



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:18 AM UTC

PDB ID : 7ZVE / pdb\_00007zve  
Title : K403 acetylated glucose-6-phosphate dehydrogenase (G6PD)  
Authors : Wu, F.; Muskat, N.H.; Shahar, A.; Arbely, E.  
Deposited on : 2022-05-15  
Resolution : 2.28 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

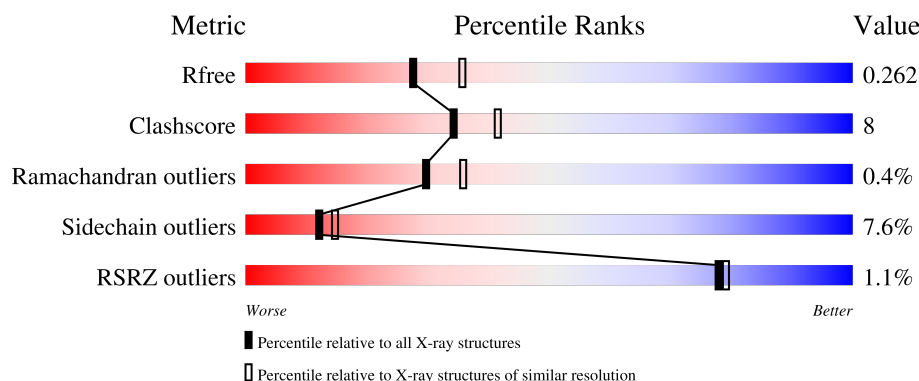
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.28 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                      | 9078 (2.30-2.26)                                      |
| Clashscore            | 190562                      | 9802 (2.30-2.26)                                      |
| Ramachandran outliers | 187476                      | 9690 (2.30-2.26)                                      |
| Sidechain outliers    | 187428                      | 9691 (2.30-2.26)                                      |
| RSRZ outliers         | 180081                      | 9085 (2.30-2.26)                                      |

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     | 501    | <div> <div>%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div>..</div> </div> </div> |
| 2   | B     | 498    | <div> <div>%</div> <div> <div></div> <div>74%</div> <div>21%</div> <div>..</div> </div> </div> |
| 3   | C     | 497    | <div> <div>%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>..</div> </div> </div> |
| 4   | D     | 499    | <div> <div></div> <div> <div>76%</div> <div>20%</div> <div>..</div> </div> </div>              |
| 4   | H     | 499    | <div> <div>%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div>..</div> </div> </div> |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 5   | E     | 500    |  |
| 6   | F     | 497    |  |
| 7   | G     | 496    |  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | ALY  | B     | 403 | -         | -        | X       | -                |
| 8   | GOL  | B     | 602 | -         | -        | X       | -                |
| 8   | GOL  | E     | 601 | -         | -        | X       | -                |

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 32772 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 Glucose-6-phosphate 1-dehydrogenase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 501      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4053  | 2582 | 706 | 744 | 21 |         |         |       |

- Molecule 2 is a protein called Glucose-6-phosphate 1-dehydrogenase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 498      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4036  | 2572 | 703 | 740 | 21 |         |         |       |

- Molecule 3 is a protein called Glucose-6-phosphate 1-dehydrogenase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | C     | 497      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 4039  | 2574 | 705 | 739 | 21 |         |         |       |

- Molecule 4 is a protein called Glucose-6-phosphate 1-dehydrogenase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4   | D     | 499      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 4051  | 2582 | 707 | 741 | 21 |         |         |       |
| 4   | H     | 499      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4043  | 2577 | 704 | 741 | 21 |         |         |       |

- Molecule 5 is a protein called Glucose-6-phosphate 1-dehydrogenase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 5   | E     | 500      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4052  | 2582 | 705 | 744 | 21 |         |         |       |

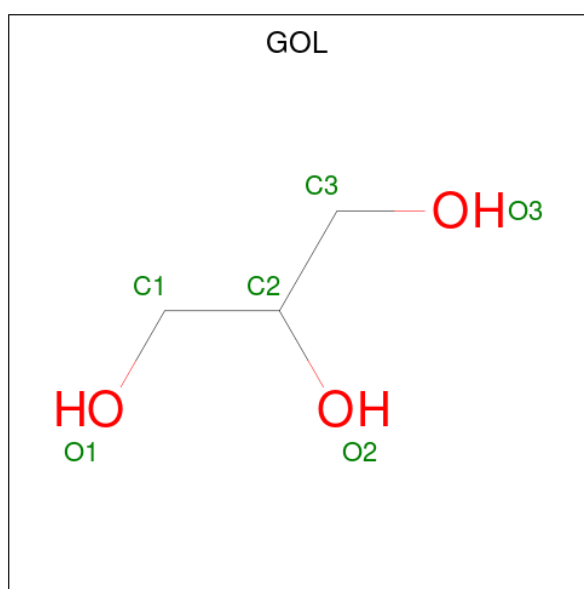
- Molecule 6 is a protein called Glucose-6-phosphate 1-dehydrogenase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 6   | F     | 497      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4028  | 2567 | 702 | 738 | 21 |         |         |       |

- Molecule 7 is a protein called Glucose-6-phosphate 1-dehydrogenase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 7   | G     | 496      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4023  | 2563 | 701 | 738 | 21 |         |         |       |

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 8   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 8   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 8   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 8   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 8   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 8   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 8   | G     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 8   | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |

- Molecule 9 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 9   | J     | 1        | Total | Cu | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

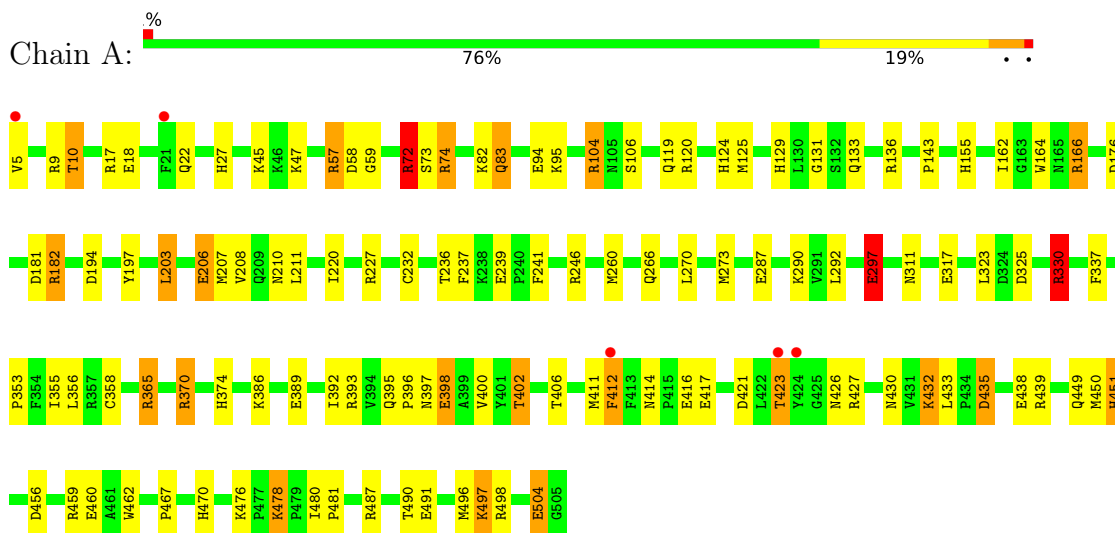
- Molecule 10 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 10  | I     | 398      | Total | O   | 0       | 0       |
|     |       |          | 398   | 398 |         |         |

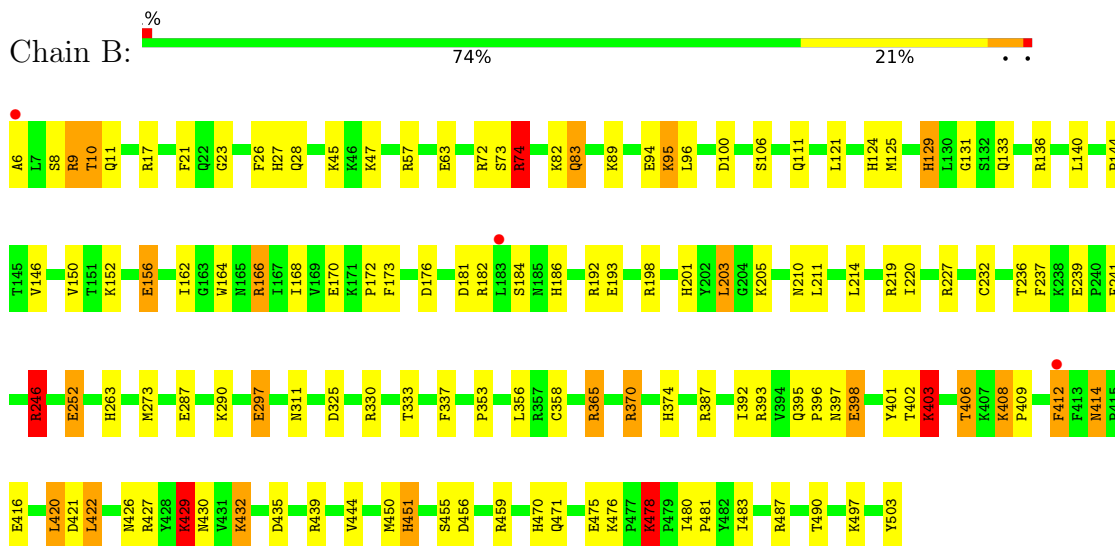
### 3 Residue-property plots [i](#)

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.

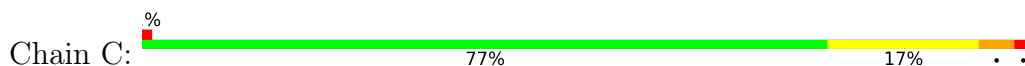
- Molecule 1: Glucose-6-phosphate 1-dehydrogenase

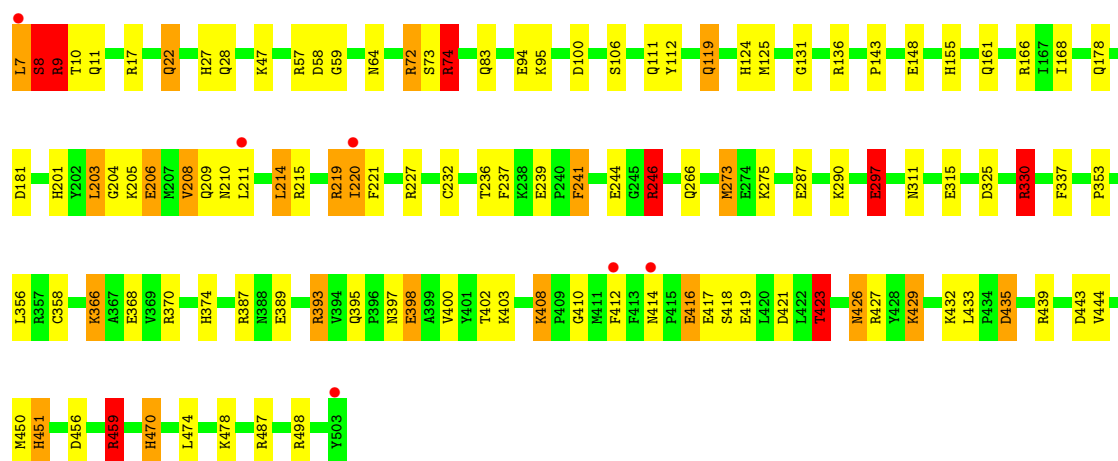


- Molecule 2: Glucose-6-phosphate 1-dehydrogenase



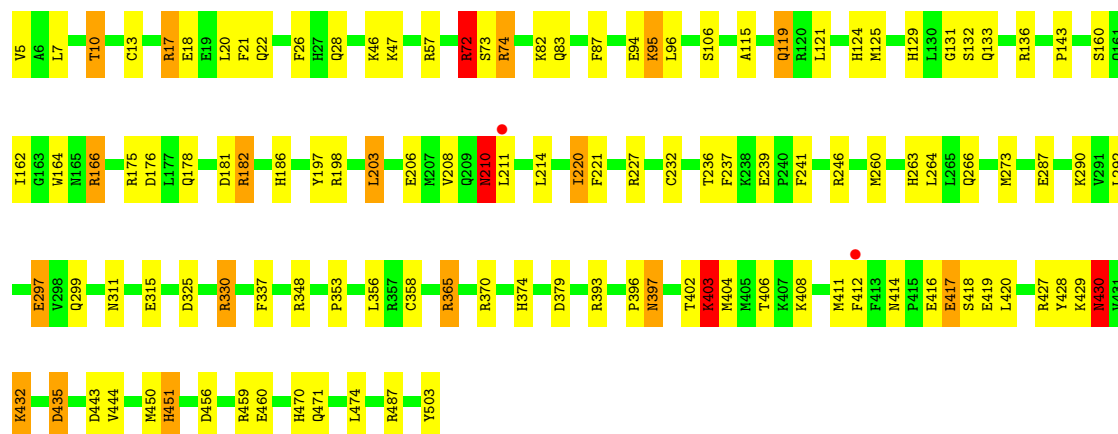
- Molecule 3: Glucose-6-phosphate 1-dehydrogenase





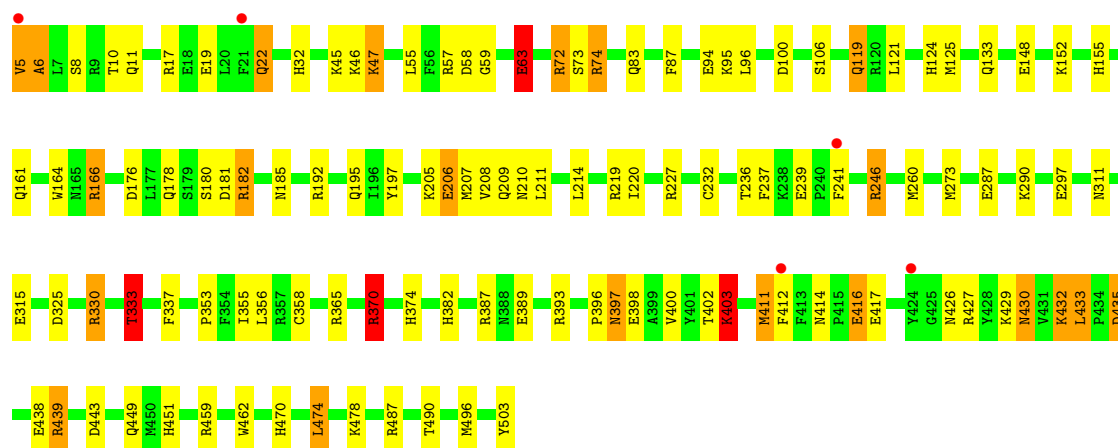
• Molecule 4: Glucose-6-phosphate 1-dehydrogenase

Chain D: 76% 20%

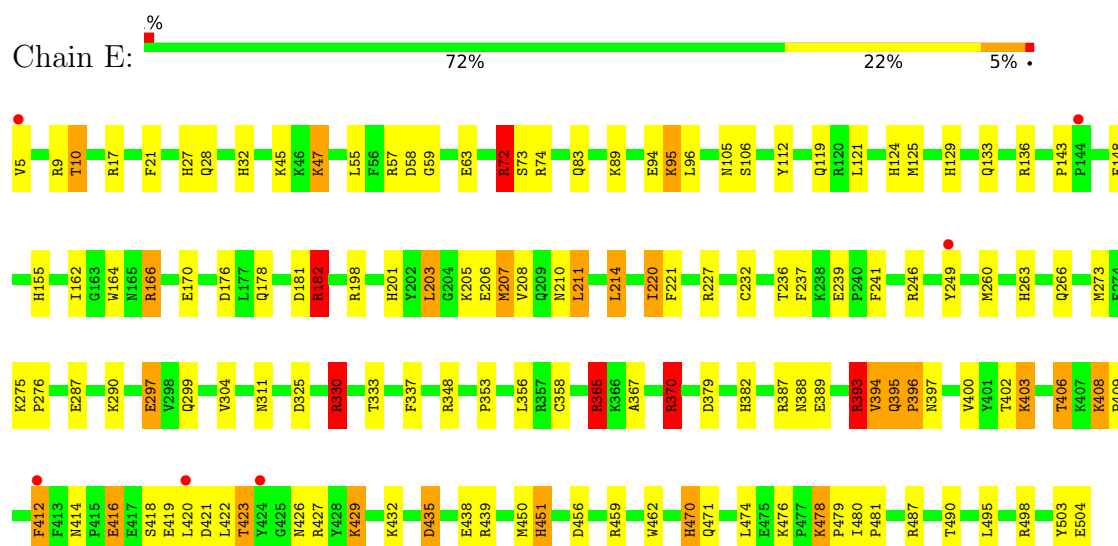


• Molecule 4: Glucose-6-phosphate 1-dehydrogenase

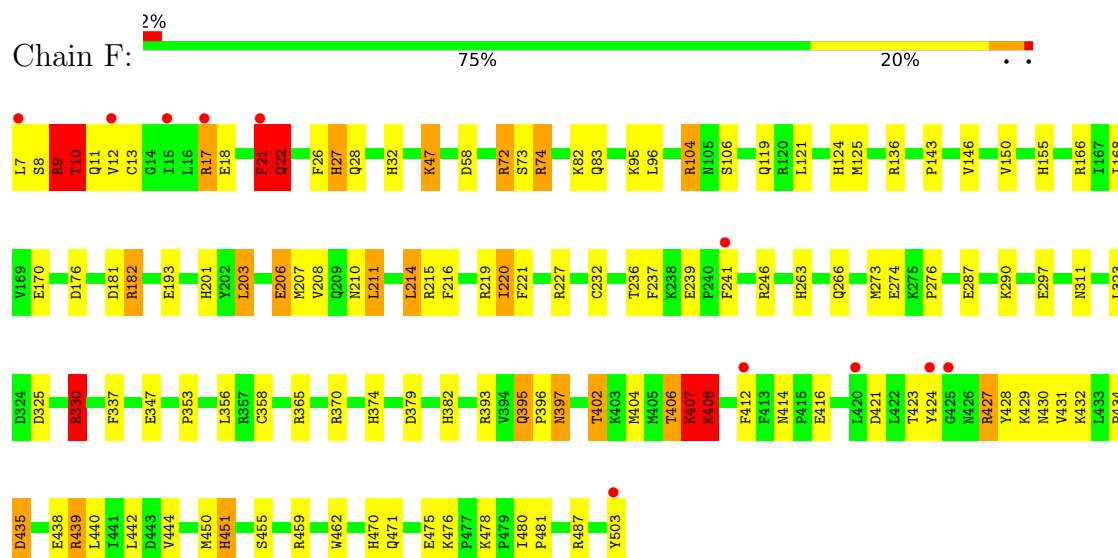
Chain H: 76% 19%



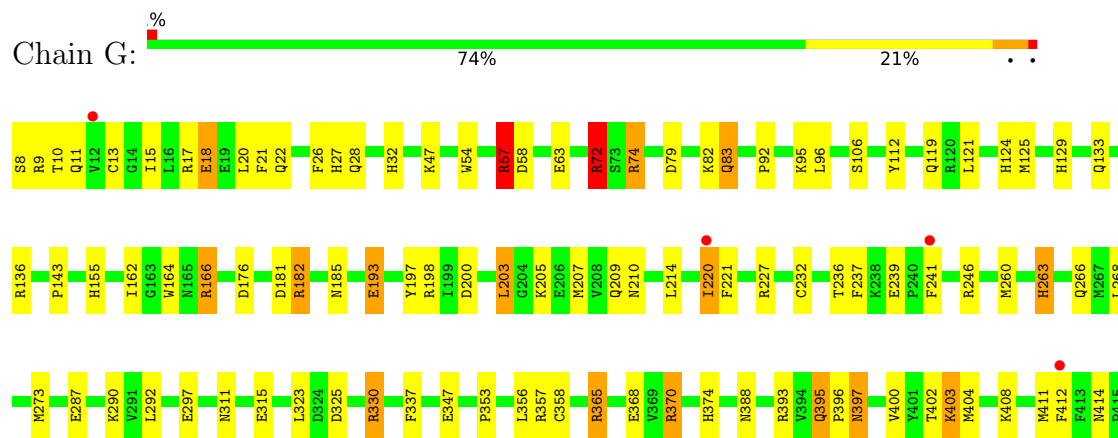
• Molecule 5: Glucose-6-phosphate 1-dehydrogenase

