CG2  | 2.22                     | 0.70              |
| 1:F:76:VAL:HB    | 1:F:79:LEU:HD12  | 1.74                     | 0.70              |
| 1:B:196:VAL:HG21 | 1:B:285:ILE:HD11 | 1.73                     | 0.70              |
| 1:H:227:GLU:O    | 1:H:231:LEU:HG   | 1.92                     | 0.69              |
| 1:D:229:ARG:HH11 | 1:D:229:ARG:HG2  | 1.57                     | 0.69              |
| 1:E:101:PHE:O    | 1:E:102:LEU:HD23 | 1.93                     | 0.69              |
| 1:G:174:GLY:HA2  | 1:G:323:ARG:HH21 | 1.56                     | 0.69              |
| 1:H:243:HIS:HA   | 1:H:300:MET:HG3  | 1.74                     | 0.69              |
| 1:D:266:ARG:HG3  | 1:D:323:ARG:HH12 | 1.56                     | 0.69              |
| 1:B:267:ARG:HG2  | 1:B:332:LEU:HG   | 1.75                     | 0.68              |
| 1:G:310:GLU:O    | 1:G:314:LYS:HD3  | 1.94                     | 0.68              |
| 1:C:165:ILE:HG13 | 1:C:170:ARG:HH11 | 1.58                     | 0.68              |
| 1:D:214:LYS:HD3  | 1:D:218:LEU:HD12 | 1.73                     | 0.68              |
| 1:B:201:ASP:OD2  | 1:B:204:ALA:HB2  | 1.93                     | 0.68              |
| 1:E:306:GLN:NE2  | 1:E:323:ARG:HH11 | 1.93                     | 0.67              |
| 1:E:55:VAL:HG21  | 1:H:99:LEU:HD21  | 1.77                     | 0.67              |
| 1:B:275:VAL:O    | 1:B:279:LEU:HG   | 1.94                     | 0.67              |
| 1:G:202:LEU:HA   | 1:G:213:LEU:HB3  | 1.75                     | 0.67              |
| 1:D:214:LYS:HD2  | 1:D:214:LYS:C    | 2.20                     | 0.67              |
| 1:B:98:PRO:HD3   | 3:B:627:HOH:O    | 1.94                     | 0.67              |
| 1:B:226:LYS:HD2  | 3:B:673:HOH:O    | 1.95                     | 0.66              |
| 1:D:249:LEU:HB3  | 1:D:250:PRO:HD3  | 1.76                     | 0.66              |
| 1:G:255:ARG:HG2  | 1:G:255:ARG:HH11 | 1.60                     | 0.66              |
| 1:A:249:LEU:HD13 | 1:A:298:LEU:HD13 | 1.77                     | 0.66              |
| 1:F:178:LEU:HD11 | 1:F:313:LEU:HD21 | 1.77                     | 0.66              |
| 1:F:138:THR:HG23 | 3:F:644:HOH:O    | 1.94                     | 0.66              |
| 1:H:120:ALA:O    | 1:H:124:GLU:HG2  | 1.95                     | 0.66              |
| 1:A:213:LEU:HD23 | 3:A:501:HOH:O    | 1.96                     | 0.66              |
| 1:B:266:ARG:HA   | 1:B:333:VAL:O    | 1.96                     | 0.66              |
| 1:D:267:ARG:NH2  | 1:D:287:GLU:OE2  | 2.29                     | 0.66              |
| 1:E:132:PRO:HG3  | 3:G:501:HOH:O    | 1.95                     | 0.65              |
| 1:B:227:GLU:HG3  | 1:B:316:VAL:HG23 | 1.79                     | 0.64              |
| 1:F:205:PRO:HB3  | 3:F:676:HOH:O    | 1.96                     | 0.64              |
| 1:D:65:THR:CG2   | 1:D:194:ARG:HE   | 2.10                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:178:LEU:HD13 | 1:A:313:LEU:HD11 | 1.80                     | 0.64              |
| 1:C:249:LEU:HD11 | 1:C:253:LEU:HD12 | 1.79                     | 0.64              |
| 1:D:84:VAL:O     | 1:D:88:VAL:HG23  | 1.98                     | 0.64              |
| 1:B:280:GLN:HG3  | 1:B:285:ILE:O    | 1.98                     | 0.64              |
| 1:G:294:PHE:HB2  | 1:G:296:MET:CE   | 2.25                     | 0.63              |
| 1:F:138:THR:HG22 | 3:F:543:HOH:O    | 1.97                     | 0.63              |
| 1:E:97:GLU:HG2   | 1:E:98:PRO:HD2   | 1.80                     | 0.63              |
| 1:B:331:ARG:H    | 1:B:331:ARG:HD2  | 1.64                     | 0.63              |
| 1:H:89:ASN:HB2   | 1:H:243:HIS:CE1  | 2.34                     | 0.62              |
| 1:A:173:GLU:CD   | 1:A:326:PRO:HG3  | 2.23                     | 0.62              |
| 1:G:278:TYR:CE2  | 1:G:282:LEU:HD22 | 2.35                     | 0.62              |
| 1:E:306:GLN:NE2  | 1:E:323:ARG:HD3  | 2.15                     | 0.62              |
| 1:F:68:LEU:O     | 1:F:72:GLU:HG3   | 1.99                     | 0.62              |
| 1:H:115:LEU:O    | 1:H:119:LEU:HD13 | 2.00                     | 0.62              |
| 1:C:307:GLU:H    | 1:C:307:GLU:CD   | 2.07                     | 0.62              |
| 1:F:105:LEU:CD2  | 1:F:152:ILE:HG23 | 2.29                     | 0.62              |
| 1:B:280:GLN:HB2  | 1:B:290:MET:HE2  | 1.82                     | 0.61              |
| 1:G:88:VAL:O     | 1:G:92:LEU:HG    | 2.00                     | 0.61              |
| 1:C:249:LEU:HB3  | 1:C:250:PRO:HD3  | 1.82                     | 0.61              |
| 1:H:53:GLU:HG2   | 1:H:161:GLU:OE2  | 2.01                     | 0.61              |
| 1:B:107:ALA:HB2  | 1:B:150:TRP:CD2  | 2.35                     | 0.61              |
| 1:G:227:GLU:HG3  | 1:G:316:VAL:HB   | 1.81                     | 0.61              |
| 1:H:126:CYS:HB3  | 1:H:131:ILE:O    | 2.01                     | 0.61              |
| 1:G:141:MET:HE3  | 1:H:64:GLY:C     | 2.26                     | 0.61              |
| 1:D:266:ARG:HH11 | 1:D:323:ARG:NH1  | 1.98                     | 0.60              |
| 1:G:304:LEU:HD13 | 1:G:309:ALA:HB2  | 1.83                     | 0.60              |
| 1:E:102:LEU:HD22 | 3:F:661:HOH:O    | 2.01                     | 0.60              |
| 1:B:169:GLU:CD   | 1:B:169:GLU:H    | 2.09                     | 0.60              |
| 1:E:249:LEU:HB3  | 1:E:250:PRO:HD3  | 1.83                     | 0.60              |
| 1:B:249:LEU:HB3  | 1:B:250:PRO:HD3  | 1.82                     | 0.60              |
| 1:E:53:GLU:HB3   | 3:E:538:HOH:O    | 2.01                     | 0.60              |
| 1:H:327:GLY:O    | 1:H:328:GLU:HB2  | 2.01                     | 0.60              |
| 1:C:143:GLY:HA2  | 1:D:146:ARG:NH1  | 2.16                     | 0.60              |
| 1:A:60:THR:HG22  | 1:A:155:THR:OG1  | 2.01                     | 0.60              |
| 1:A:289:GLU:HG3  | 1:A:292:ARG:NH2  | 2.17                     | 0.60              |
| 1:C:225:LEU:O    | 1:C:229:ARG:HG3  | 2.01                     | 0.59              |
| 1:G:255:ARG:HG2  | 1:G:255:ARG:NH1  | 2.15                     | 0.59              |
| 1:G:307:GLU:HG3  | 3:G:565:HOH:O    | 2.01                     | 0.59              |
| 1:B:263:ALA:O    | 1:B:331:ARG:HD2  | 2.01                     | 0.59              |
| 1:C:276:PHE:CE1  | 1:C:294:PHE:HB3  | 2.37                     | 0.59              |
| 1:A:285:ILE:N    | 1:A:285:ILE:HD12 | 2.17                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:275:VAL:O    | 1:A:279:LEU:HG   | 2.02                     | 0.59              |
| 1:F:321:VAL:HG12 | 1:F:321:VAL:O    | 2.01                     | 0.59              |
| 1:B:258:PRO:CG   | 1:B:261:LEU:HD12 | 2.33                     | 0.59              |
| 1:E:306:GLN:NE2  | 1:E:323:ARG:CD   | 2.65                     | 0.59              |
| 1:H:202:LEU:O    | 1:H:212:SER:HB2  | 2.02                     | 0.59              |
| 1:H:267:ARG:HG3  | 1:H:333:VAL:OXT  | 2.02                     | 0.59              |
| 1:C:173:GLU:OE1  | 1:C:326:PRO:HG3  | 2.02                     | 0.59              |
| 1:H:197:VAL:O    | 1:H:200:GLN:HB2  | 2.02                     | 0.59              |
| 1:A:178:LEU:HD12 | 1:A:319:PHE:O    | 2.02                     | 0.58              |
| 1:F:319:PHE:O    | 1:F:321:VAL:HG23 | 2.03                     | 0.58              |
| 1:G:249:LEU:HB3  | 1:G:250:PRO:HD3  | 1.85                     | 0.58              |
| 1:H:224:TYR:CD2  | 1:H:300:MET:HE3  | 2.39                     | 0.58              |
