



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:08 PM UTC

PDB ID : 3AIE / pdb\_00003aie  
Title : Crystal Structure of glucansucrase from Streptococcus mutans  
Authors : Ito, K.; Ito, S.; Shimamura, T.; Iwata, S.  
Deposited on : 2010-05-12  
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

<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                                                             |

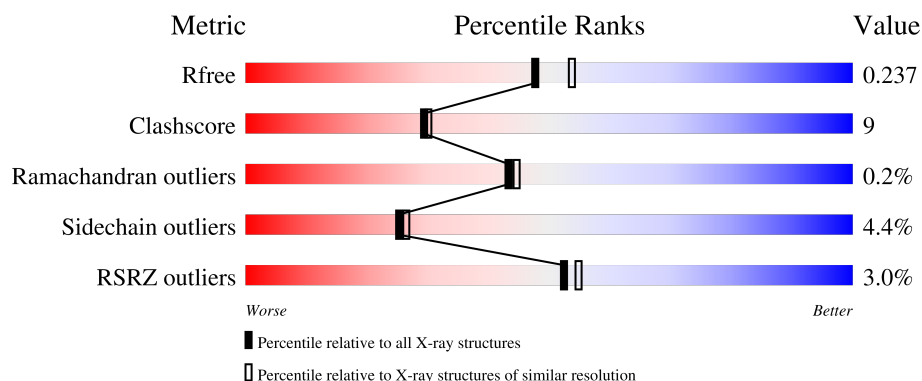
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 6658 (2.10-2.10)                                      |
| Clashscore            | 190562                      | 7164 (2.10-2.10)                                      |
| Ramachandran outliers | 187476                      | 7099 (2.10-2.10)                                      |
| Sidechain outliers    | 187428                      | 7100 (2.10-2.10)                                      |
| RSRZ outliers         | 180081                      | 6662 (2.10-2.10)                                      |

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     | 844    | <div> <div>2%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div>.</div> </div> </div> |
| 1   | B     | 844    | <div> <div>4%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div>.</div> </div> </div> |
| 1   | C     | 844    | <div> <div>2%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>.</div> </div> </div> |
| 1   | D     | 844    | <div> <div>2%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>.</div> </div> </div> |
| 1   | E     | 844    | <div> <div>4%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>.</div> </div> </div> |

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| Mol | Chain | Length | Quality of chain                                                                                              |
|-----|-------|--------|---------------------------------------------------------------------------------------------------------------|
| 1   | F     | 844    | <div><div></div><div>4%</div><div></div><div>78%</div><div></div><div>19%</div><div></div><div>.</div></div>  |
| 1   | G     | 844    | <div><div></div><div>2%</div><div></div><div>79%</div><div></div><div>17%</div><div></div><div>..</div></div> |
| 1   | H     | 844    | <div><div></div><div>2%</div><div></div><div>81%</div><div></div><div>16%</div><div></div><div>.</div></div>  |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 57830 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 Glucosyltransferase-SI.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1   | A     | 844      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6660  | 4196 | 1143 | 1305 | 16 |         |         |       |
| 1   | B     | 844      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6659  | 4196 | 1143 | 1304 | 16 |         |         |       |
| 1   | C     | 844      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6660  | 4196 | 1143 | 1305 | 16 |         |         |       |
| 1   | D     | 844      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6660  | 4196 | 1143 | 1305 | 16 |         |         |       |
| 1   | E     | 844      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6660  | 4196 | 1143 | 1305 | 16 |         |         |       |
| 1   | F     | 844      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6660  | 4196 | 1143 | 1305 | 16 |         |         |       |
| 1   | G     | 844      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6660  | 4196 | 1143 | 1305 | 16 |         |         |       |
| 1   | H     | 844      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6660  | 4196 | 1143 | 1305 | 16 |         |         |       |

There are 32 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 597     | ASP      | ASN    | SEE REMARK 999 | UNP P13470 |
| A     | 600     | LYS      | ARG    | SEE REMARK 999 | UNP P13470 |
| A     | 727     | ILE      | THR    | SEE REMARK 999 | UNP P13470 |
| A     | 734     | VAL      | ALA    | SEE REMARK 999 | UNP P13470 |
| B     | 597     | ASP      | ASN    | SEE REMARK 999 | UNP P13470 |
| B     | 600     | LYS      | ARG    | SEE REMARK 999 | UNP P13470 |
| B     | 727     | ILE      | THR    | SEE REMARK 999 | UNP P13470 |
| B     | 734     | VAL      | ALA    | SEE REMARK 999 | UNP P13470 |
| C     | 597     | ASP      | ASN    | SEE REMARK 999 | UNP P13470 |
| C     | 600     | LYS      | ARG    | SEE REMARK 999 | UNP P13470 |
| C     | 727     | ILE      | THR    | SEE REMARK 999 | UNP P13470 |
| C     | 734     | VAL      | ALA    | SEE REMARK 999 | UNP P13470 |
| D     | 597     | ASP      | ASN    | SEE REMARK 999 | UNP P13470 |

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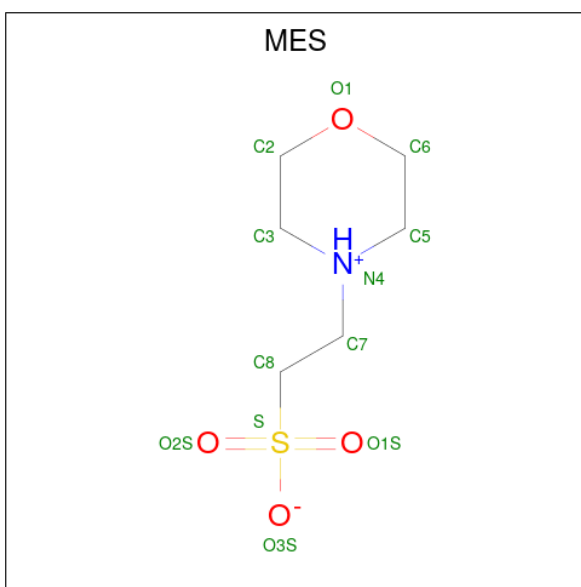
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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| D     | 600     | LYS      | ARG    | SEE REMARK 999 | UNP P13470 |
| D     | 727     | ILE      | THR    | SEE REMARK 999 | UNP P13470 |
| D     | 734     | VAL      | ALA    | SEE REMARK 999 | UNP P13470 |
| E     | 597     | ASP      | ASN    | SEE REMARK 999 | UNP P13470 |
| E     | 600     | LYS      | ARG    | SEE REMARK 999 | UNP P13470 |
| E     | 727     | ILE      | THR    | SEE REMARK 999 | UNP P13470 |
| E     | 734     | VAL      | ALA    | SEE REMARK 999 | UNP P13470 |
| F     | 597     | ASP      | ASN    | SEE REMARK 999 | UNP P13470 |
| F     | 600     | LYS      | ARG    | SEE REMARK 999 | UNP P13470 |
| F     | 727     | ILE      | THR    | SEE REMARK 999 | UNP P13470 |
| F     | 734     | VAL      | ALA    | SEE REMARK 999 | UNP P13470 |
| G     | 597     | ASP      | ASN    | SEE REMARK 999 | UNP P13470 |
| G     | 600     | LYS      | ARG    | SEE REMARK 999 | UNP P13470 |
| G     | 727     | ILE      | THR    | SEE REMARK 999 | UNP P13470 |
| G     | 734     | VAL      | ALA    | SEE REMARK 999 | UNP P13470 |
| H     | 597     | ASP      | ASN    | SEE REMARK 999 | UNP P13470 |
| H     | 600     | LYS      | ARG    | SEE REMARK 999 | UNP P13470 |
| H     | 727     | ILE      | THR    | SEE REMARK 999 | UNP P13470 |
| H     | 734     | VAL      | ALA    | SEE REMARK 999 | UNP P13470 |

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 2   | A     | 1        | Total Ca<br>1 1 | 0       | 0       |
| 2   | B     | 1        | Total Ca<br>1 1 | 0       | 0       |
| 2   | C     | 1        | Total Ca<br>1 1 | 0       | 0       |
| 2   | D     | 1        | Total Ca<br>1 1 | 0       | 0       |
| 2   | E     | 1        | Total Ca<br>1 1 | 0       | 0       |
| 2   | F     | 1        | Total Ca<br>1 1 | 0       | 0       |
| 2   | G     | 1        | Total Ca<br>1 1 | 0       | 0       |
| 2   | H     | 1        | Total Ca<br>1 1 | 0       | 0       |

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 3   | A     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 4 | 1 |         |         |
| 3   | B     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 4 | 1 |         |         |
| 3   | C     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 4 | 1 |         |         |
| 3   | D     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 4 | 1 |         |         |
| 3   | E     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 4 | 1 |         |         |
| 3   | F     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 4 | 1 |         |         |
| 3   | G     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 4 | 1 |         |         |
| 3   | H     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 4 | 1 |         |         |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 4   | A     | 529      | Total | O   | 0       | 0       |
|     |       |          | 529   | 529 |         |         |
| 4   | B     | 528      | Total | O   | 0       | 0       |
|     |       |          | 528   | 528 |         |         |
| 4   | C     | 593      | Total | O   | 0       | 0       |
|     |       |          | 593   | 593 |         |         |
| 4   | D     | 592      | Total | O   | 0       | 0       |
|     |       |          | 592   | 592 |         |         |

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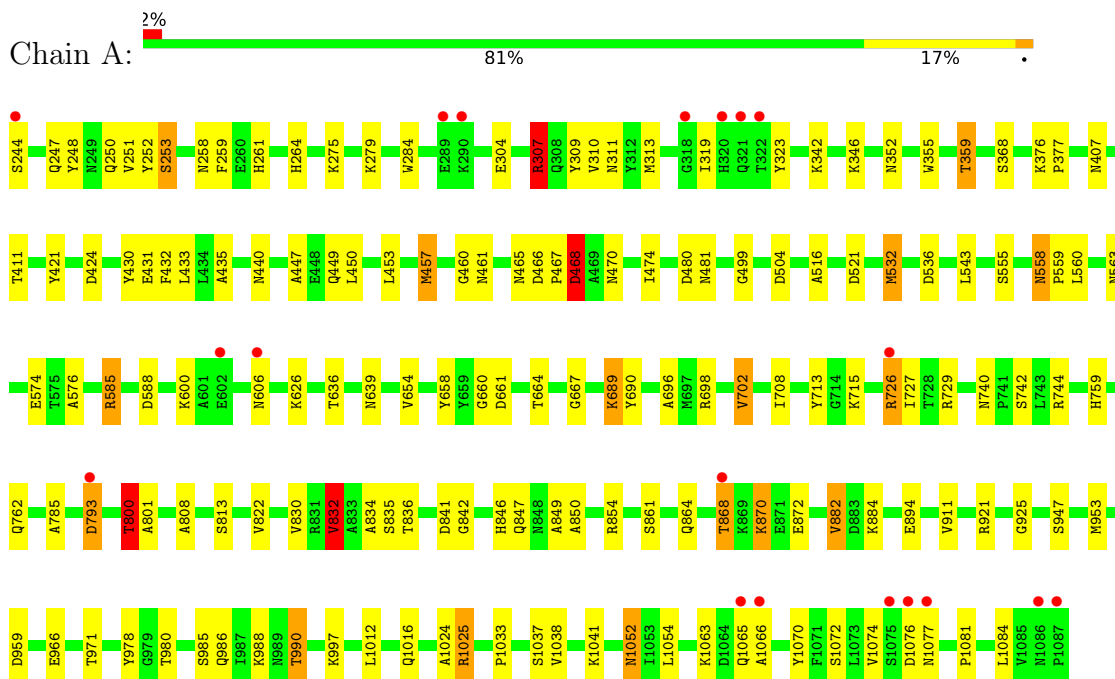
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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 4   | E     | 523      | Total<br>523 | O<br>523 | 0       | 0       |
| 4   | F     | 485      | Total<br>485 | O<br>485 | 0       | 0       |
| 4   | G     | 622      | Total<br>622 | O<br>622 | 0       | 0       |
| 4   | H     | 575      | Total<br>575 | O<br>575 | 0       | 0       |

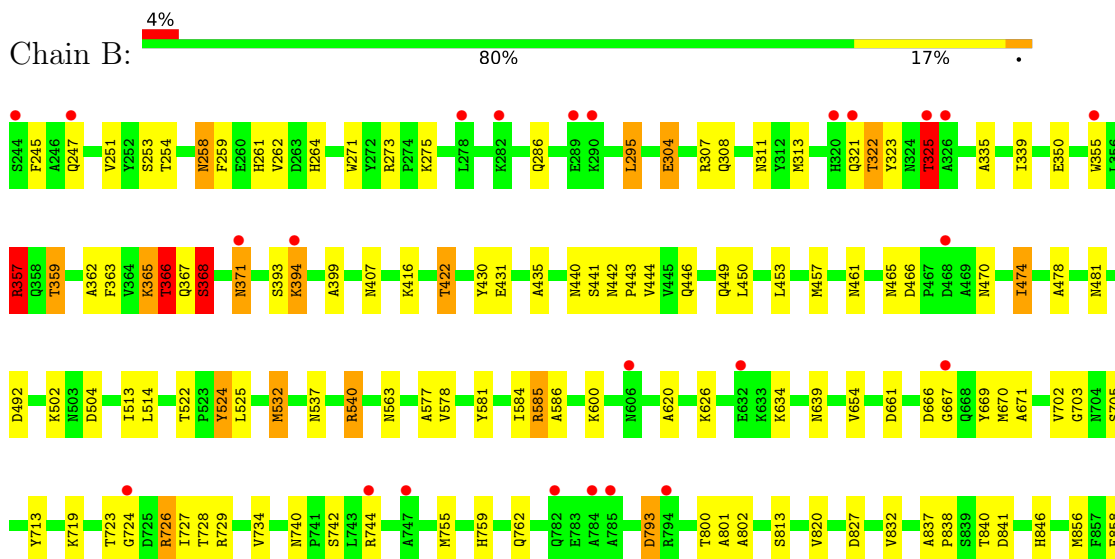
### 3 Residue-property plots [i](#)

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.

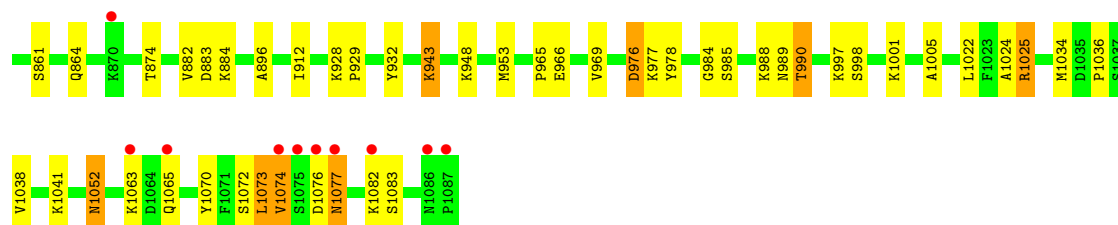
#### • Molecule 1: Glucosyltransferase-SI



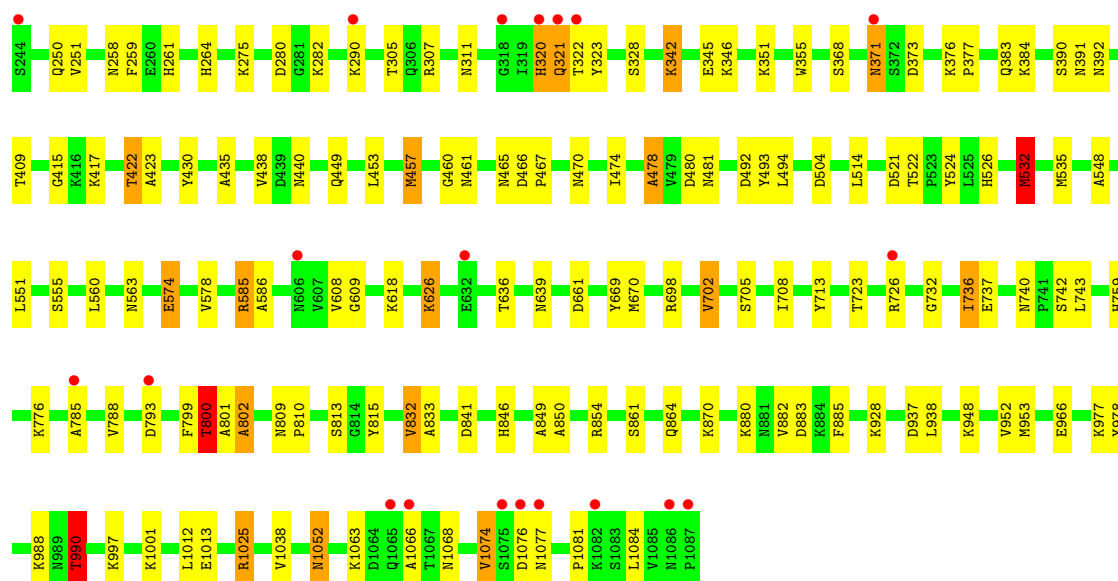
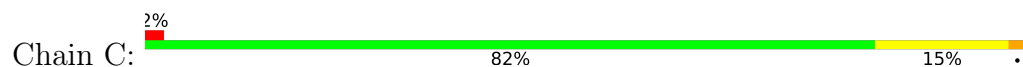
#### • Molecule 1: Glucosyltransferase-SI



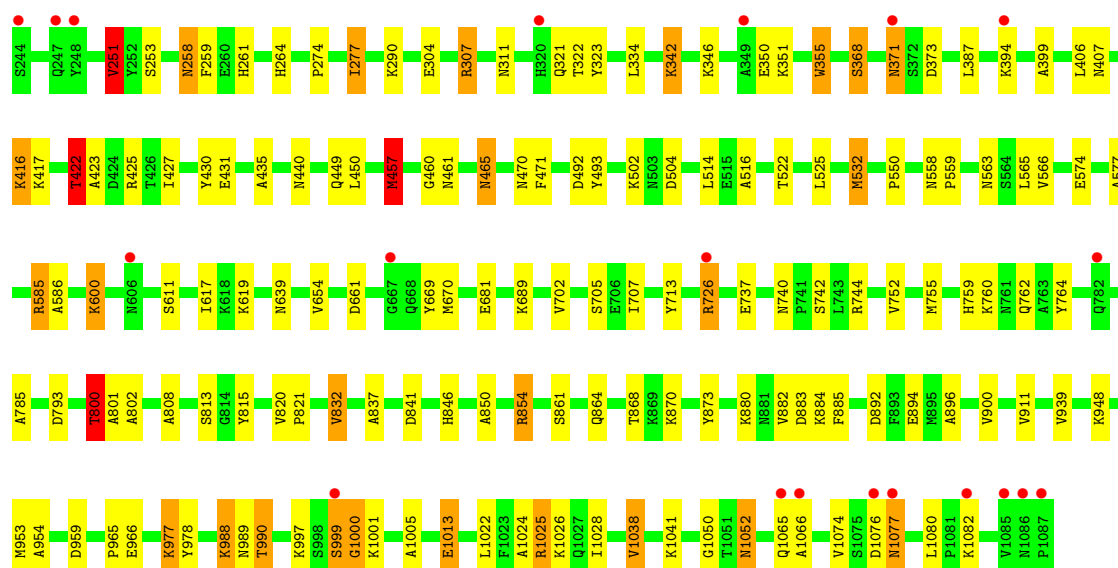
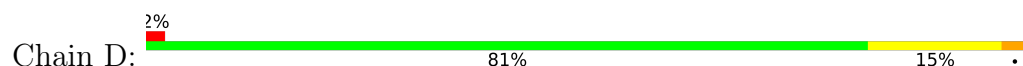




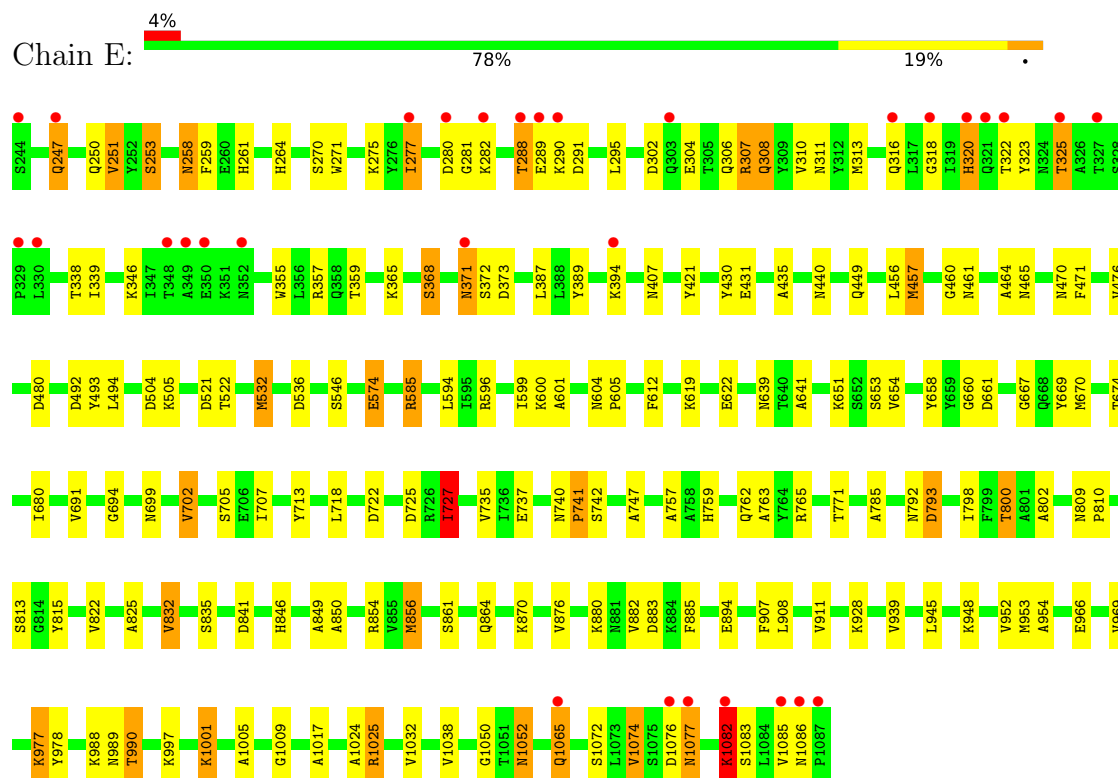
• Molecule 1: Glucosyltransferase-SI



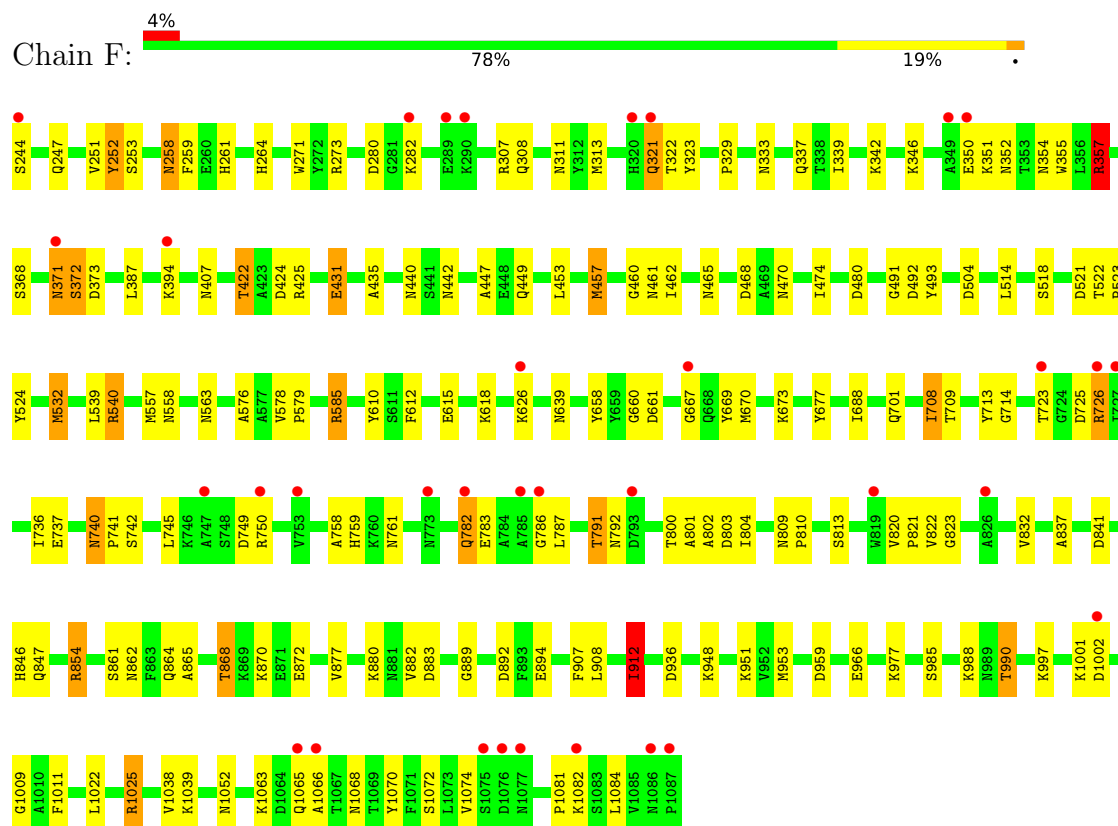
• Molecule 1: Glucosyltransferase-SI



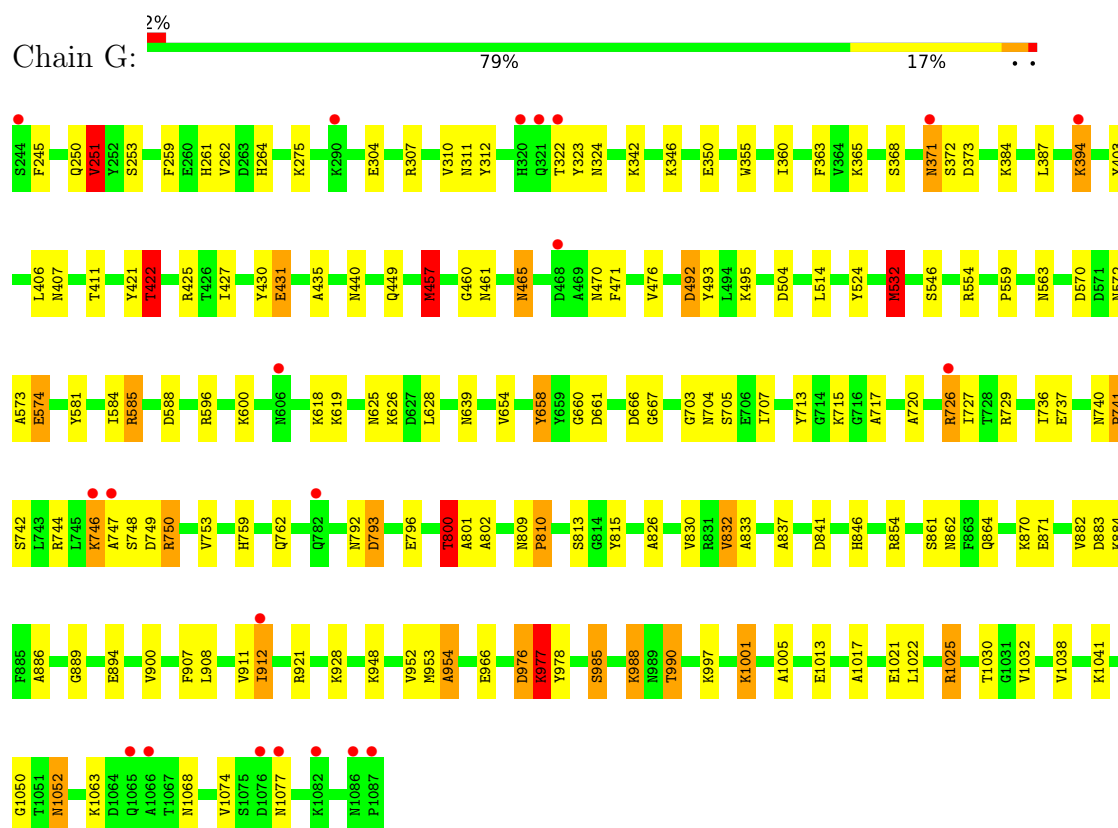
• Molecule 1: Glucosyltransferase-SI



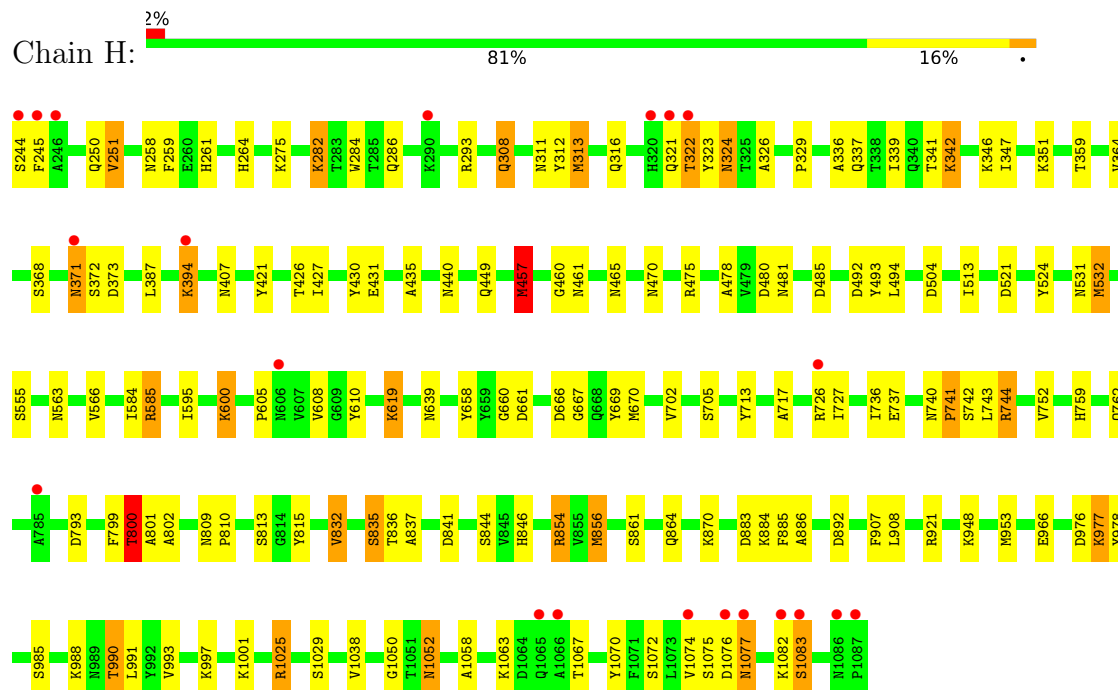
• Molecule 1: Glucosyltransferase-SI



• Molecule 1: Glucosyltransferase-SI



• Molecule 1: Glucosyltransferase-SI



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 2                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 293.88Å 215.42Å 218.95Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 50.00 – 2.10<br>50.00 – 2.10                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.6 (50.00-2.10)<br>99.5 (50.00-2.10)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.91 (at 2.10Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.5.0066                                             | Depositor        |
| R, $R_{free}$                                                           | 0.203 , 0.236<br>(Not available) , 0.237                    | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 39655 reflections (4.98%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 27.3                                                        | Xtriage          |
| Anisotropy                                                              | 0.023                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.38 , 46.7                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | 0.000 for -h,l,k                                            | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 57830                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 33.0                                                        | 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 43.73 % 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 1.6894e-04. 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: MES, CA