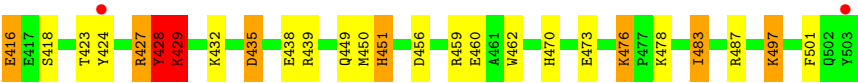


• Molecule 6: Glucose-6-phosphate 1-dehydrogenase



• Molecule 7: Glucose-6-phosphate 1-dehydrogenase





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1                                                         | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 64.36Å 122.61Å 161.31Å<br>77.23° 80.99° 77.40°              | Depositor        |
| Resolution (Å)                                                          | 50.01 – 2.28<br>50.01 – 2.28                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 96.9 (50.01-2.28)<br>96.9 (50.01-2.28)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.59 (at 2.29Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.8.0352                                             | Depositor        |
| R, $R_{free}$                                                           | 0.211 , 0.261<br>0.219 , 0.262                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 10333 reflections (4.88%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 43.7                                                        | Xtriage          |
| Anisotropy                                                              | 0.042                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 35.9                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.96                                                        | EDS              |
| Total number of atoms                                                   | 32772                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 58.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ALY, CU

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

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$     | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 0.94         | 8/4147 (0.2%)   | 1.38        | 30/5606 (0.5%)   |
| 2   | B     | 0.94         | 8/4117 (0.2%)   | 1.35        | 30/5565 (0.5%)   |
| 3   | C     | 0.97         | 11/4123 (0.3%)  | 1.37        | 32/5572 (0.6%)   |
| 4   | D     | 0.92         | 6/4135 (0.1%)   | 1.34        | 25/5589 (0.4%)   |
| 4   | H     | 0.93         | 8/4124 (0.2%)   | 1.35        | 23/5575 (0.4%)   |
| 5   | E     | 0.90         | 10/4133 (0.2%)  | 1.33        | 32/5587 (0.6%)   |
| 6   | F     | 0.99         | 14/4122 (0.3%)  | 1.40        | 27/5572 (0.5%)   |
| 7   | G     | 0.89         | 9/4104 (0.2%)   | 1.35        | 23/5547 (0.4%)   |
| All | All   | 0.94         | 74/33005 (0.2%) | 1.36        | 222/44613 (0.5%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 17                  |
| 2   | B     | 0                   | 16                  |
| 3   | C     | 0                   | 18                  |
| 4   | D     | 0                   | 18                  |
| 4   | H     | 0                   | 16                  |
| 5   | E     | 0                   | 18                  |
| 6   | F     | 0                   | 17                  |
| 7   | G     | 0                   | 19                  |
| All | All   | 0                   | 139                 |

All (74) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | C     | 155 | HIS  | CE1-NE2 | 11.86 | 1.44        | 1.32     |
| 4   | H     | 374 | HIS  | CE1-NE2 | 11.66 | 1.44        | 1.32     |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 4   | H     | 155 | HIS  | CE1-NE2 | 11.02  | 1.43        | 1.32     |
| 6   | F     | 402 | THR  | C-O     | -10.36 | 1.12        | 1.24     |
| 3   | C     | 374 | HIS  | CE1-NE2 | 10.02  | 1.42        | 1.32     |
| 3   | C     | 451 | HIS  | CE1-NE2 | 9.82   | 1.42        | 1.32     |
| 3   | C     | 470 | HIS  | CE1-NE2 | 9.79   | 1.42        | 1.32     |
| 6   | F     | 470 | HIS  | CE1-NE2 | 9.62   | 1.42        | 1.32     |
| 1   | A     | 470 | HIS  | CE1-NE2 | 9.37   | 1.42        | 1.32     |
| 2   | B     | 451 | HIS  | CE1-NE2 | 9.30   | 1.41        | 1.32     |
| 5   | E     | 451 | HIS  | CE1-NE2 | 8.88   | 1.41        | 1.32     |
| 4   | D     | 451 | HIS  | CE1-NE2 | 8.73   | 1.41        | 1.32     |
| 7   | G     | 451 | HIS  | CE1-NE2 | 8.68   | 1.41        | 1.32     |
| 7   | G     | 155 | HIS  | CE1-NE2 | 8.52   | 1.41        | 1.32     |
| 2   | B     | 374 | HIS  | CE1-NE2 | 8.09   | 1.40        | 1.32     |
| 5   | E     | 32  | HIS  | CE1-NE2 | 8.05   | 1.40        | 1.32     |
| 4   | D     | 470 | HIS  | CE1-NE2 | 8.04   | 1.40        | 1.32     |
| 6   | F     | 374 | HIS  | CE1-NE2 | 8.01   | 1.40        | 1.32     |
| 7   | G     | 193 | GLU  | CD-OE2  | 7.90   | 1.40        | 1.25     |
| 1   | A     | 155 | HIS  | CE1-NE2 | 7.83   | 1.40        | 1.32     |
| 1   | A     | 451 | HIS  | CE1-NE2 | 7.52   | 1.40        | 1.32     |
| 6   | F     | 206 | GLU  | CD-OE1  | 7.32   | 1.39        | 1.25     |
| 6   | F     | 155 | HIS  | CE1-NE2 | 7.27   | 1.39        | 1.32     |
| 3   | C     | 27  | HIS  | CE1-NE2 | 7.23   | 1.39        | 1.32     |
| 5   | E     | 155 | HIS  | CE1-NE2 | 7.16   | 1.39        | 1.32     |
| 6   | F     | 402 | THR  | CA-C    | -7.01  | 1.44        | 1.52     |
| 6   | F     | 274 | GLU  | CD-OE1  | 6.93   | 1.38        | 1.25     |
| 6   | F     | 263 | HIS  | CE1-NE2 | 6.92   | 1.39        | 1.32     |
| 4   | D     | 374 | HIS  | CE1-NE2 | 6.77   | 1.39        | 1.32     |
| 1   | A     | 27  | HIS  | CE1-NE2 | 6.77   | 1.39        | 1.32     |
| 2   | B     | 470 | HIS  | CE1-NE2 | 6.72   | 1.39        | 1.32     |
| 6   | F     | 451 | HIS  | CE1-NE2 | 6.71   | 1.39        | 1.32     |
| 4   | D     | 263 | HIS  | CE1-NE2 | 6.61   | 1.39        | 1.32     |
| 7   | G     | 374 | HIS  | CE1-NE2 | 6.59   | 1.39        | 1.32     |
| 1   | A     | 129 | HIS  | CE1-NE2 | 6.57   | 1.39        | 1.32     |
| 2   | B     | 27  | HIS  | CE1-NE2 | 6.47   | 1.39        | 1.32     |
| 5   | E     | 263 | HIS  | CE1-NE2 | 6.39   | 1.39        | 1.32     |
| 3   | C     | 201 | HIS  | CE1-NE2 | 6.21   | 1.38        | 1.32     |
| 4   | H     | 451 | HIS  | CE1-NE2 | 6.19   | 1.38        | 1.32     |
| 7   | G     | 27  | HIS  | CE1-NE2 | 6.18   | 1.38        | 1.32     |
| 6   | F     | 382 | HIS  | CE1-NE2 | 6.14   | 1.38        | 1.32     |
| 7   | G     | 129 | HIS  | CE1-NE2 | 6.08   | 1.38        | 1.32     |
| 4   | H     | 470 | HIS  | CE1-NE2 | 6.02   | 1.38        | 1.32     |
| 3   | C     | 416 | GLU  | CD-OE2  | 5.96   | 1.36        | 1.25     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4   | H     | 32  | HIS  | CE1-NE2 | 5.94 | 1.38        | 1.32     |
| 4   | H     | 148 | GLU  | CD-OE1  | 5.94 | 1.36        | 1.25     |
| 4   | H     | 382 | HIS  | CE1-NE2 | 5.83 | 1.38        | 1.32     |
| 6   | F     | 32  | HIS  | CE1-NE2 | 5.83 | 1.38        | 1.32     |
| 4   | D     | 417 | GLU  | CD-OE2  | 5.76 | 1.36        | 1.25     |
| 5   | E     | 470 | HIS  | CE1-NE2 | 5.67 | 1.38        | 1.32     |
| 6   | F     | 347 | GLU  | CD-OE1  | 5.60 | 1.35        | 1.25     |
| 7   | G     | 470 | HIS  | CE1-NE2 | 5.53 | 1.38        | 1.32     |
| 4   | H     | 416 | GLU  | CD-OE2  | 5.49 | 1.35        | 1.25     |
| 4   | D     | 186 | HIS  | CE1-NE2 | 5.45 | 1.38        | 1.32     |
| 2   | B     | 263 | HIS  | CE1-NE2 | 5.45 | 1.38        | 1.32     |
| 5   | E     | 382 | HIS  | CE1-NE2 | 5.42 | 1.38        | 1.32     |
| 3   | C     | 297 | GLU  | CD-OE1  | 5.38 | 1.35        | 1.25     |
| 3   | C     | 148 | GLU  | CD-OE1  | 5.34 | 1.35        | 1.25     |
| 3   | C     | 143 | PRO  | CA-C    | 5.32 | 1.54        | 1.51     |
| 7   | G     | 263 | HIS  | CE1-NE2 | 5.29 | 1.37        | 1.32     |
| 1   | A     | 374 | HIS  | CE1-NE2 | 5.26 | 1.37        | 1.32     |
| 1   | A     | 297 | GLU  | CD-OE2  | 5.22 | 1.35        | 1.25     |
| 5   | E     | 143 | PRO  | CA-C    | 5.21 | 1.54        | 1.51     |
| 5   | E     | 416 | GLU  | CD-OE2  | 5.16 | 1.35        | 1.25     |
| 2   | B     | 297 | GLU  | CD-OE2  | 5.15 | 1.35        | 1.25     |
| 5   | E     | 129 | HIS  | CE1-NE2 | 5.13 | 1.37        | 1.32     |
| 2   | B     | 129 | HIS  | CE1-NE2 | 5.11 | 1.37        | 1.32     |
| 5   | E     | 27  | HIS  | CE1-NE2 | 5.09 | 1.37        | 1.32     |
| 1   | A     | 491 | GLU  | CD-OE1  | 5.08 | 1.35        | 1.25     |
| 6   | F     | 207 | MET  | CG-SD   | 5.05 | 1.93        | 1.80     |
| 6   | F     | 27  | HIS  | CE1-NE2 | 5.04 | 1.37        | 1.32     |
| 3   | C     | 273 | MET  | CG-SD   | 5.04 | 1.93        | 1.80     |
| 2   | B     | 186 | HIS  | CE1-NE2 | 5.02 | 1.37        | 1.32     |
| 7   | G     | 32  | HIS  | CE1-NE2 | 5.01 | 1.37        | 1.32     |