| 1:E:239:HIS:CE1  | 1:E:305:PRO:HG3  | 2.39                     | 0.58              |
| 1:A:66:LYS:HE2   | 1:A:190:TYR:OH   | 2.04                     | 0.58              |
| 1:A:189:GLY:O    | 1:A:193:ILE:HG13 | 2.03                     | 0.58              |
| 1:B:83:LEU:HD22  | 1:B:152:ILE:HG22 | 1.85                     | 0.58              |
| 1:F:72:GLU:OE2   | 1:F:194:ARG:NH2  | 2.36                     | 0.58              |
| 1:D:202:LEU:HD23 | 1:D:213:LEU:HD23 | 1.85                     | 0.58              |
| 1:C:118:LEU:O    | 1:C:122:LEU:HD23 | 2.05                     | 0.57              |
| 1:F:146:ARG:NH2  | 3:F:501:HOH:O    | 2.37                     | 0.57              |
| 1:G:309:ALA:HB1  | 1:G:320:LEU:HD21 | 1.87                     | 0.57              |
| 1:F:51:LEU:N     | 3:F:502:HOH:O    | 2.37                     | 0.57              |
| 1:F:89:ASN:HB2   | 1:F:243:HIS:CE1  | 2.39                     | 0.57              |
| 1:D:89:ASN:HB2   | 1:D:243:HIS:CE1  | 2.38                     | 0.57              |
| 1:A:276:PHE:CE1  | 1:A:294:PHE:HB3  | 2.40                     | 0.57              |
| 1:A:70:ALA:HB1   | 1:A:75:ASP:O     | 2.04                     | 0.57              |
| 1:H:266:ARG:HB2  | 1:H:269:SER:HB3  | 1.86                     | 0.57              |
| 1:C:267:ARG:HD2  | 1:C:333:VAL:O    | 2.04                     | 0.56              |
| 1:E:132:PRO:HD3  | 1:G:164:ARG:NH2  | 2.20                     | 0.56              |
| 1:D:51:LEU:HA    | 3:D:653:HOH:O    | 2.04                     | 0.56              |
| 1:E:60:THR:HG23  | 1:F:102:LEU:HD12 | 1.86                     | 0.56              |
| 1:A:190:TYR:HA   | 1:A:193:ILE:HB   | 1.85                     | 0.56              |
| 1:C:57:VAL:HG12  | 1:C:58:ALA:N     | 2.20                     | 0.56              |
| 1:D:52:GLU:HA    | 3:D:660:HOH:O    | 2.05                     | 0.56              |
| 1:B:288:GLU:HG2  | 3:B:611:HOH:O    | 2.05                     | 0.56              |
| 1:G:307:GLU:O    | 1:G:311:GLU:HG3  | 2.05                     | 0.56              |
| 1:H:292:ARG:HG3  | 3:H:556:HOH:O    | 2.05                     | 0.56              |
| 1:A:249:LEU:N    | 1:A:250:PRO:HD2  | 2.20                     | 0.56              |
| 1:A:177:LEU:HD11 | 1:A:263:ALA:HB1  | 1.87                     | 0.56              |
| 1:D:229:ARG:O    | 1:D:233:GLU:HG3  | 2.06                     | 0.56              |
| 1:F:201:ASP:OD2  | 1:F:204:ALA:HB2  | 2.05                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:83:LEU:HD22  | 1:C:152:ILE:HG22 | 1.87                     | 0.56              |
| 1:E:105:LEU:HD22 | 1:E:152:ILE:HD12 | 1.87                     | 0.56              |
| 1:E:134:LEU:HD21 | 3:G:501:HOH:O    | 2.06                     | 0.56              |
| 1:H:224:TYR:HD2  | 1:H:300:MET:HE3  | 1.71                     | 0.56              |
| 1:D:183:SER:O    | 1:D:219:ARG:NE   | 2.31                     | 0.55              |
| 1:A:280:GLN:HA   | 1:A:285:ILE:HD13 | 1.86                     | 0.55              |
| 1:C:107:ALA:HB2  | 1:C:150:TRP:CD2  | 2.41                     | 0.55              |
| 1:D:185:PRO:HB2  | 1:D:190:TYR:OH   | 2.07                     | 0.55              |
| 1:H:177:LEU:HD11 | 1:H:263:ALA:HB1  | 1.89                     | 0.55              |
| 1:H:161:GLU:HB2  | 1:H:164:ARG:HD3  | 1.88                     | 0.55              |
| 1:D:53:GLU:N     | 1:D:54:PRO:CD    | 2.69                     | 0.55              |
| 1:D:323:ARG:HD3  | 1:D:323:ARG:N    | 2.22                     | 0.55              |
| 1:A:304:LEU:CD1  | 1:A:309:ALA:HB2  | 2.35                     | 0.55              |
| 1:B:162:ARG:HD2  | 1:C:169:GLU:OE2  | 2.06                     | 0.55              |
| 1:F:283:GLY:C    | 1:F:285:ILE:HD12 | 2.32                     | 0.55              |
| 1:G:216:ALA:HB1  | 1:G:275:VAL:CG2  | 2.37                     | 0.55              |
| 1:G:264:GLU:HG3  | 3:G:550:HOH:O    | 2.05                     | 0.55              |
| 1:B:267:ARG:HG3  | 1:B:333:VAL:O    | 2.05                     | 0.55              |
| 1:F:249:LEU:HD22 | 1:F:298:LEU:CD1  | 2.37                     | 0.55              |
| 1:H:105:LEU:HD22 | 1:H:152:ILE:HG23 | 1.89                     | 0.55              |
| 1:B:66:LYS:HB2   | 3:B:538:HOH:O    | 2.06                     | 0.54              |
| 1:F:251:GLU:O    | 1:F:255:ARG:HG3  | 2.07                     | 0.54              |
| 1:C:304:LEU:HD23 | 1:C:304:LEU:H    | 1.72                     | 0.54              |
| 1:D:258:PRO:HG2  | 1:D:261:LEU:HD12 | 1.88                     | 0.54              |
| 1:E:145:TYR:CE1  | 1:E:151:ASP:HB2  | 2.43                     | 0.54              |
| 1:F:83:LEU:HD22  | 1:F:152:ILE:HG22 | 1.89                     | 0.54              |
| 1:F:120:ALA:HB2  | 3:F:524:HOH:O    | 2.05                     | 0.54              |
| 1:D:328:GLU:HG3  | 3:D:552:HOH:O    | 2.08                     | 0.54              |
| 1:G:289:GLU:O    | 1:G:293:VAL:HG23 | 2.07                     | 0.54              |
| 1:B:267:ARG:NH2  | 1:B:287:GLU:OE1  | 2.41                     | 0.54              |
| 1:D:266:ARG:NH1  | 1:D:323:ARG:NH1  | 2.56                     | 0.54              |
| 1:F:206:VAL:HB   | 1:F:209:LEU:HB2  | 1.89                     | 0.54              |
| 1:F:332:LEU:HD12 | 1:F:332:LEU:N    | 2.21                     | 0.54              |
| 1:G:278:TYR:HE2  | 1:G:282:LEU:HD22 | 1.72                     | 0.54              |
| 1:A:247:GLY:HA3  | 1:A:251:GLU:OE1  | 2.07                     | 0.54              |
| 1:F:307:GLU:O    | 1:F:311:GLU:HG3  | 2.06                     | 0.54              |
| 1:G:290:MET:HG3  | 1:G:296:MET:CE   | 2.37                     | 0.54              |
| 1:E:60:THR:HG23  | 1:F:102:LEU:CD1  | 2.38                     | 0.54              |
| 1:G:65:THR:HB    | 1:G:194:ARG:NE   | 2.22                     | 0.54              |
| 1:G:99:LEU:O     | 1:G:132:PRO:HD2  | 2.07                     | 0.54              |
| 1:B:319:PHE:O    | 1:B:321:VAL:HG13 | 2.08                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:99:LEU:O     | 1:D:132:PRO:HD2  | 2.08                     | 0.54              |
| 1:H:185:PRO:HB2  | 1:H:190:TYR:OH   | 2.08                     | 0.54              |
| 1:E:307:GLU:HB3  | 3:E:681:HOH:O    | 2.06                     | 0.54              |
| 1:H:92:LEU:HD13  | 3:H:529:HOH:O    | 2.08                     | 0.54              |
| 1:D:313:LEU:HD11 | 1:D:320:LEU:CG   | 2.38                     | 0.53              |
| 1:F:285:ILE:HD12 | 1:F:285:ILE:N    | 2.22                     | 0.53              |
| 1:G:144:VAL:HG22 | 1:H:68:LEU:HD11  | 1.89                     | 0.53              |
| 1:G:239:HIS:CE1  | 1:G:305:PRO:HG3  | 2.43                     | 0.53              |
| 1:D:284:GLY:O    | 1:D:286:PRO:HD3  | 2.08                     | 0.53              |
| 1:G:285:ILE:CB   | 1:G:290:MET:HE1  | 2.30                     | 0.53              |
| 1:H:249:LEU:N    | 1:H:250:PRO:HD2  | 2.22                     | 0.53              |
| 1:C:181:PRO:HD2  | 3:C:524:HOH:O    | 2.09                     | 0.53              |
| 1:G:180:LEU:HB3  | 1:G:224:TYR:CE1  | 2.43                     | 0.53              |
| 1:G:333:VAL:HG22 | 1:G:333:VAL:OXT  | 2.08                     | 0.53              |
| 1:B:52:GLU:O     | 1:B:52:GLU:HG2   | 2.09                     | 0.53              |
| 1:G:201:ASP:OD2  | 1:G:204:ALA:HB2  | 2.09                     | 0.53              |
| 1:A:171:VAL:HB   | 1:A:258:PRO:HD3  | 1.89                     | 0.53              |