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

| Mol | Chain | Bond lengths |                  | Bond angles |                  |
|-----|-------|--------------|------------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5          |
| 1   | A     | 1.58         | 43/6802 (0.6%)   | 1.35        | 44/9237 (0.5%)   |
| 1   | B     | 1.42         | 19/6801 (0.3%)   | 1.30        | 29/9237 (0.3%)   |
| 1   | C     | 1.54         | 34/6802 (0.5%)   | 1.30        | 39/9237 (0.4%)   |
| 1   | D     | 1.55         | 33/6802 (0.5%)   | 1.31        | 44/9237 (0.5%)   |
| 1   | E     | 1.61         | 54/6802 (0.8%)   | 1.37        | 54/9237 (0.6%)   |
| 1   | F     | 1.36         | 14/6802 (0.2%)   | 1.25        | 30/9237 (0.3%)   |
| 1   | G     | 1.65         | 50/6802 (0.7%)   | 1.37        | 43/9237 (0.5%)   |
| 1   | H     | 1.51         | 26/6802 (0.4%)   | 1.30        | 37/9237 (0.4%)   |
| All | All   | 1.53         | 273/54415 (0.5%) | 1.32        | 320/73896 (0.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | E     | 1                   | 0                   |

All (273) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 1   | F     | 540  | ARG  | C-N   | 16.80  | 1.56        | 1.34     |
| 1   | H     | 313  | MET  | SD-CE | -11.84 | 1.50        | 1.79     |
| 1   | B     | 667  | GLY  | N-CA  | 11.67  | 1.58        | 1.45     |
| 1   | C     | 371  | ASN  | CA-CB | 11.14  | 1.71        | 1.53     |
| 1   | C     | 478  | ALA  | CA-CB | 10.65  | 1.69        | 1.53     |
| 1   | D     | 854  | ARG  | CD-NE | -9.98  | 1.32        | 1.46     |
| 1   | B     | 540  | ARG  | CD-NE | -9.51  | 1.32        | 1.46     |
| 1   | A     | 1024 | ALA  | C-N   | 9.37   | 1.46        | 1.33     |
| 1   | C     | 854  | ARG  | CD-NE | -9.37  | 1.33        | 1.46     |
| 1   | H     | 371  | ASN  | CB-CG | -9.33  | 1.28        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | G     | 667  | GLY  | N-CA   | 9.13  | 1.54        | 1.45     |
| 1   | C     | 953  | MET  | C-N    | -8.95 | 1.20        | 1.33     |
| 1   | E     | 854  | ARG  | CD-NE  | -8.94 | 1.33        | 1.46     |
| 1   | G     | 854  | ARG  | CD-NE  | -8.61 | 1.34        | 1.46     |
| 1   | A     | 558  | ASN  | N-CA   | 8.60  | 1.55        | 1.46     |
| 1   | C     | 849  | ALA  | CA-CB  | 8.43  | 1.67        | 1.53     |
| 1   | D     | 1025 | ARG  | CD-NE  | -8.39 | 1.34        | 1.46     |
| 1   | G     | 886  | ALA  | CA-CB  | 8.26  | 1.66        | 1.53     |
| 1   | G     | 573  | ALA  | CA-CB  | 8.13  | 1.65        | 1.53     |
| 1   | H     | 1083 | SER  | CB-OG  | 8.12  | 1.58        | 1.42     |
| 1   | F     | 1002 | ASP  | CA-CB  | 8.09  | 1.66        | 1.53     |
| 1   | D     | 371  | ASN  | CA-CB  | 7.87  | 1.67        | 1.54     |
| 1   | A     | 1038 | VAL  | C-N    | -7.86 | 1.22        | 1.33     |
| 1   | H     | 371  | ASN  | CA-CB  | 7.85  | 1.67        | 1.54     |
| 1   | A     | 433  | LEU  | CA-C   | -7.82 | 1.46        | 1.52     |
| 1   | B     | 896  | ALA  | CA-CB  | 7.77  | 1.65        | 1.53     |
| 1   | C     | 952  | VAL  | C-N    | -7.72 | 1.22        | 1.33     |
| 1   | H     | 364  | VAL  | CA-CB  | 7.72  | 1.63        | 1.54     |
| 1   | E     | 604  | ASN  | C-O    | -7.67 | 1.17        | 1.24     |
| 1   | D     | 585  | ARG  | CD-NE  | -7.66 | 1.35        | 1.46     |
| 1   | A     | 636  | THR  | N-CA   | 7.51  | 1.55        | 1.45     |
| 1   | E     | 798  | ILE  | C-O    | 7.48  | 1.32        | 1.24     |
| 1   | H     | 800  | THR  | CB-CG2 | -7.42 | 1.28        | 1.52     |
| 1   | G     | 371  | ASN  | CA-CB  | 7.41  | 1.69        | 1.54     |
| 1   | C     | 585  | ARG  | CD-NE  | -7.39 | 1.35        | 1.46     |
| 1   | G     | 457  | MET  | SD-CE  | -7.30 | 1.61        | 1.79     |
| 1   | G     | 954  | ALA  | CA-CB  | 7.28  | 1.63        | 1.53     |
| 1   | A     | 588  | ASP  | C-O    | 7.23  | 1.32        | 1.23     |
| 1   | G     | 1025 | ARG  | CD-NE  | -7.20 | 1.36        | 1.46     |
| 1   | E     | 371  | ASN  | CA-CB  | 7.19  | 1.66        | 1.54     |
| 1   | F     | 447  | ALA  | CA-CB  | 7.15  | 1.64        | 1.53     |
| 1   | C     | 833  | ALA  | CA-CB  | 7.12  | 1.64        | 1.53     |
| 1   | F     | 1025 | ARG  | CD-NE  | -7.10 | 1.36        | 1.46     |
| 1   | A     | 696  | ALA  | CA-CB  | 7.06  | 1.67        | 1.53     |
| 1   | G     | 371  | ASN  | CB-CG  | -7.03 | 1.34        | 1.52     |
| 1   | C     | 422  | THR  | CB-CG2 | -6.96 | 1.29        | 1.52     |
| 1   | E     | 574  | GLU  | CB-CG  | -6.94 | 1.31        | 1.52     |
| 1   | E     | 585  | ARG  | CD-NE  | -6.92 | 1.36        | 1.46     |
| 1   | A     | 307  | ARG  | CG-CD  | 6.89  | 1.73        | 1.52     |
| 1   | G     | 912  | ILE  | CA-CB  | 6.87  | 1.63        | 1.54     |
| 1   | E     | 856  | MET  | SD-CE  | -6.82 | 1.62        | 1.79     |
| 1   | E     | 546  | SER  | N-CA   | 6.76  | 1.55        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | E     | 421  | TYR  | N-CA   | 6.75  | 1.54        | 1.46     |
| 1   | B     | 371  | ASN  | CB-CG  | -6.74 | 1.35        | 1.52     |
| 1   | G     | 585  | ARG  | CD-NE  | -6.71 | 1.36        | 1.46     |
| 1   | C     | 802  | ALA  | CA-CB  | 6.69  | 1.65        | 1.53     |
| 1   | E     | 476  | VAL  | CA-CB  | 6.68  | 1.60        | 1.53     |
| 1   | C     | 574  | GLU  | CB-CG  | -6.67 | 1.32        | 1.52     |
| 1   | C     | 371  | ASN  | CB-CG  | -6.67 | 1.35        | 1.52     |
| 1   | F     | 371  | ASN  | CB-CG  | -6.63 | 1.35        | 1.52     |
| 1   | E     | 680  | ILE  | CA-CB  | 6.63  | 1.62        | 1.54     |
| 1   | E     | 850  | ALA  | CA-CB  | 6.61  | 1.63        | 1.53     |
| 1   | B     | 976  | ASP  | CA-C   | 6.61  | 1.62        | 1.53     |
| 1   | A     | 850  | ALA  | CA-CB  | 6.60  | 1.63        | 1.53     |
| 1   | A     | 849  | ALA  | CA-CB  | 6.57  | 1.64        | 1.53     |
| 1   | E     | 969  | VAL  | CA-CB  | 6.55  | 1.62        | 1.54     |
| 1   | A     | 433  | LEU  | N-CA   | -6.55 | 1.40        | 1.46     |
| 1   | G     | 921  | ARG  | CD-NE  | 6.53  | 1.55        | 1.46     |
| 1   | E     | 1025 | ARG  | CD-NE  | -6.53 | 1.37        | 1.46     |
| 1   | H     | 667  | GLY  | N-CA   | 6.52  | 1.52        | 1.45     |
| 1   | E     | 641  | ALA  | CA-CB  | 6.46  | 1.64        | 1.53     |
| 1   | D     | 457  | MET  | CB-CG  | -6.44 | 1.33        | 1.52     |
| 1   | A     | 310  | VAL  | CA-CB  | 6.43  | 1.61        | 1.54     |
| 1   | A     | 457  | MET  | SD-CE  | -6.39 | 1.63        | 1.79     |
| 1   | E     | 307  | ARG  | C-N    | -6.38 | 1.25        | 1.33     |
| 1   | E     | 371  | ASN  | N-CA   | 6.38  | 1.54        | 1.45     |
| 1   | E     | 785  | ALA  | CA-CB  | 6.29  | 1.64        | 1.53     |
| 1   | H     | 991  | LEU  | N-CA   | 6.29  | 1.53        | 1.46     |
| 1   | A     | 667  | GLY  | N-CA   | 6.28  | 1.52        | 1.45     |
| 1   | E     | 763  | ALA  | CA-CB  | 6.26  | 1.63        | 1.53     |
| 1   | G     | 628  | LEU  | N-CA   | 6.24  | 1.54        | 1.46     |
| 1   | G     | 554  | ARG  | C-O    | -6.24 | 1.16        | 1.23     |
| 1   | E     | 757  | ALA  | CA-CB  | 6.23  | 1.64        | 1.53     |
| 1   | G     | 476  | VAL  | C-O    | 6.23  | 1.31        | 1.23     |
| 1   | E     | 1024 | ALA  | CA-CB  | 6.21  | 1.63        | 1.53     |
| 1   | A     | 481  | ASN  | CG-ND2 | -6.19 | 1.20        | 1.33     |
| 1   | C     | 417  | LYS  | N-CA   | -6.18 | 1.38        | 1.46     |
| 1   | D     | 1024 | ALA  | CA-C   | 6.16  | 1.61        | 1.52     |
| 1   | C     | 990  | THR  | CA-C   | 6.15  | 1.60        | 1.52     |
| 1   | A     | 432  | PHE  | N-CA   | 6.15  | 1.53        | 1.46     |
| 1   | A     | 421  | TYR  | N-CA   | 6.14  | 1.53        | 1.46     |
| 1   | C     | 586  | ALA  | CA-CB  | 6.13  | 1.64        | 1.53     |
| 1   | B     | 441  | SER  | CA-C   | 6.12  | 1.61        | 1.52     |
| 1   | C     | 438  | VAL  | CA-CB  | 6.12  | 1.61        | 1.54     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | A     | 424  | ASP  | CA-CB  | 6.12  | 1.61        | 1.53     |
| 1   | G     | 830  | VAL  | CA-CB  | 6.12  | 1.62        | 1.54     |
| 1   | G     | 832  | VAL  | CA-CB  | 6.11  | 1.62        | 1.54     |
| 1   | G     | 837  | ALA  | CA-CB  | 6.11  | 1.62        | 1.53     |
| 1   | F     | 424  | ASP  | N-CA   | 6.11  | 1.53        | 1.46     |
| 1   | G     | 717  | ALA  | CA-CB  | 6.08  | 1.63        | 1.53     |
| 1   | H     | 584  | ILE  | CA-CB  | 6.08  | 1.62        | 1.54     |
| 1   | C     | 1066 | ALA  | N-CA   | 6.07  | 1.53        | 1.46     |
| 1   | D     | 417  | LYS  | C-O    | -6.04 | 1.16        | 1.23     |
| 1   | E     | 601  | ALA  | CA-CB  | 6.01  | 1.63        | 1.53     |
| 1   | B     | 366  | THR  | CB-OG1 | -6.01 | 1.34        | 1.43     |
| 1   | C     | 800  | THR  | CB-CG2 | -6.00 | 1.32        | 1.52     |
| 1   | D     | 1024 | ALA  | CA-CB  | 5.99  | 1.62        | 1.53     |
| 1   | G     | 889  | GLY  | N-CA   | 5.99  | 1.53        | 1.45     |
| 1   | E     | 371  | ASN  | CA-C   | -5.95 | 1.45        | 1.52     |
| 1   | D     | 566  | VAL  | CA-CB  | 5.93  | 1.61        | 1.54     |
| 1   | F     | 387  | LEU  | C-O    | -5.92 | 1.17        | 1.24     |
| 1   | B     | 585  | ARG  | CD-NE  | -5.92 | 1.38        | 1.46     |
| 1   | E     | 1017 | ALA  | CA-CB  | 5.90  | 1.62        | 1.53     |
| 1   | H     | 585  | ARG  | CD-NE  | -5.90 | 1.38        | 1.46     |
| 1   | D     | 808  | ALA  | CA-CB  | 5.89  | 1.62        | 1.53     |
| 1   | A     | 664  | THR  | CA-CB  | 5.88  | 1.63        | 1.53     |
| 1   | D     | 586  | ALA  | CA-CB  | 5.88  | 1.63        | 1.53     |
| 1   | D     | 450  | LEU  | CA-C   | 5.86  | 1.60        | 1.52     |
| 1   | H     | 608  | VAL  | CA-CB  | 5.86  | 1.61        | 1.54     |
| 1   | A     | 854  | ARG  | CD-NE  | -5.86 | 1.38        | 1.46     |
| 1   | B     | 444  | VAL  | CA-CB  | 5.85  | 1.61        | 1.54     |
| 1   | A     | 457  | MET  | CB-CG  | -5.84 | 1.34        | 1.52     |
| 1   | G     | 793  | ASP  | CB-CG  | -5.82 | 1.37        | 1.52     |
| 1   | D     | 355  | TRP  | CA-C   | 5.80  | 1.60        | 1.52     |
| 1   | B     | 620  | ALA  | CA-CB  | 5.80  | 1.62        | 1.53     |
| 1   | A     | 447  | ALA  | CA-CB  | 5.80  | 1.62        | 1.53     |
| 1   | E     | 667  | GLY  | N-CA   | 5.79  | 1.51        | 1.45     |
| 1   | D     | 900  | VAL  | CA-CB  | 5.78  | 1.60        | 1.54     |
| 1   | G     | 658  | TYR  | CA-CB  | 5.78  | 1.61        | 1.53     |
| 1   | G     | 411  | THR  | CA-CB  | 5.77  | 1.62        | 1.53     |
| 1   | D     | 896  | ALA  | CA-CB  | 5.76  | 1.62        | 1.53     |
| 1   | D     | 939  | VAL  | CA-CB  | 5.76  | 1.60        | 1.54     |
| 1   | E     | 306  | GLN  | C-N    | -5.76 | 1.26        | 1.33     |
| 1   | E     | 651  | LYS  | CA-C   | 5.75  | 1.60        | 1.53     |
| 1   | C     | 850  | ALA  | CA-CB  | 5.75  | 1.62        | 1.53     |
| 1   | A     | 560  | LEU  | N-CA   | 5.73  | 1.53        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | C     | 785  | ALA  | CA-CB   | 5.73  | 1.62        | 1.53     |
| 1   | A     | 971  | THR  | C-O     | 5.72  | 1.31        | 1.24     |
| 1   | A     | 830  | VAL  | CA-CB   | 5.71  | 1.62        | 1.54     |
| 1   | H     | 1058 | ALA  | CA-CB   | 5.71  | 1.63        | 1.53     |
| 1   | G     | 900  | VAL  | CA-CB   | 5.69  | 1.60        | 1.54     |
| 1   | G     | 833  | ALA  | CA-CB   | 5.68  | 1.62        | 1.53     |
| 1   | D     | 989  | ASN  | C-O     | -5.68 | 1.16        | 1.23     |
| 1   | A     | 499  | GLY  | N-CA    | 5.67  | 1.53        | 1.45     |
| 1   | E     | 1082 | LYS  | CB-CG   | 5.67  | 1.69        | 1.52     |
| 1   | B     | 362  | ALA  | CA-CB   | 5.65  | 1.62        | 1.53     |
| 1   | A     | 585  | ARG  | CD-NE   | -5.64 | 1.38        | 1.46     |
| 1   | A     | 947  | SER  | C-O     | -5.63 | 1.16        | 1.24     |
| 1   | H     | 293  | ARG  | N-CA    | 5.62  | 1.50        | 1.45     |
| 1   | B     | 1025 | ARG  | CD-NE   | -5.62 | 1.38        | 1.46     |
| 1   | C     | 415  | GLY  | N-CA    | 5.61  | 1.53        | 1.45     |
| 1   | A     | 702  | VAL  | CA-CB   | 5.59  | 1.62        | 1.54     |
| 1   | D     | 800  | THR  | CB-CG2  | -5.58 | 1.34        | 1.52     |
| 1   | E     | 691  | VAL  | CA-CB   | 5.57  | 1.60        | 1.53     |
| 1   | A     | 536  | ASP  | CA-CB   | 5.55  | 1.61        | 1.52     |
| 1   | A     | 959  | ASP  | CA-C    | 5.55  | 1.59        | 1.52     |
| 1   | G     | 977  | LYS  | CB-CG   | -5.52 | 1.35        | 1.52     |
| 1   | E     | 771  | THR  | CA-CB   | 5.50  | 1.61        | 1.53     |
| 1   | C     | 555  | SER  | N-CA    | 5.50  | 1.52        | 1.45     |
| 1   | A     | 1025 | ARG  | C-N     | -5.49 | 1.25        | 1.33     |
| 1   | C     | 423  | ALA  | C-O     | -5.49 | 1.17        | 1.24     |
| 1   | G     | 546  | SER  | N-CA    | 5.48  | 1.53        | 1.46     |
| 1   | C     | 532  | MET  | CB-CG   | -5.47 | 1.36        | 1.52     |
| 1   | G     | 421  | TYR  | N-CA    | 5.45  | 1.52        | 1.46     |
| 1   | E     | 735  | VAL  | C-O     | 5.45  | 1.30        | 1.24     |
| 1   | A     | 555  | SER  | CB-OG   | -5.43 | 1.31        | 1.42     |
| 1   | C     | 736  | ILE  | CA-CB   | 5.42  | 1.61        | 1.54     |
| 1   | B     | 365  | LYS  | N-CA    | 5.42  | 1.53        | 1.46     |
| 1   | E     | 747  | ALA  | CA-CB   | 5.41  | 1.62        | 1.53     |
| 1   | A     | 980  | THR  | CA-C    | 5.41  | 1.59        | 1.52     |
| 1   | B     | 399  | ALA  | CA-CB   | 5.41  | 1.61        | 1.53     |
| 1   | G     | 406  | LEU  | C-O     | -5.41 | 1.17        | 1.23     |
| 1   | E     | 464  | ALA  | CA-CB   | 5.40  | 1.60        | 1.53     |
| 1   | G     | 952  | VAL  | C-N     | -5.39 | 1.26        | 1.33     |
| 1   | H     | 427  | ILE  | CG1-CD1 | 5.39  | 1.72        | 1.51     |
| 1   | E     | 800  | THR  | CB-CG2  | -5.38 | 1.34        | 1.52     |
| 1   | H     | 426  | THR  | CB-CG2  | 5.38  | 1.70        | 1.52     |
| 1   | G     | 618  | LYS  | CB-CG   | 5.38  | 1.68        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | G     | 1017 | ALA  | CA-CB  | 5.38  | 1.61        | 1.53     |
| 1   | F     | 371  | ASN  | CA-CB  | 5.37  | 1.64        | 1.54     |
| 1   | H     | 457  | MET  | SD-CE  | -5.37 | 1.66        | 1.79     |
| 1   | C     | 560  | LEU  | C-O    | -5.36 | 1.17        | 1.24     |
| 1   | D     | 959  | ASP  | C-O    | -5.36 | 1.17        | 1.24     |
| 1   | D     | 465  | ASN  | CB-CG  | -5.34 | 1.38        | 1.52     |
| 1   | E     | 792  | ASN  | C-O    | 5.33  | 1.30        | 1.23     |
| 1   | G     | 720  | ALA  | CA-CB  | 5.32  | 1.62        | 1.53     |
| 1   | D     | 550  | PRO  | CA-C   | 5.32  | 1.58        | 1.52     |
| 1   | G     | 810  | PRO  | C-O    | -5.32 | 1.17        | 1.24     |
| 1   | D     | 837  | ALA  | CA-CB  | 5.31  | 1.61        | 1.53     |
| 1   | H     | 532  | MET  | CB-CG  | -5.31 | 1.36        | 1.52     |
| 1   | A     | 411  | THR  | CA-C   | 5.30  | 1.59        | 1.52     |
| 1   | E     | 622  | GLU  | C-O    | -5.29 | 1.18        | 1.24     |
| 1   | H     | 793  | ASP  | CB-CG  | -5.29 | 1.38        | 1.52     |
| 1   | G     | 588  | ASP  | C-O    | 5.29  | 1.30        | 1.23     |
| 1   | H     | 886  | ALA  | CA-CB  | 5.29  | 1.61        | 1.53     |
| 1   | H     | 717  | ALA  | CA-CB  | 5.27  | 1.62        | 1.53     |
| 1   | F     | 714  | GLY  | N-CA   | 5.27  | 1.50        | 1.45     |
| 1   | G     | 365  | LYS  | CG-CD  | 5.26  | 1.68        | 1.52     |
| 1   | A     | 847  | GLN  | CB-CG  | 5.26  | 1.68        | 1.52     |
| 1   | C     | 626  | LYS  | CA-C   | 5.26  | 1.59        | 1.52     |
| 1   | E     | 456  | LEU  | CA-C   | 5.25  | 1.59        | 1.52     |
| 1   | D     | 577  | ALA  | CA-CB  | 5.24  | 1.61        | 1.53     |
| 1   | E     | 802  | ALA  | CA-CB  | 5.24  | 1.61        | 1.53     |
| 1   | E     | 1032 | VAL  | N-CA   | 5.24  | 1.51        | 1.46     |
| 1   | G     | 403  | TYR  | N-CA   | 5.24  | 1.49        | 1.46     |
| 1   | C     | 578  | VAL  | CA-CB  | 5.24  | 1.60        | 1.54     |
| 1   | C     | 636  | THR  | CA-C   | 5.23  | 1.59        | 1.52     |
| 1   | F     | 442  | ASN  | CA-C   | 5.22  | 1.58        | 1.52     |
| 1   | G     | 854  | ARG  | CB-CG  | 5.22  | 1.68        | 1.52     |
| 1   | E     | 722  | ASP  | N-CA   | 5.22  | 1.52        | 1.46     |
| 1   | E     | 599  | ILE  | CA-CB  | -5.22 | 1.48        | 1.54     |
| 1   | D     | 850  | ALA  | CA-C   | 5.22  | 1.59        | 1.52     |
| 1   | C     | 1025 | ARG  | CD-NE  | -5.21 | 1.39        | 1.46     |
| 1   | E     | 654  | VAL  | CA-CB  | 5.21  | 1.59        | 1.53     |
| 1   | G     | 619  | LYS  | C-O    | -5.21 | 1.18        | 1.24     |
| 1   | A     | 834  | ALA  | C-O    | -5.21 | 1.17        | 1.23     |
| 1   | D     | 516  | ALA  | CA-CB  | 5.18  | 1.61        | 1.53     |
| 1   | C     | 526  | HIS  | C-O    | 5.18  | 1.30        | 1.24     |
| 1   | G     | 403  | TYR  | C-O    | -5.17 | 1.19        | 1.23     |
| 1   | G     | 800  | THR  | CB-CG2 | -5.16 | 1.35        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | G     | 421  | TYR  | CD2-CE2 | 5.16  | 1.54        | 1.38     |
| 1   | G     | 360  | ILE  | N-CA    | 5.16  | 1.52        | 1.46     |
| 1   | G     | 1021 | GLU  | CA-C    | 5.16  | 1.59        | 1.52     |
| 1   | D     | 854  | ARG  | CB-CG   | 5.15  | 1.68        | 1.52     |
| 1   | A     | 576  | ALA  | N-CA    | 5.15  | 1.52        | 1.45     |
| 1   | H     | 336  | ALA  | CA-C    | 5.15  | 1.59        | 1.52     |
| 1   | G     | 372  | SER  | N-CA    | 5.15  | 1.52        | 1.46     |
| 1   | D     | 1000 | GLY  | N-CA    | 5.14  | 1.52        | 1.45     |
| 1   | C     | 409  | THR  | CA-C    | 5.14  | 1.59        | 1.52     |
| 1   | D     | 1038 | VAL  | CA-CB   | 5.14  | 1.61        | 1.54     |
| 1   | C     | 702  | VAL  | CA-CB   | 5.14  | 1.62        | 1.54     |
| 1   | E     | 822  | VAL  | CA-CB   | 5.14  | 1.59        | 1.54     |
| 1   | A     | 1054 | LEU  | CG-CD2  | 5.13  | 1.69        | 1.52     |
| 1   | E     | 945  | LEU  | C-O     | 5.13  | 1.30        | 1.24     |
| 1   | F     | 342  | LYS  | CA-C    | 5.13  | 1.59        | 1.52     |
| 1   | B     | 584  | ILE  | CA-C    | 5.13  | 1.57        | 1.52     |
| 1   | A     | 450  | LEU  | CA-C    | 5.12  | 1.59        | 1.52     |
| 1   | C     | 788  | VAL  | CA-CB   | 5.12  | 1.60        | 1.54     |
| 1   | G     | 427  | ILE  | CG1-CD1 | 5.11  | 1.71        | 1.51     |
| 1   | H     | 566  | VAL  | CB-CG1  | 5.11  | 1.69        | 1.52     |
| 1   | E     | 325  | THR  | CA-CB   | 5.10  | 1.61        | 1.53     |
| 1   | D     | 399  | ALA  | CA-CB   | 5.09  | 1.61        | 1.53     |
| 1   | E     | 849  | ALA  | CA-CB   | 5.09  | 1.61        | 1.53     |
| 1   | E     | 825  | ALA  | CA-CB   | 5.09  | 1.61        | 1.53     |
| 1   | B     | 1024 | ALA  | CA-CB   | 5.09  | 1.61        | 1.53     |
| 1   | A     | 352  | ASN  | CA-C    | 5.09  | 1.58        | 1.52     |
| 1   | B     | 820  | VAL  | CA-C    | 5.08  | 1.58        | 1.52     |
| 1   | E     | 532  | MET  | CB-CG   | -5.08 | 1.37        | 1.52     |
| 1   | E     | 1005 | ALA  | CA-CB   | 5.08  | 1.61        | 1.53     |
| 1   | D     | 611  | SER  | CA-C    | -5.07 | 1.47        | 1.53     |
| 1   | H     | 555  | SER  | N-CA    | 5.07  | 1.52        | 1.45     |
| 1   | D     | 619  | LYS  | C-O     | -5.07 | 1.18        | 1.24     |
| 1   | G     | 310  | VAL  | CA-C    | 5.07  | 1.59        | 1.52     |
| 1   | H     | 993  | VAL  | C-O     | 5.06  | 1.29        | 1.24     |
| 1   | F     | 1002 | ASP  | CB-CG   | -5.06 | 1.39        | 1.52     |
| 1   | B     | 422  | THR  | CB-CG2  | -5.05 | 1.35        | 1.52     |
| 1   | H     | 244  | SER  | N-CA    | 5.05  | 1.55        | 1.46     |
| 1   | E     | 707  | ILE  | C-O     | 5.05  | 1.29        | 1.23     |
| 1   | E     | 802  | ALA  | C-O     | -5.04 | 1.17        | 1.24     |
| 1   | A     | 468  | ASP  | CB-CG   | -5.04 | 1.39        | 1.52     |
| 1   | D     | 522  | THR  | N-CA    | -5.04 | 1.42        | 1.46     |
| 1   | D     | 1028 | ILE  | CA-CB   | 5.03  | 1.60        | 1.54     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | H     | 977 | LYS  | CB-CG | -5.03 | 1.37        | 1.52     |
| 1   | G     | 492 | ASP  | CA-CB | 5.03  | 1.61        | 1.53     |
| 1   | E     | 793 | ASP  | CB-CG | -5.03 | 1.39        | 1.52     |
| 1   | A     | 808 | ALA  | CA-CB | 5.02  | 1.61        | 1.53     |
| 1   | E     | 310 | VAL  | CA-CB | -5.02 | 1.48        | 1.54     |
| 1   | F     | 518 | SER  | CA-C  | 5.02  | 1.58        | 1.52     |
| 1   | B     | 671 | ALA  | CA-CB | 5.02  | 1.61        | 1.53     |
| 1   | G     | 826 | ALA  | CA-CB | 5.01  | 1.61        | 1.53     |
| 1   | F     | 491 | GLY  | N-CA  | 5.01  | 1.52        | 1.45     |
| 1   | G     | 559 | PRO  | CA-CB | 5.00  | 1.60        | 1.53     |
| 1   | E     | 536 | ASP  | CA-CB | 5.00  | 1.60        | 1.52     |