All (222) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 6   | F     | 402 | THR  | CA-C-O    | -21.53 | 97.42       | 120.24   |
| 1   | A     | 10  | THR  | CA-CB-OG1 | -13.53 | 89.31       | 109.60   |
| 3   | C     | 423 | THR  | CB-CA-C   | 11.14  | 128.12      | 110.96   |
| 1   | A     | 423 | THR  | CB-CA-C   | 10.85  | 127.67      | 110.96   |
| 7   | G     | 10  | THR  | N-CA-CB   | 10.70  | 126.33      | 110.49   |
| 7   | G     | 193 | GLU  | CB-CG-CD  | 9.98   | 129.57      | 112.60   |
| 6   | F     | 21  | PHE  | CA-CB-CG  | -9.98  | 103.82      | 113.80   |
| 1   | A     | 414 | ASN  | CB-CA-C   | 9.88   | 120.40      | 110.33   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 7   | G     | 395 | GLN  | CB-CG-CD  | 9.83  | 129.31      | 112.60   |
| 6   | F     | 330 | ARG  | CB-CA-C   | 9.70  | 126.24      | 109.65   |
| 4   | D     | 414 | ASN  | CB-CA-C   | 9.41  | 119.93      | 110.33   |
| 3   | C     | 22  | GLN  | CB-CG-CD  | 9.31  | 128.42      | 112.60   |
| 6   | F     | 402 | THR  | O-C-N     | 9.22  | 134.06      | 123.27   |
| 7   | G     | 414 | ASN  | CB-CA-C   | 8.97  | 119.48      | 110.33   |
| 5   | E     | 414 | ASN  | CB-CA-C   | 8.96  | 119.47      | 110.33   |
| 3   | C     | 414 | ASN  | CB-CA-C   | 8.56  | 119.06      | 110.33   |
| 6   | F     | 414 | ASN  | CB-CA-C   | 8.55  | 119.05      | 110.33   |
| 1   | A     | 435 | ASP  | CB-CA-C   | -8.55 | 93.41       | 110.42   |
| 4   | D     | 435 | ASP  | CA-CB-CG  | -8.46 | 104.14      | 112.60   |
| 1   | A     | 83  | GLN  | CB-CG-CD  | 8.16  | 126.47      | 112.60   |
| 2   | B     | 397 | ASN  | CB-CA-C   | -8.12 | 98.36       | 110.62   |
| 3   | C     | 74  | ARG  | CB-CG-CD  | 8.00  | 129.71      | 111.30   |
| 4   | H     | 414 | ASN  | CB-CA-C   | 7.99  | 118.48      | 110.33   |
| 5   | E     | 395 | GLN  | CB-CG-CD  | 7.96  | 126.13      | 112.60   |
| 7   | G     | 412 | PHE  | CA-CB-CG  | 7.87  | 121.67      | 113.80   |
| 7   | G     | 18  | GLU  | CB-CA-C   | 7.85  | 125.74      | 110.67   |
| 5   | E     | 83  | GLN  | CB-CG-CD  | 7.83  | 125.91      | 112.60   |
| 6   | F     | 236 | THR  | CA-CB-OG1 | -7.82 | 97.86       | 109.60   |
| 1   | A     | 10  | THR  | CA-CB-CG2 | 7.81  | 123.78      | 110.50   |
| 7   | G     | 429 | LYS  | CB-CA-C   | 7.78  | 125.90      | 110.42   |
| 4   | H     | 333 | THR  | CA-CB-OG1 | -7.76 | 97.96       | 109.60   |
| 4   | D     | 503 | TYR  | CA-C-O    | -7.63 | 107.83      | 120.80   |
| 3   | C     | 443 | ASP  | CA-CB-CG  | 7.61  | 120.21      | 112.60   |
| 3   | C     | 236 | THR  | CA-CB-OG1 | -7.61 | 98.19       | 109.60   |
| 4   | H     | 503 | TYR  | CA-C-O    | -7.57 | 107.93      | 120.80   |
| 2   | B     | 414 | ASN  | CB-CA-C   | 7.54  | 118.02      | 110.33   |
| 2   | B     | 156 | GLU  | CB-CG-CD  | 7.51  | 125.36      | 112.60   |
| 3   | C     | 397 | ASN  | CA-CB-CG  | -7.41 | 105.19      | 112.60   |
| 2   | B     | 236 | THR  | CA-CB-OG1 | -7.41 | 98.48       | 109.60   |
| 6   | F     | 9   | ARG  | CB-CG-CD  | 7.34  | 128.18      | 111.30   |
| 1   | A     | 236 | THR  | CA-CB-OG1 | -7.31 | 98.63       | 109.60   |
| 4   | D     | 236 | THR  | CA-CB-OG1 | -7.28 | 98.67       | 109.60   |
| 4   | H     | 10  | THR  | N-CA-CB   | 7.15  | 121.07      | 110.49   |
| 4   | D     | 21  | PHE  | CA-CB-CG  | 7.08  | 120.88      | 113.80   |
| 1   | A     | 72  | ARG  | CB-CG-CD  | 7.04  | 127.48      | 111.30   |
| 5   | E     | 423 | THR  | CA-CB-OG1 | -6.97 | 99.15       | 109.60   |
| 2   | B     | 83  | GLN  | CB-CG-CD  | 6.94  | 124.40      | 112.60   |
| 4   | H     | 325 | ASP  | CB-CA-C   | 6.92  | 121.24      | 109.82   |
| 1   | A     | 402 | THR  | CB-CA-C   | 6.92  | 122.23      | 109.70   |
| 2   | B     | 311 | ASN  | CB-CA-C   | 6.89  | 117.70      | 109.85   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | H     | 63  | GLU  | CB-CG-CD   | 6.89  | 124.31      | 112.60   |
| 4   | H     | 236 | THR  | CA-CB-OG1  | -6.87 | 99.29       | 109.60   |
| 6   | F     | 330 | ARG  | NE-CZ-NH2  | 6.86  | 125.37      | 119.20   |
| 3   | C     | 83  | GLN  | CB-CG-CD   | 6.84  | 124.23      | 112.60   |
| 4   | D     | 412 | PHE  | CB-CA-C    | 6.81  | 123.97      | 110.42   |
| 7   | G     | 325 | ASP  | CB-CA-C    | 6.81  | 121.05      | 109.82   |
| 1   | A     | 365 | ARG  | CB-CG-CD   | 6.76  | 126.84      | 111.30   |
| 6   | F     | 325 | ASP  | CB-CA-C    | 6.75  | 120.95      | 109.82   |
| 6   | F     | 83  | GLN  | OE1-CD-NE2 | -6.72 | 115.88      | 122.60   |
| 4   | D     | 22  | GLN  | CB-CA-C    | -6.58 | 100.28      | 110.81   |
| 2   | B     | 370 | ARG  | CB-CA-C    | 6.52  | 120.57      | 110.14   |
| 4   | D     | 325 | ASP  | CB-CA-C    | 6.43  | 120.43      | 109.82   |
| 1   | A     | 325 | ASP  | CB-CA-C    | 6.43  | 120.42      | 109.82   |
| 3   | C     | 325 | ASP  | CB-CA-C    | 6.42  | 120.41      | 109.82   |
| 5   | E     | 311 | ASN  | CB-CA-C    | 6.41  | 116.51      | 110.17   |
| 1   | A     | 476 | LYS  | O-C-N      | -6.38 | 118.60      | 121.53   |
| 2   | B     | 325 | ASP  | CB-CA-C    | 6.34  | 120.28      | 109.82   |
| 4   | H     | 47  | LYS  | CB-CG-CD   | 6.33  | 125.86      | 111.30   |
| 5   | E     | 236 | THR  | CA-CB-OG1  | -6.28 | 100.18      | 109.60   |
| 3   | C     | 311 | ASN  | CB-CA-C    | 6.27  | 116.38      | 110.17   |
| 2   | B     | 21  | PHE  | CA-CB-CG   | 6.27  | 120.07      | 113.80   |
| 7   | G     | 412 | PHE  | CB-CA-C    | 6.26  | 122.88      | 110.42   |
| 2   | B     | 252 | GLU  | CB-CG-CD   | 6.19  | 123.12      | 112.60   |
| 1   | A     | 74  | ARG  | CG-CD-NE   | -6.18 | 98.41       | 112.00   |
| 3   | C     | 395 | GLN  | O-C-N      | -6.18 | 116.73      | 121.55   |
| 6   | F     | 476 | LYS  | O-C-N      | -6.15 | 118.70      | 121.53   |
| 1   | A     | 417 | GLU  | CB-CG-CD   | 6.13  | 123.03      | 112.60   |
| 3   | C     | 456 | ASP  | CA-C-N     | 6.13  | 128.40      | 120.44   |
| 3   | C     | 456 | ASP  | C-N-CA     | 6.13  | 128.40      | 120.44   |
| 1   | A     | 504 | GLU  | CB-CG-CD   | 6.11  | 122.99      | 112.60   |
| 5   | E     | 10  | THR  | CB-CA-C    | 6.11  | 122.84      | 110.38   |
| 5   | E     | 325 | ASP  | CB-CA-C    | 6.09  | 119.87      | 109.82   |
| 2   | B     | 100 | ASP  | CB-CA-C    | 6.04  | 120.82      | 110.79   |
| 3   | C     | 8   | SER  | N-CA-C     | 6.04  | 117.57      | 108.46   |
| 2   | B     | 397 | ASN  | CA-C-O     | -6.03 | 113.82      | 120.33   |
| 1   | A     | 435 | ASP  | CA-CB-CG   | 5.98  | 118.58      | 112.60   |
| 4   | H     | 185 | ASN  | OD1-CG-ND2 | -5.97 | 116.62      | 122.60   |
| 7   | G     | 236 | THR  | CA-CB-OG1  | -5.97 | 100.65      | 109.60   |
| 3   | C     | 412 | PHE  | CB-CA-C    | 5.95  | 122.27      | 110.42   |
| 5   | E     | 395 | GLN  | OE1-CD-NE2 | -5.93 | 116.67      | 122.60   |
| 4   | D     | 10  | THR  | CB-CA-C    | 5.93  | 122.48      | 110.38   |
| 5   | E     | 429 | LYS  | CB-CG-CD   | 5.92  | 124.91      | 111.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 7   | G     | 185 | ASN  | OD1-CG-ND2 | -5.92 | 116.68      | 122.60   |
| 6   | F     | 143 | PRO  | O-C-N      | -5.91 | 118.59      | 121.31   |
| 4   | D     | 83  | GLN  | CB-CG-CD   | 5.89  | 122.61      | 112.60   |
| 6   | F     | 407 | LYS  | CB-CG-CD   | 5.85  | 124.76      | 111.30   |
| 7   | G     | 428 | TYR  | CA-C-N     | 5.85  | 132.72      | 121.54   |
| 7   | G     | 428 | TYR  | C-N-CA     | 5.85  | 132.72      | 121.54   |
| 6   | F     | 311 | ASN  | CB-CA-C    | 5.84  | 115.95      | 110.17   |
| 4   | H     | 417 | GLU  | CB-CG-CD   | 5.83  | 122.51      | 112.60   |
| 1   | A     | 143 | PRO  | O-C-N      | -5.81 | 118.64      | 121.31   |
| 2   | B     | 471 | GLN  | OE1-CD-NE2 | -5.79 | 116.81      | 122.60   |
| 5   | E     | 397 | ASN  | CB-CA-C    | -5.77 | 100.91      | 110.14   |
| 2   | B     | 490 | THR  | N-CA-C     | -5.76 | 105.51      | 112.54   |
| 4   | H     | 161 | GLN  | CB-CG-CD   | 5.75  | 122.38      | 112.60   |
| 2   | B     | 176 | ASP  | CA-CB-CG   | 5.75  | 118.35      | 112.60   |
| 1   | A     | 22  | GLN  | CB-CG-CD   | -5.75 | 102.83      | 112.60   |
| 3   | C     | 417 | GLU  | CB-CG-CD   | 5.73  | 122.34      | 112.60   |
| 5   | E     | 393 | ARG  | NE-CZ-NH1  | -5.72 | 115.78      | 121.50   |
| 2   | B     | 429 | LYS  | CA-CB-CG   | 5.71  | 125.51      | 114.10   |
| 3   | C     | 426 | ASN  | CA-CB-CG   | 5.69  | 118.29      | 112.60   |
| 7   | G     | 83  | GLN  | CB-CG-CD   | 5.67  | 122.24      | 112.60   |
| 7   | G     | 435 | ASP  | CA-CB-CG   | 5.67  | 118.27      | 112.60   |
| 2   | B     | 412 | PHE  | CB-CA-C    | 5.67  | 121.70      | 110.42   |
| 7   | G     | 370 | ARG  | CB-CA-C    | 5.66  | 119.20      | 110.14   |
| 5   | E     | 435 | ASP  | CA-CB-CG   | 5.65  | 118.25      | 112.60   |
| 5   | E     | 105 | ASN  | OD1-CG-ND2 | 5.64  | 128.24      | 122.60   |
| 3   | C     | 370 | ARG  | CB-CA-C    | 5.63  | 119.14      | 110.14   |
| 5   | E     | 379 | ASP  | CA-CB-CG   | 5.62  | 118.22      | 112.60   |
| 3   | C     | 100 | ASP  | CB-CA-C    | 5.62  | 120.11      | 110.79   |
| 6   | F     | 435 | ASP  | CA-CB-CG   | 5.62  | 118.22      | 112.60   |
| 3   | C     | 206 | GLU  | CB-CG-CD   | 5.61  | 122.14      | 112.60   |
| 7   | G     | 143 | PRO  | O-C-N      | -5.60 | 118.73      | 121.31   |
| 4   | H     | 412 | PHE  | CB-CA-C    | 5.60  | 121.56      | 110.42   |
| 3   | C     | 416 | GLU  | CB-CG-CD   | -5.59 | 103.09      | 112.60   |
| 4   | D     | 210 | ASN  | OD1-CG-ND2 | 5.59  | 128.19      | 122.60   |
| 1   | A     | 370 | ARG  | CB-CA-C    | 5.58  | 119.07      | 110.14   |
| 5   | E     | 370 | ARG  | CB-CA-C    | 5.57  | 119.05      | 110.14   |
| 6   | F     | 412 | PHE  | CB-CA-C    | 5.56  | 121.49      | 110.42   |
| 1   | A     | 456 | ASP  | CA-C-N     | 5.56  | 127.66      | 120.44   |
| 1   | A     | 456 | ASP  | C-N-CA     | 5.56  | 127.66      | 120.44   |
| 4   | D     | 18  | GLU  | CB-CG-CD   | 5.56  | 122.05      | 112.60   |
| 5   | E     | 435 | ASP  | CB-CA-C    | 5.56  | 121.48      | 110.42   |
| 3   | C     | 429 | LYS  | CB-CG-CD   | 5.55  | 124.08      | 111.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | C     | 435 | ASP  | CB-CA-C    | 5.55  | 121.47      | 110.42   |
| 7   | G     | 395 | GLN  | OE1-CD-NE2 | -5.55 | 117.05      | 122.60   |
| 4   | D     | 311 | ASN  | CB-CA-C    | 5.54  | 115.66      | 110.17   |
| 4   | H     | 490 | THR  | N-CA-C     | -5.54 | 105.79      | 112.54   |
| 6   | F     | 402 | THR  | CB-CA-C    | 5.53  | 118.98      | 110.14   |
| 6   | F     | 104 | ARG  | CG-CD-NE   | -5.52 | 99.86       | 112.00   |
| 7   | G     | 435 | ASP  | CB-CA-C    | 5.51  | 121.39      | 110.42   |
| 4   | H     | 22  | GLN  | CB-CG-CD   | 5.51  | 121.97      | 112.60   |
| 3   | C     | 330 | ARG  | NE-CZ-NH2  | -5.49 | 114.26      | 119.20   |
| 1   | A     | 426 | ASN  | CA-CB-CG   | 5.48  | 118.08      | 112.60   |
| 2   | B     | 398 | GLU  | CA-CB-CG   | 5.48  | 125.06      | 114.10   |
| 5   | E     | 330 | ARG  | CB-CA-C    | 5.46  | 118.78      | 109.72   |
| 4   | H     | 435 | ASP  | CB-CA-C    | 5.45  | 121.27      | 110.42   |
| 5   | E     | 456 | ASP  | CA-C-N     | 5.45  | 127.52      | 120.44   |
| 5   | E     | 456 | ASP  | C-N-CA     | 5.45  | 127.52      | 120.44   |
| 2   | B     | 426 | ASN  | CA-CB-CG   | 5.44  | 118.04      | 112.60   |
| 1   | A     | 412 | PHE  | CB-CA-C    | 5.44  | 121.24      | 110.42   |
| 7   | G     | 311 | ASN  | CB-CA-C    | 5.43  | 115.55      | 110.17   |
| 1   | A     | 206 | GLU  | CB-CG-CD   | 5.42  | 121.82      | 112.60   |
| 4   | D     | 143 | PRO  | O-C-N      | -5.41 | 118.82      | 121.31   |
| 2   | B     | 406 | THR  | CA-CB-OG1  | -5.41 | 101.49      | 109.60   |
| 4   | D     | 206 | GLU  | CB-CG-CD   | 5.41  | 121.79      | 112.60   |
| 6   | F     | 408 | LYS  | CB-CG-CD   | 5.40  | 123.73      | 111.30   |
| 2   | B     | 478 | LYS  | CG-CD-CE   | 5.39  | 123.70      | 111.30   |
| 5   | E     | 388 | ASN  | CA-CB-CG   | 5.38  | 117.98      | 112.60   |
| 1   | A     | 497 | LYS  | CB-CG-CD   | 5.38  | 123.67      | 111.30   |
| 3   | C     | 387 | ARG  | NE-CZ-NH2  | -5.38 | 114.36      | 119.20   |
| 4   | D     | 471 | GLN  | OE1-CD-NE2 | 5.37  | 127.97      | 122.60   |
| 4   | H     | 435 | ASP  | CA-CB-CG   | 5.36  | 117.96      | 112.60   |
| 7   | G     | 456 | ASP  | CA-C-N     | 5.36  | 127.40      | 120.44   |
| 7   | G     | 456 | ASP  | C-N-CA     | 5.36  | 127.40      | 120.44   |
| 4   | D     | 417 | GLU  | CB-CG-CD   | 5.35  | 121.69      | 112.60   |
| 6   | F     | 10  | THR  | CB-CA-C    | 5.35  | 121.29      | 110.38   |
| 3   | C     | 435 | ASP  | CA-CB-CG   | 5.34  | 117.94      | 112.60   |
| 4   | H     | 19  | GLU  | CB-CG-CD   | 5.34  | 121.68      | 112.60   |
| 6   | F     | 430 | ASN  | CA-CB-CG   | 5.32  | 117.92      | 112.60   |
| 3   | C     | 8   | SER  | N-CA-CB    | -5.32 | 101.94      | 110.77   |
| 4   | D     | 370 | ARG  | CB-CA-C    | 5.31  | 118.64      | 110.14   |
| 3   | C     | 410 | GLY  | CA-C-N     | 5.29  | 127.64      | 120.65   |
| 3   | C     | 410 | GLY  | C-N-CA     | 5.29  | 127.64      | 120.65   |
| 5   | E     | 412 | PHE  | CB-CA-C    | 5.29  | 120.95      | 110.42   |
| 4   | H     | 311 | ASN  | CB-CA-C    | 5.29  | 115.41      | 110.17   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | B     | 21  | PHE  | CB-CA-C    | 5.29  | 119.18      | 110.88   |
| 2   | B     | 497 | LYS  | CA-CB-CG   | 5.29  | 124.67      | 114.10   |
| 4   | D     | 129 | HIS  | CB-CA-C    | 5.28  | 120.93      | 110.42   |
| 5   | E     | 21  | PHE  | CB-CA-C    | 5.28  | 119.17      | 110.88   |
| 4   | D     | 430 | ASN  | CB-CA-C    | -5.27 | 99.94       | 110.42   |
| 4   | D     | 443 | ASP  | CA-CB-CG   | 5.26  | 117.86      | 112.60   |
| 4   | D     | 456 | ASP  | CA-C-N     | 5.25  | 127.26      | 120.44   |
| 4   | D     | 456 | ASP  | C-N-CA     | 5.25  | 127.26      | 120.44   |
| 5   | E     | 387 | ARG  | NE-CZ-NH2  | -5.24 | 114.48      | 119.20   |
| 2   | B     | 503 | TYR  | CA-C-O     | -5.24 | 111.89      | 120.80   |
| 6   | F     | 27  | HIS  | CA-C-N     | 5.24  | 127.83      | 120.28   |
| 6   | F     | 27  | HIS  | C-N-CA     | 5.24  | 127.83      | 120.28   |
| 5   | E     | 426 | ASN  | CA-CB-CG   | 5.24  | 117.84      | 112.60   |
| 5   | E     | 406 | THR  | CA-CB-OG1  | -5.22 | 101.77      | 109.60   |
| 2   | B     | 100 | ASP  | CA-CB-CG   | 5.20  | 117.80      | 112.60   |
| 4   | H     | 443 | ASP  | CA-CB-CG   | 5.20  | 117.80      | 112.60   |
| 3   | C     | 178 | GLN  | CB-CG-CD   | -5.20 | 103.77      | 112.60   |
| 5   | E     | 394 | VAL  | N-CA-C     | -5.19 | 107.09      | 111.56   |
| 5   | E     | 348 | ARG  | NE-CZ-NH1  | 5.19  | 126.69      | 121.50   |
| 4   | H     | 426 | ASN  | CA-CB-CG   | 5.18  | 117.78      | 112.60   |
| 2   | B     | 95  | LYS  | CB-CG-CD   | 5.17  | 123.20      | 111.30   |
| 4   | H     | 100 | ASP  | CB-CA-C    | 5.17  | 119.38      | 110.79   |
| 2   | B     | 10  | THR  | CB-CA-C    | 5.16  | 120.90      | 110.38   |
| 6   | F     | 412 | PHE  | CA-CB-CG   | 5.16  | 118.96      | 113.80   |
| 3   | C     | 412 | PHE  | CA-CB-CG   | 5.16  | 118.96      | 113.80   |
| 4   | H     | 5   | VAL  | CB-CA-C    | 5.15  | 121.18      | 111.40   |
| 2   | B     | 430 | ASN  | OD1-CG-ND2 | -5.14 | 117.46      | 122.60   |
| 5   | E     | 412 | PHE  | CA-CB-CG   | 5.14  | 118.94      | 113.80   |
| 1   | A     | 490 | THR  | N-CA-C     | -5.13 | 106.28      | 112.54   |
| 5   | E     | 330 | ARG  | CB-CG-CD   | 5.13  | 123.09      | 111.30   |
| 7   | G     | 57  | ARG  | CG-CD-NE   | 5.12  | 123.28      | 112.00   |
| 5   | E     | 423 | THR  | CA-CB-CG2  | 5.11  | 119.18      | 110.50   |
| 6   | F     | 104 | ARG  | CB-CG-CD   | 5.11  | 123.04      | 111.30   |
| 6   | F     | 435 | ASP  | CB-CA-C    | 5.09  | 120.55      | 110.42   |
| 5   | E     | 490 | THR  | N-CA-C     | -5.07 | 106.35      | 112.54   |
| 1   | A     | 194 | ASP  | CA-CB-CG   | 5.07  | 117.67      | 112.60   |
| 1   | A     | 395 | GLN  | CB-CG-CD   | 5.07  | 121.21      | 112.60   |
| 2   | B     | 456 | ASP  | CA-C-N     | 5.06  | 127.02      | 120.44   |
| 2   | B     | 456 | ASP  | C-N-CA     | 5.06  | 127.02      | 120.44   |
| 6   | F     | 406 | THR  | CA-CB-OG1  | -5.05 | 102.02      | 109.60   |
| 1   | A     | 311 | ASN  | CB-CA-C    | 5.04  | 115.16      | 110.17   |
| 3   | C     | 241 | PHE  | CB-CA-C    | 5.04  | 118.12      | 109.51   |

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| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 4   | H     | 370 | ARG  | CB-CA-C  | 5.02 | 118.18      | 110.14   |
| 4   | D     | 176 | ASP  | CA-CB-CG | 5.01 | 117.61      | 112.60   |
| 4   | D     | 379 | ASP  | CA-CB-CG | 5.01 | 117.61      | 112.60   |
| 1   | A     | 104 | ARG  | CB-CG-CD | 5.00 | 122.81      | 111.30   |

There are no chirality outliers.

All (139) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 104 | ARG  | Sidechain |
| 1   | A     | 120 | ARG  | Sidechain |
| 1   | A     | 136 | ARG  | Sidechain |
| 1   | A     | 166 | ARG  | Sidechain |
| 1   | A     | 182 | ARG  | Sidechain |
| 1   | A     | 227 | ARG  | Sidechain |
| 1   | A     | 246 | ARG  | Sidechain |
| 1   | A     | 330 | ARG  | Sidechain |
| 1   | A     | 365 | ARG  | Sidechain |
| 1   | A     | 370 | ARG  | Sidechain |
| 1   | A     | 427 | ARG  | Sidechain |
| 1   | A     | 439 | ARG  | Sidechain |
| 1   | A     | 487 | ARG  | Sidechain |
| 1   | A     | 498 | ARG  | Sidechain |
| 1   | A     | 57  | ARG  | Sidechain |
| 1   | A     | 72  | ARG  | Sidechain |
| 1   | A     | 74  | ARG  | Sidechain |
| 2   | B     | 136 | ARG  | Sidechain |
| 2   | B     | 166 | ARG  | Sidechain |
| 2   | B     | 17  | ARG  | Sidechain |
| 2   | B     | 182 | ARG  | Sidechain |
| 2   | B     | 219 | ARG  | Sidechain |
| 2   | B     | 227 | ARG  | Sidechain |
| 2   | B     | 246 | ARG  | Sidechain |
| 2   | B     | 330 | ARG  | Sidechain |
| 2   | B     | 365 | ARG  | Sidechain |
| 2   | B     | 387 | ARG  | Sidechain |
| 2   | B     | 403 | ALY  | Mainchain |
| 2   | B     | 427 | ARG  | Sidechain |
| 2   | B     | 487 | ARG  | Sidechain |
| 2   | B     | 72  | ARG  | Sidechain |
| 2   | B     | 74  | ARG  | Sidechain |
| 2   | B     | 9   | ARG  | Sidechain |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Group</b> |
|------------|--------------|------------|-------------|--------------|
| 3          | C            | 136        | ARG         | Sidechain    |
| 3          | C            | 166        | ARG         | Sidechain    |
| 3          | C            | 219        | ARG         | Sidechain    |
| 3          | C            | 227        | ARG         | Sidechain    |
| 3          | C            | 246        | ARG         | Sidechain    |
| 3          | C            | 330        | ARG         | Sidechain    |
| 3          | C            | 393        | ARG         | Sidechain    |
| 3          | C            | 402        | THR         | Mainchain    |
| 3          | C            | 427        | ARG         | Sidechain    |
| 3          | C            | 439        | ARG         | Sidechain    |
| 3          | C            | 459        | ARG         | Sidechain    |
| 3          | C            | 487        | ARG         | Sidechain    |
| 3          | C            | 498        | ARG         | Sidechain    |
| 3          | C            | 72[A]      | ARG         | Sidechain    |
| 3          | C            | 72[B]      | ARG         | Sidechain    |
| 3          | C            | 74         | ARG         | Sidechain    |
| 3          | C            | 8          | SER         | Peptide      |
| 3          | C            | 9          | ARG         | Sidechain    |
| 4          | D            | 136        | ARG         | Sidechain    |
| 4          | D            | 166        | ARG         | Sidechain    |
| 4          | D            | 17         | ARG         | Sidechain    |
| 4          | D            | 175        | ARG         | Sidechain    |
| 4          | D            | 182        | ARG         | Sidechain    |
| 4          | D            | 198        | ARG         | Sidechain    |
| 4          | D            | 227        | ARG         | Sidechain    |
| 4          | D            | 246        | ARG         | Sidechain    |
| 4          | D            | 330        | ARG         | Sidechain    |
| 4          | D            | 365[A]     | ARG         | Sidechain    |
| 4          | D            | 365[B]     | ARG         | Sidechain    |
| 4          | D            | 402        | THR         | Mainchain    |
| 4          | D            | 403        | ALY         | Mainchain    |
| 4          | D            | 427        | ARG         | Sidechain    |
| 4          | D            | 430        | ASN         | Mainchain    |
| 4          | D            | 487        | ARG         | Sidechain    |
| 4          | D            | 72         | ARG         | Sidechain    |
| 4          | D            | 74         | ARG         | Sidechain    |
| 5          | E            | 136        | ARG         | Sidechain    |
| 5          | E            | 166        | ARG         | Sidechain    |
| 5          | E            | 182        | ARG         | Sidechain    |
| 5          | E            | 198        | ARG         | Sidechain    |
| 5          | E            | 227        | ARG         | Sidechain    |
| 5          | E            | 246        | ARG         | Sidechain    |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 5   | E     | 330 | ARG  | Sidechain |
| 5   | E     | 365 | ARG  | Sidechain |
| 5   | E     | 370 | ARG  | Sidechain |
| 5   | E     | 393 | ARG  | Sidechain |
| 5   | E     | 394 | VAL  | Peptide   |
| 5   | E     | 402 | THR  | Mainchain |
| 5   | E     | 427 | ARG  | Sidechain |
| 5   | E     | 487 | ARG  | Sidechain |
| 5   | E     | 498 | ARG  | Sidechain |
| 5   | E     | 72  | ARG  | Sidechain |
| 5   | E     | 74  | ARG  | Sidechain |
| 5   | E     | 9   | ARG  | Sidechain |
| 6   | F     | 104 | ARG  | Sidechain |
| 6   | F     | 136 | ARG  | Sidechain |
| 6   | F     | 166 | ARG  | Sidechain |
| 6   | F     | 219 | ARG  | Sidechain |
| 6   | F     | 22  | GLN  | Peptide   |
| 6   | F     | 227 | ARG  | Sidechain |
| 6   | F     | 246 | ARG  | Sidechain |
| 6   | F     | 330 | ARG  | Sidechain |
| 6   | F     | 365 | ARG  | Sidechain |
| 6   | F     | 370 | ARG  | Sidechain |
| 6   | F     | 402 | THR  | Mainchain |
| 6   | F     | 427 | ARG  | Sidechain |
| 6   | F     | 439 | ARG  | Sidechain |
| 6   | F     | 487 | ARG  | Sidechain |
| 6   | F     | 72  | ARG  | Sidechain |
| 6   | F     | 74  | ARG  | Sidechain |
| 6   | F     | 9   | ARG  | Sidechain |
| 7   | G     | 136 | ARG  | Sidechain |
| 7   | G     | 166 | ARG  | Sidechain |
| 7   | G     | 182 | ARG  | Sidechain |
| 7   | G     | 198 | ARG  | Sidechain |
| 7   | G     | 227 | ARG  | Sidechain |
| 7   | G     | 246 | ARG  | Sidechain |
| 7   | G     | 330 | ARG  | Sidechain |
| 7   | G     | 357 | ARG  | Sidechain |
| 7   | G     | 365 | ARG  | Sidechain |
| 7   | G     | 402 | THR  | Mainchain |
| 7   | G     | 403 | ALY  | Mainchain |
| 7   | G     | 427 | ARG  | Sidechain |
| 7   | G     | 428 | TYR  | Peptide   |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 7   | G     | 439 | ARG  | Sidechain |
| 7   | G     | 487 | ARG  | Sidechain |
| 7   | G     | 57  | ARG  | Sidechain |
| 7   | G     | 72  | ARG  | Sidechain |
| 7   | G     | 74  | ARG  | Sidechain |
| 7   | G     | 9   | ARG  | Sidechain |
| 4   | H     | 166 | ARG  | Sidechain |
| 4   | H     | 182 | ARG  | Sidechain |
| 4   | H     | 219 | ARG  | Sidechain |
| 4   | H     | 227 | ARG  | Sidechain |
| 4   | H     | 246 | ARG  | Sidechain |
| 4   | H     | 330 | ARG  | Sidechain |
| 4   | H     | 365 | ARG  | Sidechain |
| 4   | H     | 370 | ARG  | Sidechain |
| 4   | H     | 387 | ARG  | Sidechain |
| 4   | H     | 402 | THR  | Mainchain |
| 4   | H     | 403 | ALY  | Mainchain |
| 4   | H     | 427 | ARG  | Sidechain |
| 4   | H     | 439 | ARG  | Sidechain |
| 4   | H     | 487 | ARG  | Sidechain |
| 4   | H     | 72  | ARG  | Sidechain |
| 4   | H     | 74  | ARG  | Sidechain |