| 1:C:126:CYS:HB3  | 1:C:131:ILE:O    | 2.09                     | 0.53              |
| 1:D:323:ARG:N    | 1:D:323:ARG:CD   | 2.72                     | 0.53              |
| 1:G:104:TYR:HB2  | 1:H:60:THR:HG21  | 1.91                     | 0.53              |
| 1:C:60:THR:HG23  | 1:D:102:LEU:CD1  | 2.39                     | 0.53              |
| 1:D:190:TYR:HA   | 1:D:193:ILE:HB   | 1.90                     | 0.53              |
| 1:E:104:TYR:HB2  | 1:F:60:THR:HG21  | 1.91                     | 0.53              |
| 1:A:206:VAL:HG13 | 1:A:207:PRO:HD2  | 1.91                     | 0.52              |
| 1:D:120:ALA:O    | 1:D:124:GLU:HG2  | 2.09                     | 0.52              |
| 1:C:60:THR:HG23  | 1:D:102:LEU:HD12 | 1.92                     | 0.52              |
| 1:E:128:ALA:HB3  | 3:E:531:HOH:O    | 2.08                     | 0.52              |
| 1:F:280:GLN:HG3  | 1:F:285:ILE:O    | 2.08                     | 0.52              |
| 1:E:145:TYR:HE1  | 1:E:151:ASP:HB2  | 1.74                     | 0.52              |
| 1:G:83:LEU:HD22  | 1:G:152:ILE:HG22 | 1.92                     | 0.52              |
| 1:D:323:ARG:HD3  | 1:D:323:ARG:H    | 1.73                     | 0.52              |
| 1:E:53:GLU:N     | 1:E:54:PRO:CD    | 2.72                     | 0.52              |
| 1:F:265:VAL:HG13 | 1:F:321:VAL:CG1  | 2.37                     | 0.52              |
| 1:C:327:GLY:C    | 1:C:328:GLU:HG3  | 2.34                     | 0.52              |
| 1:C:213:LEU:O    | 1:C:217:LEU:HB2  | 2.10                     | 0.52              |
| 1:A:206:VAL:CG1  | 1:A:207:PRO:HD2  | 2.40                     | 0.52              |
| 1:F:196:VAL:HG21 | 1:F:285:ILE:HD11 | 1.91                     | 0.52              |
| 1:A:214:LYS:O    | 1:A:218:LEU:HB2  | 2.10                     | 0.52              |
| 1:F:328:GLU:HB2  | 3:F:630:HOH:O    | 2.09                     | 0.52              |
| 1:D:304:LEU:N    | 1:D:304:LEU:HD12 | 2.25                     | 0.52              |
| 1:A:66:LYS:HG3   | 1:A:190:TYR:CE2  | 2.45                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:253:LEU:HD12 | 1:A:253:LEU:O    | 2.10                     | 0.51              |
| 1:E:165:ILE:O    | 1:E:166:LEU:HD23 | 2.11                     | 0.51              |
| 1:F:171:VAL:HB   | 1:F:258:PRO:HD3  | 1.92                     | 0.51              |
| 1:G:323:ARG:HG3  | 1:G:323:ARG:HH11 | 1.74                     | 0.51              |
| 1:B:104:TYR:HD1  | 1:B:137:GLU:HB2  | 1.75                     | 0.51              |
| 1:B:296:MET:HE2  | 1:B:296:MET:CA   | 2.39                     | 0.51              |
| 1:C:89:ASN:HB2   | 1:C:243:HIS:CE1  | 2.45                     | 0.51              |
| 1:D:214:LYS:HD2  | 1:D:214:LYS:O    | 2.11                     | 0.51              |
| 1:F:178:LEU:CD1  | 1:F:313:LEU:HD21 | 2.39                     | 0.51              |
| 1:G:249:LEU:HD11 | 1:G:253:LEU:HD22 | 1.93                     | 0.51              |
| 1:H:331:ARG:NH1  | 1:H:333:VAL:HG12 | 2.22                     | 0.51              |
| 1:A:285:ILE:HD12 | 1:A:285:ILE:H    | 1.74                     | 0.51              |
| 1:A:325:VAL:HG22 | 1:A:326:PRO:HD2  | 1.92                     | 0.51              |
| 1:F:141:MET:HE3  | 1:F:145:TYR:HE1  | 1.74                     | 0.51              |
| 1:F:169:GLU:HG3  | 1:G:172:ARG:NH2  | 2.23                     | 0.51              |
| 1:H:280:GLN:HG3  | 1:H:285:ILE:O    | 2.10                     | 0.51              |
| 1:A:304:LEU:HD12 | 1:A:304:LEU:H    | 1.75                     | 0.51              |
| 1:B:227:GLU:HG3  | 1:B:316:VAL:HG21 | 1.92                     | 0.51              |
| 1:D:111:ASP:HB3  | 3:D:661:HOH:O    | 2.10                     | 0.51              |
| 1:G:105:LEU:O    | 1:G:138:THR:HA   | 2.11                     | 0.51              |
| 1:A:258:PRO:CG   | 1:A:261:LEU:HD12 | 2.41                     | 0.51              |
| 1:G:258:PRO:HG2  | 1:G:261:LEU:HD12 | 1.92                     | 0.51              |
| 1:A:189:GLY:HA3  | 1:A:294:PHE:CE1  | 2.46                     | 0.51              |
| 1:C:307:GLU:CD   | 1:C:307:GLU:N    | 2.69                     | 0.51              |
| 1:E:126:CYS:HB3  | 1:E:131:ILE:O    | 2.10                     | 0.51              |
| 1:C:265:VAL:O    | 1:C:332:LEU:HA   | 2.10                     | 0.51              |
| 1:F:169:GLU:HB2  | 3:F:604:HOH:O    | 2.11                     | 0.51              |
| 1:H:183:SER:HB2  | 1:H:222:ARG:HB2  | 1.93                     | 0.51              |
| 1:H:254:PRO:HG3  | 1:H:330:VAL:HG23 | 1.93                     | 0.51              |
| 1:F:323:ARG:CB   | 3:F:680:HOH:O    | 2.58                     | 0.51              |
| 1:G:76:VAL:CG2   | 1:G:79:LEU:HD12  | 2.41                     | 0.51              |
| 1:A:76:VAL:HB    | 1:A:118:LEU:CD1  | 2.42                     | 0.50              |
| 1:E:306:GLN:HE21 | 1:E:323:ARG:HH11 | 1.59                     | 0.50              |
| 1:G:215:GLU:HG2  | 3:G:660:HOH:O    | 2.10                     | 0.50              |
| 1:B:68:LEU:O     | 1:B:72:GLU:HG3   | 2.10                     | 0.50              |
| 1:G:141:MET:HE3  | 1:H:65:THR:N     | 2.26                     | 0.50              |
| 1:G:205:PRO:HB3  | 3:G:671:HOH:O    | 2.10                     | 0.50              |
| 1:A:279:LEU:HD12 | 1:A:280:GLN:N    | 2.25                     | 0.50              |
| 1:A:309:ALA:O    | 1:A:313:LEU:HD13 | 2.12                     | 0.50              |
| 1:D:141:MET:HE2  | 1:D:144:VAL:CG2  | 2.40                     | 0.50              |
| 1:H:304:LEU:HD13 | 1:H:309:ALA:HB2  | 1.94                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:207:PRO:HG2  | 1:B:208:GLU:H    | 1.75                     | 0.50              |
| 1:B:316:VAL:HG22 | 1:B:317:GLU:N    | 2.25                     | 0.50              |
| 1:E:84:VAL:O     | 1:E:88:VAL:HG23  | 2.12                     | 0.50              |
| 1:G:81:PHE:CE1   | 1:G:125:ALA:HA   | 2.46                     | 0.50              |
| 1:H:63:VAL:HG11  | 1:H:79:LEU:HD22  | 1.92                     | 0.50              |
| 1:H:200:GLN:HG3  | 1:H:282:LEU:HD21 | 1.92                     | 0.50              |
| 1:D:280:GLN:HB2  | 1:D:290:MET:SD   | 2.52                     | 0.50              |
| 1:B:120:ALA:O    | 1:B:124:GLU:HG3  | 2.10                     | 0.50              |
| 1:F:306:GLN:O    | 1:F:310:GLU:HG2  | 2.12                     | 0.50              |
| 1:G:192:LEU:HD21 | 1:G:285:ILE:HD13 | 1.94                     | 0.50              |
| 1:G:216:ALA:HB1  | 1:G:275:VAL:HG22 | 1.94                     | 0.50              |
| 1:E:102:LEU:HD13 | 3:F:661:HOH:O    | 2.11                     | 0.50              |
| 1:G:306:GLN:HE21 | 1:G:310:GLU:HG3  | 1.77                     | 0.50              |
| 1:D:190:TYR:O    | 1:D:194:ARG:HG3  | 2.12                     | 0.50              |
| 1:F:162:ARG:NH1  | 1:G:169:GLU:OE1  | 2.45                     | 0.50              |
| 1:G:98:PRO:HB2   | 1:G:131:ILE:HG21 | 1.93                     | 0.50              |
| 1:H:109:HIS:HA   | 1:H:140:GLU:HG3  | 1.94                     | 0.50              |
| 1:H:166:LEU:HD23 | 1:H:170:ARG:HH11 | 1.77                     | 0.50              |
| 1:H:288:GLU:HG3  | 1:H:292:ARG:NH1  | 2.27                     | 0.50              |
| 1:F:267:ARG:HG2  | 1:F:333:VAL:O    | 2.11                     | 0.49              |
| 1:F:276:PHE:CE1  | 1:F:294:PHE:HB3  | 2.47                     | 0.49              |
| 1:H:99:LEU:HB2   | 1:H:158:GLY:HA2  | 1.94                     | 0.49              |