All (320) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|--------|-------------|----------|
| 1   | G     | 854  | ARG  | NE-CZ-NH2 | -18.23 | 102.79      | 119.20   |
| 1   | A     | 854  | ARG  | NE-CZ-NH2 | -17.29 | 103.64      | 119.20   |
| 1   | D     | 854  | ARG  | NE-CZ-NH2 | -17.25 | 103.67      | 119.20   |
| 1   | E     | 854  | ARG  | NE-CZ-NH2 | -16.60 | 104.26      | 119.20   |
| 1   | B     | 540  | ARG  | NE-CZ-NH2 | -16.34 | 104.50      | 119.20   |
| 1   | G     | 1025 | ARG  | NE-CZ-NH2 | -16.19 | 104.63      | 119.20   |
| 1   | B     | 666  | ASP  | CA-C-N    | -14.62 | 100.99      | 122.04   |
| 1   | B     | 666  | ASP  | C-N-CA    | -14.62 | 100.99      | 122.04   |
| 1   | E     | 1025 | ARG  | NE-CZ-NH2 | -14.16 | 106.46      | 119.20   |
| 1   | D     | 1025 | ARG  | NE-CZ-NH2 | -13.90 | 106.69      | 119.20   |
| 1   | H     | 854  | ARG  | NE-CZ-NH2 | -13.64 | 106.92      | 119.20   |
| 1   | C     | 854  | ARG  | NE-CZ-NH2 | -13.32 | 107.21      | 119.20   |
| 1   | H     | 1025 | ARG  | NE-CZ-NH2 | -12.45 | 108.00      | 119.20   |
| 1   | C     | 1025 | ARG  | NE-CZ-NH2 | -12.19 | 108.23      | 119.20   |
| 1   | F     | 1025 | ARG  | NE-CZ-NH2 | -11.58 | 108.78      | 119.20   |
| 1   | G     | 854  | ARG  | NE-CZ-NH1 | 11.32  | 132.82      | 121.50   |
| 1   | G     | 585  | ARG  | NE-CZ-NH2 | -10.83 | 109.45      | 119.20   |
| 1   | D     | 371  | ASN  | CB-CA-C   | -10.53 | 89.45       | 110.30   |
| 1   | A     | 585  | ARG  | NE-CZ-NH2 | -10.23 | 109.99      | 119.20   |
| 1   | A     | 854  | ARG  | NE-CZ-NH1 | 9.94   | 131.44      | 121.50   |
| 1   | A     | 854  | ARG  | CD-NE-CZ  | 9.85   | 138.19      | 124.40   |
| 1   | B     | 1025 | ARG  | NE-CZ-NH2 | -9.76  | 110.42      | 119.20   |
| 1   | D     | 1025 | ARG  | NE-CZ-NH1 | 9.72   | 131.22      | 121.50   |
| 1   | H     | 1025 | ARG  | NE-CZ-NH1 | 9.70   | 131.19      | 121.50   |
| 1   | E     | 854  | ARG  | NE-CZ-NH1 | 9.38   | 130.88      | 121.50   |
| 1   | B     | 522  | THR  | CA-C-N    | -9.34  | 110.12      | 119.56   |
| 1   | B     | 522  | THR  | C-N-CA    | -9.34  | 110.12      | 119.56   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | A     | 1025 | ARG  | O-C-N      | 9.31  | 134.23      | 123.06   |
| 1   | F     | 854  | ARG  | NE-CZ-NH2  | -8.93 | 111.17      | 119.20   |
| 1   | G     | 1025 | ARG  | NE-CZ-NH1  | 8.90  | 130.40      | 121.50   |
| 1   | G     | 585  | ARG  | NE-CZ-NH1  | 8.88  | 130.38      | 121.50   |
| 1   | G     | 1025 | ARG  | CG-CD-NE   | -8.87 | 92.48       | 112.00   |
| 1   | D     | 1025 | ARG  | CD-NE-CZ   | 8.68  | 136.55      | 124.40   |
| 1   | G     | 1025 | ARG  | CD-NE-CZ   | 8.64  | 136.50      | 124.40   |
| 1   | E     | 911  | VAL  | N-CA-C     | -8.41 | 103.63      | 111.45   |
| 1   | E     | 1025 | ARG  | NE-CZ-NH1  | 8.40  | 129.90      | 121.50   |
| 1   | F     | 357  | ARG  | CD-NE-CZ   | 8.34  | 136.07      | 124.40   |
| 1   | H     | 854  | ARG  | NE-CZ-NH1  | 8.27  | 129.77      | 121.50   |
| 1   | H     | 585  | ARG  | NE-CZ-NH2  | -8.26 | 111.77      | 119.20   |
| 1   | D     | 585  | ARG  | NE-CZ-NH2  | -8.19 | 111.83      | 119.20   |
| 1   | B     | 540  | ARG  | CD-NE-CZ   | 8.16  | 135.83      | 124.40   |
| 1   | C     | 953  | MET  | O-C-N      | -8.14 | 113.94      | 123.22   |
| 1   | G     | 912  | ILE  | CA-CB-CG1  | -8.13 | 96.58       | 110.40   |
| 1   | D     | 999  | SER  | N-CA-C     | -8.11 | 96.00       | 109.46   |
| 1   | E     | 854  | ARG  | CD-NE-CZ   | 7.99  | 135.59      | 124.40   |
| 1   | E     | 727  | ILE  | CB-CA-C    | -7.97 | 99.36       | 112.26   |
| 1   | C     | 371  | ASN  | CA-CB-CG   | -7.93 | 104.67      | 112.60   |
| 1   | E     | 1025 | ARG  | CD-NE-CZ   | 7.89  | 135.44      | 124.40   |
| 1   | E     | 585  | ARG  | NE-CZ-NH2  | -7.86 | 112.12      | 119.20   |
| 1   | G     | 854  | ARG  | CD-NE-CZ   | 7.84  | 135.37      | 124.40   |
| 1   | H     | 1025 | ARG  | CD-NE-CZ   | 7.73  | 135.22      | 124.40   |
| 1   | E     | 288  | THR  | CB-CA-C    | -7.72 | 96.17       | 111.60   |
| 1   | H     | 793  | ASP  | N-CA-CB    | -7.71 | 97.59       | 110.39   |
| 1   | C     | 1025 | ARG  | CG-CD-NE   | -7.69 | 95.09       | 112.00   |
| 1   | H     | 856  | MET  | CG-SD-CE   | -7.67 | 84.02       | 100.90   |
| 1   | A     | 1024 | ALA  | O-C-N      | -7.66 | 111.48      | 122.36   |
| 1   | B     | 977  | LYS  | CA-CB-CG   | 7.58  | 129.25      | 114.10   |
| 1   | E     | 1025 | ARG  | CG-CD-NE   | -7.57 | 95.35       | 112.00   |
| 1   | D     | 752  | VAL  | CA-C-N     | -7.54 | 113.84      | 123.19   |
| 1   | D     | 752  | VAL  | C-N-CA     | -7.54 | 113.84      | 123.19   |
| 1   | D     | 854  | ARG  | CD-NE-CZ   | 7.52  | 134.93      | 124.40   |
| 1   | G     | 422  | THR  | N-CA-CB    | -7.50 | 100.53      | 110.88   |
| 1   | C     | 320  | HIS  | N-CA-C     | 7.48  | 119.52      | 111.36   |
| 1   | A     | 247  | GLN  | N-CA-C     | 7.41  | 119.00      | 111.07   |
| 1   | H     | 585  | ARG  | NE-CZ-NH1  | 7.41  | 128.91      | 121.50   |
| 1   | H     | 854  | ARG  | CG-CD-NE   | -7.41 | 95.71       | 112.00   |
| 1   | F     | 307  | ARG  | NE-CZ-NH2  | -7.40 | 112.54      | 119.20   |
| 1   | D     | 854  | ARG  | NE-CZ-NH1  | 7.39  | 128.89      | 121.50   |
| 1   | G     | 422  | THR  | OG1-CB-CG2 | 7.36  | 124.03      | 109.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | B     | 540  | ARG  | NE-CZ-NH1  | 7.34  | 128.84      | 121.50   |
| 1   | G     | 748  | SER  | N-CA-C     | -7.31 | 104.51      | 113.50   |
| 1   | F     | 540  | ARG  | O-C-N      | 7.28  | 129.87      | 122.08   |
| 1   | D     | 422  | THR  | N-CA-CB    | -7.24 | 100.88      | 110.88   |
| 1   | A     | 1025 | ARG  | CA-C-N     | -7.24 | 112.52      | 122.30   |
| 1   | A     | 1025 | ARG  | C-N-CA     | -7.24 | 112.52      | 122.30   |
| 1   | C     | 952  | VAL  | CA-C-N     | 7.21  | 132.36      | 122.77   |
| 1   | C     | 952  | VAL  | C-N-CA     | 7.21  | 132.36      | 122.77   |
| 1   | G     | 976  | ASP  | CA-C-N     | 7.20  | 130.89      | 120.38   |
| 1   | G     | 976  | ASP  | C-N-CA     | 7.20  | 130.89      | 120.38   |
| 1   | D     | 854  | ARG  | CG-CD-NE   | -7.09 | 96.41       | 112.00   |
| 1   | E     | 977  | LYS  | CD-CE-NZ   | -7.06 | 89.32       | 111.90   |
| 1   | G     | 800  | THR  | N-CA-CB    | -7.05 | 99.53       | 111.31   |
| 1   | H     | 976  | ASP  | CA-C-N     | 7.04  | 130.66      | 120.38   |
| 1   | H     | 976  | ASP  | C-N-CA     | 7.04  | 130.66      | 120.38   |
| 1   | E     | 674  | THR  | N-CA-C     | -7.02 | 101.48      | 110.53   |
| 1   | F     | 1025 | ARG  | NE-CZ-NH1  | 6.99  | 128.49      | 121.50   |
| 1   | D     | 1025 | ARG  | CG-CD-NE   | -6.99 | 96.63       | 112.00   |
| 1   | C     | 1025 | ARG  | NE-CZ-NH1  | 6.98  | 128.48      | 121.50   |
| 1   | E     | 800  | THR  | N-CA-CB    | -6.97 | 99.67       | 111.31   |
| 1   | F     | 1001 | LYS  | CA-C-N     | 6.95  | 136.33      | 121.45   |
| 1   | F     | 1001 | LYS  | C-N-CA     | 6.95  | 136.33      | 121.45   |
| 1   | C     | 854  | ARG  | CG-CD-NE   | -6.95 | 96.71       | 112.00   |
| 1   | D     | 999  | SER  | O-C-N      | -6.94 | 115.31      | 123.22   |
| 1   | H     | 371  | ASN  | CA-CB-CG   | -6.93 | 105.67      | 112.60   |
| 1   | B     | 540  | ARG  | CG-CD-NE   | -6.87 | 96.88       | 112.00   |
| 1   | E     | 800  | THR  | OG1-CB-CG2 | 6.82  | 122.95      | 109.30   |
| 1   | C     | 732  | GLY  | N-CA-C     | -6.79 | 104.11      | 112.33   |
| 1   | C     | 854  | ARG  | NE-CZ-NH1  | 6.77  | 128.27      | 121.50   |
| 1   | B     | 723  | THR  | N-CA-C     | -6.77 | 101.42      | 110.55   |
| 1   | G     | 1005 | ALA  | N-CA-C     | -6.75 | 103.99      | 111.82   |
| 1   | F     | 357  | ARG  | CG-CD-NE   | 6.75  | 126.84      | 112.00   |
| 1   | G     | 911  | VAL  | N-CA-C     | -6.72 | 105.29      | 111.67   |
| 1   | F     | 422  | THR  | N-CA-CB    | -6.71 | 101.98      | 110.90   |
| 1   | A     | 585  | ARG  | NE-CZ-NH1  | 6.68  | 128.18      | 121.50   |
| 1   | B     | 422  | THR  | N-CA-CB    | -6.66 | 102.04      | 110.90   |
| 1   | F     | 252  | TYR  | N-CA-C     | -6.66 | 104.02      | 111.28   |
| 1   | C     | 522  | THR  | CA-C-N     | -6.65 | 111.96      | 119.28   |
| 1   | C     | 522  | THR  | C-N-CA     | -6.65 | 111.96      | 119.28   |
| 1   | H     | 372  | SER  | CA-CB-OG   | -6.62 | 97.86       | 111.10   |
| 1   | C     | 1025 | ARG  | CD-NE-CZ   | 6.61  | 133.65      | 124.40   |
| 1   | H     | 585  | ARG  | CD-NE-CZ   | 6.55  | 133.57      | 124.40   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | G     | 585  | ARG  | CD-NE-CZ   | 6.53  | 133.54      | 124.40   |
| 1   | D     | 502  | LYS  | CB-CG-CD   | -6.52 | 96.31       | 111.30   |
| 1   | G     | 262  | VAL  | N-CA-C     | -6.52 | 98.12       | 107.77   |
| 1   | F     | 585  | ARG  | NE-CZ-NH2  | -6.51 | 113.34      | 119.20   |
| 1   | F     | 357  | ARG  | NE-CZ-NH2  | -6.49 | 113.36      | 119.20   |
| 1   | A     | 359  | THR  | OG1-CB-CG2 | -6.48 | 96.34       | 109.30   |
| 1   | E     | 585  | ARG  | CD-NE-CZ   | 6.47  | 133.46      | 124.40   |
| 1   | F     | 431  | GLU  | N-CA-C     | 6.43  | 118.37      | 111.36   |
| 1   | G     | 666  | ASP  | CA-C-N     | -6.40 | 112.77      | 122.06   |
| 1   | G     | 666  | ASP  | C-N-CA     | -6.40 | 112.77      | 122.06   |
| 1   | E     | 522  | THR  | CA-C-N     | -6.39 | 112.41      | 119.19   |
| 1   | E     | 522  | THR  | C-N-CA     | -6.39 | 112.41      | 119.19   |
| 1   | A     | 1038 | VAL  | O-C-N      | -6.38 | 116.43      | 123.20   |
| 1   | C     | 928  | LYS  | N-CA-C     | -6.38 | 102.39      | 108.13   |
| 1   | H     | 371  | ASN  | CB-CG-OD1  | -6.36 | 108.08      | 120.80   |
| 1   | C     | 371  | ASN  | CB-CG-ND2  | 6.35  | 125.93      | 116.40   |
| 1   | H     | 854  | ARG  | CD-NE-CZ   | 6.35  | 133.29      | 124.40   |
| 1   | C     | 585  | ARG  | NE-CZ-NH2  | -6.34 | 113.50      | 119.20   |
| 1   | H     | 595  | ILE  | N-CA-C     | -6.34 | 104.32      | 110.72   |
| 1   | F     | 1025 | ARG  | CG-CD-NE   | -6.33 | 98.06       | 112.00   |
| 1   | B     | 357  | ARG  | CD-NE-CZ   | 6.28  | 133.19      | 124.40   |
| 1   | H     | 1025 | ARG  | CG-CD-NE   | -6.25 | 98.24       | 112.00   |
| 1   | D     | 368  | SER  | N-CA-C     | 6.24  | 118.60      | 111.11   |
| 1   | F     | 372  | SER  | CB-CA-C    | -6.24 | 97.16       | 110.32   |
| 1   | C     | 1074 | VAL  | N-CA-CB    | 6.21  | 117.94      | 110.31   |
| 1   | F     | 1002 | ASP  | N-CA-CB    | -6.20 | 101.58      | 110.44   |
| 1   | B     | 325  | THR  | CB-CA-C    | -6.19 | 98.11       | 110.42   |
| 1   | A     | 832  | VAL  | CB-CA-C    | 6.17  | 120.01      | 110.50   |
| 1   | B     | 666  | ASP  | O-C-N      | -6.17 | 114.72      | 122.19   |
| 1   | C     | 953  | MET  | CA-C-N     | 6.16  | 130.88      | 122.19   |
| 1   | C     | 953  | MET  | C-N-CA     | 6.16  | 130.88      | 122.19   |
| 1   | B     | 984  | GLY  | N-CA-C     | -6.16 | 106.58      | 115.27   |
| 1   | E     | 702  | VAL  | CB-CA-C    | -6.16 | 99.69       | 110.71   |
| 1   | E     | 594  | LEU  | N-CA-C     | -6.15 | 104.12      | 111.69   |
| 1   | D     | 585  | ARG  | NE-CZ-NH1  | 6.15  | 127.65      | 121.50   |
| 1   | G     | 854  | ARG  | CG-CD-NE   | -6.15 | 98.48       | 112.00   |
| 1   | H     | 1083 | SER  | N-CA-C     | -6.14 | 103.89      | 111.75   |
| 1   | F     | 837  | ALA  | CA-C-N     | -6.13 | 113.44      | 119.76   |
| 1   | F     | 837  | ALA  | C-N-CA     | -6.13 | 113.44      | 119.76   |
| 1   | A     | 726  | ARG  | CB-CA-C    | -6.11 | 101.29      | 110.88   |
| 1   | E     | 653  | SER  | CA-C-N     | -6.10 | 118.20      | 122.59   |
| 1   | E     | 653  | SER  | C-N-CA     | -6.10 | 118.20      | 122.59   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | G     | 371  | ASN  | CA-CB-CG   | -6.08 | 106.52      | 112.60   |
| 1   | G     | 532  | MET  | CB-CG-SD   | 6.05  | 130.85      | 112.70   |
| 1   | A     | 585  | ARG  | CD-NE-CZ   | 6.05  | 132.87      | 124.40   |
| 1   | A     | 800  | THR  | N-CA-CB    | -6.04 | 101.22      | 111.31   |
| 1   | C     | 371  | ASN  | CB-CA-C    | -6.04 | 98.89       | 110.24   |
| 1   | F     | 357  | ARG  | NE-CZ-NH1  | 6.02  | 127.52      | 121.50   |
| 1   | H     | 347  | ILE  | N-CA-C     | -6.01 | 104.65      | 110.42   |
| 1   | A     | 990  | THR  | OG1-CB-CG2 | -6.00 | 97.31       | 109.30   |
| 1   | A     | 543  | LEU  | N-CA-C     | -5.99 | 104.84      | 111.36   |
| 1   | B     | 585  | ARG  | NE-CZ-NH2  | -5.99 | 113.81      | 119.20   |
| 1   | E     | 371  | ASN  | CA-CB-CG   | -5.99 | 106.61      | 112.60   |
| 1   | C     | 422  | THR  | N-CA-CB    | -5.98 | 102.63      | 110.88   |
| 1   | C     | 328  | SER  | CA-C-N     | 5.97  | 125.45      | 119.24   |
| 1   | C     | 328  | SER  | C-N-CA     | 5.97  | 125.45      | 119.24   |
| 1   | E     | 585  | ARG  | NE-CZ-NH1  | 5.91  | 127.41      | 121.50   |
| 1   | G     | 625  | ASN  | N-CA-C     | 5.89  | 117.70      | 111.28   |
| 1   | D     | 999  | SER  | CA-C-N     | -5.88 | 109.88      | 121.41   |
| 1   | D     | 999  | SER  | C-N-CA     | -5.88 | 109.88      | 121.41   |
| 1   | C     | 548  | ALA  | N-CA-C     | 5.87  | 119.62      | 112.23   |
| 1   | H     | 832  | VAL  | CG1-CB-CG2 | 5.85  | 123.67      | 110.80   |
| 1   | E     | 307  | ARG  | N-CA-C     | -5.84 | 104.83      | 111.14   |
| 1   | G     | 792  | ASN  | CA-C-N     | 5.83  | 128.89      | 120.38   |
| 1   | G     | 792  | ASN  | C-N-CA     | 5.83  | 128.89      | 120.38   |
| 1   | H     | 741  | PRO  | CA-C-N     | -5.83 | 112.54      | 122.56   |
| 1   | H     | 741  | PRO  | C-N-CA     | -5.83 | 112.54      | 122.56   |
| 1   | G     | 584  | ILE  | N-CA-C     | -5.81 | 107.15      | 112.96   |
| 1   | H     | 752  | VAL  | CA-C-N     | -5.79 | 115.59      | 123.12   |
| 1   | H     | 752  | VAL  | C-N-CA     | -5.79 | 115.59      | 123.12   |
| 1   | E     | 368  | SER  | N-CA-C     | 5.79  | 118.06      | 111.11   |
| 1   | E     | 1085 | VAL  | N-CA-C     | -5.79 | 107.86      | 113.53   |
| 1   | C     | 585  | ARG  | NE-CZ-NH1  | 5.78  | 127.28      | 121.50   |
| 1   | E     | 800  | THR  | CA-CB-CG2  | 5.76  | 120.29      | 110.50   |
| 1   | D     | 585  | ARG  | CG-CD-NE   | -5.74 | 99.36       | 112.00   |
| 1   | C     | 854  | ARG  | CD-NE-CZ   | 5.73  | 132.43      | 124.40   |
| 1   | E     | 952  | VAL  | CA-C-N     | 5.73  | 130.40      | 122.77   |
| 1   | E     | 952  | VAL  | C-N-CA     | 5.73  | 130.40      | 122.77   |
| 1   | G     | 251  | VAL  | N-CA-CB    | -5.73 | 100.92      | 110.14   |
| 1   | F     | 1025 | ARG  | CD-NE-CZ   | 5.72  | 132.41      | 124.40   |
| 1   | D     | 465  | ASN  | CB-CA-C    | -5.71 | 103.79      | 111.89   |
| 1   | C     | 422  | THR  | CA-CB-CG2  | 5.68  | 120.16      | 110.50   |
| 1   | D     | 965  | PRO  | CA-C-N     | -5.68 | 114.42      | 122.94   |
| 1   | D     | 965  | PRO  | C-N-CA     | -5.68 | 114.42      | 122.94   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | D     | 1080 | LEU  | CA-C-N     | -5.68 | 113.70      | 119.83   |
| 1   | D     | 1080 | LEU  | C-N-CA     | -5.68 | 113.70      | 119.83   |
| 1   | B     | 368  | SER  | N-CA-C     | 5.67  | 117.91      | 111.11   |
| 1   | B     | 1025 | ARG  | CG-CD-NE   | -5.67 | 99.53       | 112.00   |
| 1   | H     | 666  | ASP  | CA-C-N     | -5.67 | 114.82      | 121.85   |
| 1   | H     | 666  | ASP  | C-N-CA     | -5.67 | 114.82      | 121.85   |
| 1   | E     | 832  | VAL  | N-CA-CB    | -5.65 | 102.19      | 111.45   |
| 1   | E     | 338  | THR  | N-CA-C     | -5.64 | 105.21      | 111.36   |
| 1   | G     | 431  | GLU  | N-CA-C     | 5.63  | 117.22      | 111.14   |
| 1   | A     | 252  | TYR  | N-CA-C     | -5.63 | 105.23      | 111.36   |
| 1   | C     | 371  | ASN  | CB-CG-OD1  | -5.62 | 109.55      | 120.80   |
| 1   | E     | 727  | ILE  | CG1-CB-CG2 | 5.62  | 127.57      | 110.70   |
| 1   | A     | 854  | ARG  | CG-CD-NE   | -5.61 | 99.66       | 112.00   |
| 1   | H     | 977  | LYS  | N-CA-CB    | -5.60 | 101.29      | 110.14   |
| 1   | A     | 868  | THR  | CB-CA-C    | -5.59 | 98.43       | 109.67   |
| 1   | A     | 532  | MET  | CA-CB-CG   | 5.59  | 125.28      | 114.10   |
| 1   | A     | 911  | VAL  | N-CA-C     | -5.58 | 106.37      | 111.67   |
| 1   | E     | 854  | ARG  | CG-CD-NE   | -5.58 | 99.73       | 112.00   |
| 1   | B     | 1025 | ARG  | NE-CZ-NH1  | 5.57  | 127.07      | 121.50   |
| 1   | E     | 1032 | VAL  | CA-C-N     | -5.56 | 114.87      | 120.21   |
| 1   | E     | 1032 | VAL  | C-N-CA     | -5.56 | 114.87      | 120.21   |
| 1   | A     | 842  | GLY  | N-CA-C     | -5.55 | 107.66      | 115.32   |
| 1   | G     | 748  | SER  | CA-C-N     | 5.55  | 128.59      | 120.71   |
| 1   | G     | 748  | SER  | C-N-CA     | 5.55  | 128.59      | 120.71   |
| 1   | E     | 989  | ASN  | CA-C-N     | -5.53 | 113.99      | 122.62   |
| 1   | E     | 989  | ASN  | C-N-CA     | -5.53 | 113.99      | 122.62   |
| 1   | F     | 578  | VAL  | CB-CA-C    | -5.52 | 101.31      | 111.36   |
| 1   | D     | 368  | SER  | CA-CB-OG   | -5.51 | 100.07      | 111.10   |
| 1   | D     | 585  | ARG  | CD-NE-CZ   | 5.51  | 132.12      | 124.40   |
| 1   | H     | 800  | THR  | N-CA-CB    | -5.51 | 102.52      | 111.22   |
| 1   | E     | 741  | PRO  | CA-C-N     | -5.51 | 113.84      | 122.65   |
| 1   | E     | 741  | PRO  | C-N-CA     | -5.51 | 113.84      | 122.65   |
| 1   | D     | 681  | GLU  | N-CA-C     | -5.51 | 105.36      | 111.36   |
| 1   | A     | 702  | VAL  | CB-CA-C    | -5.50 | 101.12      | 111.30   |
| 1   | C     | 800  | THR  | N-CA-CB    | -5.50 | 102.12      | 111.31   |
| 1   | E     | 307  | ARG  | O-C-N      | 5.50  | 128.04      | 122.09   |
| 1   | C     | 832  | VAL  | CB-CA-C    | 5.50  | 118.98      | 110.50   |
| 1   | C     | 832  | VAL  | N-CA-CB    | -5.50 | 102.42      | 111.44   |
| 1   | E     | 876  | VAL  | N-CA-C     | -5.49 | 105.17      | 110.72   |
| 1   | D     | 422  | THR  | OG1-CB-CG2 | 5.47  | 120.23      | 109.30   |
| 1   | A     | 1037 | SER  | CA-C-N     | 5.46  | 130.37      | 123.10   |
| 1   | A     | 1037 | SER  | C-N-CA     | 5.46  | 130.37      | 123.10   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | D     | 522  | THR  | CA-C-N    | -5.46 | 113.40      | 119.19   |
| 1   | D     | 522  | THR  | C-N-CA    | -5.46 | 113.40      | 119.19   |
| 1   | E     | 281  | GLY  | N-CA-C    | -5.46 | 108.10      | 115.36   |
| 1   | D     | 334  | LEU  | N-CA-C    | -5.45 | 105.42      | 111.36   |
| 1   | B     | 585  | ARG  | NE-CZ-NH1 | 5.44  | 126.94      | 121.50   |
| 1   | D     | 371  | ASN  | N-CA-C    | -5.44 | 101.14      | 109.41   |
| 1   | D     | 911  | VAL  | N-CA-C    | -5.42 | 106.52      | 111.67   |
| 1   | C     | 938  | LEU  | N-CA-C    | -5.42 | 105.29      | 111.14   |
| 1   | E     | 372  | SER  | CB-CA-C   | -5.42 | 100.61      | 110.63   |
| 1   | B     | 357  | ARG  | NE-CZ-NH1 | 5.39  | 126.89      | 121.50   |
| 1   | C     | 618  | LYS  | CG-CD-CE  | -5.39 | 98.91       | 111.30   |
| 1   | D     | 832  | VAL  | N-CA-CB   | -5.38 | 102.62      | 111.45   |
| 1   | A     | 835  | SER  | N-CA-CB   | -5.38 | 102.11      | 110.29   |
| 1   | H     | 371  | ASN  | CB-CA-C   | -5.36 | 99.68       | 110.30   |
| 1   | H     | 1067 | THR  | N-CA-C    | -5.33 | 106.79      | 113.72   |
| 1   | E     | 765  | ARG  | CA-C-N    | -5.32 | 114.48      | 119.85   |
| 1   | E     | 765  | ARG  | C-N-CA    | -5.32 | 114.48      | 119.85   |
| 1   | A     | 585  | ARG  | CB-CG-CD  | -5.29 | 99.13       | 111.30   |
| 1   | B     | 474  | ILE  | CB-CA-C   | -5.29 | 102.51      | 110.55   |
| 1   | C     | 535  | MET  | N-CA-C    | -5.29 | 103.42      | 110.55   |
| 1   | E     | 1009 | GLY  | N-CA-C    | -5.28 | 108.33      | 115.36   |
| 1   | G     | 245  | PHE  | N-CA-C    | -5.27 | 106.81      | 113.18   |
| 1   | H     | 921  | ARG  | N-CA-C    | 5.26  | 117.76      | 111.71   |
| 1   | B     | 1025 | ARG  | CD-NE-CZ  | 5.26  | 131.76      | 124.40   |
| 1   | B     | 245  | PHE  | N-CA-C    | -5.25 | 106.88      | 113.28   |
| 1   | B     | 295  | LEU  | CA-CB-CG  | 5.24  | 134.65      | 116.30   |
| 1   | H     | 584  | ILE  | N-CA-C    | -5.23 | 107.73      | 112.96   |
| 1   | F     | 468  | ASP  | N-CA-CB   | -5.23 | 102.72      | 110.61   |
| 1   | A     | 785  | ALA  | N-CA-C    | 5.21  | 116.96      | 111.28   |
| 1   | C     | 305  | THR  | N-CA-C    | -5.21 | 105.78      | 111.82   |
| 1   | C     | 391  | ASN  | N-CA-C    | 5.20  | 117.69      | 111.71   |
| 1   | F     | 936  | ASP  | N-CA-C    | 5.20  | 117.03      | 111.36   |
| 1   | B     | 1036 | PRO  | N-CA-C    | -5.20 | 108.73      | 114.92   |
| 1   | A     | 986  | GLN  | CA-C-N    | -5.20 | 116.03      | 123.10   |
| 1   | A     | 986  | GLN  | C-N-CA    | -5.20 | 116.03      | 123.10   |
| 1   | A     | 921  | ARG  | N-CA-C    | 5.20  | 117.68      | 111.71   |
| 1   | A     | 793  | ASP  | CB-CG-OD1 | -5.18 | 106.48      | 118.40   |
| 1   | D     | 785  | ALA  | N-CA-C    | 5.18  | 119.92      | 111.37   |
| 1   | A     | 836  | THR  | N-CA-C    | -5.18 | 106.55      | 112.92   |
| 1   | D     | 251  | VAL  | N-CA-CB   | -5.17 | 103.19      | 110.13   |
| 1   | G     | 372  | SER  | CB-CA-C   | -5.17 | 98.59       | 110.18   |
| 1   | D     | 654  | VAL  | N-CA-C    | -5.15 | 102.56      | 107.76   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 1   | G     | 465  | ASN  | CB-CA-C    | -5.13 | 104.30      | 111.80   |
| 1   | A     | 1041 | LYS  | N-CA-C     | -5.12 | 107.16      | 113.41   |
| 1   | E     | 585  | ARG  | CB-CG-CD   | -5.11 | 99.55       | 111.30   |
| 1   | G     | 715  | LYS  | CD-CE-NZ   | -5.11 | 95.55       | 111.90   |
| 1   | A     | 882  | VAL  | N-CA-CB    | -5.11 | 104.08      | 110.47   |
| 1   | B     | 727  | ILE  | N-CA-C     | 5.11  | 115.88      | 110.72   |
| 1   | A     | 606  | ASN  | CB-CA-C    | -5.10 | 103.16      | 111.06   |
| 1   | A     | 654  | VAL  | N-CA-C     | -5.09 | 102.61      | 107.76   |
| 1   | D     | 423  | ALA  | CA-C-N     | -5.09 | 115.92      | 123.05   |
| 1   | D     | 423  | ALA  | C-N-CA     | -5.09 | 115.92      | 123.05   |
| 1   | A     | 690  | TYR  | CA-C-N     | -5.09 | 116.02      | 122.43   |
| 1   | A     | 690  | TYR  | C-N-CA     | -5.09 | 116.02      | 122.43   |
| 1   | C     | 422  | THR  | OG1-CB-CG2 | 5.09  | 119.48      | 109.30   |
| 1   | A     | 822  | VAL  | N-CA-C     | 5.08  | 116.78      | 109.51   |
| 1   | D     | 689  | LYS  | N-CA-C     | 5.07  | 116.89      | 111.36   |
| 1   | E     | 699  | ASN  | N-CA-C     | -5.07 | 100.02      | 108.34   |
| 1   | B     | 977  | LYS  | CB-CA-C    | -5.07 | 100.33      | 110.42   |
| 1   | G     | 371  | ASN  | CB-CA-C    | -5.07 | 99.40       | 109.79   |
| 1   | F     | 912  | ILE  | CG1-CB-CG2 | 5.07  | 125.90      | 110.70   |
| 1   | G     | 704  | ASN  | N-CA-C     | 5.06  | 119.10      | 113.02   |
| 1   | E     | 939  | VAL  | N-CA-C     | -5.06 | 105.56      | 110.42   |
| 1   | H     | 836  | THR  | N-CA-C     | -5.06 | 106.70      | 112.92   |
| 1   | F     | 307  | ARG  | CG-CD-NE   | -5.05 | 100.88      | 112.00   |
| 1   | G     | 371  | ASN  | CB-CG-ND2  | 5.05  | 123.97      | 116.40   |
| 1   | A     | 925  | GLY  | N-CA-C     | -5.04 | 107.31      | 115.08   |
| 1   | E     | 318  | GLY  | CA-C-N     | -5.04 | 115.86      | 122.37   |
| 1   | E     | 318  | GLY  | C-N-CA     | -5.04 | 115.86      | 122.37   |
| 1   | E     | 325  | THR  | CB-CA-C    | -5.04 | 101.00      | 110.67   |
| 1   | F     | 959  | ASP  | N-CA-C     | 5.03  | 116.45      | 111.07   |
| 1   | F     | 626  | LYS  | N-CA-C     | -5.03 | 105.88      | 111.36   |
| 1   | D     | 868  | THR  | N-CA-C     | -5.03 | 107.18      | 113.72   |
| 1   | E     | 320  | HIS  | N-CA-C     | 5.03  | 118.56      | 112.93   |
| 1   | G     | 741  | PRO  | CA-C-N     | -5.03 | 113.92      | 122.56   |
| 1   | G     | 741  | PRO  | C-N-CA     | -5.03 | 113.92      | 122.56   |
| 1   | F     | 558  | ASN  | CA-C-N     | -5.02 | 114.44      | 119.56   |
| 1   | F     | 558  | ASN  | C-N-CA     | -5.02 | 114.44      | 119.56   |
| 1   | G     | 1041 | LYS  | N-CA-C     | -5.02 | 107.29      | 113.41   |
| 1   | A     | 744  | ARG  | CB-CA-C    | -5.02 | 100.87      | 109.65   |
| 1   | H     | 282  | LYS  | CA-C-N     | -5.01 | 115.71      | 122.77   |
| 1   | H     | 282  | LYS  | C-N-CA     | -5.01 | 115.71      | 122.77   |
| 1   | D     | 617  | ILE  | N-CA-C     | 5.00  | 115.22      | 110.42   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1   | E     | 800 | THR  | CB   |