## 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     | 4053  | 0        | 3996     | 51      | 0            |
| 2   | B     | 4036  | 0        | 3979     | 81      | 0            |
| 3   | C     | 4039  | 0        | 3987     | 58      | 0            |
| 4   | D     | 4051  | 0        | 4001     | 45      | 0            |
| 4   | H     | 4043  | 0        | 3988     | 62      | 0            |
| 5   | E     | 4052  | 0        | 3994     | 68      | 0            |
| 6   | F     | 4028  | 0        | 3973     | 72      | 0            |
| 7   | G     | 4023  | 0        | 3963     | 62      | 0            |
| 8   | B     | 12    | 0        | 16       | 6       | 0            |
| 8   | C     | 6     | 0        | 8        | 1       | 0            |
| 8   | D     | 6     | 0        | 8        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 8   | E     | 6     | 0        | 8        | 4       | 0            |
| 8   | F     | 6     | 0        | 8        | 2       | 0            |
| 8   | G     | 6     | 0        | 8        | 1       | 0            |
| 8   | H     | 6     | 0        | 8        | 2       | 0            |
| 9   | J     | 1     | 0        | 0        | 0       | 0            |
| 10  | I     | 398   | 0        | 0        | 30      | 0            |
| All | All   | 32772 | 0        | 31945    | 489     | 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 8.