| 1:E:333:VAL:OXT  | 1:E:333:VAL:HG12 | 2.11                     | 0.49              |
| 1:G:196:VAL:HG21 | 1:G:285:ILE:HD11 | 1.94                     | 0.49              |
| 1:A:280:GLN:HB2  | 1:A:290:MET:HE2  | 1.92                     | 0.49              |
| 1:B:176:ALA:HB1  | 1:B:320:LEU:CD1  | 2.43                     | 0.49              |
| 1:E:136:GLY:O    | 1:E:137:GLU:HB2  | 2.11                     | 0.49              |
| 1:F:126:CYS:SG   | 1:F:133:LEU:HD13 | 2.52                     | 0.49              |
| 1:C:333:VAL:OXT  | 1:C:333:VAL:HG12 | 2.13                     | 0.49              |
| 1:E:107:ALA:HB2  | 1:E:150:TRP:CD2  | 2.47                     | 0.49              |
| 1:G:280:GLN:HE22 | 1:G:287:GLU:HB2  | 1.78                     | 0.49              |
| 1:D:304:LEU:HD13 | 1:D:309:ALA:HB2  | 1.94                     | 0.49              |
| 1:H:313:LEU:HD11 | 1:H:320:LEU:CG   | 2.41                     | 0.49              |
| 1:C:193:ILE:O    | 1:C:197:VAL:HG22 | 2.12                     | 0.49              |
| 1:F:169:GLU:HG2  | 1:G:172:ARG:HH21 | 1.75                     | 0.49              |
| 1:H:111:ASP:HB3  | 3:H:566:HOH:O    | 2.11                     | 0.49              |
| 1:D:323:ARG:HB3  | 3:D:532:HOH:O    | 2.13                     | 0.49              |
| 1:F:261:LEU:HD13 | 1:F:324:VAL:HG11 | 1.94                     | 0.49              |
| 1:F:304:LEU:HB2  | 1:F:305:PRO:HD2  | 1.93                     | 0.49              |
| 1:G:126:CYS:HB3  | 1:G:131:ILE:O    | 2.12                     | 0.49              |
| 1:D:171:VAL:HB   | 1:D:258:PRO:HD3  | 1.95                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:82:ASP:OD1   | 1:F:220:PRO:HA   | 2.13                     | 0.49              |
| 1:A:114:VAL:HG12 | 1:A:118:LEU:HD22 | 1.94                     | 0.48              |
| 1:A:178:LEU:CD1  | 1:A:313:LEU:HD11 | 2.42                     | 0.48              |
| 1:A:222:ARG:HD2  | 3:A:622:HOH:O    | 2.12                     | 0.48              |
| 1:B:333:VAL:OXT  | 1:B:333:VAL:HG12 | 2.13                     | 0.48              |
| 1:C:304:LEU:HD23 | 1:C:304:LEU:N    | 2.28                     | 0.48              |
| 1:F:305:PRO:HG2  | 1:F:308:ALA:CB   | 2.43                     | 0.48              |
| 1:G:141:MET:HE2  | 1:G:144:VAL:CG2  | 2.42                     | 0.48              |
| 1:G:272:ILE:O    | 1:G:273:PRO:C    | 2.56                     | 0.48              |
| 1:B:294:PHE:CB   | 1:B:296:MET:HE3  | 2.34                     | 0.48              |
| 1:D:185:PRO:O    | 1:D:186:HIS:HB2  | 2.13                     | 0.48              |
| 1:A:76:VAL:HB    | 1:A:118:LEU:HD11 | 1.94                     | 0.48              |
| 1:A:306:GLN:OE1  | 1:A:323:ARG:NE   | 2.45                     | 0.48              |
| 1:E:101:PHE:C    | 1:E:102:LEU:HD23 | 2.37                     | 0.48              |
| 1:F:105:LEU:HD22 | 1:F:152:ILE:HG23 | 1.94                     | 0.48              |
| 1:A:266:ARG:NH2  | 1:A:320:LEU:O    | 2.47                     | 0.48              |
| 1:C:205:PRO:HG3  | 1:F:120:ALA:HA   | 1.94                     | 0.48              |
| 1:B:104:TYR:CD1  | 1:B:137:GLU:HB2  | 2.48                     | 0.48              |
| 1:B:316:VAL:CG2  | 1:B:317:GLU:N    | 2.76                     | 0.48              |
| 1:F:190:TYR:O    | 1:F:194:ARG:HG3  | 2.14                     | 0.48              |
| 1:H:304:LEU:N    | 1:H:304:LEU:HD12 | 2.28                     | 0.48              |
| 1:A:325:VAL:HG22 | 1:A:326:PRO:CD   | 2.44                     | 0.48              |
| 1:F:304:LEU:HD23 | 1:F:304:LEU:H    | 1.78                     | 0.48              |
| 1:E:193:ILE:O    | 1:E:197:VAL:HG22 | 2.14                     | 0.48              |
| 1:G:280:GLN:CD   | 1:G:290:MET:HE3  | 2.39                     | 0.48              |
| 1:E:169:GLU:OE2  | 1:H:162:ARG:HD2  | 2.15                     | 0.47              |
| 1:F:239:HIS:HB2  | 1:F:303:VAL:O    | 2.14                     | 0.47              |
| 1:F:249:LEU:HB3  | 1:F:250:PRO:HD3  | 1.95                     | 0.47              |
| 1:A:323:ARG:HB2  | 1:A:323:ARG:CZ   | 2.43                     | 0.47              |
| 1:B:286:PRO:HD2  | 1:B:289:GLU:OE1  | 2.14                     | 0.47              |
| 1:B:310:GLU:O    | 1:B:314:LYS:HG3  | 2.14                     | 0.47              |
| 1:C:280:GLN:HG3  | 1:C:285:ILE:O    | 2.15                     | 0.47              |
| 1:B:249:LEU:CD2  | 1:B:253:LEU:HD12 | 2.39                     | 0.47              |
| 1:D:295:ASN:HB2  | 1:D:298:LEU:O    | 2.15                     | 0.47              |
| 1:G:314:LYS:HD2  | 1:G:314:LYS:N    | 2.28                     | 0.47              |
| 1:C:102:LEU:HB3  | 1:D:60:THR:HG23  | 1.96                     | 0.47              |
| 1:D:83:LEU:HD22  | 1:D:152:ILE:HG22 | 1.96                     | 0.47              |
| 1:H:189:GLY:O    | 1:H:193:ILE:HG13 | 2.15                     | 0.47              |
| 1:B:95:GLY:CA    | 1:B:166:LEU:HD22 | 2.44                     | 0.47              |
| 1:B:193:ILE:O    | 1:B:197:VAL:HG22 | 2.13                     | 0.47              |
| 1:E:189:GLY:O    | 1:E:193:ILE:HG13 | 2.13                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:304:LEU:HD12 | 1:G:304:LEU:N    | 2.29                     | 0.47              |
| 1:H:105:LEU:CD2  | 1:H:152:ILE:HG23 | 2.44                     | 0.47              |
| 1:D:51:LEU:N     | 3:D:510:HOH:O    | 2.47                     | 0.47              |
| 1:D:104:TYR:C    | 1:D:105:LEU:HD12 | 2.40                     | 0.47              |
| 1:D:266:ARG:HG3  | 1:D:323:ARG:NH1  | 2.28                     | 0.47              |
| 1:E:274:PRO:O    | 1:E:277:PRO:HG2  | 2.15                     | 0.47              |
| 1:F:254:PRO:HG3  | 1:F:330:VAL:HG23 | 1.95                     | 0.47              |
| 1:G:181:PRO:HG2  | 1:G:222:ARG:NH1  | 2.30                     | 0.47              |
| 1:H:171:VAL:HG21 | 1:H:256:ALA:O    | 2.15                     | 0.47              |
| 1:B:304:LEU:HD12 | 1:B:304:LEU:O    | 2.14                     | 0.47              |
| 1:G:178:LEU:C    | 1:G:178:LEU:HD23 | 2.40                     | 0.47              |
| 1:A:93:ALA:HB2   | 1:A:300:MET:CE   | 2.43                     | 0.47              |
| 1:A:162:ARG:HB3  | 1:C:134:LEU:HD11 | 1.95                     | 0.47              |
| 1:D:285:ILE:HG22 | 1:D:290:MET:HG2  | 1.95                     | 0.47              |
| 1:F:267:ARG:HD3  | 1:F:332:LEU:HB3  | 1.97                     | 0.47              |
| 1:A:97:GLU:CD    | 1:A:229:ARG:HH22 | 2.22                     | 0.47              |
| 1:B:57:VAL:HG12  | 1:C:162:ARG:HB2  | 1.96                     | 0.47              |
| 3:B:550:HOH:O    | 1:C:57:VAL:HG13  | 2.15                     | 0.47              |
| 1:B:226:LYS:O    | 1:B:230:LEU:HG   | 2.15                     | 0.46              |
| 1:D:229:ARG:HG2  | 1:D:229:ARG:NH1  | 2.29                     | 0.46              |
| 1:F:305:PRO:HG2  | 1:F:308:ALA:HB2  | 1.97                     | 0.46              |
| 1:B:89:ASN:HB2   | 1:B:243:HIS:CE1  | 2.50                     | 0.46              |
| 1:E:238:LEU:HD23 | 1:E:304:LEU:HD23 | 1.96                     | 0.46              |
| 1:G:96:ALA:HB2   | 1:G:160:VAL:CG2  | 2.45                     | 0.46              |
| 1:A:185:PRO:O    | 1:A:186:HIS:HB2  | 2.15                     | 0.46              |
| 1:C:91:LEU:HB3   | 1:C:96:ALA:HB3   | 1.98                     | 0.46              |
| 1:H:83:LEU:HD23  | 1:H:122:LEU:CD2  | 2.46                     | 0.46              |