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     | 6660  | 0        | 6489     | 79      | 0            |
| 1   | B     | 6659  | 0        | 6489     | 130     | 0            |
| 1   | C     | 6660  | 0        | 6489     | 100     | 0            |
| 1   | D     | 6660  | 0        | 6489     | 107     | 0            |
| 1   | E     | 6660  | 0        | 6489     | 115     | 0            |
| 1   | F     | 6660  | 0        | 6489     | 142     | 0            |
| 1   | G     | 6660  | 0        | 6489     | 112     | 0            |
| 1   | H     | 6660  | 0        | 6489     | 121     | 0            |
| 2   | A     | 1     | 0        | 0        | 0       | 0            |
| 2   | B     | 1     | 0        | 0        | 0       | 0            |
| 2   | C     | 1     | 0        | 0        | 0       | 0            |
| 2   | D     | 1     | 0        | 0        | 0       | 0            |
| 2   | E     | 1     | 0        | 0        | 0       | 0            |
| 2   | F     | 1     | 0        | 0        | 0       | 0            |
| 2   | G     | 1     | 0        | 0        | 0       | 0            |
| 2   | H     | 1     | 0        | 0        | 0       | 0            |
| 3   | A     | 12    | 0        | 12       | 0       | 0            |
| 3   | B     | 12    | 0        | 12       | 2       | 0            |
| 3   | C     | 12    | 0        | 12       | 0       | 0            |
| 3   | D     | 12    | 0        | 12       | 1       | 0            |
| 3   | E     | 12    | 0        | 12       | 0       | 0            |
| 3   | F     | 12    | 0        | 12       | 0       | 0            |
| 3   | G     | 12    | 0        | 12       | 0       | 0            |
| 3   | H     | 12    | 0        | 12       | 1       | 0            |
| 4   | A     | 529   | 0        | 0        | 8       | 0            |
| 4   | B     | 528   | 0        | 0        | 15      | 0            |
| 4   | C     | 593   | 0        | 0        | 11      | 0            |
| 4   | D     | 592   | 0        | 0        | 15      | 0            |
| 4   | E     | 523   | 0        | 0        | 2       | 0            |
| 4   | F     | 485   | 0        | 0        | 10      | 0            |
| 4   | G     | 622   | 0        | 0        | 14      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | H     | 575   | 0        | 0        | 5       | 0            |
| All | All   | 57830 | 0        | 52008    | 907     | 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 9.