All (489) 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) |
|-----------------|---------------------|--------------------------|-------------------|
| 3:C:7:LEU:HD13  | 3:C:11:GLN:HE21     | 0.93                     | 1.09              |
| 5:E:408:LYS:CE  | 5:E:409:PRO:O       | 2.01                     | 1.08              |
| 3:C:421:ASP:OD1 | 3:C:423:THR:HG22    | 1.54                     | 1.06              |
| 1:A:421:ASP:OD1 | 1:A:423:THR:HG22    | 1.57                     | 1.04              |
| 3:C:7:LEU:HD13  | 3:C:11:GLN:NE2      | 1.74                     | 1.02              |
| 4:D:72:ARG:HH21 | 4:D:72:ARG:HG2      | 1.22                     | 1.01              |
| 3:C:7:LEU:CD1   | 3:C:11:GLN:HE21     | 1.78                     | 0.96              |
| 7:G:193:GLU:CG  | 10:I:219:HOH:O      | 2.16                     | 0.94              |
| 5:E:408:LYS:HE3 | 5:E:409:PRO:O       | 1.66                     | 0.93              |
| 5:E:333:THR:OG1 | 5:E:476:LYS:HE3     | 1.69                     | 0.92              |
| 2:B:408:LYS:HE2 | 2:B:409:PRO:O       | 1.68                     | 0.91              |
| 5:E:206:GLU:HB2 | 8:E:601:GOL:H2      | 1.48                     | 0.91              |
| 5:E:367:ALA:HB3 | 5:E:395:GLN:HB2     | 1.51                     | 0.91              |
| 3:C:7:LEU:C     | 3:C:8:SER:OG        | 2.13                     | 0.90              |
| 3:C:398:GLU:OE1 | 3:C:433:LEU:HD12    | 1.70                     | 0.90              |
| 7:G:54:TRP:CD1  | 7:G:57:ARG:HH21     | 1.91                     | 0.89              |
| 4:D:408:LYS:HD3 | 4:D:416:GLU:OE1     | 1.73                     | 0.89              |
| 7:G:193:GLU:OE1 | 10:I:219:HOH:O      | 1.91                     | 0.88              |
| 7:G:368:GLU:OE2 | 7:G:370:ARG:NH1     | 2.08                     | 0.87              |
| 2:B:241:PHE:CE2 | 2:B:365:ARG:NH2     | 2.43                     | 0.87              |
| 1:A:411:MET:HE2 | 1:A:411:MET:HA      | 1.57                     | 0.86              |
| 6:F:9:ARG:NH2   | 6:F:11:GLN:HE22     | 1.74                     | 0.86              |
| 4:D:72:ARG:HG2  | 4:D:72:ARG:NH2      | 1.83                     | 0.86              |
| 4:D:241:PHE:HE2 | 4:D:365[B]:ARG:HH12 | 1.23                     | 0.86              |
| 2:B:408:LYS:CE  | 2:B:409:PRO:O       | 2.24                     | 0.85              |
| 5:E:408:LYS:HE2 | 5:E:409:PRO:O       | 1.77                     | 0.83              |
| 4:H:182:ARG:NH1 | 4:H:182:ARG:HB3     | 1.94                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:E:478:LYS:HE2  | 5:E:479:PRO:HD2  | 1.61                     | 0.82              |
| 2:B:370:ARG:HH12 | 2:B:403:ALY:HZ   | 1.28                     | 0.80              |
| 1:A:182:ARG:HE   | 4:H:119:GLN:NE2  | 1.80                     | 0.79              |
| 2:B:192:ARG:HH22 | 8:B:602:GOL:C3   | 1.97                     | 0.78              |
| 1:A:182:ARG:HE   | 4:H:119:GLN:CD   | 1.91                     | 0.78              |
| 6:F:211:LEU:HD11 | 10:I:54:HOH:O    | 1.84                     | 0.78              |
| 4:H:182:ARG:HH11 | 4:H:182:ARG:CB   | 1.96                     | 0.78              |
| 2:B:8:SER:H      | 2:B:11:GLN:HE21  | 1.33                     | 0.77              |
| 1:A:211:LEU:HD13 | 1:A:392:ILE:HG12 | 1.67                     | 0.77              |
| 6:F:21:PHE:CZ    | 6:F:442:LEU:HD11 | 2.20                     | 0.77              |
| 2:B:241:PHE:CZ   | 2:B:365:ARG:NH2  | 2.53                     | 0.77              |
| 4:H:45:LYS:HE2   | 4:H:83:GLN:NE2   | 2.00                     | 0.76              |
| 2:B:370:ARG:HH12 | 2:B:403:ALY:HH31 | 1.50                     | 0.76              |
| 6:F:17:ARG:CG    | 6:F:17:ARG:HH21  | 1.98                     | 0.76              |
| 4:D:95:LYS:HE3   | 4:D:95:LYS:HA    | 1.69                     | 0.74              |
| 7:G:193:GLU:CD   | 10:I:219:HOH:O   | 2.27                     | 0.74              |
| 5:E:297:GLU:HG2  | 10:I:307:HOH:O   | 1.85                     | 0.74              |
| 1:A:430:ASN:OD1  | 1:A:432:LYS:HE2  | 1.87                     | 0.74              |
| 3:C:17:ARG:NH1   | 3:C:58:ASP:O     | 2.20                     | 0.74              |
| 7:G:497:LYS:HE2  | 7:G:501:PHE:O    | 1.87                     | 0.74              |
| 4:H:17:ARG:NH1   | 4:H:58:ASP:O     | 2.20                     | 0.74              |
| 3:C:7:LEU:C      | 3:C:8:SER:HG     | 1.94                     | 0.74              |
| 3:C:215:ARG:NH2  | 8:C:601:GOL:O2   | 2.20                     | 0.74              |
| 5:E:17:ARG:NH1   | 5:E:58:ASP:O     | 2.20                     | 0.74              |
| 5:E:367:ALA:CB   | 5:E:395:GLN:HB2  | 2.16                     | 0.74              |
| 6:F:407:LYS:HD2  | 6:F:408:LYS:O    | 1.87                     | 0.73              |
| 2:B:241:PHE:HE2  | 2:B:365:ARG:NH2  | 1.86                     | 0.73              |
| 1:A:323:LEU:HB3  | 1:A:330:ARG:HH22 | 1.53                     | 0.73              |
| 6:F:17:ARG:HH21  | 6:F:17:ARG:HG3   | 1.52                     | 0.73              |
| 2:B:370:ARG:NH1  | 2:B:403:ALY:HH31 | 2.04                     | 0.73              |
| 3:C:28:GLN:OE1   | 10:I:449:HOH:O   | 2.07                     | 0.72              |
| 4:H:182:ARG:HB3  | 4:H:182:ARG:HH11 | 1.53                     | 0.72              |
| 2:B:333:THR:HG22 | 2:B:478:LYS:HE2  | 1.72                     | 0.71              |
| 2:B:192:ARG:HH22 | 8:B:602:GOL:H32  | 1.55                     | 0.71              |
| 6:F:10:THR:HA    | 6:F:13:CYS:SG    | 2.31                     | 0.71              |
| 4:D:178:GLN:HG2  | 4:D:182:ARG:HH11 | 1.56                     | 0.71              |
| 2:B:211:LEU:HD13 | 2:B:392:ILE:HG12 | 1.73                     | 0.70              |
| 6:F:211:LEU:CD1  | 10:I:54:HOH:O    | 2.40                     | 0.69              |
| 7:G:8:SER:CB     | 7:G:11:GLN:HE21  | 2.06                     | 0.69              |
| 6:F:17:ARG:NH1   | 6:F:439:ARG:NH1  | 2.40                     | 0.69              |
| 2:B:370:ARG:NH1  | 2:B:403:ALY:HZ   | 1.90                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:G:8:SER:HB3    | 7:G:11:GLN:HE21  | 1.58                     | 0.69              |
| 3:C:119:GLN:NE2  | 6:F:182:ARG:CZ   | 2.56                     | 0.69              |
| 2:B:144:PRO:HG3  | 2:B:172:PRO:HG2  | 1.75                     | 0.68              |
| 1:A:207:MET:HE3  | 1:A:398:GLU:HG3  | 1.75                     | 0.68              |
| 5:E:95:LYS:HA    | 5:E:95:LYS:HE3   | 1.74                     | 0.68              |
| 6:F:450:MET:HE2  | 6:F:451:HIS:NE2  | 2.09                     | 0.68              |
| 4:D:397:ASN:ND2  | 4:D:397:ASN:O    | 2.27                     | 0.68              |
| 3:C:450:MET:HE2  | 3:C:451:HIS:NE2  | 2.09                     | 0.68              |
| 1:A:17:ARG:NH1   | 1:A:58:ASP:O     | 2.28                     | 0.67              |
| 4:H:397:ASN:O    | 4:H:397:ASN:ND2  | 2.28                     | 0.67              |
| 4:D:220:ILE:HD11 | 4:D:221:PHE:CE2  | 2.29                     | 0.67              |
| 5:E:450:MET:HE2  | 5:E:451:HIS:NE2  | 2.10                     | 0.67              |
| 6:F:397:ASN:ND2  | 6:F:397:ASN:O    | 2.28                     | 0.67              |
| 2:B:401:TYR:OH   | 2:B:403:ALY:HH32 | 1.94                     | 0.67              |
| 6:F:13:CYS:SG    | 6:F:434:PRO:HD3  | 2.35                     | 0.66              |
| 3:C:220:ILE:HD11 | 3:C:221:PHE:CE2  | 2.30                     | 0.66              |
| 7:G:397:ASN:O    | 7:G:397:ASN:ND2  | 2.28                     | 0.66              |
| 6:F:21:PHE:CZ    | 6:F:442:LEU:HD21 | 2.29                     | 0.66              |
| 5:E:181:ASP:OD2  | 5:E:459:ARG:NH1  | 2.30                     | 0.65              |
| 3:C:64:ASN:HB3   | 10:I:510:HOH:O   | 1.96                     | 0.65              |
| 4:D:115:ALA:O    | 4:D:119:GLN:HG2  | 1.98                     | 0.64              |
| 5:E:220:ILE:HD11 | 5:E:221:PHE:CE2  | 2.32                     | 0.64              |
| 2:B:483:ILE:HD12 | 2:B:483:ILE:H    | 1.61                     | 0.64              |
| 2:B:28:GLN:OE1   | 10:I:451:HOH:O   | 2.14                     | 0.64              |
| 2:B:370:ARG:HH22 | 2:B:403:ALY:CH3  | 2.12                     | 0.63              |
| 7:G:193:GLU:CB   | 10:I:219:HOH:O   | 2.41                     | 0.63              |
| 7:G:220:ILE:HD11 | 7:G:221:PHE:CE2  | 2.34                     | 0.63              |
| 6:F:220:ILE:HD11 | 6:F:221:PHE:CE2  | 2.34                     | 0.63              |
| 7:G:181:ASP:OD2  | 7:G:459:ARG:NH1  | 2.32                     | 0.62              |
| 4:D:181:ASP:OD1  | 4:D:459:ARG:HD2  | 1.99                     | 0.62              |
| 6:F:395:GLN:NE2  | 10:I:491:HOH:O   | 2.32                     | 0.62              |
| 2:B:23:GLY:O     | 10:I:451:HOH:O   | 2.16                     | 0.61              |
| 3:C:7:LEU:HD13   | 3:C:11:GLN:HG2   | 1.82                     | 0.60              |
| 7:G:450:MET:HE2  | 7:G:451:HIS:NE2  | 2.15                     | 0.60              |
| 7:G:497:LYS:CE   | 7:G:501:PHE:O    | 2.49                     | 0.60              |
| 4:H:182:ARG:HH11 | 4:H:182:ARG:HB2  | 1.65                     | 0.60              |
| 2:B:393:ARG:HD3  | 10:I:122:HOH:O   | 2.01                     | 0.60              |
| 4:D:403:ALY:HH31 | 4:D:419:GLU:OE2  | 2.01                     | 0.60              |
| 4:D:450:MET:HE2  | 4:D:451:HIS:NE2  | 2.17                     | 0.60              |
| 4:H:182:ARG:HB3  | 4:H:182:ARG:CZ   | 2.27                     | 0.60              |
| 4:H:429:LYS:O    | 4:H:430:ASN:O    | 2.19                     | 0.60              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 6:F:182:ARG:HH11  | 6:F:182:ARG:CG   | 2.14                     | 0.60              |
| 2:B:192:ARG:HH22  | 8:B:602:GOL:H31  | 1.66                     | 0.59              |
| 4:H:195:GLN:NE2   | 8:H:601:GOL:H31  | 2.18                     | 0.59              |
| 2:B:6:ALA:HA      | 2:B:429:LYS:HD3  | 1.84                     | 0.59              |
| 5:E:471:GLN:HE21  | 6:F:471:GLN:HE22 | 1.50                     | 0.59              |
| 1:A:182:ARG:NE    | 4:H:119:GLN:NE2  | 2.49                     | 0.59              |
| 6:F:21:PHE:HZ     | 6:F:442:LEU:CG   | 2.15                     | 0.59              |
| 6:F:393:ARG:HD2   | 6:F:396:PRO:HD2  | 1.85                     | 0.58              |
| 5:E:403:ALY:HH31  | 5:E:419:GLU:OE2  | 2.02                     | 0.58              |
| 7:G:193:GLU:HB2   | 10:I:219:HOH:O   | 2.03                     | 0.58              |
| 5:E:181:ASP:OD1   | 5:E:459:ARG:HD2  | 2.01                     | 0.58              |
| 2:B:170:GLU:OE2   | 2:B:201:HIS:HE1  | 1.85                     | 0.58              |
| 2:B:408:LYS:HE3   | 2:B:409:PRO:O    | 2.03                     | 0.57              |
| 2:B:450:MET:HE2   | 2:B:451:HIS:NE2  | 2.19                     | 0.57              |
| 4:D:393:ARG:HD2   | 4:D:396:PRO:HD2  | 1.86                     | 0.57              |
| 3:C:72[B]:ARG:NH1 | 3:C:112:TYR:H    | 2.02                     | 0.57              |
| 4:D:348:ARG:HA    | 8:D:601:GOL:H31  | 1.85                     | 0.57              |
| 5:E:206:GLU:H     | 8:E:601:GOL:H2   | 1.70                     | 0.57              |
| 6:F:21:PHE:HZ     | 6:F:442:LEU:HD21 | 1.70                     | 0.57              |
| 7:G:393:ARG:HD2   | 7:G:396:PRO:HD2  | 1.86                     | 0.57              |
| 7:G:79:ASP:O      | 7:G:82:LYS:HG2   | 2.05                     | 0.57              |
| 6:F:407:LYS:NZ    | 6:F:407:LYS:HB3  | 2.19                     | 0.57              |
| 7:G:13:CYS:O      | 7:G:17:ARG:HG3   | 2.05                     | 0.57              |
| 5:E:58:ASP:OD2    | 5:E:438:GLU:OE2  | 2.24                     | 0.56              |
| 5:E:422:LEU:N     | 5:E:422:LEU:HD12 | 2.20                     | 0.56              |
| 4:H:330:ARG:HA    | 4:H:330:ARG:HH21 | 1.70                     | 0.56              |
| 4:H:474:LEU:HD22  | 4:H:474:LEU:O    | 2.05                     | 0.56              |
| 2:B:246:ARG:HB2   | 2:B:246:ARG:CZ   | 2.36                     | 0.56              |
| 2:B:422:LEU:N     | 2:B:422:LEU:CD1  | 2.69                     | 0.56              |
| 5:E:450:MET:HE2   | 5:E:451:HIS:HE2  | 1.70                     | 0.56              |
| 7:G:181:ASP:OD1   | 7:G:459:ARG:HD2  | 2.06                     | 0.56              |
| 2:B:26:PHE:O      | 10:I:451:HOH:O   | 2.18                     | 0.55              |
| 4:D:13:CYS:O      | 4:D:17:ARG:HG3   | 2.06                     | 0.55              |
| 2:B:370:ARG:NH2   | 2:B:403:ALY:HH31 | 2.22                     | 0.55              |
| 2:B:370:ARG:HH12  | 2:B:403:ALY:CH3  | 2.17                     | 0.55              |
| 5:E:47:LYS:HE2    | 5:E:201:HIS:HD2  | 1.72                     | 0.55              |
| 6:F:170:GLU:OE2   | 6:F:201:HIS:HE1  | 1.89                     | 0.55              |
| 7:G:483:ILE:HD12  | 7:G:483:ILE:H    | 1.70                     | 0.55              |
| 4:H:192:ARG:HH22  | 8:H:601:GOL:H11  | 1.70                     | 0.55              |
| 1:A:182:ARG:HH21  | 4:H:119:GLN:NE2  | 2.04                     | 0.55              |
| 6:F:239:GLU:HG2   | 6:F:241:PHE:CE1  | 2.42                     | 0.55              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:A:393:ARG:HD2  | 1:A:396:PRO:HD2    | 1.89                     | 0.54              |
| 4:D:72:ARG:NH2   | 4:D:72:ARG:CG      | 2.65                     | 0.54              |
| 5:E:421:ASP:OD2  | 5:E:423:THR:HB     | 2.08                     | 0.54              |
| 5:E:170:GLU:OE2  | 5:E:201:HIS:HE1    | 1.91                     | 0.54              |
| 7:G:323:LEU:HB3  | 7:G:330:ARG:HH22   | 1.71                     | 0.54              |
| 2:B:422:LEU:N    | 2:B:422:LEU:HD12   | 2.23                     | 0.54              |
| 6:F:203:LEU:HD22 | 6:F:451:HIS:HB3    | 1.90                     | 0.54              |
| 5:E:422:LEU:N    | 5:E:422:LEU:CD1    | 2.70                     | 0.54              |
| 6:F:9:ARG:HH22   | 6:F:11:GLN:HE22    | 1.50                     | 0.54              |
| 2:B:241:PHE:HE2  | 2:B:365:ARG:CZ     | 2.20                     | 0.54              |
| 2:B:241:PHE:HE2  | 2:B:365:ARG:HH22   | 1.47                     | 0.54              |
| 4:H:393:ARG:HD2  | 4:H:396:PRO:HD2    | 1.90                     | 0.54              |
| 3:C:206:GLU:HG2  | 3:C:433:LEU:HD11   | 1.91                     | 0.53              |
| 7:G:497:LYS:HE2  | 7:G:497:LYS:HA     | 1.89                     | 0.53              |
| 3:C:9:ARG:HB2    | 3:C:432:LYS:HB2    | 1.90                     | 0.53              |
| 3:C:72[A]:ARG:CZ | 10:I:530:HOH:O     | 2.56                     | 0.53              |
| 2:B:241:PHE:CE2  | 2:B:365:ARG:CZ     | 2.91                     | 0.53              |
| 6:F:26:PHE:O     | 6:F:28:GLN:NE2     | 2.41                     | 0.53              |
| 6:F:424:TYR:HB3  | 6:F:428:TYR:HD2    | 1.73                     | 0.53              |
| 2:B:192:ARG:NH2  | 8:B:602:GOL:H32    | 2.23                     | 0.53              |
| 6:F:21:PHE:CE2   | 6:F:442:LEU:HD11   | 2.43                     | 0.53              |
| 1:A:450:MET:HE3  | 1:A:451:HIS:NE2    | 2.23                     | 0.53              |
| 4:H:46:LYS:HD3   | 4:H:87:PHE:CE1     | 2.44                     | 0.53              |
| 5:E:203:LEU:HD22 | 5:E:451:HIS:HB3    | 1.90                     | 0.52              |
| 4:H:6:ALA:HB2    | 4:H:429:LYS:HG2    | 1.91                     | 0.52              |
| 4:H:181:ASP:OD1  | 4:H:459:ARG:HD2    | 2.10                     | 0.52              |
| 2:B:370:ARG:HH22 | 2:B:403:ALY:HH31   | 1.73                     | 0.52              |
| 4:D:241:PHE:HE2  | 4:D:365[B]:ARG:NH1 | 2.02                     | 0.52              |
| 7:G:408:LYS:HE3  | 7:G:416:GLU:OE1    | 2.09                     | 0.52              |
| 2:B:239:GLU:HG2  | 2:B:241:PHE:CE1    | 2.44                     | 0.52              |
| 5:E:333:THR:OG1  | 5:E:476:LYS:CE     | 2.52                     | 0.52              |
| 7:G:239:GLU:HG2  | 7:G:241:PHE:CE1    | 2.45                     | 0.52              |
| 3:C:239:GLU:HG2  | 3:C:241:PHE:CE1    | 2.45                     | 0.52              |
| 5:E:273:MET:HE3  | 5:E:287:GLU:HB2    | 1.92                     | 0.52              |
| 4:H:330:ARG:HA   | 4:H:330:ARG:NH2    | 2.24                     | 0.52              |
| 4:D:181:ASP:OD2  | 4:D:459:ARG:NH1    | 2.42                     | 0.52              |
| 5:E:370:ARG:HH12 | 5:E:403:ALY:HE3    | 1.75                     | 0.52              |
| 5:E:421:ASP:C    | 5:E:422:LEU:HD12   | 2.35                     | 0.52              |
| 7:G:450:MET:HE2  | 7:G:451:HIS:HE2    | 1.75                     | 0.51              |
| 1:A:400:VAL:H    | 1:A:423:THR:HB     | 1.75                     | 0.51              |
| 2:B:393:ARG:HD2  | 2:B:396:PRO:HD2    | 1.91                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:181:ASP:OD2  | 3:C:459:ARG:NH1  | 2.43                     | 0.51              |
| 3:C:400:VAL:H    | 3:C:423:THR:HB   | 1.75                     | 0.51              |
| 2:B:412:PHE:CD1  | 2:B:414:ASN:OD1  | 2.63                     | 0.51              |
| 3:C:119:GLN:NE2  | 6:F:182:ARG:NH2  | 2.58                     | 0.51              |
| 3:C:450:MET:HE2  | 3:C:451:HIS:HE2  | 1.73                     | 0.51              |
| 7:G:207:MET:HE1  | 7:G:400:VAL:HG23 | 1.91                     | 0.51              |
| 6:F:273:MET:HE3  | 6:F:287:GLU:HB2  | 1.93                     | 0.51              |
| 7:G:200:ASP:OD2  | 7:G:263:HIS:HD2  | 1.93                     | 0.51              |
| 4:H:273:MET:HE3  | 4:H:287:GLU:HB2  | 1.93                     | 0.51              |
| 4:H:207:MET:SD   | 4:H:398:GLU:HB3  | 2.51                     | 0.51              |
| 1:A:181:ASP:OD2  | 1:A:459:ARG:NH1  | 2.43                     | 0.51              |
| 2:B:241:PHE:HZ   | 2:B:365:ARG:NH2  | 2.07                     | 0.51              |
| 3:C:74:ARG:HD2   | 3:C:74:ARG:O     | 2.11                     | 0.51              |
| 6:F:106:SER:OG   | 6:F:124:HIS:HE1  | 1.94                     | 0.51              |
| 2:B:237:PHE:O    | 2:B:358:CYS:HA   | 2.11                     | 0.50              |
| 2:B:370:ARG:CZ   | 2:B:403:ALY:HH31 | 2.41                     | 0.50              |
| 3:C:408:LYS:HG3  | 3:C:416:GLU:OE1  | 2.12                     | 0.50              |
| 6:F:176:ASP:HA   | 6:F:462:TRP:CE3  | 2.46                     | 0.50              |
| 3:C:206:GLU:HG2  | 3:C:433:LEU:CD1  | 2.41                     | 0.50              |
| 4:D:432:LYS:HE3  | 4:D:432:LYS:HA   | 1.94                     | 0.50              |
| 6:F:18:GLU:O     | 6:F:21:PHE:HB2   | 2.11                     | 0.50              |
| 1:A:239:GLU:HG2  | 1:A:241:PHE:CE1  | 2.47                     | 0.50              |
| 4:D:160:SER:OG   | 10:I:436:HOH:O   | 2.20                     | 0.50              |
| 4:D:239:GLU:HG2  | 4:D:241:PHE:CE1  | 2.47                     | 0.50              |
| 4:D:237:PHE:O    | 4:D:358:CYS:HA   | 2.12                     | 0.50              |
| 7:G:205:LYS:HE2  | 7:G:209:GLN:NE2  | 2.26                     | 0.50              |
| 4:D:26:PHE:O     | 4:D:28:GLN:NE2   | 2.42                     | 0.50              |
| 4:D:197:TYR:CD2  | 4:D:444:VAL:HG22 | 2.47                     | 0.50              |
| 7:G:26:PHE:O     | 7:G:28:GLN:NE2   | 2.42                     | 0.50              |
| 7:G:58:ASP:OD2   | 7:G:438:GLU:OE2  | 2.29                     | 0.50              |
| 2:B:475:GLU:OE2  | 3:C:470:HIS:ND1  | 2.41                     | 0.50              |
| 5:E:478:LYS:HE2  | 5:E:479:PRO:CD   | 2.35                     | 0.50              |
| 6:F:237:PHE:O    | 6:F:358:CYS:HA   | 2.11                     | 0.50              |
| 1:A:203:LEU:CD1  | 1:A:203:LEU:C    | 2.85                     | 0.50              |
| 1:A:273:MET:HE3  | 1:A:287:GLU:HB2  | 1.93                     | 0.50              |
| 2:B:370:ARG:HH22 | 2:B:403:ALY:HH33 | 1.77                     | 0.49              |
| 4:H:205:LYS:HE2  | 4:H:209:GLN:NE2  | 2.27                     | 0.49              |
| 3:C:106:SER:OG   | 3:C:124:HIS:HE1  | 1.95                     | 0.49              |
| 1:A:207:MET:CE   | 1:A:398:GLU:HG3  | 2.41                     | 0.49              |
| 4:H:206:GLU:HG2  | 4:H:439:ARG:HH12 | 1.76                     | 0.49              |
| 7:G:237:PHE:O    | 7:G:358:CYS:HA   | 2.13                     | 0.49              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:58:ASP:OD2    | 1:A:438:GLU:OE2  | 2.31                     | 0.49              |
| 1:A:237:PHE:O     | 1:A:358:CYS:HA   | 2.12                     | 0.49              |
| 4:H:205:LYS:HE2   | 4:H:209:GLN:HE22 | 1.78                     | 0.49              |
| 7:G:176:ASP:HA    | 7:G:462:TRP:CE3  | 2.47                     | 0.49              |
| 7:G:388:ASN:ND2   | 7:G:404:MET:HA   | 2.27                     | 0.49              |
| 4:H:176:ASP:HA    | 4:H:462:TRP:CE3  | 2.48                     | 0.49              |
| 2:B:273:MET:HE3   | 2:B:287:GLU:HB2  | 1.93                     | 0.49              |
| 2:B:74:ARG:HB2    | 2:B:74:ARG:CZ    | 2.43                     | 0.49              |
| 3:C:168:ILE:HD11  | 3:C:444:VAL:HG21 | 1.95                     | 0.49              |
| 4:D:203:LEU:HD22  | 4:D:451:HIS:HB3  | 1.95                     | 0.49              |
| 5:E:17:ARG:HD3    | 5:E:59:GLY:O     | 2.13                     | 0.49              |
| 7:G:273:MET:HE3   | 7:G:287:GLU:HB2  | 1.94                     | 0.49              |
| 2:B:181:ASP:OD1   | 2:B:459:ARG:HD2  | 2.13                     | 0.48              |
| 2:B:401:TYR:CE2   | 2:B:403:ALY:HH32 | 2.48                     | 0.48              |
| 7:G:197:TYR:CE2   | 7:G:449:GLN:HG2  | 2.48                     | 0.48              |
| 3:C:273:MET:HE3   | 3:C:287:GLU:HB2  | 1.95                     | 0.48              |
| 4:D:273:MET:HE3   | 4:D:287:GLU:HB2  | 1.94                     | 0.48              |
| 5:E:237:PHE:O     | 5:E:358:CYS:HA   | 2.13                     | 0.48              |
| 5:E:239:GLU:HG2   | 5:E:241:PHE:CE1  | 2.48                     | 0.48              |
| 7:G:330:ARG:HA    | 7:G:330:ARG:NH2  | 2.27                     | 0.48              |
| 4:H:239:GLU:HG2   | 4:H:241:PHE:CE1  | 2.47                     | 0.48              |
| 6:F:206:GLU:CD    | 6:F:206:GLU:H    | 2.22                     | 0.48              |
| 4:D:160:SER:CB    | 10:I:436:HOH:O   | 2.62                     | 0.48              |
| 5:E:393:ARG:HD3   | 5:E:396:PRO:HG2  | 1.94                     | 0.48              |
| 6:F:21:PHE:HZ     | 6:F:442:LEU:CD2  | 2.25                     | 0.48              |
| 4:H:74:ARG:HH11   | 4:H:74:ARG:HB3   | 1.78                     | 0.48              |
| 3:C:72[B]:ARG:CD  | 3:C:111:GLN:OE1  | 2.61                     | 0.48              |
| 1:A:297:GLU:HG2   | 1:A:467:PRO:HG2  | 1.96                     | 0.48              |
| 7:G:424:TYR:HB2   | 7:G:428:TYR:CB   | 2.44                     | 0.48              |
| 1:A:330:ARG:NH2   | 1:A:330:ARG:HA   | 2.28                     | 0.48              |
| 6:F:421:ASP:OD1   | 6:F:423:THR:OG1  | 2.30                     | 0.48              |
| 4:H:181:ASP:OD2   | 4:H:459:ARG:NH1  | 2.44                     | 0.48              |
| 3:C:356:LEU:HD12  | 3:C:356:LEU:N    | 2.29                     | 0.48              |
| 5:E:232:CYS:HB3   | 5:E:353:PRO:HG2  | 1.96                     | 0.48              |
| 4:H:333:THR:HG23  | 4:H:333:THR:O    | 2.13                     | 0.48              |
| 3:C:72[A]:ARG:NH2 | 10:I:530:HOH:O   | 2.47                     | 0.48              |
| 3:C:366:LYS:HD3   | 3:C:368:GLU:OE2  | 2.14                     | 0.48              |
| 3:C:205:LYS:HE2   | 3:C:209:GLN:NE2  | 2.28                     | 0.47              |
| 6:F:181:ASP:OD2   | 6:F:459:ARG:NH1  | 2.47                     | 0.47              |
| 6:F:216:PHE:HE1   | 8:F:601:GOL:H12  | 1.79                     | 0.47              |
| 3:C:237:PHE:O     | 3:C:358:CYS:HA   | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:5:VAL:O      | 4:D:428:TYR:HA   | 2.14                     | 0.47              |
| 4:H:237:PHE:O    | 4:H:358:CYS:HA   | 2.13                     | 0.47              |
| 4:H:106:SER:OG   | 4:H:124:HIS:HE1  | 1.98                     | 0.47              |
| 5:E:370:ARG:NH1  | 5:E:403:ALY:HE3  | 2.28                     | 0.47              |
| 4:D:232:CYS:HB3  | 4:D:353:PRO:HG2  | 1.96                     | 0.47              |
| 5:E:206:GLU:HG2  | 5:E:439:ARG:HH12 | 1.80                     | 0.47              |
| 6:F:58:ASP:OD2   | 6:F:438:GLU:OE2  | 2.33                     | 0.47              |
| 6:F:121:LEU:HG   | 6:F:125:MET:HE2  | 1.97                     | 0.47              |
| 4:H:182:ARG:NH1  | 4:H:182:ARG:CB   | 2.62                     | 0.47              |
| 7:G:106:SER:OG   | 7:G:124:HIS:HE1  | 1.98                     | 0.47              |
| 1:A:478:LYS:HD3  | 1:A:478:LYS:C    | 2.40                     | 0.47              |
| 7:G:330:ARG:HA   | 7:G:330:ARG:HH21 | 1.79                     | 0.47              |
| 1:A:57:ARG:HD2   | 1:A:94:GLU:OE2   | 2.16                     | 0.46              |
| 1:A:72:ARG:NH2   | 10:I:381:HOH:O   | 2.44                     | 0.46              |
| 5:E:164:TRP:CE3  | 5:E:166:ARG:HD2  | 2.50                     | 0.46              |
| 4:H:207:MET:HE1  | 4:H:400:VAL:HG23 | 1.95                     | 0.46              |
| 2:B:421:ASP:C    | 2:B:422:LEU:HD12 | 2.40                     | 0.46              |
| 3:C:7:LEU:HD13   | 3:C:11:GLN:CG    | 2.46                     | 0.46              |
| 4:D:46:LYS:HD3   | 4:D:87:PHE:CE1   | 2.51                     | 0.46              |
| 6:F:356:LEU:N    | 6:F:356:LEU:HD12 | 2.30                     | 0.46              |
| 4:H:356:LEU:HD12 | 4:H:356:LEU:N    | 2.31                     | 0.46              |
| 5:E:176:ASP:HA   | 5:E:462:TRP:CE3  | 2.50                     | 0.46              |
| 5:E:211:LEU:HD11 | 10:I:32:HOH:O    | 2.16                     | 0.46              |
| 4:H:430:ASN:HD21 | 4:H:432:LYS:CD   | 2.29                     | 0.46              |
| 7:G:21:PHE:CD1   | 7:G:28:GLN:HG2   | 2.50                     | 0.46              |
| 3:C:9:ARG:NH2    | 3:C:10:THR:HG22  | 2.31                     | 0.46              |
| 5:E:106:SER:OG   | 5:E:124:HIS:HE1  | 1.98                     | 0.46              |
| 5:E:133:GLN:HA   | 5:E:162:ILE:HB   | 1.98                     | 0.46              |
| 5:E:176:ASP:OD2  | 5:E:470:HIS:NE2  | 2.41                     | 0.46              |
| 6:F:47:LYS:NZ    | 10:I:392:HOH:O   | 2.49                     | 0.46              |
| 2:B:181:ASP:OD2  | 2:B:459:ARG:NH1  | 2.49                     | 0.46              |
| 5:E:57:ARG:HD2   | 5:E:94:GLU:OE2   | 2.16                     | 0.46              |
| 6:F:21:PHE:CZ    | 6:F:442:LEU:CD1  | 2.97                     | 0.46              |
| 7:G:473:GLU:O    | 7:G:476:LYS:CD   | 2.64                     | 0.46              |
| 2:B:106:SER:OG   | 2:B:124:HIS:HE1  | 1.99                     | 0.46              |
| 3:C:57:ARG:HD2   | 3:C:94:GLU:OE2   | 2.16                     | 0.46              |
| 4:D:356:LEU:N    | 4:D:356:LEU:HD12 | 2.30                     | 0.46              |
| 5:E:72:ARG:NH1   | 5:E:112:TYR:OH   | 2.48                     | 0.46              |
| 2:B:412:PHE:CE1  | 2:B:414:ASN:OD1  | 2.69                     | 0.45              |
| 4:D:337:PHE:CD1  | 4:D:337:PHE:C    | 2.95                     | 0.45              |
| 1:A:182:ARG:NE   | 4:H:119:GLN:CD   | 2.68                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:176:ASP:HA   | 1:A:462:TRP:CE3  | 2.51                     | 0.45              |
| 6:F:9:ARG:NH2    | 6:F:11:GLN:NE2   | 2.54                     | 0.45              |
| 4:H:17:ARG:HD3   | 4:H:59:GLY:O     | 2.16                     | 0.45              |
| 5:E:260:MET:HG3  | 5:E:356:LEU:HD23 | 1.99                     | 0.45              |
| 4:H:429:LYS:O    | 4:H:430:ASN:C    | 2.58                     | 0.45              |
| 6:F:239:GLU:HG2  | 6:F:241:PHE:CZ   | 2.51                     | 0.45              |
| 7:G:323:LEU:HB3  | 7:G:330:ARG:NH2  | 2.31                     | 0.45              |
| 4:H:355:ILE:HD13 | 4:H:496:MET:HG2  | 1.97                     | 0.45              |
| 2:B:401:TYR:OH   | 2:B:403:ALY:CH3  | 2.62                     | 0.45              |
| 5:E:148:GLU:OE2  | 5:E:182:ARG:NH1  | 2.49                     | 0.45              |
| 7:G:82:LYS:HG3   | 7:G:83:GLN:N     | 2.32                     | 0.45              |
| 1:A:106:SER:OG   | 1:A:124:HIS:HE1  | 2.00                     | 0.45              |
| 2:B:211:LEU:HD12 | 2:B:211:LEU:HA   | 1.72                     | 0.45              |
| 4:H:411:MET:HE3  | 4:H:411:MET:HB2  | 1.83                     | 0.45              |
| 4:D:239:GLU:HG2  | 4:D:241:PHE:CZ   | 2.52                     | 0.45              |
| 5:E:206:GLU:H    | 8:E:601:GOL:C2   | 2.29                     | 0.45              |
| 1:A:208:VAL:HG11 | 1:A:451:HIS:CE1  | 2.52                     | 0.45              |
| 2:B:45:LYS:HD2   | 2:B:83:GLN:HB2   | 1.98                     | 0.45              |
| 3:C:232:CYS:HB3  | 3:C:353:PRO:HG2  | 1.99                     | 0.45              |
| 4:D:210:ASN:ND2  | 10:I:422:HOH:O   | 2.49                     | 0.45              |
| 1:A:45:LYS:HD2   | 1:A:83:GLN:HB2   | 1.99                     | 0.44              |
| 2:B:239:GLU:HG2  | 2:B:241:PHE:CZ   | 2.53                     | 0.44              |
| 3:C:205:LYS:HE2  | 3:C:209:GLN:HE22 | 1.82                     | 0.44              |
| 4:D:121:LEU:HG   | 4:D:125:MET:HE2  | 1.99                     | 0.44              |
| 5:E:420:LEU:O    | 5:E:422:LEU:CD1  | 2.65                     | 0.44              |
| 1:A:17:ARG:HD3   | 1:A:59:GLY:O     | 2.16                     | 0.44              |
| 1:A:432:LYS:HE3  | 1:A:432:LYS:N    | 2.33                     | 0.44              |
| 3:C:17:ARG:HD3   | 3:C:59:GLY:O     | 2.17                     | 0.44              |
| 4:H:430:ASN:HD21 | 4:H:432:LYS:HE3  | 1.82                     | 0.44              |
| 6:F:323:LEU:O    | 10:I:476:HOH:O   | 2.21                     | 0.44              |
| 4:D:164:TRP:CE3  | 4:D:166:ARG:HD2  | 2.52                     | 0.44              |
| 5:E:207:MET:HE1  | 5:E:400:VAL:HG23 | 2.00                     | 0.44              |
| 5:E:337:PHE:CD1  | 5:E:337:PHE:C    | 2.96                     | 0.44              |
| 6:F:8:SER:HB3    | 6:F:431:VAL:HG13 | 2.00                     | 0.44              |
| 6:F:503:TYR:C    | 10:I:330:HOH:O   | 2.61                     | 0.44              |
| 3:C:337:PHE:CD1  | 3:C:337:PHE:C    | 2.95                     | 0.44              |
| 6:F:182:ARG:CG   | 6:F:182:ARG:NH1  | 2.77                     | 0.44              |
| 1:A:239:GLU:HG2  | 1:A:241:PHE:CZ   | 2.52                     | 0.44              |
| 1:A:356:LEU:N    | 1:A:356:LEU:HD12 | 2.33                     | 0.44              |
| 2:B:401:TYR:CZ   | 2:B:403:ALY:HH32 | 2.53                     | 0.44              |
| 1:A:260:MET:HG3  | 1:A:356:LEU:HD23 | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:337:PHE:CD1  | 2:B:337:PHE:C    | 2.96                     | 0.44              |
| 4:H:55:LEU:HG    | 4:H:438:GLU:HG3  | 1.99                     | 0.44              |
| 5:E:389:GLU:O    | 5:E:403:ALY:N    | 2.51                     | 0.44              |
| 5:E:470:HIS:ND1  | 6:F:475:GLU:OE2  | 2.51                     | 0.43              |
| 7:G:203:LEU:HD22 | 7:G:451:HIS:HB3  | 1.98                     | 0.43              |
| 2:B:173:PHE:HB3  | 8:B:601:GOL:H2   | 1.99                     | 0.43              |
| 4:H:337:PHE:CD1  | 4:H:337:PHE:C    | 2.96                     | 0.43              |
| 1:A:197:TYR:CZ   | 1:A:449:GLN:HG2  | 2.53                     | 0.43              |
| 2:B:193:GLU:OE1  | 2:B:455:SER:OG   | 2.19                     | 0.43              |
| 3:C:214:LEU:HD23 | 3:C:214:LEU:HA   | 1.90                     | 0.43              |
| 3:C:421:ASP:OD1  | 3:C:423:THR:CG2  | 2.45                     | 0.43              |
| 6:F:17:ARG:CG    | 6:F:17:ARG:NH2   | 2.66                     | 0.43              |
| 1:A:232:CYS:HB3  | 1:A:353:PRO:HG2  | 2.00                     | 0.43              |
| 2:B:9:ARG:HA     | 2:B:432:LYS:O    | 2.18                     | 0.43              |
| 6:F:232:CYS:HB3  | 6:F:353:PRO:HG2  | 2.00                     | 0.43              |
| 7:G:92:PRO:HA    | 10:I:288:HOH:O   | 2.18                     | 0.43              |
| 7:G:411:MET:HE3  | 7:G:411:MET:HB3  | 1.73                     | 0.43              |
| 4:H:121:LEU:HG   | 4:H:125:MET:HE2  | 2.01                     | 0.43              |
| 2:B:121:LEU:HG   | 2:B:125:MET:HE2  | 2.01                     | 0.43              |
| 3:C:393:ARG:HD3  | 10:I:171:HOH:O   | 2.18                     | 0.43              |
| 5:E:121:LEU:HG   | 5:E:125:MET:HE2  | 2.01                     | 0.43              |
| 1:A:206:GLU:HG2  | 1:A:433:LEU:CD1  | 2.48                     | 0.43              |
| 1:A:389:GLU:O    | 1:A:402:THR:HA   | 2.19                     | 0.43              |
| 5:E:239:GLU:HG2  | 5:E:241:PHE:CZ   | 2.54                     | 0.43              |
| 7:G:121:LEU:HG   | 7:G:125:MET:HE2  | 2.00                     | 0.43              |
| 7:G:356:LEU:N    | 7:G:356:LEU:HD12 | 2.34                     | 0.43              |
| 7:G:473:GLU:O    | 7:G:476:LYS:HD2  | 2.19                     | 0.43              |
| 1:A:337:PHE:CD1  | 1:A:337:PHE:C    | 2.95                     | 0.43              |
| 2:B:356:LEU:N    | 2:B:356:LEU:HD12 | 2.34                     | 0.43              |
| 3:C:9:ARG:HH22   | 3:C:10:THR:HG22  | 1.84                     | 0.43              |
| 5:E:356:LEU:HD12 | 5:E:356:LEU:N    | 2.34                     | 0.43              |
| 2:B:133:GLN:HA   | 2:B:162:ILE:HB   | 2.00                     | 0.43              |
| 2:B:420:LEU:O    | 2:B:422:LEU:CD1  | 2.67                     | 0.43              |
| 5:E:55:LEU:HG    | 5:E:438:GLU:HG3  | 2.01                     | 0.43              |
| 7:G:337:PHE:CD1  | 7:G:337:PHE:C    | 2.96                     | 0.43              |
| 4:H:246:ARG:CZ   | 4:H:246:ARG:HB2  | 2.49                     | 0.43              |
| 3:C:239:GLU:HG2  | 3:C:241:PHE:CZ   | 2.54                     | 0.42              |
| 4:H:197:TYR:CZ   | 4:H:449:GLN:HG2  | 2.53                     | 0.42              |
| 7:G:133:GLN:HA   | 7:G:162:ILE:HB   | 2.01                     | 0.42              |
| 2:B:8:SER:OG     | 2:B:11:GLN:HG3   | 2.19                     | 0.42              |
| 2:B:57:ARG:HD2   | 2:B:94:GLU:OE2   | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:244:GLU:O    | 3:C:246:ARG:HD3  | 2.19                     | 0.42              |
| 4:D:106:SER:OG   | 4:D:124:HIS:HE1  | 2.01                     | 0.42              |
| 5:E:47:LYS:HE2   | 5:E:201:HIS:CD2  | 2.51                     | 0.42              |
| 6:F:182:ARG:HH11 | 6:F:182:ARG:HG2  | 1.83                     | 0.42              |
| 4:H:57:ARG:HD2   | 4:H:94:GLU:OE2   | 2.20                     | 0.42              |
| 3:C:297:GLU:H    | 3:C:297:GLU:HG2  | 1.62                     | 0.42              |
| 6:F:9:ARG:HB2    | 6:F:12:VAL:HG23  | 2.02                     | 0.42              |
| 6:F:215:ARG:HH21 | 8:F:601:GOL:H11  | 1.83                     | 0.42              |
| 7:G:164:TRP:CE3  | 7:G:166:ARG:HD2  | 2.55                     | 0.42              |
| 7:G:365:ARG:HH21 | 7:G:395:GLN:HB2  | 1.83                     | 0.42              |
| 5:E:205:LYS:N    | 8:E:601:GOL:O2   | 2.53                     | 0.42              |
| 6:F:478:LYS:HD2  | 6:F:478:LYS:HA   | 1.91                     | 0.42              |
| 7:G:205:LYS:HE2  | 7:G:209:GLN:HE22 | 1.83                     | 0.42              |
| 2:B:370:ARG:HH12 | 2:B:403:ALY:CH   | 2.32                     | 0.42              |
| 3:C:203:LEU:HD21 | 3:C:208:VAL:HG11 | 2.01                     | 0.42              |
| 4:D:57:ARG:HD2   | 4:D:94:GLU:OE2   | 2.20                     | 0.42              |
| 5:E:480:ILE:HA   | 5:E:481:PRO:HD3  | 1.91                     | 0.42              |
| 4:H:239:GLU:HG2  | 4:H:241:PHE:CZ   | 2.55                     | 0.42              |
| 4:D:125:MET:O    | 4:D:131:GLY:HA3  | 2.20                     | 0.42              |
| 6:F:337:PHE:CD1  | 6:F:337:PHE:C    | 2.97                     | 0.42              |
| 2:B:203:LEU:HD22 | 2:B:451:HIS:HB3  | 2.02                     | 0.42              |
| 4:D:297:GLU:H    | 4:D:297:GLU:HG2  | 1.61                     | 0.42              |
| 6:F:10:THR:HG22  | 6:F:432:LYS:HZ3  | 1.85                     | 0.42              |
| 1:A:197:TYR:CE2  | 1:A:449:GLN:HG2  | 2.54                     | 0.42              |
| 2:B:89:LYS:HB2   | 2:B:89:LYS:HE3   | 1.80                     | 0.42              |
| 2:B:164:TRP:CE3  | 2:B:166:ARG:HD2  | 2.55                     | 0.42              |
| 2:B:168:ILE:HD11 | 2:B:444:VAL:HG21 | 2.02                     | 0.42              |
| 2:B:246:ARG:CZ   | 2:B:246:ARG:CB   | 2.97                     | 0.42              |
| 6:F:182:ARG:HH11 | 6:F:182:ARG:HG3  | 1.85                     | 0.42              |
| 6:F:379:ASP:O    | 10:I:183:HOH:O   | 2.22                     | 0.42              |
| 7:G:260:MET:HG3  | 7:G:356:LEU:HD23 | 2.00                     | 0.42              |
| 2:B:146:VAL:O    | 2:B:150:VAL:HG23 | 2.20                     | 0.42              |
| 3:C:64:ASN:CB    | 10:I:510:HOH:O   | 2.62                     | 0.42              |
| 5:E:214:LEU:HD23 | 5:E:214:LEU:HA   | 1.94                     | 0.42              |
| 6:F:480:ILE:HA   | 6:F:481:PRO:HD3  | 1.93                     | 0.42              |
| 4:D:292:LEU:HB3  | 4:D:460:GLU:HB3  | 2.02                     | 0.41              |
| 5:E:297:GLU:HG2  | 5:E:297:GLU:H    | 1.65                     | 0.41              |
| 1:A:181:ASP:OD1  | 1:A:459:ARG:HD2  | 2.20                     | 0.41              |
| 1:A:480:ILE:HA   | 1:A:481:PRO:HD3  | 1.92                     | 0.41              |
| 3:C:204:GLY:O    | 3:C:208:VAL:HG12 | 2.20                     | 0.41              |
| 2:B:198:ARG:NE   | 8:B:601:GOL:O2   | 2.47                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:330:ARG:HH21 | 4:D:330:ARG:HA   | 1.85                     | 0.41              |
| 7:G:292:LEU:HB3  | 7:G:460:GLU:HB3  | 2.03                     | 0.41              |
| 4:H:370:ARG:HH12 | 4:H:403:ALY:HE3  | 1.85                     | 0.41              |
| 4:H:389:GLU:O    | 4:H:403:ALY:N    | 2.54                     | 0.41              |
| 4:H:232:CYS:HB3  | 4:H:353:PRO:HG2  | 2.01                     | 0.41              |
| 2:B:232:CYS:HB3  | 2:B:353:PRO:HG2  | 2.02                     | 0.41              |
| 3:C:125:MET:O    | 3:C:131:GLY:HA3  | 2.21                     | 0.41              |
| 1:A:133:GLN:HA   | 1:A:162:ILE:HB   | 2.02                     | 0.41              |
| 7:G:347:GLU:CD   | 8:G:601:GOL:O2   | 2.63                     | 0.41              |
| 2:B:241:PHE:HE2  | 2:B:365:ARG:NH1  | 2.19                     | 0.41              |
| 3:C:7:LEU:CD1    | 3:C:11:GLN:HG2   | 2.49                     | 0.41              |
| 3:C:389:GLU:O    | 3:C:403:ALY:N    | 2.54                     | 0.41              |
| 5:E:420:LEU:O    | 5:E:422:LEU:HD13 | 2.20                     | 0.41              |
| 7:G:268:LEU:C    | 7:G:268:LEU:HD23 | 2.45                     | 0.41              |
| 1:A:164:TRP:CE3  | 1:A:166:ARG:HD2  | 2.56                     | 0.41              |
| 1:A:355:ILE:HD13 | 1:A:496:MET:HG2  | 2.03                     | 0.41              |
| 2:B:480:ILE:HA   | 2:B:481:PRO:HD3  | 1.95                     | 0.41              |
| 4:D:133:GLN:HA   | 4:D:162:ILE:HB   | 2.03                     | 0.41              |
| 4:D:260:MET:HG3  | 4:D:356:LEU:HD23 | 2.02                     | 0.41              |
| 6:F:214:LEU:HD23 | 6:F:214:LEU:HA   | 1.96                     | 0.41              |
| 7:G:239:GLU:HG2  | 7:G:241:PHE:CZ   | 2.55                     | 0.41              |
| 1:A:330:ARG:HA   | 1:A:330:ARG:HH21 | 1.85                     | 0.41              |
| 4:D:264:LEU:HD23 | 4:D:264:LEU:HA   | 1.89                     | 0.41              |
| 5:E:273:MET:HE2  | 5:E:276:PRO:HD3  | 2.03                     | 0.41              |
| 6:F:21:PHE:HD1   | 6:F:21:PHE:HA    | 1.37                     | 0.41              |
| 6:F:193:GLU:OE1  | 6:F:455:SER:OG   | 2.30                     | 0.41              |
| 2:B:125:MET:O    | 2:B:131:GLY:HA3  | 2.21                     | 0.41              |
| 2:B:205:LYS:HE3  | 2:B:439:ARG:HH21 | 1.86                     | 0.41              |
| 5:E:181:ASP:CG   | 5:E:459:ARG:HH11 | 2.29                     | 0.41              |
| 5:E:365:ARG:CZ   | 5:E:365:ARG:HB3  | 2.51                     | 0.41              |
| 4:H:63:GLU:N     | 4:H:63:GLU:CD    | 2.78                     | 0.41              |
| 4:H:164:TRP:CE3  | 4:H:166:ARG:HD2  | 2.56                     | 0.41              |
| 4:H:260:MET:HG3  | 4:H:356:LEU:HD23 | 2.03                     | 0.41              |
| 1:A:292:LEU:HB3  | 1:A:460:GLU:HB3  | 2.04                     | 0.40              |
| 1:A:317:GLU:HA   | 1:A:317:GLU:OE1  | 2.21                     | 0.40              |
| 3:C:9:ARG:HH22   | 3:C:10:THR:CG2   | 2.34                     | 0.40              |
| 4:H:8:SER:H      | 4:H:11:GLN:NE2   | 2.19                     | 0.40              |
| 4:H:398:GLU:OE1  | 4:H:433:LEU:HD23 | 2.22                     | 0.40              |
| 6:F:168:ILE:HD11 | 6:F:444:VAL:HG21 | 2.04                     | 0.40              |
| 7:G:428:TYR:N    | 7:G:428:TYR:CD1  | 2.89                     | 0.40              |
| 6:F:27:HIS:HD2   | 10:I:448:HOH:O   | 2.05                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:H:246:ARG:CZ   | 4:H:246:ARG:CB   | 2.99                     | 0.40              |
| 1:A:125:MET:O    | 1:A:131:GLY:HA3  | 2.21                     | 0.40              |
| 5:E:304:VAL:HG23 | 5:E:495:LEU:HD22 | 2.04                     | 0.40              |
| 6:F:9:ARG:HB2    | 6:F:12:VAL:H     | 1.85                     | 0.40              |
| 6:F:22:GLN:NE2   | 6:F:22:GLN:N     | 2.68                     | 0.40              |
| 6:F:273:MET:HE2  | 6:F:276:PRO:HD3  | 2.03                     | 0.40              |
| 6:F:146:VAL:O    | 6:F:150:VAL:HG23 | 2.22                     | 0.40              |
| 7:G:72:ARG:NH1   | 7:G:112:TYR:OH   | 2.55                     | 0.40              |
| 7:G:232:CYS:HB3  | 7:G:353:PRO:HG2  | 2.02                     | 0.40              |
| 4:H:180:SER:HG   | 4:H:462:TRP:CD1  | 2.38                     | 0.40              |
| 4:H:197:TYR:CE2  | 4:H:449:GLN:HG2  | 2.56                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed         | Favoured   | Allowed | Outliers | Percentiles |    |
|-----|-------|------------------|------------|---------|----------|-------------|----|
| 1   | A     | 499/501 (100%)   | 484 (97%)  | 14 (3%) | 1 (0%)   | 43          | 53 |
| 2   | B     | 495/498 (99%)    | 483 (98%)  | 10 (2%) | 2 (0%)   | 30          | 36 |
| 3   | C     | 495/497 (100%)   | 483 (98%)  | 10 (2%) | 2 (0%)   | 30          | 36 |
| 4   | D     | 497/499 (100%)   | 486 (98%)  | 9 (2%)  | 2 (0%)   | 30          | 36 |
| 4   | H     | 496/499 (99%)    | 482 (97%)  | 11 (2%) | 3 (1%)   | 21          | 25 |
| 5   | E     | 497/500 (99%)    | 485 (98%)  | 10 (2%) | 2 (0%)   | 30          | 36 |
| 6   | F     | 495/497 (100%)   | 477 (96%)  | 16 (3%) | 2 (0%)   | 30          | 36 |
| 7   | G     | 493/496 (99%)    | 481 (98%)  | 10 (2%) | 2 (0%)   | 30          | 36 |
| All | All   | 3967/3987 (100%) | 3861 (97%) | 90 (2%) | 16 (0%)  | 30          | 36 |