| 1:C:105:LEU:O    | 1:C:138:THR:HA   | 2.16                     | 0.46              |
| 1:C:112:GLU:HG2  | 3:E:502:HOH:O    | 2.15                     | 0.46              |
| 1:D:333:VAL:HG22 | 1:D:333:VAL:OXT  | 2.14                     | 0.46              |
| 1:H:110:LEU:O    | 1:H:111:ASP:C    | 2.59                     | 0.46              |
| 1:H:265:VAL:HG13 | 1:H:321:VAL:O    | 2.15                     | 0.46              |
| 1:A:110:LEU:HD21 | 1:A:139:ALA:O    | 2.16                     | 0.46              |
| 1:E:253:LEU:N    | 1:E:254:PRO:CD   | 2.78                     | 0.46              |
| 1:G:171:VAL:HB   | 1:G:258:PRO:CD   | 2.40                     | 0.46              |
| 1:H:164:ARG:NH1  | 3:H:504:HOH:O    | 2.47                     | 0.46              |
| 1:E:177:LEU:HD11 | 1:E:263:ALA:HB1  | 1.96                     | 0.46              |
| 1:H:89:ASN:HB3   | 1:H:300:MET:HE2  | 1.98                     | 0.46              |
| 1:E:306:GLN:NE2  | 1:E:323:ARG:HD2  | 2.30                     | 0.46              |
| 1:F:82:ASP:HB3   | 1:F:187:THR:HG21 | 1.97                     | 0.46              |
| 1:A:267:ARG:HA   | 3:A:574:HOH:O    | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:70:ALA:HB1   | 1:D:75:ASP:O     | 2.16                     | 0.46              |
| 1:B:304:LEU:HD11 | 1:B:309:ALA:HB2  | 1.98                     | 0.46              |
| 1:B:185:PRO:HB2  | 1:B:190:TYR:CZ   | 2.51                     | 0.46              |
| 1:D:258:PRO:CG   | 1:D:261:LEU:HD12 | 2.46                     | 0.46              |
| 1:G:319:PHE:O    | 1:G:321:VAL:HG13 | 2.15                     | 0.46              |
| 1:H:306:GLN:HG2  | 3:H:528:HOH:O    | 2.16                     | 0.46              |
| 1:A:102:LEU:HG   | 1:A:135:GLY:H    | 1.80                     | 0.45              |
| 1:A:323:ARG:HB2  | 1:A:323:ARG:NH1  | 2.32                     | 0.45              |
| 1:C:311:GLU:HG2  | 3:C:711:HOH:O    | 2.15                     | 0.45              |
| 1:D:213:LEU:HB2  | 3:D:519:HOH:O    | 2.16                     | 0.45              |
| 1:E:96:ALA:HB2   | 1:E:160:VAL:HG22 | 1.97                     | 0.45              |
| 1:H:261:LEU:HD12 | 1:H:261:LEU:N    | 2.31                     | 0.45              |
| 1:G:258:PRO:CG   | 1:G:261:LEU:HD12 | 2.47                     | 0.45              |
| 1:H:295:ASN:HB2  | 1:H:298:LEU:O    | 2.16                     | 0.45              |
| 1:A:304:LEU:HD12 | 1:A:304:LEU:N    | 2.32                     | 0.45              |
| 1:B:51:LEU:HA    | 3:B:669:HOH:O    | 2.16                     | 0.45              |
| 1:F:178:LEU:HD12 | 1:F:319:PHE:O    | 2.16                     | 0.45              |
| 1:B:82:ASP:HB3   | 1:B:187:THR:HG21 | 1.99                     | 0.45              |
| 1:F:213:LEU:HB2  | 3:F:513:HOH:O    | 2.17                     | 0.45              |
| 1:G:323:ARG:HD3  | 3:G:510:HOH:O    | 2.15                     | 0.45              |
| 1:E:176:ALA:HB2  | 1:E:306:GLN:NE2  | 2.31                     | 0.45              |
| 1:F:267:ARG:CD   | 1:F:332:LEU:HD23 | 2.44                     | 0.45              |
| 1:G:181:PRO:HG3  | 1:G:317:GLU:CD   | 2.42                     | 0.45              |
| 1:A:238:LEU:CD2  | 1:A:304:LEU:HD23 | 2.46                     | 0.45              |
| 1:F:82:ASP:HB3   | 1:F:187:THR:CG2  | 2.46                     | 0.45              |
| 1:G:204:ALA:HA   | 1:G:205:PRO:HD3  | 1.83                     | 0.45              |
| 1:H:172:ARG:HH11 | 1:H:172:ARG:HG3  | 1.81                     | 0.45              |
| 1:A:253:LEU:N    | 1:A:254:PRO:CD   | 2.80                     | 0.45              |
| 1:C:137:GLU:HG3  | 1:C:138:THR:N    | 2.32                     | 0.45              |
| 1:D:253:LEU:HB3  | 1:D:254:PRO:HD3  | 1.98                     | 0.45              |
| 1:F:106:ALA:HA   | 1:F:139:ALA:O    | 2.16                     | 0.45              |
| 1:E:174:GLY:O    | 1:E:323:ARG:NH1  | 2.50                     | 0.45              |
| 1:H:229:ARG:NH2  | 3:H:507:HOH:O    | 2.50                     | 0.45              |
| 1:A:311:GLU:O    | 1:A:315:LEU:HD13 | 2.17                     | 0.45              |
| 1:B:189:GLY:HA2  | 3:B:617:HOH:O    | 2.16                     | 0.45              |
| 1:B:227:GLU:CG   | 1:B:316:VAL:HG21 | 2.46                     | 0.45              |
| 1:C:60:THR:HG22  | 1:C:155:THR:OG1  | 2.17                     | 0.45              |
| 1:C:285:ILE:HG23 | 1:C:289:GLU:OE1  | 2.17                     | 0.44              |
| 1:D:259:PRO:HG3  | 3:D:724:HOH:O    | 2.16                     | 0.44              |
| 1:G:175:ASP:OD2  | 1:G:239:HIS:ND1  | 2.49                     | 0.44              |
| 1:H:171:VAL:HB   | 1:H:258:PRO:HD3  | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:151:ASP:OD1  | 1:B:141:MET:HE1  | 2.17                     | 0.44              |
| 1:A:249:LEU:HD13 | 1:A:298:LEU:CD1  | 2.45                     | 0.44              |
| 1:B:249:LEU:HD23 | 1:B:253:LEU:HB2  | 2.00                     | 0.44              |
| 1:C:311:GLU:OE2  | 1:C:315:LEU:HD11 | 2.17                     | 0.44              |
| 1:E:102:LEU:HD11 | 1:F:58:ALA:HB1   | 1.98                     | 0.44              |
| 1:F:88:VAL:O     | 1:F:92:LEU:HG    | 2.18                     | 0.44              |
| 1:G:53:GLU:N     | 3:G:517:HOH:O    | 2.50                     | 0.44              |
| 1:G:190:TYR:O    | 1:G:194:ARG:HG3  | 2.17                     | 0.44              |
| 1:H:109:HIS:HA   | 1:H:140:GLU:CG   | 2.47                     | 0.44              |
| 1:H:191:SER:O    | 1:H:195:LYS:HG3  | 2.16                     | 0.44              |
| 1:H:253:LEU:HB3  | 1:H:254:PRO:HD3  | 1.98                     | 0.44              |
| 1:F:164:ARG:NH2  | 3:F:511:HOH:O    | 2.50                     | 0.44              |
| 1:F:193:ILE:HD13 | 1:F:217:LEU:HD22 | 1.99                     | 0.44              |
| 1:F:304:LEU:HD11 | 1:F:309:ALA:HA   | 1.99                     | 0.44              |
| 1:B:190:TYR:HA   | 1:B:193:ILE:HB   | 1.99                     | 0.44              |
| 1:D:65:THR:HG21  | 1:D:194:ARG:HE   | 1.80                     | 0.44              |
| 1:E:141:MET:HE1  | 1:F:151:ASP:OD1  | 2.17                     | 0.44              |
| 1:F:65:THR:C     | 1:F:67:THR:N     | 2.72                     | 0.44              |
| 1:F:323:ARG:HD3  | 3:F:680:HOH:O    | 2.16                     | 0.44              |
| 1:A:189:GLY:HA3  | 1:A:294:PHE:HE1  | 1.82                     | 0.44              |
| 1:A:273:PRO:HA   | 1:A:274:PRO:HD3  | 1.79                     | 0.44              |
| 1:C:109:HIS:HA   | 1:C:140:GLU:HG3  | 1.98                     | 0.44              |
| 1:C:224:TYR:O    | 1:C:228:PHE:HD1  | 2.01                     | 0.44              |
| 1:H:228:PHE:C    | 1:H:230:LEU:H    | 2.25                     | 0.44              |
| 1:A:323:ARG:NH1  | 3:A:503:HOH:O    | 2.45                     | 0.44              |
| 1:C:214:LYS:HD3  | 3:C:607:HOH:O    | 2.18                     | 0.44              |
| 1:E:206:VAL:HB   | 1:E:209:LEU:HB2  | 1.99                     | 0.44              |
| 1:F:323:ARG:HB2  | 3:F:680:HOH:O    | 2.17                     | 0.44              |
| 1:C:196:VAL:HG21 | 1:C:285:ILE:HD11 | 2.00                     | 0.44              |
| 1:G:280:GLN:HB2  | 1:G:290:MET:CE   | 2.48                     | 0.44              |
| 1:B:237:GLU:OE2  | 1:B:305:PRO:HG2  | 2.18                     | 0.44              |
| 1:F:183:SER:HB3  | 1:F:222:ARG:HB2  | 1.99                     | 0.44              |