All (907) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:H:475:ARG:HB2  | 1:H:953:MET:CE    | 1.39                     | 1.52              |
| 1:G:394:LYS:H    | 1:G:394:LYS:CD    | 1.44                     | 1.27              |
| 1:H:475:ARG:CB   | 1:H:953:MET:HE2   | 1.66                     | 1.25              |
| 1:E:277:ILE:CD1  | 1:E:291:ASP:HB3   | 1.69                     | 1.20              |
| 1:A:250:GLN:NE2  | 1:A:275:LYS:HE3   | 1.56                     | 1.18              |
| 1:B:394:LYS:CE   | 1:B:394:LYS:H     | 1.55                     | 1.18              |
| 1:A:250:GLN:HE21 | 1:A:275:LYS:HE3   | 1.08                     | 1.13              |
| 1:H:250:GLN:HE21 | 1:H:275:LYS:HE3   | 1.03                     | 1.12              |
| 1:H:475:ARG:CB   | 1:H:953:MET:CE    | 2.26                     | 1.12              |
| 1:B:304:GLU:OE1  | 1:B:307:ARG:HD3   | 1.49                     | 1.11              |
| 1:H:250:GLN:NE2  | 1:H:275:LYS:HE3   | 1.65                     | 1.11              |
| 1:C:670:MET:HE1  | 1:C:885:PHE:HZ    | 1.01                     | 1.11              |
| 1:H:669:TYR:CE2  | 1:H:670:MET:HE3   | 1.85                     | 1.10              |
| 1:F:726:ARG:H    | 1:F:726:ARG:HD3   | 1.13                     | 1.10              |
| 1:E:250:GLN:NE2  | 1:E:275:LYS:HE2   | 1.67                     | 1.09              |
| 1:C:251:VAL:HG21 | 1:C:259:PHE:CZ    | 1.87                     | 1.09              |
| 1:E:1082:LYS:HD3 | 1:E:1083:SER:H    | 1.14                     | 1.08              |
| 1:E:250:GLN:HE21 | 1:E:275:LYS:HE2   | 0.96                     | 1.07              |
| 1:F:759:HIS:O    | 1:F:791:THR:HG21  | 1.53                     | 1.07              |
| 1:C:670:MET:HE1  | 1:C:885:PHE:CZ    | 1.89                     | 1.06              |
| 1:F:726:ARG:NH1  | 1:F:726:ARG:HG2   | 1.58                     | 1.06              |
| 1:E:288:THR:HG22 | 1:E:289:GLU:H     | 1.20                     | 1.06              |
| 1:G:457:MET:HE3  | 1:G:493:TYR:HE2   | 1.23                     | 1.03              |
| 1:B:394:LYS:H    | 1:B:394:LYS:HE3   | 1.24                     | 1.02              |
| 1:F:726:ARG:HD3  | 1:F:726:ARG:N     | 1.66                     | 1.02              |
| 1:G:394:LYS:H    | 1:G:394:LYS:HD2   | 1.19                     | 1.02              |
| 1:F:800:THR:HG22 | 1:F:801:ALA:N     | 1.74                     | 1.02              |
| 1:F:726:ARG:HH11 | 1:F:726:ARG:CG    | 1.73                     | 1.01              |
| 1:F:726:ARG:HG2  | 1:F:726:ARG:HH11  | 0.84                     | 1.00              |
| 1:H:669:TYR:HE2  | 1:H:670:MET:HE3   | 1.18                     | 1.00              |
| 1:F:1063:LYS:HE2 | 1:F:1068:ASN:HD21 | 1.27                     | 1.00              |
| 1:G:394:LYS:H    | 1:G:394:LYS:HD3   | 1.24                     | 1.00              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:669:TYR:CE2  | 1:E:670:MET:HE3   | 1.97                     | 0.99              |
| 1:C:861:SER:H    | 1:C:864:GLN:HE21  | 1.08                     | 0.99              |
| 1:E:277:ILE:HD11 | 1:E:291:ASP:HB3   | 1.45                     | 0.99              |
| 1:F:1063:LYS:HE2 | 1:F:1068:ASN:ND2  | 1.76                     | 0.98              |
| 1:A:251:VAL:HG21 | 1:A:259:PHE:CZ    | 1.98                     | 0.98              |
| 1:C:669:TYR:HE2  | 1:C:670:MET:HE3   | 1.28                     | 0.98              |
| 1:H:251:VAL:HG21 | 1:H:259:PHE:CZ    | 1.99                     | 0.98              |
| 1:G:394:LYS:HD2  | 1:G:394:LYS:N     | 1.77                     | 0.97              |
| 1:F:861:SER:H    | 1:F:864:GLN:HE21  | 1.04                     | 0.97              |
| 1:D:416:LYS:HE2  | 4:D:2790:HOH:O    | 1.62                     | 0.97              |
| 1:B:800:THR:HG22 | 1:B:802:ALA:H     | 1.27                     | 0.96              |
| 1:C:1081:PRO:HG2 | 1:C:1084:LEU:HD12 | 1.48                     | 0.96              |
| 1:D:669:TYR:CE2  | 1:D:670:MET:HE3   | 2.01                     | 0.95              |
| 1:C:669:TYR:CE2  | 1:C:670:MET:HE3   | 2.01                     | 0.95              |
| 1:G:394:LYS:CD   | 1:G:394:LYS:N     | 2.22                     | 0.95              |
| 1:F:670:MET:HE3  | 1:F:877:VAL:HG12  | 1.48                     | 0.95              |
| 1:H:670:MET:HE1  | 1:H:885:PHE:HZ    | 1.30                     | 0.95              |
| 1:H:513:ILE:HD13 | 1:H:856:MET:HE1   | 1.46                     | 0.94              |
| 1:B:669:TYR:CE2  | 1:B:670:MET:CE    | 2.50                     | 0.94              |
| 1:D:1013:GLU:HG2 | 4:D:3867:HOH:O    | 1.65                     | 0.94              |
| 1:H:504:ASP:OD1  | 1:H:846:HIS:HD2   | 1.51                     | 0.94              |
| 1:A:861:SER:H    | 1:A:864:GLN:HE21  | 1.15                     | 0.94              |
| 1:C:351:LYS:HE3  | 4:C:3968:HOH:O    | 1.67                     | 0.94              |
| 1:B:669:TYR:CE2  | 1:B:670:MET:HE2   | 2.02                     | 0.93              |
| 1:B:466:ASP:OD2  | 1:B:943:LYS:HE2   | 1.68                     | 0.93              |
| 1:D:639:ASN:HD21 | 1:D:813:SER:H     | 1.14                     | 0.93              |
| 1:D:669:TYR:CE2  | 1:D:670:MET:CE    | 2.52                     | 0.93              |
| 1:E:250:GLN:HE21 | 1:E:275:LYS:CE    | 1.81                     | 0.93              |
| 1:F:251:VAL:HG21 | 1:F:259:PHE:HZ    | 1.33                     | 0.93              |
| 1:B:639:ASN:HD21 | 1:B:813:SER:H     | 1.15                     | 0.93              |
| 1:H:861:SER:H    | 1:H:864:GLN:HE21  | 1.09                     | 0.92              |
| 1:D:492:ASP:HB3  | 1:D:1022:LEU:HD22 | 1.51                     | 0.92              |
| 1:E:288:THR:HG22 | 1:E:289:GLU:N     | 1.83                     | 0.92              |
| 1:F:251:VAL:HG21 | 1:F:259:PHE:CZ    | 2.05                     | 0.91              |
| 1:E:861:SER:H    | 1:E:864:GLN:HE21  | 1.13                     | 0.91              |
| 1:C:670:MET:CE   | 1:C:885:PHE:HZ    | 1.83                     | 0.90              |
| 1:D:861:SER:H    | 1:D:864:GLN:HE21  | 1.18                     | 0.90              |
| 1:A:250:GLN:HE21 | 1:A:275:LYS:CE    | 1.83                     | 0.90              |
| 1:E:440:ASN:HD21 | 1:E:449:GLN:HE21  | 1.19                     | 0.90              |
| 1:H:250:GLN:HE21 | 1:H:275:LYS:CE    | 1.85                     | 0.90              |
| 1:G:457:MET:HE3  | 1:G:493:TYR:CE2   | 2.06                     | 0.90              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:669:TYR:HE2   | 1:D:670:MET:CE    | 1.85                     | 0.90              |
| 1:G:861:SER:H     | 1:G:864:GLN:HE21  | 1.19                     | 0.89              |
| 1:B:394:LYS:CE    | 1:B:394:LYS:N     | 2.35                     | 0.89              |
| 1:B:669:TYR:HE2   | 1:B:670:MET:CE    | 1.84                     | 0.89              |
| 1:G:492:ASP:HB3   | 1:G:1022:LEU:HD22 | 1.52                     | 0.89              |
| 1:H:1074:VAL:HG23 | 1:H:1077:ASN:HB3  | 1.54                     | 0.89              |
| 1:E:669:TYR:CE2   | 1:E:670:MET:CE    | 2.55                     | 0.89              |
| 1:E:670:MET:HE1   | 1:E:885:PHE:HZ    | 1.36                     | 0.89              |
| 1:E:1082:LYS:HD3  | 1:E:1083:SER:N    | 1.86                     | 0.89              |
| 1:C:261:HIS:HD2   | 1:C:264:HIS:H     | 1.20                     | 0.88              |
| 1:F:800:THR:CG2   | 1:F:801:ALA:N     | 2.37                     | 0.88              |
| 1:D:563:ASN:HB3   | 4:D:1180:HOH:O    | 1.74                     | 0.87              |
| 1:H:513:ILE:HG12  | 1:H:953:MET:CE    | 2.04                     | 0.87              |
| 1:B:1074:VAL:CG1  | 1:B:1077:ASN:HB3  | 2.05                     | 0.87              |
| 1:C:311:ASN:HD21  | 1:C:323:TYR:H     | 1.23                     | 0.87              |
| 1:H:513:ILE:CG1   | 1:H:953:MET:HE1   | 2.04                     | 0.87              |
| 1:H:513:ILE:CD1   | 1:H:953:MET:HE1   | 2.05                     | 0.87              |
| 1:C:251:VAL:HG21  | 1:C:259:PHE:HZ    | 1.39                     | 0.86              |
| 1:C:440:ASN:HD21  | 1:C:449:GLN:HE21  | 1.22                     | 0.86              |
| 1:E:1082:LYS:CD   | 1:E:1083:SER:H    | 1.87                     | 0.86              |
| 1:H:669:TYR:CE2   | 1:H:670:MET:CE    | 2.59                     | 0.86              |
| 1:H:639:ASN:HD21  | 1:H:813:SER:H     | 1.22                     | 0.86              |
| 1:D:440:ASN:HD21  | 1:D:449:GLN:HE21  | 1.20                     | 0.86              |
| 1:B:861:SER:H     | 1:B:864:GLN:HE21  | 1.16                     | 0.86              |
| 1:G:800:THR:HG22  | 1:G:802:ALA:H     | 1.40                     | 0.86              |
| 1:C:639:ASN:HD21  | 1:C:813:SER:H     | 1.23                     | 0.85              |
| 1:E:457:MET:HE2   | 1:E:493:TYR:HE2   | 1.41                     | 0.85              |
| 1:E:669:TYR:HE2   | 1:E:670:MET:HE3   | 1.41                     | 0.85              |
| 1:B:440:ASN:HD21  | 1:B:449:GLN:HE21  | 1.18                     | 0.85              |
| 1:C:321:GLN:HG3   | 4:C:3192:HOH:O    | 1.76                     | 0.85              |
| 1:H:475:ARG:HB2   | 1:H:953:MET:HE2   | 0.84                     | 0.84              |
| 1:H:513:ILE:HD11  | 1:H:953:MET:HE1   | 1.60                     | 0.84              |
| 1:A:440:ASN:HD21  | 1:A:449:GLN:HE21  | 1.20                     | 0.84              |
| 1:F:667:GLY:O     | 1:F:865:ALA:HB3   | 1.78                     | 0.84              |
| 1:E:639:ASN:HD21  | 1:E:813:SER:H     | 1.23                     | 0.84              |
| 1:G:639:ASN:HD21  | 1:G:813:SER:H     | 1.23                     | 0.84              |
| 1:A:261:HIS:HD2   | 1:A:264:HIS:H     | 1.24                     | 0.84              |
| 1:A:460:GLY:H     | 1:A:470:ASN:HD22  | 1.25                     | 0.84              |
| 1:H:669:TYR:HE2   | 1:H:670:MET:CE    | 1.91                     | 0.84              |
| 1:H:251:VAL:HG21  | 1:H:259:PHE:HZ    | 1.40                     | 0.83              |
| 1:B:1074:VAL:HG11 | 1:B:1077:ASN:HB3  | 1.61                     | 0.83              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:988:LYS:H    | 1:B:990:THR:HG23  | 1.44                     | 0.83              |
| 1:H:313:MET:HE1  | 1:H:359:THR:HG22  | 1.61                     | 0.83              |
| 1:F:247:GLN:HG3  | 4:F:4174:HOH:O    | 1.78                     | 0.82              |
| 1:E:1072:SER:OG  | 1:E:1074:VAL:HG12 | 1.80                     | 0.82              |
| 1:A:870:LYS:HD2  | 4:A:3971:HOH:O    | 1.77                     | 0.82              |
| 1:F:1063:LYS:CE  | 1:F:1068:ASN:ND2  | 2.42                     | 0.82              |
| 1:H:1074:VAL:CG2 | 1:H:1077:ASN:HB3  | 2.10                     | 0.82              |
| 1:H:475:ARG:HB2  | 1:H:953:MET:HE1   | 1.61                     | 0.81              |
| 1:F:514:LEU:HD21 | 1:F:532:MET:HG3   | 1.62                     | 0.81              |
| 1:G:311:ASN:HD21 | 1:G:323:TYR:H     | 1.27                     | 0.81              |
| 1:B:271:TRP:CZ2  | 1:B:357:ARG:HG3   | 2.16                     | 0.81              |
| 1:A:311:ASN:HD21 | 1:A:323:TYR:H     | 1.26                     | 0.81              |
| 1:G:261:HIS:HD2  | 1:G:264:HIS:H     | 1.28                     | 0.81              |
| 1:F:669:TYR:HE2  | 1:F:670:MET:HE2   | 1.44                     | 0.80              |
| 1:A:639:ASN:HD21 | 1:A:813:SER:H     | 1.29                     | 0.80              |
| 1:C:626:LYS:HE2  | 4:C:1985:HOH:O    | 1.79                     | 0.80              |
| 1:D:883:ASP:OD1  | 1:D:948:LYS:HE3   | 1.81                     | 0.80              |
| 1:F:639:ASN:HD21 | 1:F:813:SER:H     | 1.26                     | 0.80              |
| 1:E:841:ASP:OD1  | 1:E:846:HIS:HE1   | 1.65                     | 0.80              |
| 1:B:251:VAL:HG21 | 1:B:259:PHE:CZ    | 2.17                     | 0.80              |
| 1:A:261:HIS:CD2  | 1:A:264:HIS:H     | 2.00                     | 0.80              |
| 1:D:988:LYS:H    | 1:D:990:THR:CG2   | 1.94                     | 0.80              |
| 1:D:1082:LYS:HB2 | 4:D:3996:HOH:O    | 1.81                     | 0.80              |
| 1:A:504:ASP:OD1  | 1:A:846:HIS:HD2   | 1.66                     | 0.79              |
| 1:F:261:HIS:HD2  | 1:F:264:HIS:H     | 1.28                     | 0.79              |
| 1:E:277:ILE:CD1  | 1:E:291:ASP:CB    | 2.57                     | 0.79              |
| 1:B:563:ASN:HB3  | 4:B:3514:HOH:O    | 1.81                     | 0.79              |
| 1:H:670:MET:HE1  | 1:H:885:PHE:CZ    | 2.18                     | 0.79              |
| 1:D:988:LYS:N    | 1:D:990:THR:HG23  | 1.98                     | 0.79              |
| 1:D:800:THR:HG22 | 1:D:802:ALA:H     | 1.45                     | 0.79              |
| 1:H:670:MET:CE   | 1:H:885:PHE:HZ    | 1.95                     | 0.78              |
| 1:H:563:ASN:HB3  | 4:H:1162:HOH:O    | 1.83                     | 0.78              |
| 1:E:457:MET:HE2  | 1:E:493:TYR:CE2   | 2.18                     | 0.78              |
| 1:H:430:TYR:CD1  | 1:H:977:LYS:HG2   | 2.18                     | 0.78              |
| 1:C:261:HIS:CD2  | 1:C:264:HIS:H     | 2.02                     | 0.78              |
| 1:D:311:ASN:HD21 | 1:D:323:TYR:H     | 1.31                     | 0.78              |
| 1:F:667:GLY:O    | 1:F:865:ALA:CB    | 2.32                     | 0.78              |
| 1:H:475:ARG:CA   | 1:H:953:MET:HE3   | 2.13                     | 0.78              |
| 1:C:460:GLY:H    | 1:C:470:ASN:HD22  | 1.32                     | 0.77              |
| 1:C:504:ASP:OD1  | 1:C:846:HIS:HD2   | 1.66                     | 0.77              |
| 1:F:407:ASN:ND2  | 1:F:431:GLU:H     | 1.81                     | 0.77              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:261:HIS:CD2  | 1:G:264:HIS:H     | 2.02                     | 0.77              |
| 1:F:492:ASP:HB3  | 1:F:1022:LEU:HD22 | 1.66                     | 0.77              |
| 1:F:841:ASP:OD1  | 1:F:846:HIS:HE1   | 1.68                     | 0.77              |
| 1:D:669:TYR:HE2  | 1:D:670:MET:HE3   | 1.43                     | 0.77              |
| 1:C:371:ASN:HB3  | 1:C:373:ASP:H     | 1.49                     | 0.77              |
| 1:B:304:GLU:OE1  | 1:B:307:ARG:CD    | 2.30                     | 0.76              |
| 1:E:669:TYR:HE2  | 1:E:670:MET:CE    | 1.95                     | 0.76              |
| 1:B:713:TYR:O    | 1:B:759:HIS:HE1   | 1.69                     | 0.76              |
| 1:F:261:HIS:CD2  | 1:F:264:HIS:H     | 2.03                     | 0.76              |
| 1:B:513:ILE:HG21 | 1:B:856:MET:HE1   | 1.67                     | 0.76              |
| 1:D:342:LYS:CE   | 4:D:2496:HOH:O    | 2.34                     | 0.76              |
| 1:F:435:ALA:HA   | 1:F:1052:ASN:ND2  | 1.99                     | 0.76              |
| 1:B:504:ASP:OD1  | 1:B:846:HIS:HD2   | 1.69                     | 0.76              |
| 1:G:985:SER:HB2  | 4:G:3639:HOH:O    | 1.86                     | 0.76              |
| 1:G:440:ASN:HD21 | 1:G:449:GLN:HE21  | 1.33                     | 0.75              |
| 1:E:311:ASN:HD21 | 1:E:323:TYR:H     | 1.32                     | 0.75              |
| 1:F:440:ASN:HD21 | 1:F:449:GLN:HE21  | 1.33                     | 0.75              |
| 1:A:251:VAL:HG21 | 1:A:259:PHE:HZ    | 1.50                     | 0.75              |
| 1:G:1063:LYS:HE2 | 1:G:1068:ASN:ND2  | 2.02                     | 0.75              |
| 1:B:669:TYR:CE2  | 1:B:670:MET:HE3   | 2.20                     | 0.75              |
| 1:C:1076:ASP:OD2 | 1:C:1077:ASN:HB2  | 1.87                     | 0.75              |
| 1:F:669:TYR:CE2  | 1:F:670:MET:HE2   | 2.21                     | 0.75              |
| 1:B:1076:ASP:O   | 1:B:1077:ASN:HB2  | 1.87                     | 0.75              |
| 1:D:639:ASN:ND2  | 1:D:813:SER:H     | 1.83                     | 0.74              |
| 1:B:1072:SER:OG  | 1:B:1074:VAL:HG12 | 1.87                     | 0.74              |
| 1:F:726:ARG:H    | 1:F:726:ARG:CD    | 1.97                     | 0.74              |
| 1:H:883:ASP:OD1  | 1:H:948:LYS:HE3   | 1.87                     | 0.74              |
| 1:G:251:VAL:HG21 | 1:G:259:PHE:HZ    | 1.51                     | 0.74              |
| 1:D:461:ASN:H    | 1:D:470:ASN:HD21  | 1.31                     | 0.74              |
| 1:F:861:SER:H    | 1:F:864:GLN:NE2   | 1.83                     | 0.74              |
| 1:C:713:TYR:O    | 1:C:759:HIS:HE1   | 1.71                     | 0.74              |
| 1:F:311:ASN:HD21 | 1:F:323:TYR:H     | 1.35                     | 0.73              |
| 1:F:557:MET:HE2  | 1:F:708:ILE:HD12  | 1.69                     | 0.73              |
| 1:F:563:ASN:HB3  | 4:F:3413:HOH:O    | 1.88                     | 0.73              |
| 1:B:669:TYR:HE2  | 1:B:670:MET:HE2   | 1.46                     | 0.73              |
| 1:G:504:ASP:OD1  | 1:G:846:HIS:HD2   | 1.71                     | 0.73              |
| 1:E:288:THR:CG2  | 1:E:289:GLU:H     | 2.01                     | 0.73              |
| 1:D:669:TYR:CE2  | 1:D:670:MET:HE2   | 2.22                     | 0.73              |
| 1:E:504:ASP:OD1  | 1:E:846:HIS:HD2   | 1.72                     | 0.73              |
| 1:H:513:ILE:HG12 | 1:H:953:MET:HE1   | 1.66                     | 0.73              |
| 1:B:435:ALA:HA   | 1:B:1052:ASN:ND2  | 2.04                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:639:ASN:ND2  | 1:B:813:SER:H    | 1.86                     | 0.73              |
| 1:F:726:ARG:N    | 1:F:726:ARG:CD   | 2.50                     | 0.73              |
| 1:D:504:ASP:OD1  | 1:D:846:HIS:HD2  | 1.71                     | 0.73              |
| 1:H:475:ARG:CA   | 1:H:953:MET:CE   | 2.67                     | 0.72              |
| 1:H:460:GLY:H    | 1:H:470:ASN:HD22 | 1.38                     | 0.72              |
| 1:C:321:GLN:CG   | 4:C:3192:HOH:O   | 2.36                     | 0.72              |
| 1:G:639:ASN:ND2  | 1:G:813:SER:H    | 1.87                     | 0.72              |
| 1:E:460:GLY:H    | 1:E:470:ASN:HD22 | 1.38                     | 0.72              |
| 1:B:988:LYS:H    | 1:B:990:THR:CG2  | 2.03                     | 0.72              |
| 1:F:708:ILE:HD11 | 1:F:737:GLU:HB2  | 1.71                     | 0.72              |
| 1:G:988:LYS:H    | 1:G:990:THR:HG23 | 1.55                     | 0.72              |
| 1:H:440:ASN:HD21 | 1:H:449:GLN:HE21 | 1.38                     | 0.72              |
| 1:E:988:LYS:H    | 1:E:990:THR:CG2  | 2.03                     | 0.71              |
| 1:E:261:HIS:CD2  | 1:E:264:HIS:H    | 2.08                     | 0.71              |
| 1:G:800:THR:CG2  | 1:G:802:ALA:H    | 2.04                     | 0.71              |
| 1:H:342:LYS:HE2  | 4:H:2642:HOH:O   | 1.88                     | 0.71              |
| 1:H:461:ASN:H    | 1:H:470:ASN:HD21 | 1.38                     | 0.71              |
| 1:G:883:ASP:OD1  | 1:G:948:LYS:HE3  | 1.90                     | 0.71              |
| 1:E:639:ASN:ND2  | 1:E:813:SER:H    | 1.89                     | 0.71              |
| 1:C:988:LYS:H    | 1:C:990:THR:CG2  | 2.02                     | 0.71              |
| 1:D:342:LYS:HE2  | 4:D:2496:HOH:O   | 1.90                     | 0.71              |
| 1:B:394:LYS:H    | 1:B:394:LYS:HE2  | 1.53                     | 0.70              |
| 1:B:800:THR:HG22 | 1:B:801:ALA:N    | 2.04                     | 0.70              |
| 1:D:670:MET:HE1  | 1:D:885:PHE:HZ   | 1.55                     | 0.70              |
| 1:E:247:GLN:H    | 1:E:247:GLN:HE21 | 1.37                     | 0.70              |
| 1:B:286:GLN:HB3  | 4:B:2568:HOH:O   | 1.91                     | 0.70              |
| 1:B:705:SER:HA   | 4:B:3521:HOH:O   | 1.91                     | 0.70              |
| 1:B:393:SER:HA   | 1:B:394:LYS:HE2  | 1.72                     | 0.70              |
| 1:C:988:LYS:H    | 1:C:990:THR:HG23 | 1.56                     | 0.69              |
| 1:E:261:HIS:HD2  | 1:E:264:HIS:H    | 1.41                     | 0.69              |
| 1:B:800:THR:HG22 | 1:B:802:ALA:N    | 2.05                     | 0.69              |
| 1:E:250:GLN:HG3  | 1:E:275:LYS:HG3  | 1.74                     | 0.69              |
| 1:E:670:MET:HE1  | 1:E:885:PHE:CZ   | 2.25                     | 0.69              |
| 1:D:514:LEU:HD21 | 1:D:532:MET:HG3  | 1.75                     | 0.69              |
| 1:F:861:SER:N    | 1:F:864:GLN:HE21 | 1.85                     | 0.69              |
| 1:H:639:ASN:ND2  | 1:H:813:SER:H    | 1.90                     | 0.69              |
| 1:C:861:SER:H    | 1:C:864:GLN:NE2  | 1.86                     | 0.68              |
| 1:B:394:LYS:N    | 1:B:394:LYS:CD   | 2.56                     | 0.68              |
| 1:G:841:ASP:OD1  | 1:G:846:HIS:HE1  | 1.76                     | 0.68              |
| 1:A:585:ARG:CD   | 1:A:661:ASP:OD1  | 2.41                     | 0.68              |
| 1:C:461:ASN:H    | 1:C:470:ASN:HD21 | 1.41                     | 0.68              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:585:ARG:HD3  | 1:D:661:ASP:OD1   | 1.94                     | 0.68              |
| 1:G:703:GLY:HA2  | 1:G:746:LYS:HD2   | 1.75                     | 0.68              |
| 1:D:726:ARG:H    | 1:D:726:ARG:NE    | 1.92                     | 0.68              |
| 1:F:514:LEU:CD2  | 1:F:532:MET:HG3   | 2.23                     | 0.67              |
| 1:F:740:ASN:C    | 1:F:740:ASN:HD22  | 2.01                     | 0.67              |
| 1:E:988:LYS:N    | 1:E:990:THR:HG23  | 2.10                     | 0.67              |
| 1:E:461:ASN:H    | 1:E:470:ASN:HD21  | 1.42                     | 0.67              |
| 1:B:988:LYS:N    | 1:B:990:THR:HG23  | 2.08                     | 0.67              |
| 1:F:787:LEU:HD12 | 1:F:787:LEU:N     | 2.10                     | 0.67              |
| 1:F:708:ILE:CD1  | 1:F:737:GLU:HB2   | 2.25                     | 0.67              |
| 1:B:311:ASN:HD21 | 1:B:323:TYR:H     | 1.43                     | 0.66              |
| 1:C:250:GLN:NE2  | 1:C:275:LYS:NZ    | 2.43                     | 0.66              |
| 1:F:709:THR:HG22 | 1:F:736:ILE:HD12  | 1.75                     | 0.66              |
| 1:D:422:THR:HG23 | 4:G:1164:HOH:O    | 1.96                     | 0.66              |
| 1:C:988:LYS:N    | 1:C:990:THR:HG23  | 2.11                     | 0.66              |
| 1:D:304:GLU:OE2  | 1:D:307:ARG:NH1   | 2.28                     | 0.66              |
| 1:E:1076:ASP:O   | 1:E:1077:ASN:HB2  | 1.95                     | 0.66              |
| 1:F:800:THR:CG2  | 1:F:801:ALA:H     | 2.08                     | 0.66              |
| 1:A:639:ASN:ND2  | 1:A:813:SER:H     | 1.94                     | 0.66              |
| 1:C:457:MET:HE2  | 1:C:493:TYR:HE2   | 1.61                     | 0.66              |
| 1:E:302:ASP:HB3  | 1:E:1065:GLN:HE21 | 1.59                     | 0.66              |
| 1:H:743:LEU:O    | 1:H:744:ARG:HD3   | 1.95                     | 0.66              |
| 1:F:800:THR:HG22 | 1:F:802:ALA:H     | 1.59                     | 0.66              |
| 1:D:760:LYS:HE2  | 4:D:2980:HOH:O    | 1.95                     | 0.66              |
| 1:H:513:ILE:HG12 | 1:H:953:MET:HE3   | 1.77                     | 0.66              |
| 1:A:585:ARG:HD3  | 1:A:661:ASP:OD1   | 1.95                     | 0.65              |
| 1:H:261:HIS:CD2  | 1:H:264:HIS:H     | 2.15                     | 0.65              |
| 1:C:1063:LYS:HE2 | 1:C:1068:ASN:HD21 | 1.59                     | 0.65              |
| 1:E:346:LYS:HE2  | 1:E:355:TRP:CE3   | 2.32                     | 0.65              |
| 1:G:371:ASN:HB3  | 1:G:373:ASP:H     | 1.61                     | 0.65              |
| 1:A:346:LYS:HE2  | 1:A:355:TRP:CD2   | 2.31                     | 0.65              |
| 1:A:861:SER:H    | 1:A:864:GLN:NE2   | 1.91                     | 0.65              |
| 1:B:513:ILE:CG2  | 1:B:856:MET:HE1   | 2.26                     | 0.65              |
| 1:D:261:HIS:HD2  | 1:D:264:HIS:H     | 1.44                     | 0.65              |
| 1:G:988:LYS:H    | 1:G:990:THR:CG2   | 2.10                     | 0.65              |
| 1:B:366:THR:HG21 | 4:B:3624:HOH:O    | 1.96                     | 0.65              |
| 1:B:492:ASP:HB3  | 1:B:1022:LEU:HD22 | 1.79                     | 0.65              |
| 1:E:988:LYS:H    | 1:E:990:THR:HG23  | 1.60                     | 0.65              |
| 1:H:988:LYS:H    | 1:H:990:THR:HG23  | 1.61                     | 0.65              |
| 1:A:1081:PRO:HG2 | 1:A:1084:LEU:HD12 | 1.79                     | 0.65              |
| 1:D:457:MET:HE2  | 1:D:493:TYR:HE2   | 1.62                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:1052:ASN:H    | 1:E:1052:ASN:HD22 | 1.43                     | 0.65              |
| 1:D:1052:ASN:HD22 | 1:D:1052:ASN:H    | 1.44                     | 0.65              |
| 1:D:854:ARG:HD3   | 1:D:892:ASP:OD2   | 1.96                     | 0.65              |
| 1:C:1063:LYS:CE   | 1:C:1068:ASN:ND2  | 2.60                     | 0.64              |
| 4:D:1230:HOH:O    | 1:G:422:THR:HG23  | 1.97                     | 0.64              |
| 1:G:713:TYR:O     | 1:G:759:HIS:HE1   | 1.80                     | 0.64              |
| 1:F:457:MET:HE2   | 1:F:493:TYR:HE2   | 1.61                     | 0.64              |
| 1:H:585:ARG:HD3   | 1:H:661:ASP:OD1   | 1.97                     | 0.64              |
| 1:C:585:ARG:HD3   | 1:C:661:ASP:OD1   | 1.96                     | 0.64              |
| 1:C:841:ASP:OD1   | 1:C:846:HIS:HE1   | 1.80                     | 0.64              |
| 1:C:883:ASP:OD1   | 1:C:948:LYS:HE3   | 1.98                     | 0.64              |
| 1:E:670:MET:CE    | 1:E:885:PHE:HZ    | 2.11                     | 0.64              |
| 1:F:407:ASN:HD22  | 1:F:431:GLU:H     | 1.46                     | 0.64              |
| 1:B:514:LEU:HD21  | 1:B:532:MET:HG3   | 1.79                     | 0.64              |
| 1:B:726:ARG:NH2   | 4:B:3637:HOH:O    | 2.31                     | 0.64              |
| 1:D:713:TYR:O     | 1:D:759:HIS:HE1   | 1.80                     | 0.64              |
| 1:E:280:ASP:OD2   | 1:E:282:LYS:NZ    | 2.31                     | 0.64              |
| 1:G:251:VAL:HG21  | 1:G:259:PHE:CZ    | 2.31                     | 0.64              |
| 1:F:761:ASN:N     | 1:F:791:THR:HG22  | 2.13                     | 0.64              |
| 1:E:251:VAL:HG13  | 1:E:253:SER:O     | 1.98                     | 0.63              |
| 1:E:669:TYR:CE2   | 1:E:670:MET:HE2   | 2.33                     | 0.63              |
| 1:H:245:PHE:CD1   | 1:H:284:TRP:HZ2   | 2.15                     | 0.63              |
| 1:B:1074:VAL:HG13 | 1:B:1077:ASN:HB3  | 1.79                     | 0.63              |
| 1:H:261:HIS:HD2   | 1:H:264:HIS:H     | 1.44                     | 0.63              |
| 1:B:585:ARG:HD3   | 1:B:661:ASP:OD1   | 1.99                     | 0.63              |
| 1:D:371:ASN:HB3   | 1:D:373:ASP:H     | 1.63                     | 0.63              |
| 1:E:883:ASP:OD1   | 1:E:948:LYS:HE3   | 1.99                     | 0.63              |
| 1:H:371:ASN:HB3   | 1:H:373:ASP:H     | 1.63                     | 0.63              |
| 1:C:1063:LYS:HE3  | 1:C:1068:ASN:ND2  | 2.13                     | 0.63              |
| 1:B:461:ASN:H     | 1:B:470:ASN:HD21  | 1.47                     | 0.63              |
| 1:E:435:ALA:HA    | 1:E:1052:ASN:ND2  | 2.14                     | 0.63              |
| 1:D:966:GLU:HB2   | 1:D:997:LYS:HB2   | 1.81                     | 0.62              |
| 1:C:251:VAL:CG2   | 1:C:259:PHE:CZ    | 2.76                     | 0.62              |
| 1:E:277:ILE:HD13  | 1:E:291:ASP:HB3   | 1.76                     | 0.62              |
| 1:G:460:GLY:H     | 1:G:470:ASN:HD22  | 1.48                     | 0.62              |
| 1:G:574:GLU:HG2   | 4:G:2941:HOH:O    | 1.99                     | 0.62              |
| 1:H:513:ILE:CG1   | 1:H:953:MET:CE    | 2.72                     | 0.62              |
| 1:C:280:ASP:OD2   | 1:C:282:LYS:HE3   | 2.00                     | 0.62              |
| 1:F:311:ASN:ND2   | 1:F:323:TYR:H     | 1.98                     | 0.62              |
| 1:A:440:ASN:HD21  | 1:A:449:GLN:NE2   | 1.95                     | 0.62              |
| 1:A:1052:ASN:HD22 | 1:A:1052:ASN:H    | 1.48                     | 0.62              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:277:ILE:HD12 | 1:E:291:ASP:HB3   | 1.72                     | 0.62              |
| 1:D:261:HIS:CD2  | 1:D:264:HIS:H     | 2.17                     | 0.62              |
| 1:E:861:SER:H    | 1:E:864:GLN:NE2   | 1.93                     | 0.62              |
| 1:D:435:ALA:HA   | 1:D:1052:ASN:ND2  | 2.15                     | 0.62              |
| 1:E:585:ARG:HD3  | 1:E:661:ASP:OD1   | 1.99                     | 0.62              |
| 1:D:1076:ASP:O   | 1:D:1077:ASN:HB2  | 1.99                     | 0.61              |
| 1:C:514:LEU:HD21 | 1:C:532:MET:HG3   | 1.82                     | 0.61              |
| 1:D:670:MET:CE   | 1:D:885:PHE:HZ    | 2.13                     | 0.61              |
| 1:E:313:MET:HB2  | 1:E:339:ILE:HD13  | 1.80                     | 0.61              |
| 1:H:337:GLN:O    | 1:H:341:THR:HG23  | 2.00                     | 0.61              |
| 1:D:600:LYS:HE3  | 4:D:3768:HOH:O    | 2.01                     | 0.61              |
| 1:H:740:ASN:ND2  | 1:H:742:SER:H     | 1.99                     | 0.61              |
| 1:C:321:GLN:CD   | 4:C:3192:HOH:O    | 2.43                     | 0.61              |
| 1:F:557:MET:HE2  | 1:F:708:ILE:CD1   | 2.30                     | 0.61              |
| 1:A:461:ASN:H    | 1:A:470:ASN:HD21  | 1.47                     | 0.61              |
| 1:B:800:THR:CG2  | 1:B:801:ALA:N     | 2.63                     | 0.61              |
| 1:F:658:TYR:CE2  | 1:F:660:GLY:HA3   | 2.36                     | 0.61              |
| 1:E:492:ASP:OD2  | 1:E:1025:ARG:HD2  | 1.99                     | 0.61              |
| 1:F:1081:PRO:HG2 | 1:F:1084:LEU:HD12 | 1.82                     | 0.61              |
| 1:G:492:ASP:OD2  | 1:G:1025:ARG:HD2  | 2.00                     | 0.61              |
| 1:H:475:ARG:HA   | 1:H:953:MET:HE3   | 1.81                     | 0.61              |
| 1:B:407:ASN:ND2  | 1:B:431:GLU:H     | 1.98                     | 0.61              |
| 1:G:988:LYS:N    | 1:G:990:THR:HG23  | 2.15                     | 0.61              |
| 1:F:252:TYR:HB3  | 1:F:258:ASN:HD21  | 1.65                     | 0.61              |
| 1:G:435:ALA:HA   | 1:G:1052:ASN:ND2  | 2.16                     | 0.60              |
| 1:B:363:PHE:O    | 1:B:366:THR:HG22  | 2.01                     | 0.60              |
| 1:B:513:ILE:HD13 | 1:B:856:MET:CE    | 2.31                     | 0.60              |
| 1:G:457:MET:CE   | 1:G:493:TYR:CE2   | 2.83                     | 0.60              |
| 1:B:251:VAL:HG21 | 1:B:259:PHE:HZ    | 1.67                     | 0.60              |
| 1:E:247:GLN:HE21 | 1:E:247:GLN:N     | 2.00                     | 0.60              |
| 1:C:311:ASN:ND2  | 1:C:323:TYR:H     | 1.97                     | 0.60              |
| 1:E:585:ARG:CD   | 1:E:661:ASP:OD1   | 2.49                     | 0.60              |
| 1:F:740:ASN:ND2  | 1:F:742:SER:H     | 1.99                     | 0.60              |
| 1:H:1052:ASN:H   | 1:H:1052:ASN:HD22 | 1.50                     | 0.60              |
| 1:D:585:ARG:CD   | 1:D:661:ASP:OD1   | 2.48                     | 0.60              |
| 1:G:251:VAL:CG2  | 1:G:259:PHE:CZ    | 2.84                     | 0.60              |
| 1:D:457:MET:HE2  | 1:D:493:TYR:CE2   | 2.37                     | 0.60              |
| 1:D:460:GLY:H    | 1:D:470:ASN:HD22  | 1.50                     | 0.60              |
| 1:F:251:VAL:CG2  | 1:F:259:PHE:CZ    | 2.82                     | 0.60              |
| 1:B:729:ARG:NH2  | 1:B:762:GLN:HB2   | 2.17                     | 0.59              |
| 1:E:371:ASN:HB3  | 1:E:373:ASP:H     | 1.66                     | 0.59              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:E:1074:VAL:HG13 | 1:E:1077:ASN:HB3 | 1.84                     | 0.59              |
| 1:H:740:ASN:C     | 1:H:740:ASN:HD22 | 2.09                     | 0.59              |
| 1:C:440:ASN:HD21  | 1:C:449:GLN:NE2  | 1.96                     | 0.59              |
| 1:G:407:ASN:ND2   | 1:G:431:GLU:H    | 2.00                     | 0.59              |
| 1:G:461:ASN:H     | 1:G:470:ASN:HD21 | 1.51                     | 0.59              |
| 1:B:514:LEU:CD2   | 1:B:532:MET:HG3  | 2.32                     | 0.59              |
| 1:F:460:GLY:H     | 1:F:470:ASN:HD22 | 1.48                     | 0.59              |
| 1:B:313:MET:HB2   | 1:B:339:ILE:HD13 | 1.84                     | 0.59              |
| 1:C:585:ARG:CD    | 1:C:661:ASP:OD1  | 2.50                     | 0.59              |
| 1:A:868:THR:HG22  | 1:A:868:THR:O    | 2.02                     | 0.59              |
| 1:A:1076:ASP:OD2  | 1:A:1077:ASN:HB2 | 2.02                     | 0.59              |
| 1:G:250:GLN:OE1   | 1:G:275:LYS:HE3  | 2.03                     | 0.59              |
| 1:C:311:ASN:HD21  | 1:C:323:TYR:N    | 1.97                     | 0.59              |
| 1:D:351:LYS:HE2   | 4:D:2565:HOH:O   | 2.03                     | 0.59              |
| 1:G:800:THR:HG22  | 1:G:802:ALA:N    | 2.13                     | 0.59              |
| 1:G:883:ASP:OD1   | 1:G:948:LYS:CE   | 2.51                     | 0.59              |
| 1:A:841:ASP:OD1   | 1:A:846:HIS:HE1  | 1.86                     | 0.59              |
| 1:D:407:ASN:ND2   | 1:D:431:GLU:H    | 2.01                     | 0.59              |
| 1:D:514:LEU:CD2   | 1:D:532:MET:HG3  | 2.33                     | 0.59              |
| 1:E:440:ASN:HD21  | 1:E:449:GLN:NE2  | 1.96                     | 0.59              |
| 1:C:346:LYS:HE2   | 1:C:355:TRP:CE3  | 2.38                     | 0.58              |
| 1:C:457:MET:HE2   | 1:C:493:TYR:CE2  | 2.38                     | 0.58              |
| 1:B:883:ASP:OD1   | 1:B:948:LYS:CE   | 2.51                     | 0.58              |
| 1:C:670:MET:CE    | 1:C:885:PHE:CZ   | 2.70                     | 0.58              |
| 1:F:713:TYR:O     | 1:F:759:HIS:HE1  | 1.87                     | 0.58              |
| 1:H:988:LYS:N     | 1:H:990:THR:HG23 | 2.19                     | 0.58              |
| 1:H:713:TYR:O     | 1:H:759:HIS:HE1  | 1.86                     | 0.58              |
| 1:B:394:LYS:HE3   | 1:B:394:LYS:N    | 2.07                     | 0.58              |
| 1:G:311:ASN:ND2   | 1:G:323:TYR:H    | 2.00                     | 0.58              |
| 1:A:253:SER:HB2   | 4:A:4186:HOH:O   | 2.02                     | 0.58              |
| 1:B:793:ASP:OD1   | 1:B:793:ASP:N    | 2.36                     | 0.58              |
| 1:G:884:LYS:HG3   | 4:G:3691:HOH:O   | 2.03                     | 0.58              |
| 1:H:800:THR:HG22  | 1:H:802:ALA:H    | 1.69                     | 0.58              |
| 1:C:492:ASP:OD2   | 1:C:1025:ARG:HD2 | 2.04                     | 0.58              |
| 1:F:321:GLN:HG2   | 1:F:323:TYR:CZ   | 2.39                     | 0.57              |
| 1:A:440:ASN:ND2   | 1:A:449:GLN:HE21 | 1.97                     | 0.57              |
| 1:G:430:TYR:CD1   | 1:G:977:LYS:HG2  | 2.39                     | 0.57              |
| 1:B:669:TYR:CD2   | 1:B:670:MET:HE3  | 2.38                     | 0.57              |
| 1:F:333:ASN:O     | 1:F:337:GLN:HG3  | 2.05                     | 0.57              |
| 1:F:726:ARG:NH1   | 1:F:726:ARG:CG   | 2.43                     | 0.57              |
| 1:H:658:TYR:CE2   | 1:H:660:GLY:HA3  | 2.40                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:H:5001:MES:H51 | 4:H:2109:HOH:O   | 2.04                     | 0.57              |
| 1:E:311:ASN:HD21 | 1:E:323:TYR:N    | 2.02                     | 0.57              |
| 1:H:800:THR:HG23 | 1:H:801:ALA:N    | 2.19                     | 0.57              |
| 1:H:861:SER:H    | 1:H:864:GLN:NE2  | 1.90                     | 0.57              |
| 1:D:440:ASN:ND2  | 1:D:449:GLN:HE21 | 1.96                     | 0.57              |
| 1:G:585:ARG:HD3  | 1:G:661:ASP:OD1  | 2.05                     | 0.57              |
| 1:E:600:LYS:HE2  | 1:E:605:PRO:O    | 2.05                     | 0.57              |
| 1:H:457:MET:HE2  | 1:H:493:TYR:HE2  | 1.69                     | 0.57              |
| 1:H:251:VAL:CG2  | 1:H:259:PHE:CZ   | 2.84                     | 0.57              |
| 1:B:563:ASN:CB   | 4:B:3514:HOH:O   | 2.48                     | 0.56              |
| 1:H:585:ARG:CD   | 1:H:661:ASP:OD1  | 2.53                     | 0.56              |
| 1:C:368:SER:HA   | 1:C:371:ASN:HB2  | 1.88                     | 0.56              |
| 1:B:261:HIS:HD2  | 1:B:264:HIS:H    | 1.54                     | 0.56              |
| 1:B:325:THR:HG21 | 4:B:2752:HOH:O   | 2.05                     | 0.56              |
| 1:B:840:THR:HG21 | 1:C:723:THR:OG1  | 2.06                     | 0.56              |
| 1:D:311:ASN:ND2  | 1:D:323:TYR:H    | 2.01                     | 0.56              |
| 1:F:966:GLU:HB2  | 1:F:997:LYS:HB2  | 1.88                     | 0.56              |
| 1:F:670:MET:HE3  | 1:F:877:VAL:CG1  | 2.30                     | 0.56              |
| 1:H:504:ASP:OD1  | 1:H:846:HIS:CD2  | 2.43                     | 0.56              |
| 1:E:316:GLN:HG2  | 1:E:359:THR:HG23 | 1.88                     | 0.55              |
| 1:F:321:GLN:HG3  | 1:F:322:THR:N    | 2.21                     | 0.55              |
| 1:F:639:ASN:ND2  | 1:F:813:SER:H    | 2.00                     | 0.55              |
| 1:H:286:GLN:HG3  | 4:H:1200:HOH:O   | 2.06                     | 0.55              |
| 1:E:368:SER:HA   | 1:E:371:ASN:HB2  | 1.88                     | 0.55              |
| 1:D:800:THR:CG2  | 1:D:801:ALA:N    | 2.69                     | 0.55              |
| 1:F:461:ASN:H    | 1:F:470:ASN:HD21 | 1.53                     | 0.55              |
| 1:H:988:LYS:H    | 1:H:990:THR:CG2  | 2.18                     | 0.55              |
| 1:A:988:LYS:H    | 1:A:990:THR:HG23 | 1.71                     | 0.55              |
| 1:F:540:ARG:HD2  | 4:F:1142:HOH:O   | 2.06                     | 0.55              |
| 1:F:585:ARG:HD3  | 1:F:661:ASP:OD1  | 2.06                     | 0.55              |
| 1:C:726:ARG:NH2  | 4:C:1110:HOH:O   | 2.38                     | 0.55              |
| 1:D:820:VAL:HB   | 1:D:821:PRO:HD2  | 1.89                     | 0.55              |
| 1:E:759:HIS:HD2  | 1:E:762:GLN:OE1  | 1.90                     | 0.55              |
| 1:F:740:ASN:HD22 | 1:F:741:PRO:N    | 2.03                     | 0.55              |
| 1:A:460:GLY:N    | 1:A:470:ASN:HD22 | 1.99                     | 0.55              |
| 1:E:713:TYR:O    | 1:E:759:HIS:HE1  | 1.89                     | 0.55              |
| 1:A:311:ASN:HD21 | 1:A:323:TYR:N    | 2.01                     | 0.55              |
| 1:F:407:ASN:HD22 | 1:F:431:GLU:N    | 2.03                     | 0.55              |
| 1:G:740:ASN:ND2  | 1:G:742:SER:H    | 2.05                     | 0.55              |
| 1:D:669:TYR:CD2  | 1:D:670:MET:HE3  | 2.42                     | 0.55              |
| 1:F:618:LYS:HE3  | 4:F:149:HOH:O    | 2.07                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:H:311:ASN:HD21 | 1:H:323:TYR:H     | 1.52                     | 0.55              |
| 1:D:440:ASN:HD21 | 1:D:449:GLN:NE2   | 1.96                     | 0.54              |
| 1:A:689:LYS:HE3  | 4:A:3634:HOH:O    | 2.06                     | 0.54              |
| 1:D:311:ASN:HD21 | 1:D:323:TYR:N     | 2.02                     | 0.54              |
| 1:A:504:ASP:OD1  | 1:A:846:HIS:CD2   | 2.54                     | 0.54              |
| 1:B:1005:ALA:O   | 1:B:1041:LYS:HD2  | 2.08                     | 0.54              |
| 3:B:5001:MES:C7  | 4:B:2759:HOH:O    | 2.55                     | 0.54              |
| 1:F:457:MET:CE   | 1:F:493:TYR:HE2   | 2.19                     | 0.54              |
| 1:F:809:ASN:HB2  | 1:F:810:PRO:CD    | 2.37                     | 0.54              |
| 1:H:435:ALA:HA   | 1:H:1052:ASN:ND2  | 2.23                     | 0.54              |
| 1:B:365:LYS:HD3  | 4:B:3556:HOH:O    | 2.08                     | 0.54              |
| 1:C:966:GLU:HB2  | 1:C:997:LYS:HB2   | 1.90                     | 0.54              |
| 1:E:440:ASN:ND2  | 1:E:449:GLN:HE21  | 1.97                     | 0.54              |
| 1:D:251:VAL:HG13 | 1:D:253:SER:O     | 2.08                     | 0.54              |
| 1:E:277:ILE:HD12 | 1:E:291:ASP:CB    | 2.32                     | 0.54              |
| 1:E:430:TYR:CD1  | 1:E:977:LYS:HD3   | 2.43                     | 0.54              |