All (16) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 9   | ARG  |
| 4   | D     | 430 | ASN  |
| 7   | G     | 429 | LYS  |
| 4   | H     | 430 | ASN  |
| 5   | E     | 396 | PRO  |
| 2   | B     | 435 | ASP  |
| 3   | C     | 435 | ASP  |
| 4   | D     | 435 | ASP  |
| 6   | F     | 21  | PHE  |
| 6   | F     | 435 | ASP  |
| 7   | G     | 435 | ASP  |
| 4   | H     | 6   | ALA  |
| 4   | H     | 435 | ASP  |
| 1   | A     | 435 | ASP  |
| 5   | E     | 435 | ASP  |
| 2   | B     | 129 | HIS  |

### 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     | 437/437 (100%)   | 410 (94%)  | 27 (6%)  | 16          | 21 |
| 2   | B     | 434/434 (100%)   | 401 (92%)  | 33 (8%)  | 12          | 15 |
| 3   | C     | 435/434 (100%)   | 401 (92%)  | 34 (8%)  | 11          | 14 |
| 4   | D     | 436/435 (100%)   | 403 (92%)  | 33 (8%)  | 12          | 15 |
| 4   | H     | 435/435 (100%)   | 406 (93%)  | 29 (7%)  | 15          | 19 |
| 5   | E     | 436/436 (100%)   | 396 (91%)  | 40 (9%)  | 8           | 10 |
| 6   | F     | 435/435 (100%)   | 401 (92%)  | 34 (8%)  | 11          | 14 |
| 7   | G     | 433/433 (100%)   | 400 (92%)  | 33 (8%)  | 12          | 15 |
| All | All   | 3481/3479 (100%) | 3218 (92%) | 263 (8%) | 12          | 15 |