| 1:G:177:LEU:HD11 | 1:G:263:ALA:HB1  | 1.99                     | 0.44              |
| 1:G:327:GLY:O    | 1:G:328:GLU:HB2  | 2.16                     | 0.44              |
| 1:A:84:VAL:O     | 1:A:88:VAL:HG23  | 2.18                     | 0.43              |
| 1:A:289:GLU:HG3  | 1:A:292:ARG:CZ   | 2.48                     | 0.43              |
| 1:C:94:GLN:NE2   | 3:C:512:HOH:O    | 2.48                     | 0.43              |
| 1:F:317:GLU:HG2  | 3:F:641:HOH:O    | 2.18                     | 0.43              |
| 1:G:82:ASP:HB3   | 1:G:187:THR:CG2  | 2.47                     | 0.43              |
| 1:H:331:ARG:NH1  | 1:H:333:VAL:CG1  | 2.81                     | 0.43              |
| 1:H:232:TRP:HZ3  | 3:H:530:HOH:O    | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:281:ARG:HD3  | 3:B:654:HOH:O    | 2.17                     | 0.43              |
| 1:H:123:ALA:HA   | 1:H:133:LEU:HD22 | 1.98                     | 0.43              |
| 1:H:171:VAL:HG12 | 1:H:172:ARG:N    | 2.32                     | 0.43              |
| 1:B:123:ALA:O    | 1:B:127:ARG:HG2  | 2.18                     | 0.43              |
| 1:D:253:LEU:N    | 1:D:254:PRO:CD   | 2.81                     | 0.43              |
| 1:F:206:VAL:HB   | 1:F:209:LEU:HD22 | 2.01                     | 0.43              |
| 1:F:272:ILE:O    | 1:F:273:PRO:C    | 2.60                     | 0.43              |
| 1:F:313:LEU:HD11 | 1:F:320:LEU:HG   | 2.00                     | 0.43              |
| 1:G:265:VAL:O    | 1:G:332:LEU:HA   | 2.18                     | 0.43              |
| 1:G:307:GLU:HB3  | 3:G:622:HOH:O    | 2.18                     | 0.43              |
| 1:H:204:ALA:HA   | 1:H:205:PRO:HD3  | 1.80                     | 0.43              |
| 1:B:249:LEU:N    | 1:B:250:PRO:CD   | 2.81                     | 0.43              |
| 1:B:291:TYR:CD2  | 1:B:296:MET:HG3  | 2.53                     | 0.43              |
| 1:C:57:VAL:HG12  | 1:C:58:ALA:H     | 1.84                     | 0.43              |
| 1:G:141:MET:HG2  | 1:H:65:THR:HG23  | 1.99                     | 0.43              |
| 1:G:194:ARG:HD2  | 3:G:583:HOH:O    | 2.18                     | 0.43              |
| 1:B:59:THR:CG2   | 1:B:91:LEU:HD13  | 2.43                     | 0.43              |
| 1:B:227:GLU:CG   | 1:B:316:VAL:CG2  | 2.96                     | 0.43              |
| 1:C:237:GLU:OE2  | 1:C:239:HIS:NE2  | 2.52                     | 0.43              |
| 1:D:105:LEU:HD12 | 1:D:105:LEU:N    | 2.34                     | 0.43              |
| 1:D:331:ARG:NH1  | 1:D:331:ARG:HG3  | 2.34                     | 0.43              |
| 1:B:113:GLY:HA3  | 3:B:587:HOH:O    | 2.17                     | 0.43              |
| 1:B:177:LEU:HD11 | 1:B:263:ALA:HB1  | 2.00                     | 0.43              |
| 1:B:263:ALA:O    | 1:B:331:ARG:CD   | 2.66                     | 0.43              |
| 1:F:204:ALA:HA   | 1:F:205:PRO:HD3  | 1.88                     | 0.43              |
| 3:G:617:HOH:O    | 1:H:65:THR:HG21  | 2.18                     | 0.43              |
| 1:A:194:ARG:HD2  | 3:A:630:HOH:O    | 2.18                     | 0.43              |
| 1:D:264:GLU:HA   | 1:D:331:ARG:O    | 2.19                     | 0.43              |
| 1:E:89:ASN:HB2   | 1:E:243:HIS:CE1  | 2.54                     | 0.43              |
| 1:F:311:GLU:HB3  | 3:F:551:HOH:O    | 2.18                     | 0.43              |
| 1:A:325:VAL:HG13 | 1:A:326:PRO:N    | 2.32                     | 0.43              |
| 1:B:188:ASN:ND2  | 1:B:245:THR:HB   | 2.34                     | 0.43              |
| 1:D:105:LEU:O    | 1:D:138:THR:HA   | 2.18                     | 0.43              |
| 1:D:320:LEU:HB3  | 3:D:547:HOH:O    | 2.18                     | 0.43              |
| 1:A:249:LEU:HD21 | 1:A:265:VAL:HG21 | 2.01                     | 0.42              |
| 1:B:74:GLY:HA2   | 3:B:531:HOH:O    | 2.18                     | 0.42              |
| 1:D:331:ARG:HG3  | 1:D:331:ARG:HH11 | 1.84                     | 0.42              |
| 1:F:114:VAL:HB   | 1:F:150:TRP:CH2  | 2.54                     | 0.42              |
| 1:G:226:LYS:HE2  | 3:G:681:HOH:O    | 2.19                     | 0.42              |
| 1:D:81:PHE:CE1   | 1:D:125:ALA:HA   | 2.54                     | 0.42              |
| 1:B:96:ALA:HB2   | 1:B:160:VAL:HB   | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:240:ALA:HB1  | 1:B:256:ALA:HB1  | 2.01                     | 0.42              |
| 1:G:216:ALA:HB1  | 1:G:275:VAL:HG21 | 2.02                     | 0.42              |
| 1:G:304:LEU:HD12 | 1:G:304:LEU:H    | 1.83                     | 0.42              |
| 1:H:51:LEU:N     | 3:H:509:HOH:O    | 2.51                     | 0.42              |
| 1:C:165:ILE:HG13 | 1:C:170:ARG:NH1  | 2.32                     | 0.42              |
| 1:C:178:LEU:C    | 1:C:178:LEU:HD23 | 2.44                     | 0.42              |
| 1:C:304:LEU:N    | 1:C:304:LEU:CD2  | 2.83                     | 0.42              |
| 1:F:224:TYR:OH   | 1:F:299:GLY:HA3  | 2.18                     | 0.42              |
| 1:G:86:HIS:HD2   | 1:G:86:HIS:O     | 2.03                     | 0.42              |
| 1:G:180:LEU:HD23 | 1:G:224:TYR:CG   | 2.54                     | 0.42              |
| 1:G:265:VAL:HG13 | 1:G:321:VAL:O    | 2.19                     | 0.42              |
| 1:C:137:GLU:HB2  | 1:D:60:THR:O     | 2.19                     | 0.42              |
| 1:C:225:LEU:O    | 1:C:229:ARG:CG   | 2.68                     | 0.42              |
| 1:D:66:LYS:NZ    | 1:D:186:HIS:O    | 2.52                     | 0.42              |
| 1:E:55:VAL:O     | 1:E:55:VAL:HG13  | 2.18                     | 0.42              |
| 1:F:229:ARG:HG3  | 3:F:677:HOH:O    | 2.19                     | 0.42              |
| 1:H:171:VAL:CG1  | 1:H:172:ARG:N    | 2.83                     | 0.42              |
| 1:H:186:HIS:HD2  | 3:H:543:HOH:O    | 2.03                     | 0.42              |
| 1:H:242:ALA:O    | 1:H:300:MET:HG2  | 2.19                     | 0.42              |
| 1:H:276:PHE:CE1  | 1:H:294:PHE:HB3  | 2.55                     | 0.42              |
| 1:A:291:TYR:CE1  | 1:A:296:MET:HG3  | 2.55                     | 0.42              |
| 1:B:72:GLU:CD    | 1:B:194:ARG:HH21 | 2.28                     | 0.42              |
| 1:D:107:ALA:HB2  | 1:D:150:TRP:CD2  | 2.54                     | 0.42              |
| 1:D:264:GLU:HG3  | 1:D:325:VAL:HG21 | 2.01                     | 0.42              |
| 1:E:171:VAL:HG22 | 1:E:258:PRO:CD   | 2.50                     | 0.42              |
| 1:F:321:VAL:O    | 1:F:321:VAL:CG1  | 2.68                     | 0.42              |
| 1:B:206:VAL:CG1  | 1:B:209:LEU:HG   | 2.49                     | 0.42              |
| 1:B:238:LEU:CD1  | 1:B:304:LEU:HD23 | 2.44                     | 0.42              |
| 1:C:288:GLU:HG3  | 3:C:688:HOH:O    | 2.19                     | 0.42              |
| 1:G:185:PRO:HB2  | 1:G:190:TYR:OH   | 2.20                     | 0.42              |
| 1:H:82:ASP:OD1   | 1:H:220:PRO:HA   | 2.20                     | 0.42              |
| 1:H:247:GLY:HA3  | 1:H:251:GLU:CB   | 2.50                     | 0.42              |
| 1:D:202:LEU:CD2  | 1:D:213:LEU:HD23 | 2.48                     | 0.42              |
| 1:D:213:LEU:HD12 | 1:D:213:LEU:HA   | 1.91                     | 0.42              |
| 1:A:136:GLY:HA3  | 3:A:599:HOH:O    | 2.19                     | 0.42              |
| 1:A:238:LEU:HD23 | 1:A:304:LEU:HD23 | 2.02                     | 0.42              |
| 1:H:182:SER:HA   | 1:H:224:TYR:OH   | 2.20                     | 0.42              |
| 1:H:196:VAL:C    | 1:H:198:ALA:H    | 2.28                     | 0.42              |