| 1:G:574:GLU:CG   | 4:G:2941:HOH:O    | 2.54                     | 0.54              |
| 1:G:563:ASN:HB3  | 4:G:1128:HOH:O    | 2.08                     | 0.54              |
| 1:A:868:THR:O    | 1:A:868:THR:CG2   | 2.56                     | 0.54              |
| 1:E:407:ASN:ND2  | 1:E:431:GLU:H     | 2.06                     | 0.53              |
| 1:E:966:GLU:HB2  | 1:E:997:LYS:HB2   | 1.89                     | 0.53              |
| 1:B:261:HIS:CD2  | 1:B:264:HIS:H     | 2.26                     | 0.53              |
| 1:D:800:THR:HG22 | 1:D:801:ALA:N     | 2.23                     | 0.53              |
| 1:E:669:TYR:CD2  | 1:E:670:MET:HE3   | 2.43                     | 0.53              |
| 1:B:525:LEU:HD11 | 1:B:532:MET:HG2   | 1.90                     | 0.53              |
| 1:C:563:ASN:HB3  | 4:C:1770:HOH:O    | 2.07                     | 0.53              |
| 1:F:782:GLN:HG3  | 1:F:783:GLU:N     | 2.24                     | 0.53              |
| 1:A:346:LYS:HE2  | 1:A:355:TRP:CE3   | 2.43                     | 0.53              |
| 1:F:894:GLU:HA   | 1:F:953:MET:HB3   | 1.90                     | 0.53              |
| 1:C:460:GLY:N    | 1:C:470:ASN:HD22  | 2.04                     | 0.53              |
| 1:C:1063:LYS:HE2 | 1:C:1068:ASN:ND2  | 2.22                     | 0.53              |
| 1:D:988:LYS:O    | 1:D:988:LYS:HG3   | 2.08                     | 0.53              |
| 1:G:862:ASN:O    | 1:G:912:ILE:HG12  | 2.08                     | 0.53              |
| 1:A:435:ALA:HA   | 1:A:1052:ASN:ND2  | 2.23                     | 0.53              |
| 1:C:1063:LYS:CE  | 1:C:1068:ASN:HD21 | 2.20                     | 0.53              |
| 1:D:841:ASP:OD1  | 1:D:846:HIS:HE1   | 1.91                     | 0.53              |
| 1:F:749:ASP:C    | 1:F:750:ARG:HG2   | 2.33                     | 0.53              |
| 1:A:585:ARG:HD2  | 1:A:661:ASP:OD1   | 2.07                     | 0.53              |
| 1:G:740:ASN:C    | 1:G:740:ASN:HD22  | 2.16                     | 0.53              |
| 1:C:351:LYS:CE   | 4:C:3968:HOH:O    | 2.39                     | 0.53              |
| 1:B:440:ASN:HD21 | 1:B:449:GLN:NE2   | 1.98                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:F:457:MET:HE2  | 1:F:493:TYR:CE2   | 2.42                     | 0.52              |
| 1:H:800:THR:CG2  | 1:H:801:ALA:N     | 2.72                     | 0.52              |
| 1:E:504:ASP:OD1  | 1:E:846:HIS:CD2   | 2.60                     | 0.52              |
| 1:G:746:LYS:O    | 1:G:749:ASP:HB2   | 2.10                     | 0.52              |
| 1:A:868:THR:HB   | 1:A:872:GLU:OE1   | 2.09                     | 0.52              |
| 1:D:1074:VAL:CG2 | 1:D:1077:ASN:HB3  | 2.40                     | 0.52              |
| 1:D:1082:LYS:CB  | 4:D:3996:HOH:O    | 2.51                     | 0.52              |
| 1:H:368:SER:HA   | 1:H:371:ASN:HB2   | 1.91                     | 0.52              |
| 1:C:800:THR:HG22 | 1:C:802:ALA:H     | 1.75                     | 0.52              |
| 1:E:740:ASN:HD22 | 1:E:740:ASN:C     | 2.17                     | 0.52              |
| 1:B:368:SER:HA   | 1:B:371:ASN:HB2   | 1.92                     | 0.52              |
| 1:B:513:ILE:HD13 | 1:B:856:MET:HE2   | 1.91                     | 0.52              |
| 1:C:740:ASN:C    | 1:C:740:ASN:HD22  | 2.17                     | 0.52              |
| 1:F:346:LYS:HE2  | 1:F:355:TRP:CE3   | 2.45                     | 0.51              |
| 1:B:726:ARG:NH2  | 4:B:3961:HOH:O    | 2.43                     | 0.51              |
| 1:F:688:ILE:HD11 | 1:F:889:GLY:CA    | 2.40                     | 0.51              |
| 1:C:1052:ASN:H   | 1:C:1052:ASN:HD22 | 1.59                     | 0.51              |
| 1:D:670:MET:HE1  | 1:D:885:PHE:CZ    | 2.42                     | 0.51              |
| 1:E:311:ASN:ND2  | 1:E:323:TYR:H     | 2.05                     | 0.51              |
| 1:G:425:ARG:HG2  | 4:G:1748:HOH:O    | 2.10                     | 0.51              |
| 1:B:355:TRP:O    | 1:B:359:THR:HG23  | 2.09                     | 0.51              |
| 1:C:440:ASN:ND2  | 1:C:449:GLN:HE21  | 2.00                     | 0.51              |
| 4:D:1230:HOH:O   | 1:G:422:THR:CG2   | 2.55                     | 0.51              |
| 1:F:244:SER:N    | 4:F:2541:HOH:O    | 2.44                     | 0.51              |
| 1:H:457:MET:HE2  | 1:H:493:TYR:CE2   | 2.44                     | 0.51              |
| 1:H:948:LYS:NZ   | 4:H:2486:HOH:O    | 2.44                     | 0.51              |
| 1:B:740:ASN:HD22 | 1:B:742:SER:H     | 1.59                     | 0.51              |
| 1:E:302:ASP:HB3  | 1:E:1065:GLN:NE2  | 2.26                     | 0.51              |
| 1:F:371:ASN:HB3  | 1:F:373:ASP:H     | 1.75                     | 0.51              |
| 1:E:480:ASP:OD1  | 1:E:521:ASP:OD2   | 2.28                     | 0.51              |
| 1:F:667:GLY:O    | 1:F:865:ALA:N     | 2.39                     | 0.51              |
| 1:B:577:ALA:C    | 1:B:578:VAL:HG23  | 2.36                     | 0.51              |
| 1:G:457:MET:CE   | 1:G:493:TYR:HE2   | 2.08                     | 0.51              |
| 1:F:618:LYS:CE   | 4:F:149:HOH:O     | 2.59                     | 0.51              |
| 1:G:311:ASN:HD21 | 1:G:323:TYR:N     | 2.03                     | 0.51              |
| 1:A:460:GLY:H    | 1:A:470:ASN:ND2   | 2.02                     | 0.51              |
| 1:B:357:ARG:HA   | 4:B:2535:HOH:O    | 2.09                     | 0.51              |
| 1:C:551:LEU:HD21 | 4:C:3907:HOH:O    | 2.10                     | 0.51              |
| 1:D:460:GLY:N    | 1:D:470:ASN:HD22  | 2.09                     | 0.51              |
| 1:E:883:ASP:OD1  | 1:E:948:LYS:CE    | 2.58                     | 0.51              |
| 1:B:883:ASP:OD1  | 1:B:948:LYS:HE3   | 2.10                     | 0.50              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C:435:ALA:HA    | 1:C:1052:ASN:ND2 | 2.25                     | 0.50              |
| 1:F:1052:ASN:HD22 | 1:F:1052:ASN:H   | 1.59                     | 0.50              |
| 1:A:884:LYS:CE    | 4:A:1171:HOH:O   | 2.58                     | 0.50              |
| 1:B:366:THR:HG23  | 1:B:367:GLN:OE1  | 2.11                     | 0.50              |
| 1:E:288:THR:HB    | 1:E:290:LYS:H    | 1.76                     | 0.50              |
| 1:E:304:GLU:OE2   | 1:E:307:ARG:NH2  | 2.43                     | 0.50              |
| 1:A:800:THR:HG23  | 1:A:801:ALA:N    | 2.26                     | 0.50              |
| 1:C:251:VAL:HG21  | 1:C:259:PHE:CE1  | 2.43                     | 0.50              |
| 1:G:504:ASP:OD1   | 1:G:846:HIS:CD2  | 2.59                     | 0.50              |
| 1:C:669:TYR:CE2   | 1:C:670:MET:CE   | 2.88                     | 0.50              |
| 1:E:1001:LYS:O    | 1:E:1001:LYS:HG3 | 2.11                     | 0.50              |
| 1:F:868:THR:OG1   | 1:F:872:GLU:OE1  | 2.29                     | 0.50              |
| 1:G:324:ASN:HB2   | 4:G:2423:HOH:O   | 2.12                     | 0.50              |
| 1:G:394:LYS:HD3   | 1:G:394:LYS:N    | 2.07                     | 0.50              |
| 1:E:270:SER:HB2   | 1:E:295:LEU:HD12 | 1.93                     | 0.50              |
| 1:B:586:ALA:HA    | 1:B:858:GLU:OE1  | 2.12                     | 0.50              |
| 1:B:740:ASN:HD22  | 1:B:740:ASN:C    | 2.19                     | 0.50              |
| 1:G:966:GLU:HB2   | 1:G:997:LYS:HB2  | 1.92                     | 0.50              |
| 1:D:1000:GLY:C    | 1:D:1001:LYS:HG3 | 2.37                     | 0.50              |
| 1:G:492:ASP:HB3   | 1:G:1022:LEU:CD2 | 2.34                     | 0.50              |
| 1:B:841:ASP:OD1   | 1:B:846:HIS:HE1  | 1.94                     | 0.49              |
| 1:D:988:LYS:N     | 1:D:990:THR:CG2  | 2.61                     | 0.49              |
| 1:A:740:ASN:C     | 1:A:740:ASN:HD22 | 2.20                     | 0.49              |
| 1:B:800:THR:CG2   | 1:B:802:ALA:H    | 2.13                     | 0.49              |
| 1:D:988:LYS:O     | 1:D:990:THR:HG22 | 2.11                     | 0.49              |
| 1:F:854:ARG:HD3   | 1:F:892:ASP:OD2  | 2.12                     | 0.49              |
| 1:H:460:GLY:N     | 1:H:470:ASN:HD22 | 2.07                     | 0.49              |
| 1:E:988:LYS:O     | 1:E:990:THR:HG22 | 2.12                     | 0.49              |
| 1:F:504:ASP:OD1   | 1:F:846:HIS:HD2  | 1.95                     | 0.49              |
| 1:F:723:THR:O     | 1:F:758:ALA:HB2  | 2.11                     | 0.49              |
| 1:D:274:PRO:HG2   | 1:D:277:ILE:HD12 | 1.94                     | 0.49              |
| 1:D:1065:GLN:HG3  | 1:D:1066:ALA:N   | 2.27                     | 0.49              |
| 1:G:471:PHE:CG    | 1:G:954:ALA:HB2  | 2.46                     | 0.49              |
| 1:A:516:ALA:HB1   | 1:A:521:ASP:OD2  | 2.12                     | 0.49              |
| 1:C:740:ASN:ND2   | 1:C:742:SER:H    | 2.11                     | 0.49              |
| 1:D:427:ILE:HG12  | 3:D:5001:MES:H82 | 1.95                     | 0.49              |
| 1:E:505:LYS:NZ    | 4:E:2897:HOH:O   | 2.44                     | 0.49              |
| 1:B:563:ASN:HB3   | 4:B:3350:HOH:O   | 2.13                     | 0.49              |
| 1:F:988:LYS:H     | 1:F:990:THR:CG2  | 2.25                     | 0.49              |
| 1:A:251:VAL:HG21  | 1:A:259:PHE:CE1  | 2.46                     | 0.49              |
| 1:A:870:LYS:CD    | 4:A:3971:HOH:O   | 2.49                     | 0.49              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C:809:ASN:HB2   | 1:C:810:PRO:HD2  | 1.94                     | 0.49              |
| 1:E:365:LYS:HE3   | 4:E:3590:HOH:O   | 2.13                     | 0.49              |
| 1:F:883:ASP:OD1   | 1:F:948:LYS:CE   | 2.61                     | 0.49              |
| 1:F:740:ASN:C     | 1:F:740:ASN:ND2  | 2.71                     | 0.48              |
| 1:A:248:TYR:HB3   | 1:A:284:TRP:CZ3  | 2.48                     | 0.48              |
| 1:B:304:GLU:HA    | 1:B:307:ARG:HG2  | 1.94                     | 0.48              |
| 1:D:1076:ASP:O    | 1:D:1077:ASN:CB  | 2.61                     | 0.48              |
| 1:A:311:ASN:ND2   | 1:A:323:TYR:H    | 2.02                     | 0.48              |
| 1:A:715:LYS:NZ    | 1:A:832:VAL:HG23 | 2.28                     | 0.48              |
| 1:E:856:MET:HB3   | 1:E:856:MET:HE2  | 1.47                     | 0.48              |
| 1:F:453:LEU:CD1   | 1:F:474:ILE:HG21 | 2.43                     | 0.48              |
| 1:B:740:ASN:ND2   | 1:B:742:SER:H    | 2.12                     | 0.48              |
| 1:B:861:SER:H     | 1:B:864:GLN:NE2  | 1.98                     | 0.48              |
| 1:G:750:ARG:CD    | 4:G:1546:HOH:O   | 2.61                     | 0.48              |
| 1:H:966:GLU:HB2   | 1:H:997:LYS:HB2  | 1.96                     | 0.48              |
| 1:B:394:LYS:N     | 1:B:394:LYS:HD3  | 2.27                     | 0.48              |
| 1:E:725:ASP:OD1   | 1:E:727:ILE:CD1  | 2.62                     | 0.48              |
| 1:G:800:THR:HG23  | 1:G:801:ALA:N    | 2.27                     | 0.48              |
| 1:B:513:ILE:HD13  | 1:B:856:MET:HE1  | 1.95                     | 0.48              |
| 1:B:966:GLU:HB2   | 1:B:997:LYS:HB2  | 1.96                     | 0.48              |
| 1:B:1052:ASN:HD22 | 1:B:1052:ASN:H   | 1.62                     | 0.48              |
| 1:D:565:LEU:HD11  | 4:D:3922:HOH:O   | 2.12                     | 0.48              |
| 1:F:457:MET:CE    | 1:F:493:TYR:CE2  | 2.97                     | 0.48              |
| 1:F:557:MET:CE    | 1:F:708:ILE:CD1  | 2.92                     | 0.48              |
| 1:C:460:GLY:H     | 1:C:470:ASN:ND2  | 2.08                     | 0.47              |
| 1:F:1065:GLN:HG3  | 1:F:1066:ALA:N   | 2.29                     | 0.47              |
| 1:A:1025:ARG:O    | 1:A:1033:PRO:HA  | 2.13                     | 0.47              |
| 1:B:474:ILE:O     | 1:B:953:MET:HE2  | 2.13                     | 0.47              |
| 1:D:461:ASN:H     | 1:D:470:ASN:ND2  | 2.07                     | 0.47              |
| 1:F:462:ILE:HD13  | 1:F:1011:PHE:CZ  | 2.49                     | 0.47              |
| 1:F:745:LEU:HD13  | 1:F:804:ILE:O    | 2.13                     | 0.47              |
| 1:F:800:THR:HG23  | 1:F:801:ALA:H    | 1.80                     | 0.47              |
| 1:A:250:GLN:NE2   | 1:A:275:LYS:CE   | 2.48                     | 0.47              |
| 1:E:894:GLU:HA    | 1:E:953:MET:HB3  | 1.96                     | 0.47              |
| 1:B:394:LYS:N     | 1:B:394:LYS:HE2  | 2.21                     | 0.47              |
| 1:F:761:ASN:H     | 1:F:791:THR:HG22 | 1.77                     | 0.47              |
| 1:G:626:LYS:HB3   | 1:G:626:LYS:HE3  | 1.54                     | 0.47              |
| 1:G:759:HIS:HD2   | 1:G:762:GLN:OE1  | 1.98                     | 0.47              |
| 1:D:304:GLU:CD    | 1:D:307:ARG:HH11 | 2.22                     | 0.47              |
| 1:D:759:HIS:HD2   | 1:D:762:GLN:OE1  | 1.98                     | 0.47              |
| 1:G:976:ASP:OD1   | 1:G:976:ASP:C    | 2.58                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:978:TYR:CD1  | 3:B:5001:MES:H31  | 2.50                     | 0.47              |
| 1:B:1070:TYR:HE2 | 4:B:2873:HOH:O    | 1.98                     | 0.47              |
| 1:G:261:HIS:CD2  | 1:G:264:HIS:N     | 2.78                     | 0.47              |
| 1:H:324:ASN:ND2  | 1:H:326:ALA:H     | 2.12                     | 0.47              |
| 1:E:740:ASN:ND2  | 1:E:742:SER:H     | 2.12                     | 0.46              |
| 1:F:615:GLU:HG2  | 4:F:1620:HOH:O    | 2.14                     | 0.46              |
| 1:A:319:ILE:HD11 | 1:A:342:LYS:HG3   | 1.97                     | 0.46              |
| 1:A:376:LYS:HA   | 1:A:377:PRO:C     | 2.40                     | 0.46              |
| 1:C:430:TYR:HB3  | 1:C:978:TYR:CE1   | 2.50                     | 0.46              |
| 1:F:280:ASP:OD2  | 1:F:282:LYS:HE3   | 2.15                     | 0.46              |
| 1:G:740:ASN:HD22 | 1:G:741:PRO:N     | 2.13                     | 0.46              |
| 1:F:440:ASN:HD21 | 1:F:449:GLN:NE2   | 2.07                     | 0.46              |
| 1:C:250:GLN:NE2  | 1:C:275:LYS:HZ1   | 2.12                     | 0.46              |
| 1:F:1072:SER:OG  | 1:F:1074:VAL:HG12 | 2.16                     | 0.46              |
| 1:H:245:PHE:CD2  | 1:H:337:GLN:HG2   | 2.50                     | 0.46              |
| 1:H:421:TYR:OH   | 1:H:524:TYR:HA    | 2.15                     | 0.46              |
| 1:A:1072:SER:OG  | 1:A:1074:VAL:HG12 | 2.15                     | 0.46              |
| 1:B:492:ASP:HB3  | 1:B:1022:LEU:CD2  | 2.46                     | 0.46              |
| 1:C:705:SER:HB3  | 1:C:743:LEU:HD13  | 1.96                     | 0.46              |
| 1:D:883:ASP:OD1  | 1:D:948:LYS:CE    | 2.60                     | 0.46              |
| 1:E:308:GLN:HE21 | 1:E:308:GLN:HB3   | 1.39                     | 0.46              |
| 1:G:600:LYS:HE3  | 1:G:600:LYS:HB3   | 1.61                     | 0.46              |
| 1:H:440:ASN:HD21 | 1:H:449:GLN:NE2   | 2.09                     | 0.46              |
| 1:H:883:ASP:OD1  | 1:H:948:LYS:CE    | 2.60                     | 0.46              |
| 1:B:600:LYS:NZ   | 4:B:4161:HOH:O    | 2.49                     | 0.46              |
| 1:C:809:ASN:HB2  | 1:C:810:PRO:CD    | 2.45                     | 0.46              |
| 1:D:894:GLU:HA   | 1:D:953:MET:HB3   | 1.96                     | 0.46              |
| 1:F:1063:LYS:HA  | 1:F:1070:TYR:HA   | 1.98                     | 0.46              |
| 1:G:324:ASN:C    | 1:G:324:ASN:OD1   | 2.58                     | 0.46              |
| 1:G:861:SER:O    | 1:G:864:GLN:HG3   | 2.15                     | 0.46              |
| 1:H:311:ASN:HD21 | 1:H:323:TYR:N     | 2.14                     | 0.46              |
| 1:D:740:ASN:ND2  | 1:D:742:SER:H     | 2.14                     | 0.46              |
| 1:E:471:PHE:CG   | 1:E:954:ALA:HB2   | 2.51                     | 0.46              |
| 1:F:539:LEU:O    | 1:F:540:ARG:C     | 2.58                     | 0.46              |
| 1:G:726:ARG:HG2  | 4:G:2598:HOH:O    | 2.15                     | 0.46              |
| 1:F:522:THR:HB   | 1:F:523:PRO:CD    | 2.46                     | 0.45              |
| 1:F:988:LYS:H    | 1:F:990:THR:HG23  | 1.80                     | 0.45              |
| 1:H:670:MET:CE   | 1:H:885:PHE:CZ    | 2.87                     | 0.45              |
| 1:B:407:ASN:HD22 | 1:B:431:GLU:N     | 2.15                     | 0.45              |
| 1:C:740:ASN:HD22 | 1:C:742:SER:H     | 1.63                     | 0.45              |
| 1:C:861:SER:N    | 1:C:864:GLN:HE21  | 1.92                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:524:TYR:CD2   | 1:G:524:TYR:C     | 2.94                     | 0.45              |
| 1:F:329:PRO:HD2   | 4:F:2953:HOH:O    | 2.17                     | 0.45              |
| 1:H:312:TYR:O     | 1:H:316:GLN:HG2   | 2.16                     | 0.45              |
| 1:C:376:LYS:HA    | 1:C:377:PRO:C     | 2.41                     | 0.45              |
| 1:E:740:ASN:HD22  | 1:E:741:PRO:N     | 2.14                     | 0.45              |
| 1:F:709:THR:HG22  | 1:F:736:ILE:CD1   | 2.46                     | 0.45              |
| 1:F:460:GLY:N     | 1:F:470:ASN:HD22  | 2.13                     | 0.45              |
| 1:F:1065:GLN:HG3  | 1:F:1066:ALA:H    | 1.81                     | 0.45              |
| 1:G:740:ASN:HD22  | 1:G:742:SER:H     | 1.64                     | 0.45              |
| 1:H:313:MET:HB2   | 1:H:339:ILE:HD13  | 1.99                     | 0.45              |
| 1:A:460:GLY:N     | 1:A:470:ASN:ND2   | 2.64                     | 0.45              |
| 1:B:308:GLN:HE21  | 1:B:308:GLN:HB3   | 1.62                     | 0.45              |
| 1:E:725:ASP:OD1   | 1:E:727:ILE:HD12  | 2.17                     | 0.45              |
| 1:F:610:TYR:HA    | 1:F:612:PHE:CE2   | 2.52                     | 0.45              |
| 1:H:600:LYS:HE2   | 1:H:605:PRO:O     | 2.17                     | 0.45              |
| 1:A:304:GLU:OE2   | 1:A:307:ARG:NH1   | 2.49                     | 0.45              |
| 1:B:435:ALA:HA    | 1:B:1052:ASN:HD22 | 1.79                     | 0.45              |
| 1:C:639:ASN:ND2   | 1:C:813:SER:H     | 2.03                     | 0.45              |
| 1:E:1052:ASN:HD22 | 1:E:1052:ASN:N    | 2.13                     | 0.45              |
| 1:H:485:ASP:OD2   | 1:H:1029:SER:OG   | 2.31                     | 0.45              |
| 1:A:988:LYS:N     | 1:A:990:THR:HG23  | 2.32                     | 0.45              |
| 1:F:368:SER:HA    | 1:F:371:ASN:HB2   | 1.99                     | 0.45              |
| 1:G:460:GLY:N     | 1:G:470:ASN:HD22  | 2.12                     | 0.45              |
| 1:H:457:MET:HE1   | 1:H:494:LEU:HD21  | 1.99                     | 0.45              |
| 1:H:740:ASN:HD22  | 1:H:742:SER:H     | 1.63                     | 0.45              |
| 1:A:466:ASP:C     | 1:A:468:ASP:H     | 2.25                     | 0.45              |
| 1:C:776:LYS:NZ    | 4:C:3790:HOH:O    | 2.50                     | 0.45              |
| 1:F:425:ARG:H     | 1:F:425:ARG:HG2   | 1.60                     | 0.45              |
| 1:F:809:ASN:HB2   | 1:F:810:PRO:HD2   | 1.99                     | 0.45              |
| 1:G:871:GLU:CD    | 1:G:871:GLU:H     | 2.25                     | 0.45              |
| 1:E:430:TYR:HB3   | 1:E:978:TYR:CE1   | 2.52                     | 0.45              |
| 1:E:457:MET:CE    | 1:E:493:TYR:HE2   | 2.20                     | 0.45              |
| 1:E:457:MET:HE1   | 1:E:494:LEU:HD21  | 1.99                     | 0.45              |
| 1:G:861:SER:H     | 1:G:864:GLN:NE2   | 2.01                     | 0.45              |
| 1:B:755:MET:HB3   | 1:B:755:MET:HE3   | 1.78                     | 0.44              |
| 1:C:870:LYS:NZ    | 1:C:937:ASP:OD2   | 2.44                     | 0.44              |
| 1:F:311:ASN:HD21  | 1:F:323:TYR:N     | 2.07                     | 0.44              |
| 1:G:570:ASP:HB3   | 1:G:572:ASN:HD21  | 1.81                     | 0.44              |
| 1:B:407:ASN:ND2   | 1:B:431:GLU:N     | 2.64                     | 0.44              |
| 1:C:800:THR:CG2   | 1:C:801:ALA:N     | 2.80                     | 0.44              |
| 1:G:809:ASN:HB2   | 1:G:810:PRO:CD    | 2.47                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:1001:LYS:HE2  | 1:G:1001:LYS:HB2  | 1.32                     | 0.44              |
| 1:D:346:LYS:HG2   | 1:D:355:TRP:CE2   | 2.53                     | 0.44              |
| 1:D:726:ARG:H     | 1:D:726:ARG:HE    | 1.62                     | 0.44              |
| 1:H:250:GLN:HG3   | 1:H:275:LYS:HG3   | 1.99                     | 0.44              |
| 1:B:827:ASP:OD1   | 1:B:827:ASP:N     | 2.46                     | 0.44              |
| 1:D:999:SER:O     | 1:D:1001:LYS:N    | 2.50                     | 0.44              |
| 1:G:800:THR:CG2   | 1:G:801:ALA:N     | 2.78                     | 0.44              |
| 1:A:713:TYR:O     | 1:A:759:HIS:HE1   | 2.01                     | 0.44              |
| 1:A:1012:LEU:O    | 1:A:1016:GLN:HG3  | 2.18                     | 0.44              |
| 1:B:258:ASN:ND2   | 1:B:273:ARG:HB3   | 2.33                     | 0.44              |
| 1:C:376:LYS:HB3   | 1:C:377:PRO:HA    | 1.99                     | 0.44              |
| 1:D:1052:ASN:HD22 | 1:D:1052:ASN:N    | 2.13                     | 0.44              |
| 1:H:387:LEU:O     | 1:H:1050:GLY:HA3  | 2.17                     | 0.44              |
| 1:A:466:ASP:HA    | 1:A:467:PRO:HD2   | 1.80                     | 0.44              |
| 1:C:383:GLN:O     | 1:C:384:LYS:HB2   | 2.17                     | 0.44              |
| 1:E:1001:LYS:O    | 1:E:1001:LYS:CG   | 2.66                     | 0.44              |
| 1:B:262:VAL:HG12  | 1:B:969:VAL:HG23  | 2.00                     | 0.44              |
| 1:B:724:GLY:HA3   | 1:B:728:THR:OG1   | 2.17                     | 0.44              |
| 1:F:435:ALA:HA    | 1:F:1052:ASN:HD22 | 1.81                     | 0.44              |
| 1:H:394:LYS:HB2   | 1:H:394:LYS:HE2   | 1.41                     | 0.44              |
| 1:A:430:TYR:HB3   | 1:A:978:TYR:CE1   | 2.53                     | 0.44              |
| 1:A:658:TYR:CE2   | 1:A:660:GLY:HA3   | 2.52                     | 0.44              |
| 1:E:271:TRP:CZ2   | 1:E:357:ARG:HD3   | 2.53                     | 0.44              |
| 1:F:313:MET:HB2   | 1:F:339:ILE:HD13  | 2.00                     | 0.44              |
| 1:G:304:GLU:OE2   | 1:G:307:ARG:NH1   | 2.50                     | 0.44              |
| 1:H:619:LYS:HE2   | 1:H:619:LYS:HB3   | 1.44                     | 0.44              |
| 1:C:392:ASN:ND2   | 4:C:3574:HOH:O    | 2.48                     | 0.44              |
| 1:F:907:PHE:O     | 1:F:908:LEU:C     | 2.61                     | 0.44              |
| 1:F:1063:LYS:HE3  | 1:F:1068:ASN:ND2  | 2.28                     | 0.44              |
| 1:H:854:ARG:HD3   | 1:H:892:ASP:OD2   | 2.18                     | 0.44              |
| 1:G:596:ARG:NH2   | 1:G:600:LYS:HD2   | 2.34                     | 0.43              |
| 1:G:793:ASP:HB2   | 4:G:3607:HOH:O    | 2.17                     | 0.43              |
| 1:H:861:SER:N     | 1:H:864:GLN:HE21  | 1.93                     | 0.43              |
| 1:B:703:GLY:HA3   | 1:B:744:ARG:O     | 2.19                     | 0.43              |
| 1:D:274:PRO:HG2   | 1:D:277:ILE:CD1   | 2.47                     | 0.43              |
| 1:E:457:MET:HE1   | 1:E:494:LEU:CD2   | 2.48                     | 0.43              |
| 1:F:352:ASN:OD1   | 1:F:354:ASN:N     | 2.51                     | 0.43              |
| 1:F:492:ASP:OD2   | 1:F:1025:ARG:HD2  | 2.18                     | 0.43              |
| 1:A:966:GLU:HB2   | 1:A:997:LYS:HB2   | 2.00                     | 0.43              |
| 1:B:311:ASN:ND2   | 1:B:323:TYR:H     | 2.12                     | 0.43              |
| 1:E:658:TYR:CE2   | 1:E:660:GLY:HA3   | 2.53                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:495:LYS:NZ    | 4:G:3377:HOH:O    | 2.51                     | 0.43              |
| 1:H:394:LYS:H     | 1:H:394:LYS:CE    | 2.31                     | 0.43              |
| 1:A:453:LEU:CD1   | 1:A:474:ILE:HG21  | 2.48                     | 0.43              |
| 1:G:658:TYR:CE2   | 1:G:660:GLY:HA3   | 2.52                     | 0.43              |
| 1:D:425:ARG:HH11  | 1:D:425:ARG:HD3   | 1.65                     | 0.43              |
| 1:D:884:LYS:HE3   | 4:D:1112:HOH:O    | 2.18                     | 0.43              |
| 1:D:1074:VAL:HG22 | 1:D:1077:ASN:HB3  | 2.00                     | 0.43              |
| 1:F:524:TYR:C     | 1:F:524:TYR:CD2   | 2.96                     | 0.43              |
| 1:H:430:TYR:HB3   | 1:H:978:TYR:CE1   | 2.53                     | 0.43              |
| 1:E:737:GLU:HA    | 1:E:815:TYR:O     | 2.18                     | 0.43              |
| 1:G:261:HIS:CD2   | 1:G:264:HIS:HA    | 2.54                     | 0.43              |
| 1:G:1074:VAL:CG2  | 1:G:1077:ASN:HB3  | 2.49                     | 0.43              |
| 1:C:737:GLU:HA    | 1:C:815:TYR:O     | 2.19                     | 0.43              |
| 1:E:841:ASP:OD1   | 1:E:846:HIS:CE1   | 2.57                     | 0.43              |
| 1:G:894:GLU:HA    | 1:G:953:MET:HB3   | 2.00                     | 0.43              |
| 1:H:835:SER:HG    | 1:H:837:ALA:H     | 1.66                     | 0.43              |
| 1:D:1005:ALA:O    | 1:D:1041:LYS:HD2  | 2.19                     | 0.43              |
| 1:F:673:LYS:HE2   | 1:F:677:TYR:CZ    | 2.53                     | 0.43              |
| 1:H:1076:ASP:OD1  | 1:H:1076:ASP:N    | 2.49                     | 0.43              |
| 1:B:440:ASN:ND2   | 1:B:449:GLN:HE21  | 1.98                     | 0.43              |
| 1:C:460:GLY:N     | 1:C:470:ASN:ND2   | 2.67                     | 0.43              |
| 1:C:466:ASP:HA    | 1:C:467:PRO:HD2   | 1.89                     | 0.43              |
| 1:F:688:ILE:HD11  | 1:F:889:GLY:HA3   | 2.00                     | 0.43              |
| 1:G:907:PHE:O     | 1:G:908:LEU:C     | 2.62                     | 0.43              |
| 1:H:312:TYR:HD2   | 1:H:313:MET:HE2   | 1.84                     | 0.43              |
| 1:B:478:ALA:HB1   | 1:B:481:ASN:HD22  | 1.84                     | 0.43              |
| 1:B:1074:VAL:HG13 | 1:B:1077:ASN:C    | 2.44                     | 0.43              |
| 1:E:585:ARG:HD2   | 1:E:661:ASP:OD1   | 2.19                     | 0.43              |
| 1:F:669:TYR:CE2   | 1:F:670:MET:CE    | 2.98                     | 0.43              |
| 1:H:308:GLN:HE21  | 1:H:308:GLN:HB3   | 1.68                     | 0.43              |
| 1:H:740:ASN:HD22  | 1:H:741:PRO:N     | 2.17                     | 0.43              |
| 1:B:874:THR:HB    | 1:B:932:TYR:HB3   | 2.01                     | 0.42              |
| 1:B:928:LYS:HB2   | 1:B:929:PRO:CD    | 2.49                     | 0.42              |
| 1:C:800:THR:HG23  | 1:C:801:ALA:N     | 2.34                     | 0.42              |
| 1:E:1072:SER:HG   | 1:E:1074:VAL:HG12 | 1.83                     | 0.42              |
| 1:G:753:VAL:O     | 1:G:796:GLU:HA    | 2.19                     | 0.42              |
| 1:H:461:ASN:H     | 1:H:470:ASN:ND2   | 2.11                     | 0.42              |
| 1:H:736:ILE:HD11  | 1:H:799:PHE:CE2   | 2.54                     | 0.42              |
| 1:H:809:ASN:HB2   | 1:H:810:PRO:CD    | 2.49                     | 0.42              |
| 1:H:884:LYS:HD2   | 1:H:884:LYS:HA    | 1.83                     | 0.42              |
| 1:H:1063:LYS:HA   | 1:H:1070:TYR:HA   | 2.01                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:504:ASP:OD1  | 1:B:846:HIS:CD2   | 2.60                     | 0.42              |
| 1:G:346:LYS:HG2  | 1:G:355:TRP:CE2   | 2.54                     | 0.42              |
| 1:G:977:LYS:HE2  | 1:G:977:LYS:HB2   | 1.78                     | 0.42              |
| 1:H:737:GLU:HA   | 1:H:815:TYR:O     | 2.19                     | 0.42              |
| 1:B:442:ASN:O    | 1:B:446:GLN:HG3   | 2.19                     | 0.42              |
| 1:C:736:ILE:HD11 | 1:C:799:PHE:CE2   | 2.55                     | 0.42              |
| 1:D:988:LYS:HE3  | 1:D:988:LYS:HB2   | 1.33                     | 0.42              |
| 1:E:460:GLY:N    | 1:E:470:ASN:HD22  | 2.13                     | 0.42              |
| 1:G:407:ASN:HD22 | 1:G:431:GLU:H     | 1.66                     | 0.42              |
| 1:G:1030:THR:HB  | 1:G:1032:VAL:HG22 | 2.00                     | 0.42              |
| 1:A:1063:LYS:HE3 | 1:A:1070:TYR:CZ   | 2.54                     | 0.42              |
| 1:B:321:GLN:HG3  | 1:B:322:THR:N     | 2.34                     | 0.42              |
| 1:C:342:LYS:HE2  | 1:C:345:GLU:OE1   | 2.19                     | 0.42              |
| 1:F:480:ASP:OD1  | 1:F:521:ASP:OD2   | 2.37                     | 0.42              |
| 1:D:1026:LYS:NZ  | 4:D:3568:HOH:O    | 2.45                     | 0.42              |
| 1:G:440:ASN:HD21 | 1:G:449:GLN:NE2   | 2.10                     | 0.42              |
| 1:G:585:ARG:CD   | 1:G:661:ASP:OD1   | 2.67                     | 0.42              |
| 1:H:421:TYR:CZ   | 1:H:524:TYR:HA    | 2.55                     | 0.42              |
| 1:H:1072:SER:OG  | 1:H:1074:VAL:HG22 | 2.19                     | 0.42              |
| 1:A:1065:GLN:O   | 1:A:1066:ALA:C    | 2.62                     | 0.42              |
| 1:B:537:ASN:OD1  | 1:B:540:ARG:HD3   | 2.20                     | 0.42              |
| 1:F:576:ALA:HB3  | 1:F:847:GLN:HB3   | 2.01                     | 0.42              |
| 1:F:701:GLN:HG2  | 4:F:3429:HOH:O    | 2.18                     | 0.42              |
| 1:F:725:ASP:OD1  | 1:F:725:ASP:C     | 2.60                     | 0.42              |
| 1:H:610:TYR:HB2  | 1:H:907:PHE:CE1   | 2.54                     | 0.42              |
| 1:C:453:LEU:CD1  | 1:C:474:ILE:HG21  | 2.50                     | 0.42              |
| 1:E:387:LEU:O    | 1:E:1050:GLY:HA3  | 2.19                     | 0.42              |
| 1:E:389:TYR:CE2  | 1:E:1050:GLY:HA2  | 2.54                     | 0.42              |
| 1:F:585:ARG:CD   | 1:F:661:ASP:OD1   | 2.66                     | 0.42              |
| 1:G:737:GLU:HA   | 1:G:815:TYR:O     | 2.19                     | 0.42              |
| 1:C:1076:ASP:OD2 | 1:C:1077:ASN:N    | 2.53                     | 0.42              |
| 1:D:870:LYS:HD2  | 1:D:873:TYR:HD2   | 1.85                     | 0.42              |
| 1:F:258:ASN:ND2  | 1:F:273:ARG:HB3   | 2.34                     | 0.42              |
| 1:F:271:TRP:CZ2  | 1:F:357:ARG:HD2   | 2.54                     | 0.42              |
| 1:F:820:VAL:HB   | 1:F:821:PRO:HD2   | 2.01                     | 0.42              |
| 1:H:492:ASP:OD2  | 1:H:1025:ARG:HD2  | 2.20                     | 0.42              |
| 1:A:759:HIS:HD2  | 1:A:762:GLN:OE1   | 2.03                     | 0.42              |
| 1:B:837:ALA:HA   | 1:B:838:PRO:HD3   | 1.94                     | 0.42              |
| 1:D:258:ASN:HB3  | 1:D:259:PHE:CE2   | 2.55                     | 0.42              |
| 1:E:304:GLU:O    | 1:E:308:GLN:HG2   | 2.20                     | 0.42              |
| 1:G:250:GLN:CG   | 1:G:275:LYS:HE2   | 2.48                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:368:SER:HA   | 1:G:371:ASN:HB2   | 2.01                     | 0.42              |
| 1:H:475:ARG:N    | 1:H:953:MET:HE3   | 2.34                     | 0.42              |
| 1:A:563:ASN:HB3  | 4:A:1115:HOH:O    | 2.19                     | 0.41              |
| 1:C:311:ASN:HD22 | 1:C:311:ASN:HA    | 1.70                     | 0.41              |
| 1:C:698:ARG:O    | 1:C:708:ILE:HA    | 2.20                     | 0.41              |
| 1:D:740:ASN:C    | 1:D:740:ASN:HD22  | 2.28                     | 0.41              |
| 1:D:740:ASN:HD22 | 1:D:742:SER:H     | 1.67                     | 0.41              |
| 1:G:387:LEU:O    | 1:G:1050:GLY:HA3  | 2.19                     | 0.41              |
| 1:A:480:ASP:OD1  | 1:A:521:ASP:OD2   | 2.38                     | 0.41              |
| 1:A:729:ARG:HH11 | 1:A:729:ARG:HD2   | 1.72                     | 0.41              |
| 1:B:261:HIS:HB3  | 1:B:1073:LEU:HD23 | 2.02                     | 0.41              |
| 1:C:457:MET:HE1  | 1:C:494:LEU:HD21  | 2.02                     | 0.41              |
| 1:E:694:GLY:HA3  | 1:E:718:LEU:O     | 2.20                     | 0.41              |
| 1:H:321:GLN:HG3  | 1:H:322:THR:H     | 1.85                     | 0.41              |
| 1:H:524:TYR:C    | 1:H:524:TYR:CD2   | 2.98                     | 0.41              |
| 1:H:531:ASN:ND2  | 1:H:844:SER:OG    | 2.53                     | 0.41              |
| 1:A:884:LYS:HE3  | 4:A:1171:HOH:O    | 2.18                     | 0.41              |
| 1:B:861:SER:N    | 1:B:864:GLN:HE21  | 2.00                     | 0.41              |
| 1:E:247:GLN:O    | 1:E:250:GLN:HG2   | 2.19                     | 0.41              |
| 1:B:524:TYR:CD2  | 1:B:524:TYR:C     | 2.98                     | 0.41              |
| 1:B:577:ALA:C    | 1:B:578:VAL:CG2   | 2.92                     | 0.41              |
| 1:B:581:TYR:HA   | 1:B:654:VAL:O     | 2.20                     | 0.41              |
| 1:B:988:LYS:O    | 1:B:989:ASN:C     | 2.64                     | 0.41              |
| 1:C:478:ALA:HB1  | 1:C:481:ASN:HD22  | 1.84                     | 0.41              |
| 1:D:471:PHE:CG   | 1:D:954:ALA:HB2   | 2.55                     | 0.41              |
| 1:E:258:ASN:HB3  | 1:E:259:PHE:CE2   | 2.56                     | 0.41              |
| 1:F:792:ASN:OD1  | 1:F:792:ASN:C     | 2.64                     | 0.41              |
| 1:H:478:ALA:HB1  | 1:H:481:ASN:HD22  | 1.85                     | 0.41              |
| 1:A:558:ASN:N    | 1:A:559:PRO:HD2   | 2.36                     | 0.41              |
| 1:A:894:GLU:HA   | 1:A:953:MET:HB3   | 2.02                     | 0.41              |
| 1:B:430:TYR:HB3  | 1:B:978:TYR:CE1   | 2.55                     | 0.41              |
| 1:D:504:ASP:OD1  | 1:D:846:HIS:CD2   | 2.62                     | 0.41              |
| 1:E:669:TYR:CD2  | 1:E:670:MET:HG3   | 2.55                     | 0.41              |
| 1:H:669:TYR:CE2  | 1:H:670:MET:HE2   | 2.54                     | 0.41              |
| 1:H:841:ASP:OD1  | 1:H:846:HIS:HE1   | 2.02                     | 0.41              |
| 1:C:1012:LEU:HA  | 1:C:1012:LEU:HD23 | 1.87                     | 0.41              |
| 1:E:907:PHE:O    | 1:E:908:LEU:C     | 2.60                     | 0.41              |
| 1:F:862:ASN:O    | 1:F:912:ILE:HG12  | 2.21                     | 0.41              |
| 1:G:514:LEU:HD21 | 1:G:532:MET:HG3   | 2.02                     | 0.41              |
| 1:B:965:PRO:HD2  | 1:B:998:SER:HA    | 2.03                     | 0.41              |
| 1:D:430:TYR:HB3  | 1:D:978:TYR:CE1   | 2.56                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:809:ASN:HB2  | 1:E:810:PRO:CD    | 2.51                     | 0.41              |
| 1:F:870:LYS:HG3  | 4:F:3278:HOH:O    | 2.21                     | 0.41              |
| 1:F:951:LYS:HA   | 1:F:951:LYS:HD3   | 1.94                     | 0.41              |
| 1:G:430:TYR:HB3  | 1:G:978:TYR:CE1   | 2.56                     | 0.41              |
| 1:H:407:ASN:ND2  | 1:H:431:GLU:H     | 2.19                     | 0.41              |
| 1:H:759:HIS:HD2  | 1:H:762:GLN:OE1   | 2.04                     | 0.41              |
| 1:A:251:VAL:CG2  | 1:A:259:PHE:CZ    | 2.88                     | 0.41              |
| 1:A:689:LYS:CE   | 4:A:3634:HOH:O    | 2.68                     | 0.41              |
| 1:A:698:ARG:O    | 1:A:708:ILE:HA    | 2.21                     | 0.41              |
| 1:B:450:LEU:HD22 | 1:B:1034:MET:HE1  | 2.02                     | 0.41              |
| 1:D:406:LEU:HD22 | 1:D:431:GLU:HG2   | 2.03                     | 0.41              |
| 1:D:430:TYR:CD1  | 1:D:977:LYS:HD3   | 2.55                     | 0.41              |
| 1:F:822:VAL:HG12 | 1:F:823:GLY:N     | 2.35                     | 0.41              |
| 1:G:407:ASN:HD22 | 1:G:431:GLU:N     | 2.19                     | 0.41              |
| 1:A:309:TYR:CZ   | 1:A:313:MET:HG3   | 2.56                     | 0.41              |
| 1:B:311:ASN:HD21 | 1:B:323:TYR:N     | 2.14                     | 0.41              |
| 1:B:335:ALA:O    | 1:B:339:ILE:HG13  | 2.21                     | 0.41              |
| 1:D:492:ASP:HB3  | 1:D:1022:LEU:CD2  | 2.37                     | 0.41              |
| 1:D:558:ASN:N    | 1:D:559:PRO:CD    | 2.84                     | 0.41              |
| 1:F:740:ASN:HD22 | 1:F:742:SER:H     | 1.65                     | 0.41              |
| 1:F:786:GLY:C    | 1:F:787:LEU:HD12  | 2.46                     | 0.41              |
| 1:C:608:VAL:O    | 1:C:609:GLY:C     | 2.64                     | 0.40              |
| 1:C:988:LYS:O    | 1:C:990:THR:HG22  | 2.22                     | 0.40              |
| 1:F:579:PRO:HA   | 1:F:847:GLN:OE1   | 2.21                     | 0.40              |
| 1:B:626:LYS:NZ   | 4:B:1655:HOH:O    | 2.46                     | 0.40              |
| 1:B:976:ASP:OD1  | 1:B:976:ASP:C     | 2.63                     | 0.40              |
| 1:D:394:LYS:HE2  | 1:D:394:LYS:HB2   | 1.60                     | 0.40              |
| 1:F:322:THR:CG2  | 1:F:323:TYR:N     | 2.84                     | 0.40              |
| 1:G:581:TYR:HA   | 1:G:654:VAL:O     | 2.22                     | 0.40              |
| 1:G:750:ARG:HD3  | 4:G:1546:HOH:O    | 2.21                     | 0.40              |
| 1:G:1052:ASN:H   | 1:G:1052:ASN:HD22 | 1.68                     | 0.40              |
| 1:C:524:TYR:CD2  | 1:C:524:TYR:C     | 2.99                     | 0.40              |
| 1:D:525:LEU:HD11 | 1:D:532:MET:HG2   | 2.03                     | 0.40              |
| 1:D:755:MET:HE2  | 1:D:764:TYR:CE1   | 2.57                     | 0.40              |
| 1:E:457:MET:CE   | 1:E:493:TYR:CE2   | 2.98                     | 0.40              |
| 1:E:596:ARG:HB2  | 1:E:612:PHE:HZ    | 1.87                     | 0.40              |
| 1:F:1009:GLY:O   | 1:F:1039:LYS:HE2  | 2.21                     | 0.40              |
| 1:G:729:ARG:HH11 | 1:G:729:ARG:HD2   | 1.72                     | 0.40              |
| 1:H:480:ASP:OD1  | 1:H:521:ASP:OD2   | 2.39                     | 0.40              |
| 1:B:453:LEU:HD13 | 1:B:474:ILE:HG21  | 2.03                     | 0.40              |
| 1:C:480:ASP:OD1  | 1:C:521:ASP:OD2   | 2.40                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:870:LYS:HD2  | 1:D:873:TYR:CD2  | 2.56                     | 0.40              |
| 1:G:312:TYR:CD2  | 1:G:363:PHE:HB2  | 2.56                     | 0.40              |
| 1:G:384:LYS:NZ   | 4:G:4166:HOH:O   | 2.48                     | 0.40              |
| 1:H:346:LYS:HE3  | 1:H:346:LYS:HB3  | 1.91                     | 0.40              |
| 1:H:907:PHE:O    | 1:H:908:LEU:C    | 2.64                     | 0.40              |
| 1:A:244:SER:O    | 1:A:244:SER:OG   | 2.36                     | 0.40              |
| 1:A:407:ASN:ND2  | 1:A:431:GLU:H    | 2.20                     | 0.40              |
| 1:B:442:ASN:HA   | 1:B:443:PRO:HD3  | 1.93                     | 0.40              |
| 1:C:251:VAL:HG22 | 1:C:258:ASN:HD22 | 1.86                     | 0.40              |
| 1:D:387:LEU:O    | 1:D:1050:GLY:HA3 | 2.22                     | 0.40              |
| 1:D:737:GLU:HA   | 1:D:815:TYR:O    | 2.22                     | 0.40              |
| 1:D:1013:GLU:HG2 | 1:D:1013:GLU:H   | 1.60                     | 0.40              |
| 1:D:1065:GLN:HG3 | 1:D:1066:ALA:H   | 1.86                     | 0.40              |
| 1:G:250:GLN:HG2  | 1:G:275:LYS:HE2  | 2.04                     | 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     | 842/844 (100%)   | 816 (97%)  | 25 (3%)  | 1 (0%)   | 48          | 50  |
| 1   | B     | 842/844 (100%)   | 812 (96%)  | 29 (3%)  | 1 (0%)   | 48          | 50  |
| 1   | C     | 842/844 (100%)   | 817 (97%)  | 24 (3%)  | 1 (0%)   | 48          | 50  |
| 1   | D     | 842/844 (100%)   | 815 (97%)  | 25 (3%)  | 2 (0%)   | 43          | 44  |
| 1   | E     | 842/844 (100%)   | 815 (97%)  | 25 (3%)  | 2 (0%)   | 43          | 44  |
| 1   | F     | 842/844 (100%)   | 818 (97%)  | 24 (3%)  | 0        | 100         | 100 |
| 1   | G     | 842/844 (100%)   | 817 (97%)  | 23 (3%)  | 2 (0%)   | 43          | 44  |
| 1   | H     | 842/844 (100%)   | 817 (97%)  | 23 (3%)  | 2 (0%)   | 43          | 44  |
| All | All   | 6736/6752 (100%) | 6527 (97%) | 198 (3%) | 11 (0%)  | 43          | 44  |