All (263) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 5   | VAL  |
| 1   | A     | 9   | ARG  |
| 1   | A     | 10  | THR  |
| 1   | A     | 18  | GLU  |
| 1   | A     | 47  | LYS  |
| 1   | A     | 73  | SER  |
| 1   | A     | 82  | LYS  |
| 1   | A     | 95  | LYS  |
| 1   | A     | 119 | GLN  |
| 1   | A     | 203 | LEU  |
| 1   | A     | 210 | ASN  |
| 1   | A     | 220 | ILE  |
| 1   | A     | 266 | GLN  |
| 1   | A     | 270 | LEU  |
| 1   | A     | 290 | LYS  |
| 1   | A     | 297 | GLU  |
| 1   | A     | 330 | ARG  |
| 1   | A     | 386 | LYS  |
| 1   | A     | 397 | ASN  |
| 1   | A     | 398 | GLU  |
| 1   | A     | 406 | THR  |
| 1   | A     | 412 | PHE  |
| 1   | A     | 416 | GLU  |
| 1   | A     | 432 | LYS  |
| 1   | A     | 478 | LYS  |
| 1   | A     | 497 | LYS  |
| 1   | A     | 504 | GLU  |
| 2   | B     | 10  | THR  |
| 2   | B     | 47  | LYS  |
| 2   | B     | 63  | GLU  |
| 2   | B     | 73  | SER  |
| 2   | B     | 74  | ARG  |
| 2   | B     | 82  | LYS  |
| 2   | B     | 95  | LYS  |
| 2   | B     | 96  | LEU  |
| 2   | B     | 111 | GLN  |
| 2   | B     | 140 | LEU  |
| 2   | B     | 152 | LYS  |
| 2   | B     | 156 | GLU  |
| 2   | B     | 184 | SER  |
| 2   | B     | 203 | LEU  |
| 2   | B     | 210 | ASN  |
| 2   | B     | 214 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 220 | ILE  |
| 2   | B     | 246 | ARG  |
| 2   | B     | 252 | GLU  |
| 2   | B     | 290 | LYS  |
| 2   | B     | 297 | GLU  |
| 2   | B     | 395 | GLN  |
| 2   | B     | 398 | GLU  |
| 2   | B     | 402 | THR  |
| 2   | B     | 406 | THR  |
| 2   | B     | 408 | LYS  |
| 2   | B     | 416 | GLU  |
| 2   | B     | 420 | LEU  |
| 2   | B     | 422 | LEU  |
| 2   | B     | 429 | LYS  |
| 2   | B     | 432 | LYS  |
| 2   | B     | 476 | LYS  |
| 2   | B     | 478 | LYS  |
| 3   | C     | 7   | LEU  |
| 3   | C     | 8   | SER  |
| 3   | C     | 22  | GLN  |
| 3   | C     | 47  | LYS  |
| 3   | C     | 73  | SER  |
| 3   | C     | 74  | ARG  |
| 3   | C     | 95  | LYS  |
| 3   | C     | 119 | GLN  |
| 3   | C     | 161 | GLN  |
| 3   | C     | 203 | LEU  |
| 3   | C     | 208 | VAL  |
| 3   | C     | 210 | ASN  |
| 3   | C     | 211 | LEU  |
| 3   | C     | 214 | LEU  |
| 3   | C     | 219 | ARG  |
| 3   | C     | 220 | ILE  |
| 3   | C     | 246 | ARG  |
| 3   | C     | 266 | GLN  |
| 3   | C     | 275 | LYS  |
| 3   | C     | 290 | LYS  |
| 3   | C     | 297 | GLU  |
| 3   | C     | 315 | GLU  |
| 3   | C     | 330 | ARG  |
| 3   | C     | 366 | LYS  |
| 3   | C     | 398 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 408 | LYS  |
| 3   | C     | 418 | SER  |
| 3   | C     | 419 | GLU  |
| 3   | C     | 423 | THR  |
| 3   | C     | 426 | ASN  |
| 3   | C     | 429 | LYS  |
| 3   | C     | 459 | ARG  |
| 3   | C     | 474 | LEU  |
| 3   | C     | 478 | LYS  |
| 4   | D     | 7   | LEU  |
| 4   | D     | 10  | THR  |
| 4   | D     | 20  | LEU  |
| 4   | D     | 47  | LYS  |
| 4   | D     | 72  | ARG  |
| 4   | D     | 73  | SER  |
| 4   | D     | 74  | ARG  |
| 4   | D     | 82  | LYS  |
| 4   | D     | 95  | LYS  |
| 4   | D     | 96  | LEU  |
| 4   | D     | 119 | GLN  |
| 4   | D     | 132 | SER  |
| 4   | D     | 203 | LEU  |
| 4   | D     | 208 | VAL  |
| 4   | D     | 210 | ASN  |
| 4   | D     | 211 | LEU  |
| 4   | D     | 214 | LEU  |
| 4   | D     | 220 | ILE  |
| 4   | D     | 266 | GLN  |
| 4   | D     | 290 | LYS  |
| 4   | D     | 297 | GLU  |
| 4   | D     | 299 | GLN  |
| 4   | D     | 315 | GLU  |
| 4   | D     | 397 | ASN  |
| 4   | D     | 404 | MET  |
| 4   | D     | 406 | THR  |
| 4   | D     | 411 | MET  |
| 4   | D     | 417 | GLU  |
| 4   | D     | 418 | SER  |
| 4   | D     | 420 | LEU  |
| 4   | D     | 429 | LYS  |
| 4   | D     | 432 | LYS  |
| 4   | D     | 474 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | E     | 5   | VAL  |
| 5   | E     | 10  | THR  |
| 5   | E     | 28  | GLN  |
| 5   | E     | 45  | LYS  |
| 5   | E     | 47  | LYS  |
| 5   | E     | 63  | GLU  |
| 5   | E     | 72  | ARG  |
| 5   | E     | 73  | SER  |
| 5   | E     | 89  | LYS  |
| 5   | E     | 95  | LYS  |
| 5   | E     | 96  | LEU  |
| 5   | E     | 119 | GLN  |
| 5   | E     | 178 | GLN  |
| 5   | E     | 182 | ARG  |
| 5   | E     | 203 | LEU  |
| 5   | E     | 207 | MET  |
| 5   | E     | 208 | VAL  |
| 5   | E     | 210 | ASN  |
| 5   | E     | 211 | LEU  |
| 5   | E     | 214 | LEU  |
| 5   | E     | 220 | ILE  |
| 5   | E     | 249 | TYR  |
| 5   | E     | 266 | GLN  |
| 5   | E     | 275 | LYS  |
| 5   | E     | 290 | LYS  |
| 5   | E     | 297 | GLU  |
| 5   | E     | 299 | GLN  |
| 5   | E     | 330 | ARG  |
| 5   | E     | 365 | ARG  |
| 5   | E     | 406 | THR  |
| 5   | E     | 408 | LYS  |
| 5   | E     | 412 | PHE  |
| 5   | E     | 416 | GLU  |
| 5   | E     | 418 | SER  |
| 5   | E     | 429 | LYS  |
| 5   | E     | 432 | LYS  |
| 5   | E     | 474 | LEU  |
| 5   | E     | 478 | LYS  |
| 5   | E     | 503 | TYR  |
| 5   | E     | 504 | GLU  |
| 6   | F     | 7   | LEU  |
| 6   | F     | 9   | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | F     | 10  | THR  |
| 6   | F     | 17  | ARG  |
| 6   | F     | 22  | GLN  |
| 6   | F     | 47  | LYS  |
| 6   | F     | 72  | ARG  |
| 6   | F     | 73  | SER  |
| 6   | F     | 74  | ARG  |
| 6   | F     | 82  | LYS  |
| 6   | F     | 95  | LYS  |
| 6   | F     | 96  | LEU  |
| 6   | F     | 119 | GLN  |
| 6   | F     | 182 | ARG  |
| 6   | F     | 203 | LEU  |
| 6   | F     | 208 | VAL  |
| 6   | F     | 210 | ASN  |
| 6   | F     | 211 | LEU  |
| 6   | F     | 214 | LEU  |
| 6   | F     | 220 | ILE  |
| 6   | F     | 266 | GLN  |
| 6   | F     | 290 | LYS  |
| 6   | F     | 297 | GLU  |
| 6   | F     | 330 | ARG  |
| 6   | F     | 395 | GLN  |
| 6   | F     | 397 | ASN  |
| 6   | F     | 404 | MET  |
| 6   | F     | 406 | THR  |
| 6   | F     | 407 | LYS  |
| 6   | F     | 408 | LYS  |
| 6   | F     | 416 | GLU  |
| 6   | F     | 427 | ARG  |
| 6   | F     | 429 | LYS  |
| 6   | F     | 440 | LEU  |
| 7   | G     | 15  | ILE  |
| 7   | G     | 18  | GLU  |
| 7   | G     | 20  | LEU  |
| 7   | G     | 22  | GLN  |
| 7   | G     | 47  | LYS  |
| 7   | G     | 57  | ARG  |
| 7   | G     | 63  | GLU  |
| 7   | G     | 72  | ARG  |
| 7   | G     | 74  | ARG  |
| 7   | G     | 95  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | G     | 96  | LEU  |
| 7   | G     | 119 | GLN  |
| 7   | G     | 182 | ARG  |
| 7   | G     | 203 | LEU  |
| 7   | G     | 210 | ASN  |
| 7   | G     | 214 | LEU  |
| 7   | G     | 220 | ILE  |
| 7   | G     | 266 | GLN  |
| 7   | G     | 290 | LYS  |
| 7   | G     | 297 | GLU  |
| 7   | G     | 315 | GLU  |
| 7   | G     | 397 | ASN  |
| 7   | G     | 416 | GLU  |
| 7   | G     | 418 | SER  |
| 7   | G     | 423 | THR  |
| 7   | G     | 427 | ARG  |
| 7   | G     | 428 | TYR  |
| 7   | G     | 429 | LYS  |
| 7   | G     | 432 | LYS  |
| 7   | G     | 476 | LYS  |
| 7   | G     | 478 | LYS  |
| 7   | G     | 483 | ILE  |
| 7   | G     | 497 | LYS  |
| 4   | H     | 5   | VAL  |
| 4   | H     | 22  | GLN  |
| 4   | H     | 47  | LYS  |
| 4   | H     | 63  | GLU  |
| 4   | H     | 72  | ARG  |
| 4   | H     | 73  | SER  |
| 4   | H     | 95  | LYS  |
| 4   | H     | 96  | LEU  |
| 4   | H     | 119 | GLN  |
| 4   | H     | 133 | GLN  |
| 4   | H     | 152 | LYS  |
| 4   | H     | 178 | GLN  |
| 4   | H     | 206 | GLU  |
| 4   | H     | 208 | VAL  |
| 4   | H     | 210 | ASN  |
| 4   | H     | 211 | LEU  |
| 4   | H     | 214 | LEU  |
| 4   | H     | 220 | ILE  |
| 4   | H     | 290 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | H     | 297 | GLU  |
| 4   | H     | 315 | GLU  |
| 4   | H     | 333 | THR  |
| 4   | H     | 397 | ASN  |
| 4   | H     | 411 | MET  |
| 4   | H     | 416 | GLU  |
| 4   | H     | 432 | LYS  |
| 4   | H     | 433 | LEU  |
| 4   | H     | 474 | LEU  |
| 4   | H     | 478 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 27  | HIS  |
| 1   | A     | 124 | HIS  |
| 1   | A     | 161 | GLN  |
| 1   | A     | 178 | GLN  |
| 1   | A     | 388 | ASN  |
| 1   | A     | 395 | GLN  |
| 1   | A     | 414 | ASN  |
| 1   | A     | 426 | ASN  |
| 1   | A     | 502 | GLN  |
| 2   | B     | 11  | GLN  |
| 2   | B     | 27  | HIS  |
| 2   | B     | 124 | HIS  |
| 2   | B     | 161 | GLN  |
| 2   | B     | 178 | GLN  |
| 2   | B     | 201 | HIS  |
| 2   | B     | 266 | GLN  |
| 2   | B     | 299 | GLN  |
| 2   | B     | 301 | ASN  |
| 2   | B     | 384 | GLN  |
| 2   | B     | 388 | ASN  |
| 2   | B     | 414 | ASN  |
| 2   | B     | 430 | ASN  |
| 2   | B     | 471 | GLN  |
| 3   | C     | 11  | GLN  |
| 3   | C     | 27  | HIS  |
| 3   | C     | 119 | GLN  |
| 3   | C     | 124 | HIS  |
| 3   | C     | 161 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 209 | GLN  |
| 3   | C     | 301 | ASN  |
| 3   | C     | 388 | ASN  |
| 3   | C     | 395 | GLN  |
| 3   | C     | 426 | ASN  |
| 3   | C     | 471 | GLN  |
| 4   | D     | 27  | HIS  |
| 4   | D     | 124 | HIS  |
| 4   | D     | 301 | ASN  |
| 4   | D     | 384 | GLN  |
| 4   | D     | 502 | GLN  |
| 5   | E     | 83  | GLN  |
| 5   | E     | 124 | HIS  |
| 5   | E     | 161 | GLN  |
| 5   | E     | 178 | GLN  |
| 5   | E     | 201 | HIS  |
| 5   | E     | 299 | GLN  |
| 5   | E     | 301 | ASN  |
| 5   | E     | 502 | GLN  |
| 6   | F     | 11  | GLN  |
| 6   | F     | 27  | HIS  |
| 6   | F     | 124 | HIS  |
| 6   | F     | 161 | GLN  |
| 6   | F     | 201 | HIS  |
| 6   | F     | 299 | GLN  |
| 6   | F     | 384 | GLN  |
| 6   | F     | 471 | GLN  |
| 7   | G     | 11  | GLN  |
| 7   | G     | 27  | HIS  |
| 7   | G     | 124 | HIS  |
| 7   | G     | 161 | GLN  |
| 7   | G     | 209 | GLN  |
| 7   | G     | 263 | HIS  |
| 7   | G     | 388 | ASN  |
| 7   | G     | 471 | GLN  |
| 4   | H     | 11  | GLN  |
| 4   | H     | 27  | HIS  |
| 4   | H     | 83  | GLN  |
| 4   | H     | 119 | GLN  |
| 4   | H     | 124 | HIS  |
| 4   | H     | 178 | GLN  |
| 4   | H     | 209 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | H     | 266 | GLN  |
| 4   | H     | 388 | ASN  |
| 4   | H     | 426 | ASN  |
| 4   | H     | 430 | ASN  |
| 4   | H     | 471 | GLN  |
| 4   | H     | 502 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 2   | ALY  | B     | 403 | 2    | 10,11,12     | 0.91 | 1 (10%)     | 7,12,14     | 1.79 | 2 (28%)     |
| 4   | ALY  | H     | 403 | 4    | 10,11,12     | 1.05 | 2 (20%)     | 7,12,14     | 1.24 | 1 (14%)     |
| 5   | ALY  | E     | 403 | 5    | 10,11,12     | 0.77 | 0           | 7,12,14     | 1.18 | 1 (14%)     |
| 7   | ALY  | G     | 403 | 7    | 10,11,12     | 1.16 | 1 (10%)     | 7,12,14     | 1.45 | 1 (14%)     |
| 4   | ALY  | D     | 403 | 4    | 10,11,12     | 0.46 | 0           | 7,12,14     | 0.93 | 1 (14%)     |
| 3   | ALY  | C     | 403 | 3    | 10,11,12     | 0.96 | 0           | 7,12,14     | 1.09 | 0           |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings |
|-----|------|-------|-----|------|---------|-----------|-------|
| 2   | ALY  | B     | 403 | 2    | -       | 5/9/10/12 | -     |
| 4   | ALY  | H     | 403 | 4    | -       | 2/9/10/12 | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings |
|-----|------|-------|-----|------|---------|-----------|-------|
| 5   | ALY  | E     | 403 | 5    | -       | 3/9/10/12 | -     |
| 7   | ALY  | G     | 403 | 7    | -       | 5/9/10/12 | -     |
| 4   | ALY  | D     | 403 | 4    | -       | 3/9/10/12 | -     |
| 3   | ALY  | C     | 403 | 3    | -       | 3/9/10/12 | -     |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 7   | G     | 403 | ALY  | O-C   | 2.13 | 1.28        | 1.20     |
| 4   | H     | 403 | ALY  | O-C   | 2.13 | 1.28        | 1.20     |
| 2   | B     | 403 | ALY  | O-C   | 2.12 | 1.28        | 1.20     |
| 4   | H     | 403 | ALY  | CG-CD | 2.10 | 1.62        | 1.51     |

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | B     | 403 | ALY  | CE-NZ-CH  | 2.88  | 126.81      | 122.56   |
| 5   | E     | 403 | ALY  | CE-NZ-CH  | 2.79  | 126.69      | 122.56   |
| 2   | B     | 403 | ALY  | OH-CH-CH3 | -2.62 | 117.38      | 122.05   |
| 4   | H     | 403 | ALY  | CE-NZ-CH  | 2.58  | 126.37      | 122.56   |
| 4   | D     | 403 | ALY  | CE-NZ-CH  | 2.04  | 125.57      | 122.56   |
| 7   | G     | 403 | ALY  | CG-CD-CE  | 2.02  | 122.88      | 113.56   |

There are no chirality outliers.

All (21) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 3   | C     | 403 | ALY  | C-CA-CB-CG   |
| 4   | D     | 403 | ALY  | O-C-CA-CB    |
| 7   | G     | 403 | ALY  | C-CA-CB-CG   |
| 2   | B     | 403 | ALY  | CD-CE-NZ-CH  |
| 7   | G     | 403 | ALY  | CH3-CH-NZ-CE |
| 4   | H     | 403 | ALY  | CG-CD-CE-NZ  |
| 2   | B     | 403 | ALY  | CE-CD-CG-CB  |
| 2   | B     | 403 | ALY  | CA-CB-CG-CD  |
| 2   | B     | 403 | ALY  | CH3-CH-NZ-CE |
| 3   | C     | 403 | ALY  | CH3-CH-NZ-CE |
| 4   | D     | 403 | ALY  | CA-CB-CG-CD  |
| 7   | G     | 403 | ALY  | CE-CD-CG-CB  |
| 4   | D     | 403 | ALY  | CE-CD-CG-CB  |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 5   | E     | 403 | ALY  | CE-CD-CG-CB |
| 5   | E     | 403 | ALY  | C-CA-CB-CG  |
| 4   | H     | 403 | ALY  | C-CA-CB-CG  |
| 7   | G     | 403 | ALY  | CG-CD-CE-NZ |
| 3   | C     | 403 | ALY  | CA-CB-CG-CD |
| 5   | E     | 403 | ALY  | CG-CD-CE-NZ |
| 7   | G     | 403 | ALY  | OH-CH-NZ-CE |
| 2   | B     | 403 | ALY  | C-CA-CB-CG  |

There are no ring outliers.

5 monomers are involved in 23 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | B     | 403 | ALY  | 15      | 0            |
| 4   | H     | 403 | ALY  | 2       | 0            |
| 5   | E     | 403 | ALY  | 4       | 0            |
| 4   | D     | 403 | ALY  | 1       | 0            |
| 3   | C     | 403 | ALY  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is 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 | $\# Z  > 2$ |
| 8   | GOL  | F     | 601 | -    | 5,5,5        | 0.41 | 0           | 5,5,5       | 1.69 | 1 (20%)     |
| 8   | GOL  | E     | 601 | -    | 5,5,5        | 0.30 | 0           | 5,5,5       | 0.76 | 0           |
| 8   | GOL  | B     | 601 | -    | 5,5,5        | 0.43 | 0           | 5,5,5       | 1.08 | 0           |
| 8   | GOL  | H     | 601 | -    | 5,5,5        | 0.29 | 0           | 5,5,5       | 0.71 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 8   | GOL  | D     | 601 | -    | 5,5,5        | 0.63 | 0        | 5,5,5       | 1.26 | 0        |
| 8   | GOL  | C     | 601 | -    | 5,5,5        | 0.97 | 0        | 5,5,5       | 1.34 | 1 (20%)  |
| 8   | GOL  | G     | 601 | -    | 5,5,5        | 0.68 | 0        | 5,5,5       | 1.42 | 0        |
| 8   | GOL  | B     | 602 | -    | 5,5,5        | 0.21 | 0        | 5,5,5       | 0.42 | 0        |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 8   | GOL  | F     | 601 | -    | -       | 4/4/4/4  | -     |
| 8   | GOL  | E     | 601 | -    | -       | 1/4/4/4  | -     |
| 8   | GOL  | B     | 601 | -    | -       | 2/4/4/4  | -     |
| 8   | GOL  | H     | 601 | -    | -       | 2/4/4/4  | -     |
| 8   | GOL  | D     | 601 | -    | -       | 4/4/4/4  | -     |
| 8   | GOL  | C     | 601 | -    | -       | 1/4/4/4  | -     |
| 8   | GOL  | G     | 601 | -    | -       | 4/4/4/4  | -     |
| 8   | GOL  | B     | 602 | -    | -       | 2/4/4/4  | -     |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 8   | F     | 601 | GOL  | O2-C2-C3 | -2.51 | 98.78       | 109.18   |
| 8   | C     | 601 | GOL  | O1-C1-C2 | 2.11  | 119.89      | 110.38   |

There are no chirality outliers.