| 1:A:313:LEU:HD21 | 1:A:320:LEU:HG   | 2.02                     | 0.41              |
| 1:B:272:ILE:O    | 1:B:273:PRO:C    | 2.60                     | 0.41              |
| 1:C:53:GLU:O     | 1:C:53:GLU:HG3   | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:273:PRO:HA   | 1:F:274:PRO:HD2  | 1.95                     | 0.41              |
| 1:H:323:ARG:HG3  | 3:H:528:HOH:O    | 2.19                     | 0.41              |
| 1:C:88:VAL:HA    | 1:C:156:LEU:CD2  | 2.50                     | 0.41              |
| 1:D:313:LEU:HD11 | 1:D:320:LEU:CD2  | 2.50                     | 0.41              |
| 1:F:111:ASP:N    | 1:F:150:TRP:HH2  | 2.17                     | 0.41              |
| 1:F:253:LEU:HB3  | 1:F:254:PRO:HD3  | 2.02                     | 0.41              |
| 1:A:99:LEU:O     | 1:A:132:PRO:HD2  | 2.21                     | 0.41              |
| 1:B:229:ARG:O    | 1:B:233:GLU:HG3  | 2.20                     | 0.41              |
| 1:B:312:ALA:O    | 1:B:316:VAL:HG12 | 2.21                     | 0.41              |
| 1:G:185:PRO:HB2  | 1:G:190:TYR:CZ   | 2.56                     | 0.41              |
| 1:H:51:LEU:HD23  | 3:H:644:HOH:O    | 2.20                     | 0.41              |
| 1:A:192:LEU:HD23 | 1:A:294:PHE:CZ   | 2.55                     | 0.41              |
| 1:B:190:TYR:O    | 1:B:194:ARG:HG3  | 2.20                     | 0.41              |
| 1:G:54:PRO:HA    | 3:G:577:HOH:O    | 2.19                     | 0.41              |
| 1:G:181:PRO:O    | 1:G:222:ARG:HD3  | 2.20                     | 0.41              |
| 1:A:63:VAL:HG11  | 1:A:79:LEU:HD22  | 2.03                     | 0.41              |
| 1:D:238:LEU:HA   | 1:D:304:LEU:HB3  | 2.03                     | 0.41              |
| 1:E:144:VAL:HG22 | 1:F:68:LEU:HD21  | 2.03                     | 0.41              |
| 1:F:51:LEU:HA    | 3:F:639:HOH:O    | 2.20                     | 0.41              |
| 1:G:56:LEU:HD11  | 1:H:56:LEU:HD21  | 2.02                     | 0.41              |
| 1:H:81:PHE:CE1   | 1:H:125:ALA:HA   | 2.55                     | 0.41              |
| 1:H:83:LEU:HD23  | 1:H:122:LEU:HD21 | 2.02                     | 0.41              |
| 1:A:86:HIS:CD2   | 1:A:86:HIS:C     | 2.99                     | 0.41              |
| 1:B:265:VAL:O    | 1:B:332:LEU:HD12 | 2.20                     | 0.41              |
| 1:C:93:ALA:HA    | 1:C:241:ALA:HB3  | 2.02                     | 0.41              |
| 1:G:280:GLN:HB2  | 1:G:290:MET:HE3  | 2.01                     | 0.41              |
| 1:A:53:GLU:HG3   | 3:D:542:HOH:O    | 2.21                     | 0.41              |
| 1:B:214:LYS:HD3  | 3:B:532:HOH:O    | 2.20                     | 0.41              |
| 1:B:264:GLU:O    | 1:B:322:GLY:HA3  | 2.21                     | 0.41              |
| 1:D:287:GLU:O    | 1:D:287:GLU:HG2  | 2.20                     | 0.41              |
| 1:H:172:ARG:NH1  | 3:H:511:HOH:O    | 2.53                     | 0.41              |
| 1:D:304:LEU:HD12 | 1:D:304:LEU:H    | 1.85                     | 0.41              |
| 1:F:196:VAL:CG2  | 1:F:285:ILE:HD11 | 2.51                     | 0.41              |
| 1:G:186:HIS:CD2  | 1:G:221:HIS:HA   | 2.56                     | 0.41              |
| 1:G:224:TYR:OH   | 1:G:299:GLY:HA3  | 2.21                     | 0.41              |
| 1:G:318:GLY:C    | 1:G:319:PHE:CD1  | 2.98                     | 0.41              |
| 1:H:53:GLU:N     | 1:H:54:PRO:CD    | 2.84                     | 0.41              |
| 1:H:172:ARG:O    | 1:H:175:ASP:HB2  | 2.21                     | 0.41              |
| 1:A:311:GLU:HB3  | 3:A:597:HOH:O    | 2.21                     | 0.41              |
| 1:D:229:ARG:HD2  | 3:D:539:HOH:O    | 2.19                     | 0.41              |
| 1:F:320:LEU:HD23 | 1:F:320:LEU:HA   | 1.85                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:62:GLY:HA2   | 1:B:153:ALA:HA   | 2.02                     | 0.40              |
| 1:B:102:LEU:HA   | 3:B:521:HOH:O    | 2.20                     | 0.40              |
| 1:F:249:LEU:N    | 1:F:250:PRO:CD   | 2.84                     | 0.40              |
| 1:F:285:ILE:HA   | 1:F:286:PRO:HD3  | 1.98                     | 0.40              |
| 1:F:300:MET:HE2  | 1:F:300:MET:HB3  | 1.98                     | 0.40              |
| 1:G:182:SER:HB2  | 1:G:186:HIS:CE1  | 2.56                     | 0.40              |
| 1:G:261:LEU:HD13 | 1:G:324:VAL:HG11 | 2.02                     | 0.40              |
| 1:H:94:GLN:HG2   | 3:H:570:HOH:O    | 2.22                     | 0.40              |
| 1:B:213:LEU:O    | 1:B:217:LEU:HB2  | 2.21                     | 0.40              |
| 1:B:251:GLU:OE2  | 1:B:255:ARG:NH2  | 2.53                     | 0.40              |
| 1:C:76:VAL:HB    | 1:C:79:LEU:HD12  | 2.04                     | 0.40              |
| 1:D:103:ASP:OD2  | 1:D:122:LEU:HD13 | 2.21                     | 0.40              |
| 1:D:141:MET:CE   | 1:D:144:VAL:HG21 | 2.47                     | 0.40              |
| 1:D:196:VAL:HG21 | 1:D:285:ILE:HD11 | 2.03                     | 0.40              |
| 1:D:290:MET:HE3  | 1:D:296:MET:SD   | 2.61                     | 0.40              |
| 1:F:171:VAL:HG21 | 1:F:256:ALA:O    | 2.21                     | 0.40              |
| 1:F:304:LEU:HD23 | 1:F:304:LEU:N    | 2.35                     | 0.40              |
| 1:H:249:LEU:HD12 | 1:H:253:LEU:HB2  | 2.04                     | 0.40              |
| 1:B:171:VAL:HB   | 1:B:258:PRO:HD3  | 2.03                     | 0.40              |
| 1:B:239:HIS:NE2  | 1:B:305:PRO:HD3  | 2.37                     | 0.40              |
| 1:B:304:LEU:HD13 | 1:B:305:PRO:O    | 2.22                     | 0.40              |
| 1:F:57:VAL:HG21  | 1:F:96:ALA:CB    | 2.51                     | 0.40              |
| 1:F:232:TRP:O    | 1:F:235:GLY:N    | 2.45                     | 0.40              |
| 1:E:227:GLU:HG3  | 1:E:316:VAL:HB   | 2.03                     | 0.40              |
| 1:E:314:LYS:HG3  | 3:E:724:HOH:O    | 2.20                     | 0.40              |
| 1:F:332:LEU:HD13 | 3:F:622:HOH:O    | 2.21                     | 0.40              |
| 1:G:86:HIS:C     | 1:G:86:HIS:CD2   | 3.00                     | 0.40              |
| 1:G:314:LYS:N    | 1:G:314:LYS:CD   | 2.84                     | 0.40              |
| 1:B:162:ARG:NH1  | 1:C:169:GLU:OE1  | 2.54                     | 0.40              |
| 1:F:65:THR:O     | 1:F:66:LYS:C     | 2.64                     | 0.40              |
| 1:G:91:LEU:O     | 1:G:94:GLN:HB2   | 2.21                     | 0.40              |
| 1:G:253:LEU:HB3  | 1:G:254:PRO:HD3  | 2.03                     | 0.40              |
| 1:G:265:VAL:O    | 1:G:333:VAL:N    | 2.49                     | 0.40              |
| 1:H:179:ALA:CB   | 1:H:298:LEU:HD22 | 2.51                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1   | A     | 279/333 (84%)   | 269 (96%)  | 9 (3%)  | 1 (0%)   | 30          | 34  |
| 1   | B     | 281/333 (84%)   | 268 (95%)  | 11 (4%) | 2 (1%)   | 18          | 19  |
| 1   | C     | 279/333 (84%)   | 269 (96%)  | 10 (4%) | 0        | 100         | 100 |
| 1   | D     | 281/333 (84%)   | 274 (98%)  | 7 (2%)  | 0        | 100         | 100 |
| 1   | E     | 279/333 (84%)   | 268 (96%)  | 10 (4%) | 1 (0%)   | 30          | 34  |
| 1   | F     | 281/333 (84%)   | 263 (94%)  | 18 (6%) | 0        | 100         | 100 |
| 1   | G     | 279/333 (84%)   | 263 (94%)  | 16 (6%) | 0        | 100         | 100 |
| 1   | H     | 281/333 (84%)   | 267 (95%)  | 13 (5%) | 1 (0%)   | 30          | 34  |