All (11) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 1077 | ASN  |
| 1   | D     | 1077 | ASN  |
| 1   | E     | 1077 | ASN  |
| 1   | C     | 793  | ASP  |
| 1   | G     | 747  | ALA  |
| 1   | D     | 705  | SER  |
| 1   | A     | 793  | ASP  |
| 1   | E     | 705  | SER  |
| 1   | H     | 1077 | ASN  |
| 1   | G     | 705  | SER  |
| 1   | H     | 705  | SER  |

### 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     | 715/715 (100%)   | 691 (97%)  | 24 (3%)  | 32          | 35 |
| 1   | B     | 715/715 (100%)   | 670 (94%)  | 45 (6%)  | 16          | 14 |
| 1   | C     | 715/715 (100%)   | 691 (97%)  | 24 (3%)  | 32          | 35 |
| 1   | D     | 715/715 (100%)   | 682 (95%)  | 33 (5%)  | 24          | 25 |
| 1   | E     | 715/715 (100%)   | 682 (95%)  | 33 (5%)  | 24          | 25 |
| 1   | F     | 715/715 (100%)   | 686 (96%)  | 29 (4%)  | 27          | 29 |
| 1   | G     | 715/715 (100%)   | 684 (96%)  | 31 (4%)  | 26          | 27 |
| 1   | H     | 715/715 (100%)   | 684 (96%)  | 31 (4%)  | 26          | 27 |
| All | All   | 5720/5720 (100%) | 5470 (96%) | 250 (4%) | 25          | 26 |

All (250) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 253 | SER  |
| 1   | A     | 258 | ASN  |
| 1   | A     | 279 | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 307  | ARG  |
| 1   | A     | 359  | THR  |
| 1   | A     | 368  | SER  |
| 1   | A     | 457  | MET  |
| 1   | A     | 465  | ASN  |
| 1   | A     | 468  | ASP  |
| 1   | A     | 532  | MET  |
| 1   | A     | 574  | GLU  |
| 1   | A     | 600  | LYS  |
| 1   | A     | 626  | LYS  |
| 1   | A     | 689  | LYS  |
| 1   | A     | 702  | VAL  |
| 1   | A     | 726  | ARG  |
| 1   | A     | 727  | ILE  |
| 1   | A     | 742  | SER  |
| 1   | A     | 800  | THR  |
| 1   | A     | 832  | VAL  |
| 1   | A     | 870  | LYS  |
| 1   | A     | 882  | VAL  |
| 1   | A     | 985  | SER  |
| 1   | A     | 1052 | ASN  |
| 1   | B     | 247  | GLN  |
| 1   | B     | 253  | SER  |
| 1   | B     | 254  | THR  |
| 1   | B     | 258  | ASN  |
| 1   | B     | 275  | LYS  |
| 1   | B     | 295  | LEU  |
| 1   | B     | 304  | GLU  |
| 1   | B     | 322  | THR  |
| 1   | B     | 325  | THR  |
| 1   | B     | 350  | GLU  |
| 1   | B     | 357  | ARG  |
| 1   | B     | 359  | THR  |
| 1   | B     | 366  | THR  |
| 1   | B     | 368  | SER  |
| 1   | B     | 394  | LYS  |
| 1   | B     | 416  | LYS  |
| 1   | B     | 422  | THR  |
| 1   | B     | 457  | MET  |
| 1   | B     | 465  | ASN  |
| 1   | B     | 502  | LYS  |
| 1   | B     | 524  | TYR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 532  | MET  |
| 1   | B     | 634  | LYS  |
| 1   | B     | 702  | VAL  |
| 1   | B     | 719  | LYS  |
| 1   | B     | 726  | ARG  |
| 1   | B     | 734  | VAL  |
| 1   | B     | 793  | ASP  |
| 1   | B     | 832  | VAL  |
| 1   | B     | 882  | VAL  |
| 1   | B     | 884  | LYS  |
| 1   | B     | 912  | ILE  |
| 1   | B     | 943  | LYS  |
| 1   | B     | 985  | SER  |
| 1   | B     | 990  | THR  |
| 1   | B     | 1001 | LYS  |
| 1   | B     | 1025 | ARG  |
| 1   | B     | 1038 | VAL  |
| 1   | B     | 1052 | ASN  |
| 1   | B     | 1063 | LYS  |
| 1   | B     | 1065 | GLN  |
| 1   | B     | 1073 | LEU  |
| 1   | B     | 1074 | VAL  |
| 1   | B     | 1082 | LYS  |
| 1   | B     | 1083 | SER  |
| 1   | C     | 290  | LYS  |
| 1   | C     | 307  | ARG  |
| 1   | C     | 320  | HIS  |
| 1   | C     | 321  | GLN  |
| 1   | C     | 322  | THR  |
| 1   | C     | 342  | LYS  |
| 1   | C     | 390  | SER  |
| 1   | C     | 422  | THR  |
| 1   | C     | 457  | MET  |
| 1   | C     | 465  | ASN  |
| 1   | C     | 532  | MET  |
| 1   | C     | 574  | GLU  |
| 1   | C     | 702  | VAL  |
| 1   | C     | 800  | THR  |
| 1   | C     | 832  | VAL  |
| 1   | C     | 880  | LYS  |
| 1   | C     | 882  | VAL  |
| 1   | C     | 977  | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 990  | THR  |
| 1   | C     | 1001 | LYS  |
| 1   | C     | 1013 | GLU  |
| 1   | C     | 1038 | VAL  |
| 1   | C     | 1052 | ASN  |
| 1   | C     | 1074 | VAL  |
| 1   | D     | 251  | VAL  |
| 1   | D     | 258  | ASN  |
| 1   | D     | 277  | ILE  |
| 1   | D     | 290  | LYS  |
| 1   | D     | 307  | ARG  |
| 1   | D     | 321  | GLN  |
| 1   | D     | 322  | THR  |
| 1   | D     | 342  | LYS  |
| 1   | D     | 350  | GLU  |
| 1   | D     | 368  | SER  |
| 1   | D     | 416  | LYS  |
| 1   | D     | 422  | THR  |
| 1   | D     | 457  | MET  |
| 1   | D     | 465  | ASN  |
| 1   | D     | 532  | MET  |
| 1   | D     | 574  | GLU  |
| 1   | D     | 600  | LYS  |
| 1   | D     | 702  | VAL  |
| 1   | D     | 707  | ILE  |
| 1   | D     | 726  | ARG  |
| 1   | D     | 744  | ARG  |
| 1   | D     | 793  | ASP  |
| 1   | D     | 800  | THR  |
| 1   | D     | 832  | VAL  |
| 1   | D     | 880  | LYS  |
| 1   | D     | 882  | VAL  |
| 1   | D     | 977  | LYS  |
| 1   | D     | 988  | LYS  |
| 1   | D     | 990  | THR  |
| 1   | D     | 1013 | GLU  |
| 1   | D     | 1025 | ARG  |
| 1   | D     | 1038 | VAL  |
| 1   | D     | 1052 | ASN  |
| 1   | E     | 247  | GLN  |
| 1   | E     | 251  | VAL  |
| 1   | E     | 253  | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | E     | 258  | ASN  |
| 1   | E     | 277  | ILE  |
| 1   | E     | 308  | GLN  |
| 1   | E     | 320  | HIS  |
| 1   | E     | 322  | THR  |
| 1   | E     | 325  | THR  |
| 1   | E     | 394  | LYS  |
| 1   | E     | 457  | MET  |
| 1   | E     | 465  | ASN  |
| 1   | E     | 532  | MET  |
| 1   | E     | 574  | GLU  |
| 1   | E     | 619  | LYS  |
| 1   | E     | 702  | VAL  |
| 1   | E     | 727  | ILE  |
| 1   | E     | 793  | ASP  |
| 1   | E     | 800  | THR  |
| 1   | E     | 832  | VAL  |
| 1   | E     | 835  | SER  |
| 1   | E     | 870  | LYS  |
| 1   | E     | 880  | LYS  |
| 1   | E     | 882  | VAL  |
| 1   | E     | 928  | LYS  |
| 1   | E     | 990  | THR  |
| 1   | E     | 1001 | LYS  |
| 1   | E     | 1038 | VAL  |
| 1   | E     | 1052 | ASN  |
| 1   | E     | 1065 | GLN  |
| 1   | E     | 1074 | VAL  |
| 1   | E     | 1082 | LYS  |
| 1   | E     | 1086 | ASN  |
| 1   | F     | 253  | SER  |
| 1   | F     | 258  | ASN  |
| 1   | F     | 308  | GLN  |
| 1   | F     | 321  | GLN  |
| 1   | F     | 350  | GLU  |
| 1   | F     | 351  | LYS  |
| 1   | F     | 357  | ARG  |
| 1   | F     | 372  | SER  |
| 1   | F     | 394  | LYS  |
| 1   | F     | 422  | THR  |
| 1   | F     | 457  | MET  |
| 1   | F     | 465  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | F     | 532  | MET  |
| 1   | F     | 708  | ILE  |
| 1   | F     | 726  | ARG  |
| 1   | F     | 740  | ASN  |
| 1   | F     | 782  | GLN  |
| 1   | F     | 791  | THR  |
| 1   | F     | 803  | ASP  |
| 1   | F     | 832  | VAL  |
| 1   | F     | 868  | THR  |
| 1   | F     | 880  | LYS  |
| 1   | F     | 882  | VAL  |
| 1   | F     | 912  | ILE  |
| 1   | F     | 977  | LYS  |
| 1   | F     | 985  | SER  |
| 1   | F     | 990  | THR  |
| 1   | F     | 1038 | VAL  |
| 1   | F     | 1082 | LYS  |
| 1   | G     | 251  | VAL  |
| 1   | G     | 253  | SER  |
| 1   | G     | 322  | THR  |
| 1   | G     | 342  | LYS  |
| 1   | G     | 350  | GLU  |
| 1   | G     | 394  | LYS  |
| 1   | G     | 422  | THR  |
| 1   | G     | 457  | MET  |
| 1   | G     | 465  | ASN  |
| 1   | G     | 532  | MET  |
| 1   | G     | 574  | GLU  |
| 1   | G     | 707  | ILE  |
| 1   | G     | 726  | ARG  |
| 1   | G     | 727  | ILE  |
| 1   | G     | 736  | ILE  |
| 1   | G     | 744  | ARG  |
| 1   | G     | 746  | LYS  |
| 1   | G     | 750  | ARG  |
| 1   | G     | 800  | THR  |
| 1   | G     | 832  | VAL  |
| 1   | G     | 870  | LYS  |
| 1   | G     | 882  | VAL  |
| 1   | G     | 928  | LYS  |
| 1   | G     | 977  | LYS  |
| 1   | G     | 985  | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | G     | 988  | LYS  |
| 1   | G     | 990  | THR  |
| 1   | G     | 1001 | LYS  |
| 1   | G     | 1013 | GLU  |
| 1   | G     | 1038 | VAL  |
| 1   | G     | 1052 | ASN  |
| 1   | H     | 251  | VAL  |
| 1   | H     | 258  | ASN  |
| 1   | H     | 282  | LYS  |
| 1   | H     | 308  | GLN  |
| 1   | H     | 322  | THR  |
| 1   | H     | 324  | ASN  |
| 1   | H     | 329  | PRO  |
| 1   | H     | 342  | LYS  |
| 1   | H     | 351  | LYS  |
| 1   | H     | 394  | LYS  |
| 1   | H     | 457  | MET  |
| 1   | H     | 465  | ASN  |
| 1   | H     | 532  | MET  |
| 1   | H     | 600  | LYS  |
| 1   | H     | 619  | LYS  |
| 1   | H     | 702  | VAL  |
| 1   | H     | 726  | ARG  |
| 1   | H     | 727  | ILE  |
| 1   | H     | 744  | ARG  |
| 1   | H     | 800  | THR  |
| 1   | H     | 832  | VAL  |
| 1   | H     | 835  | SER  |
| 1   | H     | 870  | LYS  |
| 1   | H     | 985  | SER  |
| 1   | H     | 990  | THR  |
| 1   | H     | 1001 | LYS  |
| 1   | H     | 1038 | VAL  |
| 1   | H     | 1052 | ASN  |
| 1   | H     | 1075 | SER  |
| 1   | H     | 1082 | LYS  |
| 1   | H     | 1083 | SER  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (213) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 258 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 261  | HIS  |
| 1   | A     | 308  | GLN  |
| 1   | A     | 311  | ASN  |
| 1   | A     | 407  | ASN  |
| 1   | A     | 440  | ASN  |
| 1   | A     | 470  | ASN  |
| 1   | A     | 481  | ASN  |
| 1   | A     | 531  | ASN  |
| 1   | A     | 558  | ASN  |
| 1   | A     | 572  | ASN  |
| 1   | A     | 639  | ASN  |
| 1   | A     | 672  | HIS  |
| 1   | A     | 699  | ASN  |
| 1   | A     | 740  | ASN  |
| 1   | A     | 759  | HIS  |
| 1   | A     | 761  | ASN  |
| 1   | A     | 773  | ASN  |
| 1   | A     | 782  | GLN  |
| 1   | A     | 846  | HIS  |
| 1   | A     | 864  | GLN  |
| 1   | A     | 986  | GLN  |
| 1   | A     | 1016 | GLN  |
| 1   | A     | 1027 | GLN  |
| 1   | A     | 1052 | ASN  |
| 1   | A     | 1068 | ASN  |
| 1   | B     | 247  | GLN  |
| 1   | B     | 250  | GLN  |
| 1   | B     | 258  | ASN  |
| 1   | B     | 261  | HIS  |
| 1   | B     | 308  | GLN  |
| 1   | B     | 311  | ASN  |
| 1   | B     | 407  | ASN  |
| 1   | B     | 440  | ASN  |
| 1   | B     | 461  | ASN  |
| 1   | B     | 470  | ASN  |
| 1   | B     | 481  | ASN  |
| 1   | B     | 531  | ASN  |
| 1   | B     | 558  | ASN  |
| 1   | B     | 592  | GLN  |
| 1   | B     | 639  | ASN  |
| 1   | B     | 699  | ASN  |
| 1   | B     | 740  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 759  | HIS  |
| 1   | B     | 773  | ASN  |
| 1   | B     | 782  | GLN  |
| 1   | B     | 811  | GLN  |
| 1   | B     | 828  | GLN  |
| 1   | B     | 846  | HIS  |
| 1   | B     | 864  | GLN  |
| 1   | B     | 881  | ASN  |
| 1   | B     | 960  | GLN  |
| 1   | B     | 1016 | GLN  |
| 1   | B     | 1052 | ASN  |
| 1   | C     | 250  | GLN  |
| 1   | C     | 261  | HIS  |
| 1   | C     | 303  | GLN  |
| 1   | C     | 308  | GLN  |
| 1   | C     | 311  | ASN  |
| 1   | C     | 407  | ASN  |
| 1   | C     | 412  | ASN  |
| 1   | C     | 440  | ASN  |
| 1   | C     | 470  | ASN  |
| 1   | C     | 481  | ASN  |
| 1   | C     | 531  | ASN  |
| 1   | C     | 558  | ASN  |
| 1   | C     | 572  | ASN  |
| 1   | C     | 592  | GLN  |
| 1   | C     | 639  | ASN  |
| 1   | C     | 740  | ASN  |
| 1   | C     | 759  | HIS  |
| 1   | C     | 761  | ASN  |
| 1   | C     | 773  | ASN  |
| 1   | C     | 782  | GLN  |
| 1   | C     | 828  | GLN  |
| 1   | C     | 846  | HIS  |
| 1   | C     | 864  | GLN  |
| 1   | C     | 881  | ASN  |
| 1   | C     | 1016 | GLN  |
| 1   | C     | 1052 | ASN  |
| 1   | C     | 1068 | ASN  |
| 1   | D     | 258  | ASN  |
| 1   | D     | 261  | HIS  |
| 1   | D     | 308  | GLN  |
| 1   | D     | 311  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 331  | GLN  |
| 1   | D     | 367  | GLN  |
| 1   | D     | 407  | ASN  |
| 1   | D     | 412  | ASN  |
| 1   | D     | 440  | ASN  |
| 1   | D     | 461  | ASN  |
| 1   | D     | 470  | ASN  |
| 1   | D     | 481  | ASN  |
| 1   | D     | 531  | ASN  |
| 1   | D     | 558  | ASN  |
| 1   | D     | 572  | ASN  |
| 1   | D     | 592  | GLN  |
| 1   | D     | 639  | ASN  |
| 1   | D     | 672  | HIS  |
| 1   | D     | 699  | ASN  |
| 1   | D     | 740  | ASN  |
| 1   | D     | 759  | HIS  |
| 1   | D     | 773  | ASN  |
| 1   | D     | 782  | GLN  |
| 1   | D     | 811  | GLN  |
| 1   | D     | 846  | HIS  |
| 1   | D     | 864  | GLN  |
| 1   | D     | 960  | GLN  |
| 1   | D     | 1016 | GLN  |
| 1   | D     | 1052 | ASN  |
| 1   | D     | 1068 | ASN  |
| 1   | E     | 247  | GLN  |
| 1   | E     | 250  | GLN  |
| 1   | E     | 261  | HIS  |
| 1   | E     | 308  | GLN  |
| 1   | E     | 311  | ASN  |
| 1   | E     | 367  | GLN  |
| 1   | E     | 407  | ASN  |
| 1   | E     | 412  | ASN  |
| 1   | E     | 440  | ASN  |
| 1   | E     | 461  | ASN  |
| 1   | E     | 470  | ASN  |
| 1   | E     | 531  | ASN  |
| 1   | E     | 558  | ASN  |
| 1   | E     | 572  | ASN  |
| 1   | E     | 592  | GLN  |
| 1   | E     | 639  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | E     | 740  | ASN  |
| 1   | E     | 759  | HIS  |
| 1   | E     | 773  | ASN  |
| 1   | E     | 828  | GLN  |
| 1   | E     | 846  | HIS  |
| 1   | E     | 864  | GLN  |
| 1   | E     | 881  | ASN  |
| 1   | E     | 1016 | GLN  |
| 1   | E     | 1027 | GLN  |
| 1   | E     | 1052 | ASN  |
| 1   | E     | 1065 | GLN  |
| 1   | F     | 258  | ASN  |
| 1   | F     | 261  | HIS  |
| 1   | F     | 308  | GLN  |
| 1   | F     | 311  | ASN  |
| 1   | F     | 407  | ASN  |
| 1   | F     | 412  | ASN  |
| 1   | F     | 440  | ASN  |
| 1   | F     | 470  | ASN  |
| 1   | F     | 481  | ASN  |
| 1   | F     | 531  | ASN  |
| 1   | F     | 592  | GLN  |
| 1   | F     | 606  | ASN  |
| 1   | F     | 639  | ASN  |
| 1   | F     | 699  | ASN  |
| 1   | F     | 740  | ASN  |
| 1   | F     | 759  | HIS  |
| 1   | F     | 782  | GLN  |
| 1   | F     | 811  | GLN  |
| 1   | F     | 846  | HIS  |
| 1   | F     | 864  | GLN  |
| 1   | F     | 1042 | GLN  |
| 1   | F     | 1052 | ASN  |
| 1   | F     | 1068 | ASN  |
| 1   | G     | 258  | ASN  |
| 1   | G     | 261  | HIS  |
| 1   | G     | 308  | GLN  |
| 1   | G     | 311  | ASN  |
| 1   | G     | 367  | GLN  |
| 1   | G     | 407  | ASN  |
| 1   | G     | 412  | ASN  |
| 1   | G     | 440  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | G     | 470  | ASN  |
| 1   | G     | 481  | ASN  |
| 1   | G     | 558  | ASN  |
| 1   | G     | 572  | ASN  |
| 1   | G     | 592  | GLN  |
| 1   | G     | 639  | ASN  |
| 1   | G     | 672  | HIS  |
| 1   | G     | 740  | ASN  |
| 1   | G     | 759  | HIS  |
| 1   | G     | 762  | GLN  |
| 1   | G     | 811  | GLN  |
| 1   | G     | 828  | GLN  |
| 1   | G     | 846  | HIS  |
| 1   | G     | 864  | GLN  |
| 1   | G     | 881  | ASN  |
| 1   | G     | 960  | GLN  |
| 1   | G     | 1052 | ASN  |
| 1   | G     | 1068 | ASN  |
| 1   | H     | 250  | GLN  |
| 1   | H     | 258  | ASN  |
| 1   | H     | 261  | HIS  |
| 1   | H     | 308  | GLN  |
| 1   | H     | 311  | ASN  |
| 1   | H     | 324  | ASN  |
| 1   | H     | 337  | GLN  |
| 1   | H     | 367  | GLN  |
| 1   | H     | 407  | ASN  |
| 1   | H     | 412  | ASN  |
| 1   | H     | 440  | ASN  |
| 1   | H     | 461  | ASN  |
| 1   | H     | 470  | ASN  |
| 1   | H     | 481  | ASN  |
| 1   | H     | 531  | ASN  |
| 1   | H     | 572  | ASN  |
| 1   | H     | 592  | GLN  |
| 1   | H     | 639  | ASN  |
| 1   | H     | 740  | ASN  |
| 1   | H     | 759  | HIS  |
| 1   | H     | 773  | ASN  |
| 1   | H     | 811  | GLN  |
| 1   | H     | 846  | HIS  |
| 1   | H     | 864  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | H     | 1003 | GLN  |
| 1   | H     | 1052 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | MES  | F     | 5001 | -    | 12,12,12     | 2.57 | 1 (8%)   | 15,16,16    | 2.57 | 6 (40%)  |
| 3   | MES  | B     | 5001 | -    | 12,12,12     | 1.85 | 1 (8%)   | 15,16,16    | 5.39 | 11 (73%) |
| 3   | MES  | A     | 5001 | -    | 12,12,12     | 2.52 | 3 (25%)  | 15,16,16    | 4.90 | 9 (60%)  |
| 3   | MES  | E     | 5001 | -    | 12,12,12     | 1.33 | 1 (8%)   | 15,16,16    | 4.33 | 11 (73%) |
| 3   | MES  | D     | 5001 | -    | 12,12,12     | 1.72 | 2 (16%)  | 15,16,16    | 5.88 | 9 (60%)  |
| 3   | MES  | C     | 5001 | -    | 12,12,12     | 2.36 | 1 (8%)   | 15,16,16    | 6.21 | 10 (66%) |
| 3   | MES  | H     | 5001 | -    | 12,12,12     | 2.38 | 1 (8%)   | 15,16,16    | 6.23 | 10 (66%) |
| 3   | MES  | G     | 5001 | -    | 12,12,12     | 2.21 | 1 (8%)   | 15,16,16    | 4.21 | 9 (60%)  |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral



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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 3   | MES  | F     | 5001 | -    | -       | 1/6/14/14 | 0/1/1/1 |
| 3   | MES  | B     | 5001 | -    | -       | 1/6/14/14 | 0/1/1/1 |
| 3   | MES  | A     | 5001 | -    | -       | 2/6/14/14 | 0/1/1/1 |
| 3   | MES  | E     | 5001 | -    | -       | 1/6/14/14 | 0/1/1/1 |
| 3   | MES  | D     | 5001 | -    | -       | 4/6/14/14 | 0/1/1/1 |
| 3   | MES  | C     | 5001 | -    | -       | 2/6/14/14 | 0/1/1/1 |
| 3   | MES  | H     | 5001 | -    | -       | 1/6/14/14 | 0/1/1/1 |
| 3   | MES  | G     | 5001 | -    | -       | 1/6/14/14 | 0/1/1/1 |

All (11) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | F     | 5001 | MES  | C8-S  | -8.16 | 1.66        | 1.77     |
| 3   | H     | 5001 | MES  | C8-S  | -7.85 | 1.66        | 1.77     |
| 3   | C     | 5001 | MES  | C8-S  | -7.82 | 1.66        | 1.77     |
| 3   | A     | 5001 | MES  | C8-S  | -7.59 | 1.66        | 1.77     |
| 3   | G     | 5001 | MES  | C8-S  | -7.31 | 1.67        | 1.77     |
| 3   | B     | 5001 | MES  | C8-S  | -6.04 | 1.69        | 1.77     |
| 3   | D     | 5001 | MES  | O3S-S | -4.41 | 1.30        | 1.47     |
| 3   | E     | 5001 | MES  | C8-S  | -3.41 | 1.72        | 1.77     |
| 3   | D     | 5001 | MES  | C8-S  | -2.77 | 1.73        | 1.77     |
| 3   | A     | 5001 | MES  | O2S-S | -2.69 | 1.37        | 1.45     |
| 3   | A     | 5001 | MES  | O1S-S | -2.12 | 1.39        | 1.45     |

All (75) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 3   | D     | 5001 | MES  | O2S-S-C8 | -16.30 | 82.10       | 106.73   |
| 3   | C     | 5001 | MES  | O2S-S-C8 | -13.67 | 86.07       | 106.73   |
| 3   | H     | 5001 | MES  | O1S-S-C8 | -13.65 | 86.11       | 106.73   |
| 3   | C     | 5001 | MES  | O1S-S-C8 | -13.64 | 86.11       | 106.73   |
| 3   | H     | 5001 | MES  | O2S-S-C8 | -13.64 | 86.12       | 106.73   |
| 3   | B     | 5001 | MES  | O1S-S-C8 | -12.56 | 87.75       | 106.73   |
| 3   | A     | 5001 | MES  | O2S-S-C8 | -11.97 | 88.64       | 106.73   |
| 3   | B     | 5001 | MES  | O3S-S-C8 | -11.89 | 82.74       | 106.00   |
| 3   | G     | 5001 | MES  | O1S-S-C8 | -10.76 | 90.47       | 106.73   |
| 3   | E     | 5001 | MES  | O3S-S-C8 | -10.31 | 85.83       | 106.00   |
| 3   | C     | 5001 | MES  | O3S-S-C8 | -10.19 | 86.07       | 106.00   |
| 3   | H     | 5001 | MES  | O3S-S-C8 | -10.18 | 86.09       | 106.00   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 3   | A     | 5001 | MES  | O1S-S-C8  | -8.71 | 93.57       | 106.73   |
| 3   | D     | 5001 | MES  | O1S-S-C8  | -8.39 | 94.06       | 106.73   |
| 3   | G     | 5001 | MES  | O2S-S-C8  | -7.80 | 94.94       | 106.73   |
| 3   | A     | 5001 | MES  | O3S-S-C8  | -7.41 | 91.51       | 106.00   |
| 3   | D     | 5001 | MES  | O3S-S-O2S | 7.12  | 129.22      | 111.40   |
| 3   | E     | 5001 | MES  | C5-N4-C3  | 6.52  | 122.89      | 108.84   |
| 3   | D     | 5001 | MES  | C5-N4-C3  | 6.07  | 121.93      | 108.84   |
| 3   | F     | 5001 | MES  | C5-N4-C3  | 5.86  | 121.46      | 108.84   |
| 3   | B     | 5001 | MES  | O2S-S-C8  | -5.74 | 98.05       | 106.73   |
| 3   | D     | 5001 | MES  | C7-N4-C5  | 5.35  | 125.50      | 111.24   |
| 3   | C     | 5001 | MES  | C5-N4-C3  | 5.18  | 120.00      | 108.84   |
| 3   | E     | 5001 | MES  | C7-N4-C5  | 4.87  | 124.23      | 111.24   |
| 3   | E     | 5001 | MES  | O3S-S-O1S | 4.84  | 123.50      | 111.40   |
| 3   | E     | 5001 | MES  | O2S-S-C8  | -4.78 | 99.50       | 106.73   |
| 3   | H     | 5001 | MES  | C5-N4-C3  | 4.78  | 119.14      | 108.84   |
| 3   | G     | 5001 | MES  | C5-N4-C3  | 4.75  | 119.07      | 108.84   |
| 3   | B     | 5001 | MES  | O3S-S-O2S | 4.71  | 123.18      | 111.40   |
| 3   | A     | 5001 | MES  | C7-N4-C3  | 4.68  | 123.72      | 111.24   |
| 3   | D     | 5001 | MES  | C6-C5-N4  | -4.49 | 103.29      | 110.12   |
| 3   | D     | 5001 | MES  | O3S-S-O1S | 4.42  | 122.45      | 111.40   |
| 3   | B     | 5001 | MES  | C5-N4-C3  | 4.39  | 118.30      | 108.84   |
| 3   | F     | 5001 | MES  | C7-N4-C3  | 4.33  | 122.78      | 111.24   |
| 3   | H     | 5001 | MES  | C2-C3-N4  | -4.25 | 103.66      | 110.12   |
| 3   | E     | 5001 | MES  | C6-C5-N4  | 4.00  | 116.20      | 110.12   |
| 3   | E     | 5001 | MES  | O1S-S-C8  | -3.92 | 100.80      | 106.73   |
| 3   | G     | 5001 | MES  | C2-C3-N4  | 3.82  | 115.93      | 110.12   |
| 3   | D     | 5001 | MES  | O3S-S-C8  | -3.79 | 98.60       | 106.00   |
| 3   | B     | 5001 | MES  | C7-N4-C5  | 3.72  | 121.16      | 111.24   |
| 3   | A     | 5001 | MES  | O3S-S-O1S | 3.70  | 120.66      | 111.40   |
| 3   | A     | 5001 | MES  | O3S-S-O2S | 3.68  | 120.60      | 111.40   |
| 3   | A     | 5001 | MES  | C5-N4-C3  | 3.57  | 116.53      | 108.84   |
| 3   | B     | 5001 | MES  | C7-N4-C3  | 3.49  | 120.53      | 111.24   |
| 3   | H     | 5001 | MES  | C7-N4-C5  | 3.46  | 120.46      | 111.24   |
| 3   | H     | 5001 | MES  | C7-N4-C3  | 3.44  | 120.40      | 111.24   |
| 3   | H     | 5001 | MES  | C6-C5-N4  | -3.43 | 104.91      | 110.12   |
| 3   | G     | 5001 | MES  | C7-N4-C3  | 3.38  | 120.24      | 111.24   |
| 3   | C     | 5001 | MES  | C6-C5-N4  | -3.37 | 105.00      | 110.12   |
| 3   | C     | 5001 | MES  | C2-C3-N4  | -3.36 | 105.02      | 110.12   |
| 3   | G     | 5001 | MES  | O3S-S-O2S | 3.36  | 119.80      | 111.40   |
| 3   | C     | 5001 | MES  | C7-N4-C3  | 3.29  | 120.00      | 111.24   |
| 3   | C     | 5001 | MES  | C7-N4-C5  | 3.29  | 120.00      | 111.24   |
| 3   | H     | 5001 | MES  | O3S-S-O1S | 3.26  | 119.55      | 111.40   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 3   | C     | 5001 | MES  | O3S-S-O2S | 3.26  | 119.54      | 111.40   |
| 3   | C     | 5001 | MES  | O3S-S-O1S | 3.25  | 119.52      | 111.40   |
| 3   | H     | 5001 | MES  | O3S-S-O2S | 3.24  | 119.50      | 111.40   |
| 3   | A     | 5001 | MES  | C7-N4-C5  | 3.19  | 119.75      | 111.24   |
| 3   | G     | 5001 | MES  | C7-N4-C5  | 3.18  | 119.71      | 111.24   |
| 3   | F     | 5001 | MES  | C6-C5-N4  | 3.16  | 114.93      | 110.12   |
| 3   | F     | 5001 | MES  | O2S-S-C8  | 2.99  | 111.25      | 106.73   |
| 3   | E     | 5001 | MES  | O1-C6-C5  | 2.99  | 118.21      | 111.77   |
| 3   | B     | 5001 | MES  | O1-C2-C3  | -2.98 | 105.36      | 111.77   |
| 3   | G     | 5001 | MES  | O3S-S-O1S | 2.96  | 118.81      | 111.40   |
| 3   | B     | 5001 | MES  | C6-C5-N4  | 2.94  | 114.59      | 110.12   |
| 3   | F     | 5001 | MES  | O3S-S-C8  | 2.79  | 111.46      | 106.00   |
| 3   | B     | 5001 | MES  | O3S-S-O1S | 2.78  | 118.36      | 111.40   |
| 3   | G     | 5001 | MES  | C8-C7-N4  | 2.56  | 122.06      | 112.36   |
| 3   | F     | 5001 | MES  | O1S-S-C8  | 2.51  | 110.53      | 106.73   |
| 3   | E     | 5001 | MES  | C2-C3-N4  | 2.51  | 113.93      | 110.12   |
| 3   | E     | 5001 | MES  | C6-O1-C2  | 2.46  | 117.84      | 109.88   |
| 3   | B     | 5001 | MES  | C2-C3-N4  | -2.38 | 106.50      | 110.12   |
| 3   | A     | 5001 | MES  | C2-C3-N4  | -2.38 | 106.50      | 110.12   |
| 3   | D     | 5001 | MES  | C2-C3-N4  | 2.12  | 113.34      | 110.12   |
| 3   | E     | 5001 | MES  | O3S-S-O2S | 2.04  | 116.51      | 111.40   |

There are no chirality outliers.

All (13) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 3   | A     | 5001 | MES  | C8-C7-N4-C3 |
| 3   | C     | 5001 | MES  | C8-C7-N4-C5 |
| 3   | D     | 5001 | MES  | C8-C7-N4-C5 |
| 3   | D     | 5001 | MES  | C7-C8-S-O1S |
| 3   | D     | 5001 | MES  | C7-C8-S-O2S |
| 3   | E     | 5001 | MES  | C8-C7-N4-C5 |
| 3   | F     | 5001 | MES  | C8-C7-N4-C3 |
| 3   | G     | 5001 | MES  | C8-C7-N4-C5 |
| 3   | H     | 5001 | MES  | C8-C7-N4-C5 |
| 3   | D     | 5001 | MES  | C7-C8-S-O3S |
| 3   | B     | 5001 | MES  | C8-C7-N4-C5 |
| 3   | C     | 5001 | MES  | C8-C7-N4-C3 |
| 3   | A     | 5001 | MES  | C8-C7-N4-C5 |

There are no ring outliers.

3 monomers are involved in 4 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | B     | 5001 | MES  | 2       | 0            |
| 3   | D     | 5001 | MES  | 1       | 0            |
| 3   | H     | 5001 | MES  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|------------------|--------|----------------|-----------------------|-------|
| 1   | A     | 844/844 (100%)   | -0.11  | 19 (2%) 61 64  | 18, 30, 49, 66        | 0     |
| 1   | B     | 844/844 (100%)   | 0.28   | 34 (4%) 42 44  | 27, 37, 52, 70        | 0     |
| 1   | C     | 844/844 (100%)   | -0.16  | 20 (2%) 59 62  | 22, 30, 45, 61        | 0     |
| 1   | D     | 844/844 (100%)   | -0.12  | 20 (2%) 59 62  | 21, 30, 47, 64        | 0     |
| 1   | E     | 844/844 (100%)   | -0.05  | 31 (3%) 45 47  | 19, 29, 53, 70        | 0     |
| 1   | F     | 844/844 (100%)   | 0.35   | 34 (4%) 42 44  | 26, 38, 54, 65        | 0     |
| 1   | G     | 844/844 (100%)   | -0.25  | 21 (2%) 58 61  | 19, 28, 45, 62        | 0     |
| 1   | H     | 844/844 (100%)   | -0.17  | 21 (2%) 58 61  | 21, 30, 44, 61        | 0     |
| All | All   | 6752/6752 (100%) | -0.03  | 200 (2%) 52 55 | 18, 32, 50, 70        | 0     |

All (200) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | F     | 667  | GLY  | 7.5  |
| 1   | C     | 320  | HIS  | 5.9  |
| 1   | H     | 245  | PHE  | 5.9  |
| 1   | A     | 320  | HIS  | 5.8  |
| 1   | E     | 320  | HIS  | 5.7  |
| 1   | B     | 1087 | PRO  | 5.6  |
| 1   | A     | 244  | SER  | 5.5  |
| 1   | D     | 1076 | ASP  | 5.4  |
| 1   | B     | 244  | SER  | 5.4  |
| 1   | D     | 320  | HIS  | 5.4  |
| 1   | B     | 1076 | ASP  | 5.4  |
| 1   | F     | 320  | HIS  | 5.3  |
| 1   | H     | 320  | HIS  | 4.8  |
| 1   | E     | 1082 | LYS  | 4.8  |
| 1   | A     | 1087 | PRO  | 4.6  |
| 1   | B     | 320  | HIS  | 4.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | C     | 244  | SER  | 4.5  |
| 1   | H     | 1083 | SER  | 4.5  |
| 1   | A     | 1076 | ASP  | 4.4  |
| 1   | H     | 1076 | ASP  | 4.4  |
| 1   | C     | 1087 | PRO  | 4.3  |
| 1   | B     | 1077 | ASN  | 4.3  |
| 1   | D     | 394  | LYS  | 4.0  |
| 1   | B     | 1075 | SER  | 4.0  |
| 1   | H     | 244  | SER  | 4.0  |
| 1   | D     | 667  | GLY  | 4.0  |
| 1   | E     | 244  | SER  | 3.9  |
| 1   | B     | 282  | LYS  | 3.9  |
| 1   | H     | 1065 | GLN  | 3.9  |
| 1   | G     | 320  | HIS  | 3.8  |
| 1   | G     | 1087 | PRO  | 3.8  |
| 1   | G     | 244  | SER  | 3.7  |
| 1   | E     | 1087 | PRO  | 3.7  |
| 1   | C     | 1086 | ASN  | 3.7  |
| 1   | F     | 785  | ALA  | 3.7  |
| 1   | C     | 1065 | GLN  | 3.7  |
| 1   | C     | 1075 | SER  | 3.7  |
| 1   | B     | 1074 | VAL  | 3.6  |
| 1   | E     | 1076 | ASP  | 3.6  |
| 1   | A     | 1086 | ASN  | 3.5  |
| 1   | F     | 1087 | PRO  | 3.5  |
| 1   | B     | 247  | GLN  | 3.5  |
| 1   | F     | 244  | SER  | 3.5  |
| 1   | D     | 1087 | PRO  | 3.4  |
| 1   | E     | 280  | ASP  | 3.4  |
| 1   | H     | 1082 | LYS  | 3.4  |
| 1   | G     | 1076 | ASP  | 3.4  |
| 1   | B     | 1065 | GLN  | 3.4  |
| 1   | D     | 782  | GLN  | 3.3  |
| 1   | E     | 1065 | GLN  | 3.3  |
| 1   | F     | 793  | ASP  | 3.3  |
| 1   | H     | 1087 | PRO  | 3.2  |
| 1   | A     | 1077 | ASN  | 3.2  |
| 1   | E     | 1086 | ASN  | 3.1  |
| 1   | F     | 1076 | ASP  | 3.1  |
| 1   | A     | 1075 | SER  | 3.1  |
| 1   | G     | 394  | LYS  | 3.1  |
| 1   | B     | 667  | GLY  | 3.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | F     | 371  | ASN  | 3.1  |
| 1   | C     | 1076 | ASP  | 3.1  |
| 1   | B     | 289  | GLU  | 3.1  |
| 1   | D     | 244  | SER  | 3.1  |
| 1   | H     | 726  | ARG  | 3.1  |
| 1   | B     | 394  | LYS  | 3.0  |
| 1   | D     | 1065 | GLN  | 3.0  |
| 1   | E     | 247  | GLN  | 3.0  |
| 1   | A     | 606  | ASN  | 3.0  |
| 1   | B     | 371  | ASN  | 3.0  |
| 1   | F     | 394  | LYS  | 3.0  |
| 1   | F     | 782  | GLN  | 3.0  |
| 1   | A     | 290  | LYS  | 3.0  |
| 1   | G     | 1065 | GLN  | 2.9  |
| 1   | B     | 747  | ALA  | 2.9  |
| 1   | F     | 1082 | LYS  | 2.9  |
| 1   | A     | 868  | THR  | 2.9  |
| 1   | E     | 288  | THR  | 2.9  |
| 1   | F     | 726  | ARG  | 2.9  |
| 1   | F     | 773  | ASN  | 2.9  |
| 1   | H     | 246  | ALA  | 2.9  |
| 1   | H     | 1086 | ASN  | 2.9  |
| 1   | E     | 318  | GLY  | 2.9  |
| 1   | E     | 321  | GLN  | 2.9  |
| 1   | G     | 747  | ALA  | 2.9  |
| 1   | F     | 1002 | ASP  | 2.8  |
| 1   | B     | 1082 | LYS  | 2.8  |
| 1   | F     | 1077 | ASN  | 2.8  |
| 1   | E     | 348  | THR  | 2.8  |
| 1   | C     | 1082 | LYS  | 2.8  |
| 1   | D     | 1086 | ASN  | 2.8  |
| 1   | B     | 794  | ARG  | 2.7  |
| 1   | E     | 352  | ASN  | 2.7  |
| 1   | E     | 371  | ASN  | 2.7  |
| 1   | E     | 349  | ALA  | 2.7  |
| 1   | B     | 325  | THR  | 2.7  |
| 1   | F     | 350  | GLU  | 2.7  |
| 1   | B     | 724  | GLY  | 2.7  |
| 1   | F     | 786  | GLY  | 2.7  |
| 1   | C     | 1077 | ASN  | 2.7  |
| 1   | G     | 371  | ASN  | 2.7  |
| 1   | F     | 747  | ALA  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | C     | 371  | ASN  | 2.7  |
| 1   | C     | 606  | ASN  | 2.7  |
| 1   | D     | 371  | ASN  | 2.7  |
| 1   | B     | 468  | ASP  | 2.7  |
| 1   | F     | 1065 | GLN  | 2.6  |
| 1   | D     | 999  | SER  | 2.6  |
| 1   | C     | 785  | ALA  | 2.6  |
| 1   | C     | 1066 | ALA  | 2.6  |
| 1   | G     | 782  | GLN  | 2.6  |
| 1   | G     | 1086 | ASN  | 2.6  |
| 1   | F     | 723  | THR  | 2.6  |
| 1   | E     | 325  | THR  | 2.6  |
| 1   | E     | 290  | LYS  | 2.5  |
| 1   | F     | 727  | ILE  | 2.5  |
| 1   | F     | 1075 | SER  | 2.5  |
| 1   | D     | 1082 | LYS  | 2.5  |
| 1   | D     | 606  | ASN  | 2.5  |
| 1   | H     | 321  | GLN  | 2.5  |
| 1   | G     | 1066 | ALA  | 2.5  |
| 1   | G     | 322  | THR  | 2.4  |
| 1   | B     | 290  | LYS  | 2.4  |
| 1   | B     | 870  | LYS  | 2.4  |
| 1   | B     | 782  | GLN  | 2.4  |
| 1   | A     | 322  | THR  | 2.4  |
| 1   | C     | 726  | ARG  | 2.4  |
| 1   | H     | 394  | LYS  | 2.4  |
| 1   | H     | 606  | ASN  | 2.4  |
| 1   | D     | 247  | GLN  | 2.4  |
| 1   | F     | 753  | VAL  | 2.4  |
| 1   | B     | 1063 | LYS  | 2.4  |
| 1   | F     | 282  | LYS  | 2.4  |
| 1   | H     | 1066 | ALA  | 2.4  |
| 1   | F     | 321  | GLN  | 2.4  |
| 1   | G     | 1077 | ASN  | 2.4  |
| 1   | B     | 321  | GLN  | 2.3  |
| 1   | F     | 1086 | ASN  | 2.3  |
| 1   | D     | 726  | ARG  | 2.3  |
| 1   | F     | 750  | ARG  | 2.3  |
| 1   | G     | 726  | ARG  | 2.3  |
| 1   | B     | 632  | GLU  | 2.3  |
| 1   | E     | 289  | GLU  | 2.3  |
| 1   | E     | 350  | GLU  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | E     | 322  | THR  | 2.3  |
| 1   | D     | 1066 | ALA  | 2.3  |
| 1   | H     | 785  | ALA  | 2.3  |
| 1   | A     | 726  | ARG  | 2.3  |
| 1   | B     | 278  | LEU  | 2.3  |
| 1   | E     | 1077 | ASN  | 2.3  |
| 1   | A     | 793  | ASP  | 2.3  |
| 1   | A     | 1066 | ALA  | 2.3  |
| 1   | G     | 290  | LYS  | 2.3  |
| 1   | E     | 330  | LEU  | 2.3  |
| 1   | A     | 321  | GLN  | 2.2  |
| 1   | B     | 1086 | ASN  | 2.2  |
| 1   | F     | 1066 | ALA  | 2.2  |
| 1   | B     | 744  | ARG  | 2.2  |
| 1   | E     | 282  | LYS  | 2.2  |
| 1   | G     | 606  | ASN  | 2.2  |
| 1   | G     | 912  | ILE  | 2.2  |
| 1   | H     | 371  | ASN  | 2.2  |
| 1   | E     | 1085 | VAL  | 2.2  |
| 1   | D     | 349  | ALA  | 2.2  |
| 1   | F     | 819  | TRP  | 2.2  |
| 1   | E     | 394  | LYS  | 2.2  |
| 1   | G     | 1082 | LYS  | 2.2  |
| 1   | D     | 1077 | ASN  | 2.2  |
| 1   | H     | 1077 | ASN  | 2.2  |
| 1   | B     | 326  | ALA  | 2.2  |
| 1   | F     | 826  | ALA  | 2.2  |
| 1   | D     | 248  | TYR  | 2.2  |
| 1   | G     | 746  | LYS  | 2.2  |
| 1   | B     | 606  | ASN  | 2.2  |
| 1   | H     | 1074 | VAL  | 2.1  |
| 1   | C     | 318  | GLY  | 2.1  |
| 1   | E     | 303  | GLN  | 2.1  |
| 1   | B     | 785  | ALA  | 2.1  |
| 1   | C     | 290  | LYS  | 2.1  |
| 1   | G     | 468  | ASP  | 2.1  |
| 1   | C     | 322  | THR  | 2.1  |
| 1   | A     | 1065 | GLN  | 2.1  |
| 1   | C     | 321  | GLN  | 2.1  |
| 1   | E     | 277  | ILE  | 2.1  |
| 1   | F     | 349  | ALA  | 2.1  |
| 1   | F     | 290  | LYS  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | F     | 626  | LYS  | 2.1  |
| 1   | H     | 290  | LYS  | 2.1  |
| 1   | E     | 329  | PRO  | 2.1  |
| 1   | D     | 1085 | VAL  | 2.1  |
| 1   | C     | 632  | GLU  | 2.1  |
| 1   | C     | 793  | ASP  | 2.1  |
| 1   | E     | 327  | THR  | 2.1  |
| 1   | H     | 322  | THR  | 2.1  |
| 1   | B     | 355  | TRP  | 2.1  |
| 1   | A     | 289  | GLU  | 2.0  |
| 1   | F     | 289  | GLU  | 2.0  |
| 1   | E     | 316  | GLN  | 2.0  |
| 1   | A     | 602  | GLU  | 2.0  |
| 1   | B     | 784  | ALA  | 2.0  |
| 1   | G     | 321  | GLN  | 2.0  |
| 1   | A     | 318  | GLY  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 3   | MES  | F     | 5001 | 12/12 | 0.91 | 0.19 | 2,16,32,98                  | 0     |
| 3   | MES  | H     | 5001 | 12/12 | 0.91 | 0.22 | 5,22,93,99                  | 0     |
| 3   | MES  | B     | 5001 | 12/12 | 0.94 | 0.22 | 6,13,15,16                  | 0     |
| 3   | MES  | C     | 5001 | 12/12 | 0.94 | 0.26 | 2,2,7,10                    | 0     |
| 3   | MES  | A     | 5001 | 12/12 | 0.96 | 0.16 | 22,22,62,81                 | 0     |
| 3   | MES  | D     | 5001 | 12/12 | 0.96 | 0.21 | 2,6,13,14                   | 0     |
| 3   | MES  | G     | 5001 | 12/12 | 0.97 | 0.14 | 4,8,15,21                   | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 3   | MES  | E     | 5001 | 12/12 | 0.97 | 0.09 | 19,24,27,28                 | 0     |
| 2   | CA   | E     | 4001 | 1/1   | 0.98 | 0.06 | 18,18,18,18                 | 0     |
| 2   | CA   | B     | 4001 | 1/1   | 0.98 | 0.12 | 19,19,19,19                 | 0     |
| 2   | CA   | D     | 4001 | 1/1   | 0.98 | 0.07 | 18,18,18,18                 | 0     |
| 2   | CA   | A     | 4001 | 1/1   | 0.99 | 0.03 | 17,17,17,17                 | 0     |
| 2   | CA   | C     | 4001 | 1/1   | 0.99 | 0.05 | 17,17,17,17                 | 0     |
| 2   | CA   | F     | 4001 | 1/1   | 0.99 | 0.09 | 16,16,16,16                 | 0     |
| 2   | CA   | H     | 4001 | 1/1   | 0.99 | 0.02 | 18,18,18,18                 | 0     |
| 2   | CA   | G     | 4001 | 1/1   | 1.00 | 0.02 | 16,16,16,16                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.