| All | All   | 2240/2664 (84%) | 2141 (96%) | 94 (4%) | 5 (0%)   | 43          | 51  |

All (5) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 134 | LEU  |
| 1   | B     | 207 | PRO  |
| 1   | H     | 328 | GLU  |
| 1   | B     | 110 | LEU  |
| 1   | E     | 137 | GLU  |

### 5.3.2 Protein sidechains

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 215/250 (86%) | 208 (97%) | 7 (3%)   | 33          | 45 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | B     | 217/250 (87%)   | 206 (95%)  | 11 (5%)  | 21          | 27 |
| 1   | C     | 215/250 (86%)   | 207 (96%)  | 8 (4%)   | 30          | 41 |
| 1   | D     | 217/250 (87%)   | 214 (99%)  | 3 (1%)   | 59          | 75 |
| 1   | E     | 215/250 (86%)   | 208 (97%)  | 7 (3%)   | 33          | 45 |
| 1   | F     | 217/250 (87%)   | 208 (96%)  | 9 (4%)   | 27          | 37 |
| 1   | G     | 215/250 (86%)   | 211 (98%)  | 4 (2%)   | 50          | 66 |
| 1   | H     | 217/250 (87%)   | 213 (98%)  | 4 (2%)   | 51          | 68 |
| All | All   | 1728/2000 (86%) | 1675 (97%) | 53 (3%)  | 35          | 48 |

All (53) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 72  | GLU  |
| 1   | A     | 97  | GLU  |
| 1   | A     | 118 | LEU  |
| 1   | A     | 119 | LEU  |
| 1   | A     | 282 | LEU  |
| 1   | A     | 304 | LEU  |
| 1   | A     | 325 | VAL  |
| 1   | B     | 53  | GLU  |
| 1   | B     | 91  | LEU  |
| 1   | B     | 111 | ASP  |
| 1   | B     | 114 | VAL  |
| 1   | B     | 138 | THR  |
| 1   | B     | 166 | LEU  |
| 1   | B     | 217 | LEU  |
| 1   | B     | 249 | LEU  |
| 1   | B     | 253 | LEU  |
| 1   | B     | 304 | LEU  |
| 1   | B     | 307 | GLU  |
| 1   | C     | 147 | GLU  |
| 1   | C     | 177 | LEU  |
| 1   | C     | 217 | LEU  |
| 1   | C     | 229 | ARG  |
| 1   | C     | 253 | LEU  |
| 1   | C     | 267 | ARG  |
| 1   | C     | 288 | GLU  |
| 1   | C     | 304 | LEU  |
| 1   | D     | 166 | LEU  |
| 1   | D     | 304 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 331 | ARG  |
| 1   | E     | 55  | VAL  |
| 1   | E     | 71  | LEU  |
| 1   | E     | 161 | GLU  |
| 1   | E     | 171 | VAL  |
| 1   | E     | 195 | LYS  |
| 1   | E     | 304 | LEU  |
| 1   | E     | 313 | LEU  |
| 1   | F     | 118 | LEU  |
| 1   | F     | 146 | ARG  |
| 1   | F     | 150 | TRP  |
| 1   | F     | 197 | VAL  |
| 1   | F     | 213 | LEU  |
| 1   | F     | 215 | GLU  |
| 1   | F     | 229 | ARG  |
| 1   | F     | 273 | PRO  |
| 1   | F     | 275 | VAL  |
| 1   | G     | 175 | ASP  |
| 1   | G     | 180 | LEU  |
| 1   | G     | 304 | LEU  |
| 1   | G     | 313 | LEU  |
| 1   | H     | 92  | LEU  |
| 1   | H     | 175 | ASP  |
| 1   | H     | 288 | GLU  |
| 1   | H     | 304 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 94  | GLN  |
| 1   | B     | 306 | GLN  |
| 1   | C     | 280 | GLN  |
| 1   | D     | 94  | GLN  |
| 1   | D     | 109 | HIS  |
| 1   | E     | 94  | GLN  |
| 1   | E     | 109 | HIS  |
| 1   | E     | 306 | GLN  |
| 1   | G     | 280 | GLN  |
| 1   | G     | 306 | GLN  |



### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

17 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 2   | SO4  | D     | 402 | -    | 4,4,4        | 0.35 | 0           | 6,6,6       | 0.09 | 0           |
| 2   | SO4  | H     | 401 | -    | 4,4,4        | 0.33 | 0           | 6,6,6       | 0.13 | 0           |
| 2   | SO4  | G     | 401 | -    | 4,4,4        | 0.37 | 0           | 6,6,6       | 0.10 | 0           |
| 2   | SO4  | G     | 402 | -    | 4,4,4        | 0.37 | 0           | 6,6,6       | 0.06 | 0           |
| 2   | SO4  | A     | 401 | -    | 4,4,4        | 0.32 | 0           | 6,6,6       | 0.20 | 0           |
| 2   | SO4  | D     | 401 | -    | 4,4,4        | 0.33 | 0           | 6,6,6       | 0.10 | 0           |
| 2   | SO4  | C     | 401 | -    | 4,4,4        | 0.33 | 0           | 6,6,6       | 0.18 | 0           |
| 2   | SO4  | G     | 403 | -    | 4,4,4        | 0.33 | 0           | 6,6,6       | 0.13 | 0           |
| 2   | SO4  | A     | 403 | -    | 4,4,4        | 0.36 | 0           | 6,6,6       | 0.09 | 0           |
| 2   | SO4  | F     | 401 | -    | 4,4,4        | 0.36 | 0           | 6,6,6       | 0.17 | 0           |
| 2   | SO4  | B     | 402 | -    | 4,4,4        | 0.39 | 0           | 6,6,6       | 0.06 | 0           |
| 2   | SO4  | A     | 402 | -    | 4,4,4        | 0.38 | 0           | 6,6,6       | 0.07 | 0           |
| 2   | SO4  | H     | 402 | -    | 4,4,4        | 0.36 | 0           | 6,6,6       | 0.07 | 0           |
| 2   | SO4  | C     | 402 | -    | 4,4,4        | 0.34 | 0           | 6,6,6       | 0.13 | 0           |
| 2   | SO4  | B     | 401 | -    | 4,4,4        | 0.39 | 0           | 6,6,6       | 0.07 | 0           |
| 2   | SO4  | E     | 401 | -    | 4,4,4        | 0.34 | 0           | 6,6,6       | 0.13 | 0           |
| 2   | SO4  | E     | 402 | -    | 4,4,4        | 0.35 | 0           | 6,6,6       | 0.07 | 0           |

There are no bond length outliers.

There are no bond angle outliers.

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 [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2   | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|-----------|-----------------------|-------|
| 1   | A     | 281/333 (84%)   | -1.38  | 0 100 100 | 16, 29, 45, 50        | 0     |
| 1   | B     | 283/333 (84%)   | -1.36  | 0 100 100 | 16, 32, 50, 66        | 0     |
| 1   | C     | 281/333 (84%)   | -1.45  | 0 100 100 | 14, 25, 38, 47        | 0     |
| 1   | D     | 283/333 (84%)   | -1.49  | 0 100 100 | 14, 23, 35, 45        | 0     |
| 1   | E     | 281/333 (84%)   | -1.50  | 0 100 100 | 15, 23, 35, 43        | 0     |
| 1   | F     | 283/333 (84%)   | -1.37  | 0 100 100 | 19, 29, 45, 61        | 0     |
| 1   | G     | 281/333 (84%)   | -1.35  | 0 100 100 | 17, 31, 47, 59        | 0     |
| 1   | H     | 283/333 (84%)   | -1.35  | 0 100 100 | 19, 34, 47, 59        | 0     |
| All | All   | 2256/2664 (84%) | -1.41  | 0 100 100 | 14, 28, 45, 66        | 0     |

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | SO4  | G     | 402 | 5/5   | 0.98 | 0.06 | 95,95,96,96                 | 0     |
| 2   | SO4  | H     | 402 | 5/5   | 0.98 | 0.05 | 67,68,68,68                 | 0     |
| 2   | SO4  | B     | 402 | 5/5   | 0.99 | 0.05 | 57,58,59,60                 | 0     |
| 2   | SO4  | D     | 402 | 5/5   | 0.99 | 0.04 | 73,73,74,75                 | 0     |
| 2   | SO4  | E     | 402 | 5/5   | 0.99 | 0.04 | 53,53,54,54                 | 0     |
| 2   | SO4  | A     | 402 | 5/5   | 0.99 | 0.04 | 64,64,65,66                 | 0     |
| 2   | SO4  | G     | 403 | 5/5   | 0.99 | 0.03 | 38,39,40,40                 | 0     |
| 2   | SO4  | A     | 403 | 5/5   | 0.99 | 0.05 | 51,53,54,54                 | 0     |
| 2   | SO4  | B     | 401 | 5/5   | 1.00 | 0.03 | 33,33,36,37                 | 0     |
| 2   | SO4  | E     | 401 | 5/5   | 1.00 | 0.03 | 26,27,29,30                 | 0     |
| 2   | SO4  | A     | 401 | 5/5   | 1.00 | 0.04 | 31,32,34,36                 | 0     |
| 2   | SO4  | F     | 401 | 5/5   | 1.00 | 0.04 | 28,30,32,33                 | 0     |
| 2   | SO4  | G     | 401 | 5/5   | 1.00 | 0.03 | 33,35,37,38                 | 0     |
| 2   | SO4  | C     | 401 | 5/5   | 1.00 | 0.03 | 26,27,30,31                 | 0     |
| 2   | SO4  | C     | 402 | 5/5   | 1.00 | 0.03 | 44,45,45,45                 | 0     |
| 2   | SO4  | H     | 401 | 5/5   | 1.00 | 0.03 | 32,33,36,37                 | 0     |
| 2   | SO4  | D     | 401 | 5/5   | 1.00 | 0.02 | 27,27,29,30                 | 0     |

## 6.5 Other polymers

There are no such residues in this entry.