All (20) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 8   | B     | 602 | GOL  | O1-C1-C2-C3 |
| 8   | D     | 601 | GOL  | O1-C1-C2-C3 |
| 8   | D     | 601 | GOL  | C1-C2-C3-O3 |
| 8   | F     | 601 | GOL  | O1-C1-C2-C3 |
| 8   | G     | 601 | GOL  | C1-C2-C3-O3 |
| 8   | F     | 601 | GOL  | O1-C1-C2-O2 |
| 8   | B     | 601 | GOL  | O1-C1-C2-C3 |
| 8   | F     | 601 | GOL  | C1-C2-C3-O3 |

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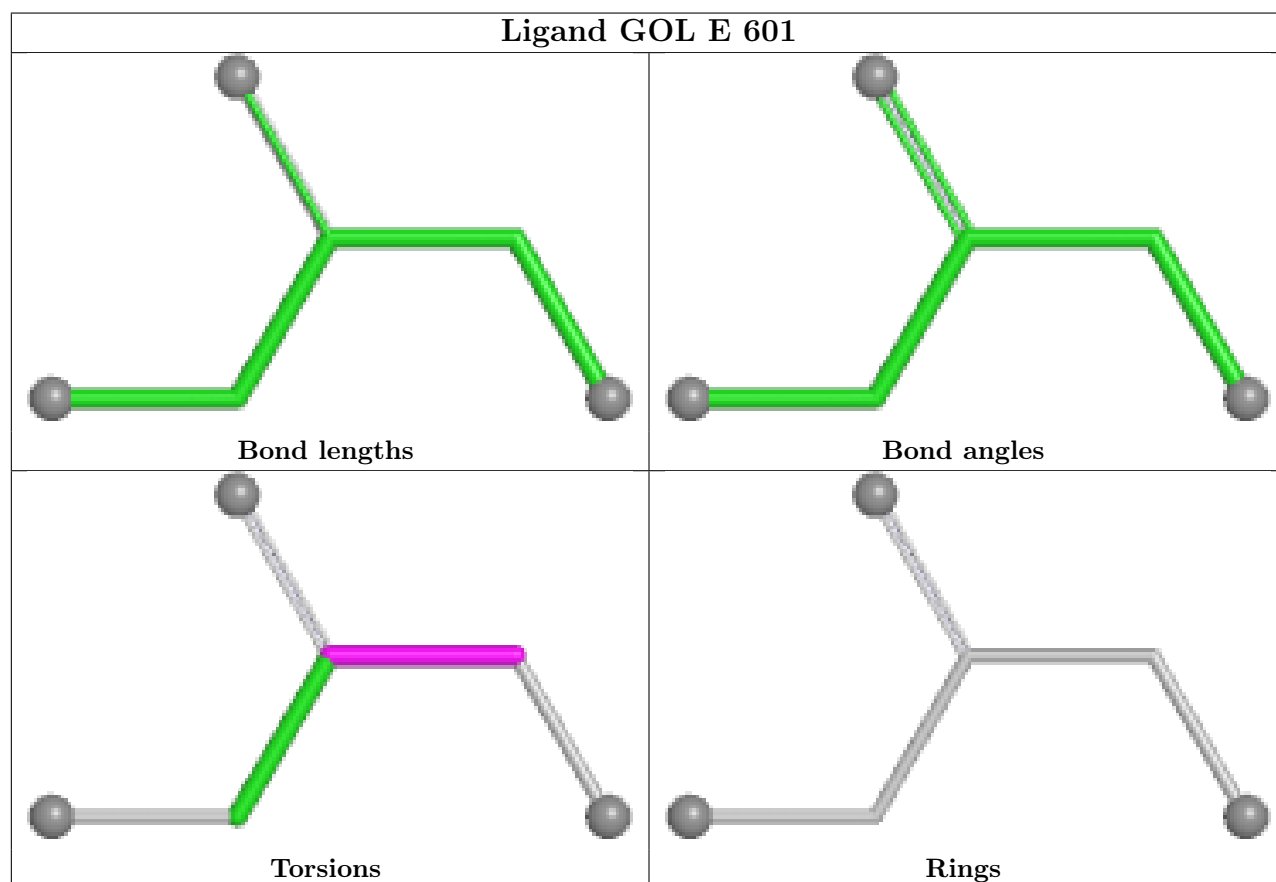
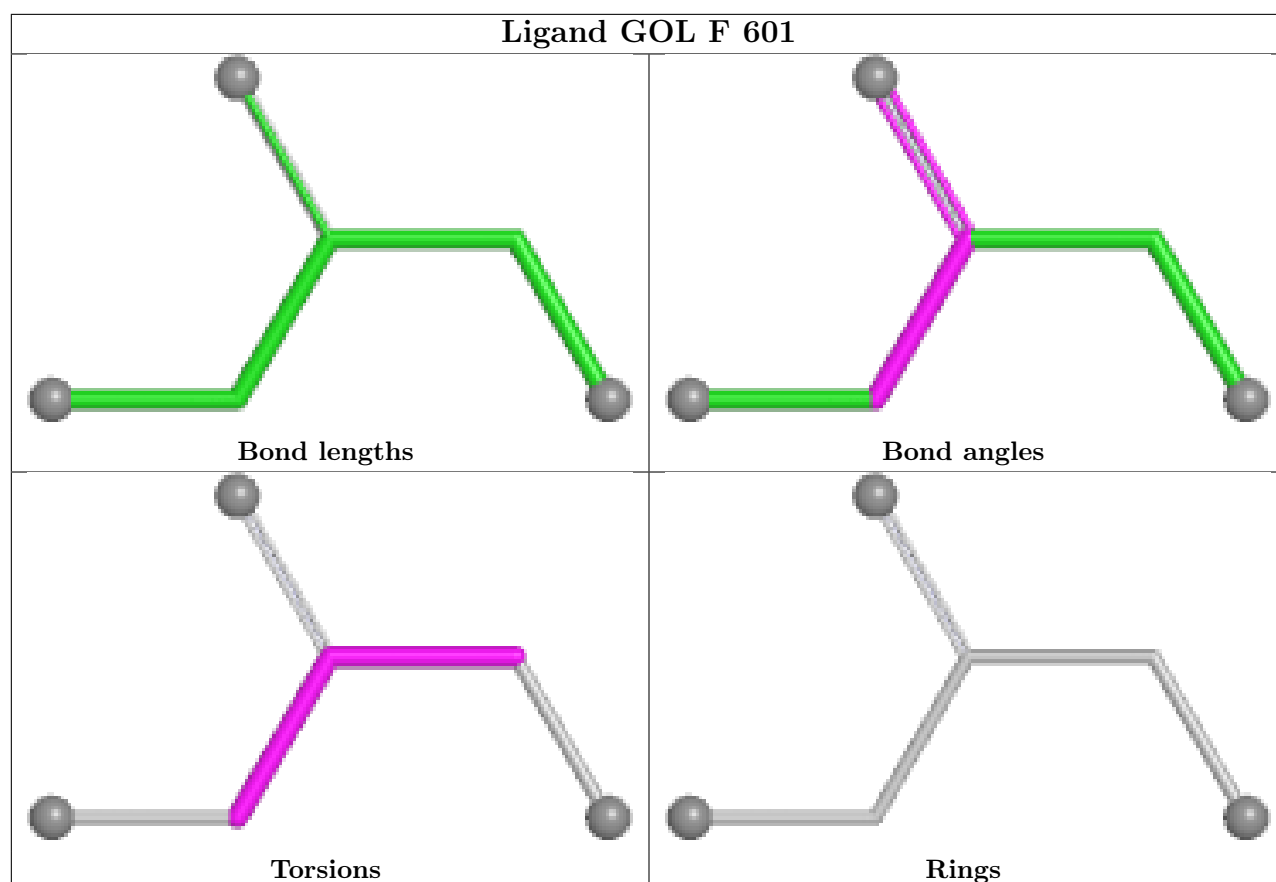
| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 8   | G     | 601 | GOL  | O1-C1-C2-C3 |
| 8   | H     | 601 | GOL  | O1-C1-C2-C3 |
| 8   | B     | 601 | GOL  | O1-C1-C2-O2 |
| 8   | B     | 602 | GOL  | O1-C1-C2-O2 |
| 8   | D     | 601 | GOL  | O1-C1-C2-O2 |
| 8   | D     | 601 | GOL  | O2-C2-C3-O3 |
| 8   | G     | 601 | GOL  | O2-C2-C3-O3 |
| 8   | C     | 601 | GOL  | O2-C2-C3-O3 |
| 8   | E     | 601 | GOL  | O1-C1-C2-O2 |
| 8   | F     | 601 | GOL  | O2-C2-C3-O3 |
| 8   | G     | 601 | GOL  | O1-C1-C2-O2 |
| 8   | H     | 601 | GOL  | O1-C1-C2-O2 |

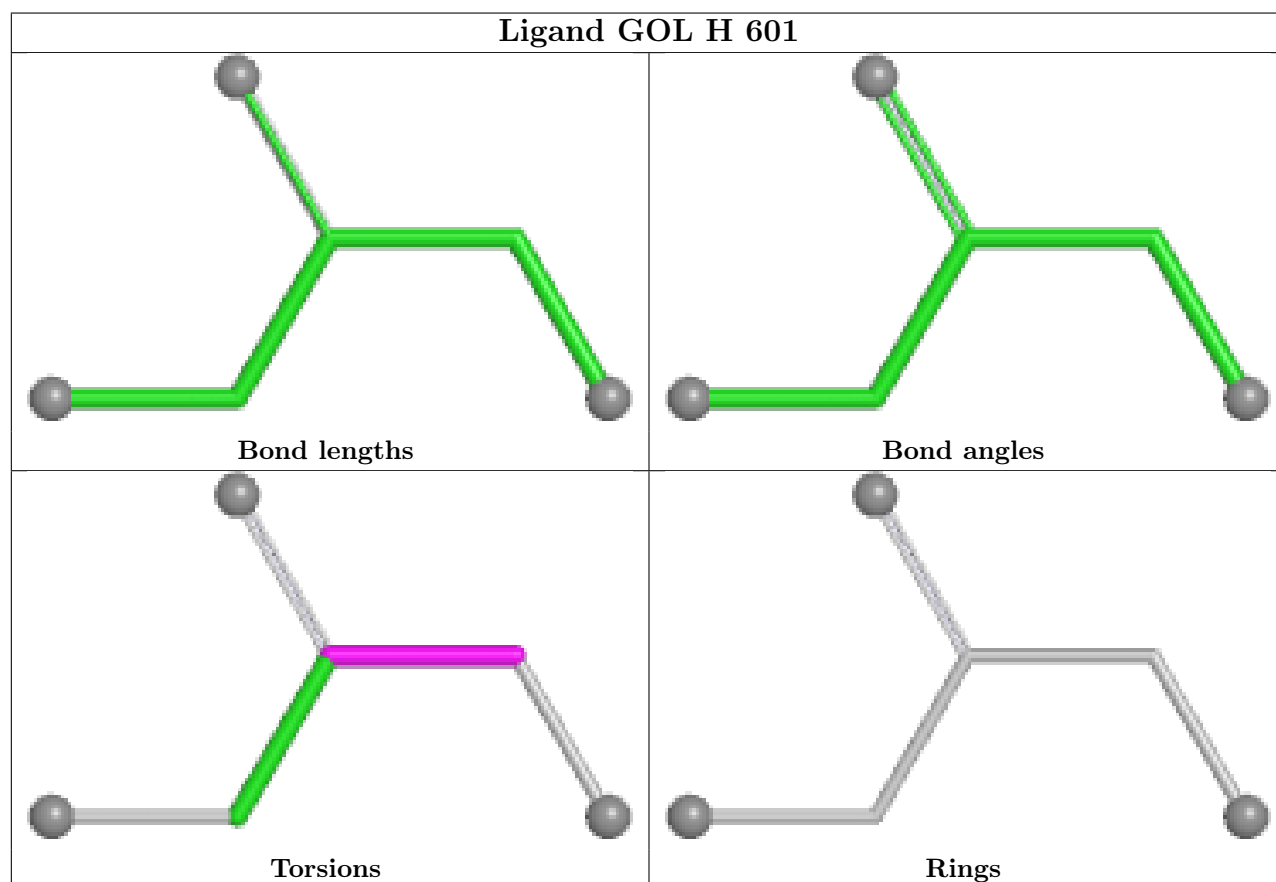
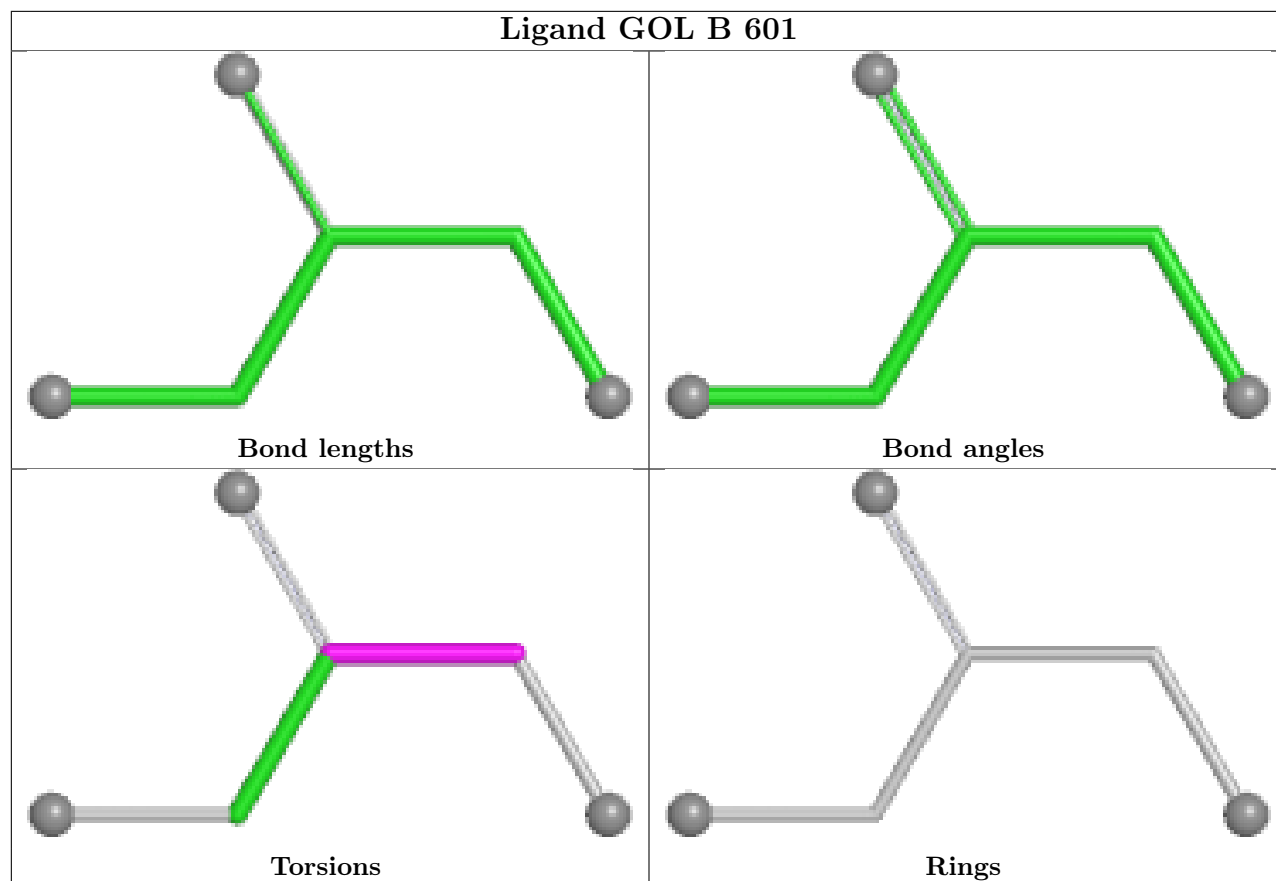
There are no ring outliers.

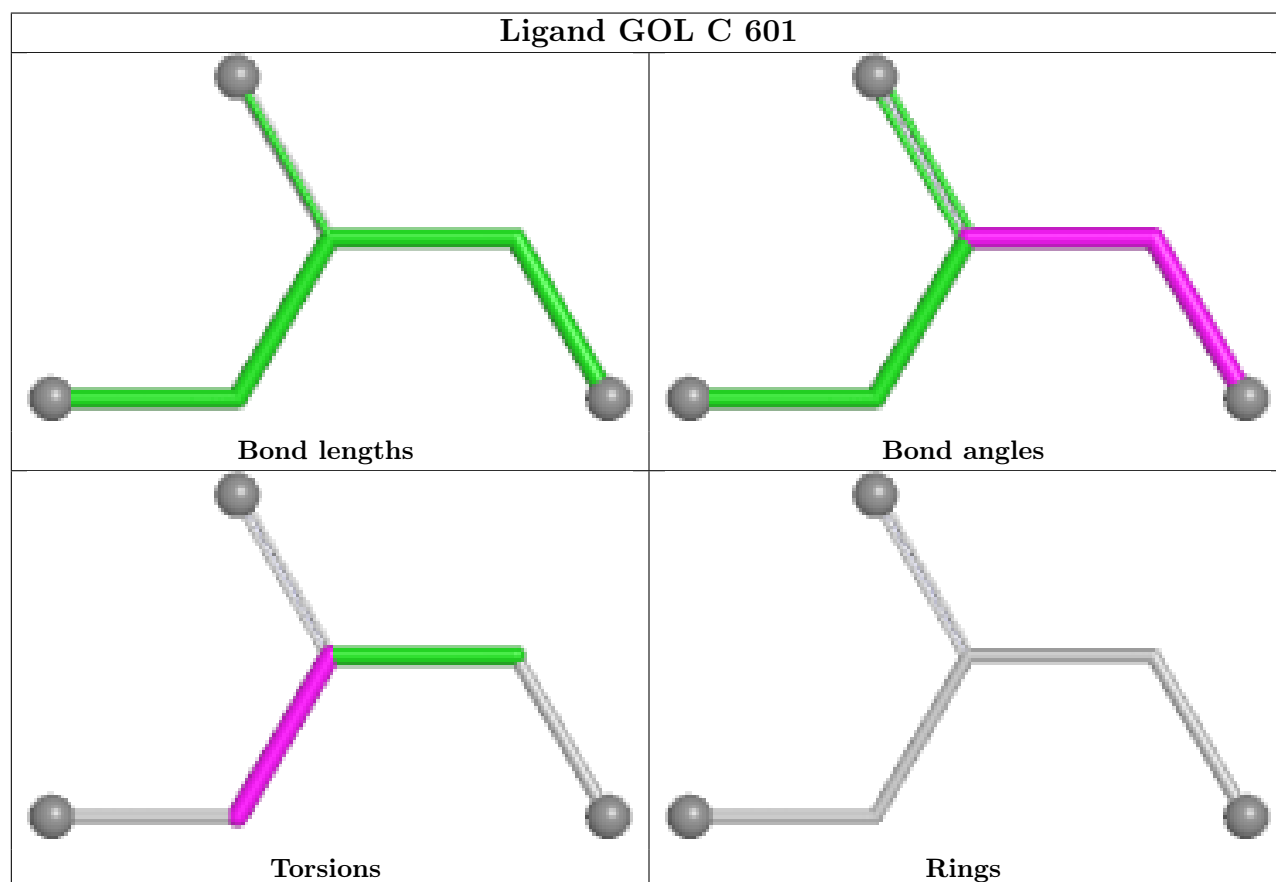
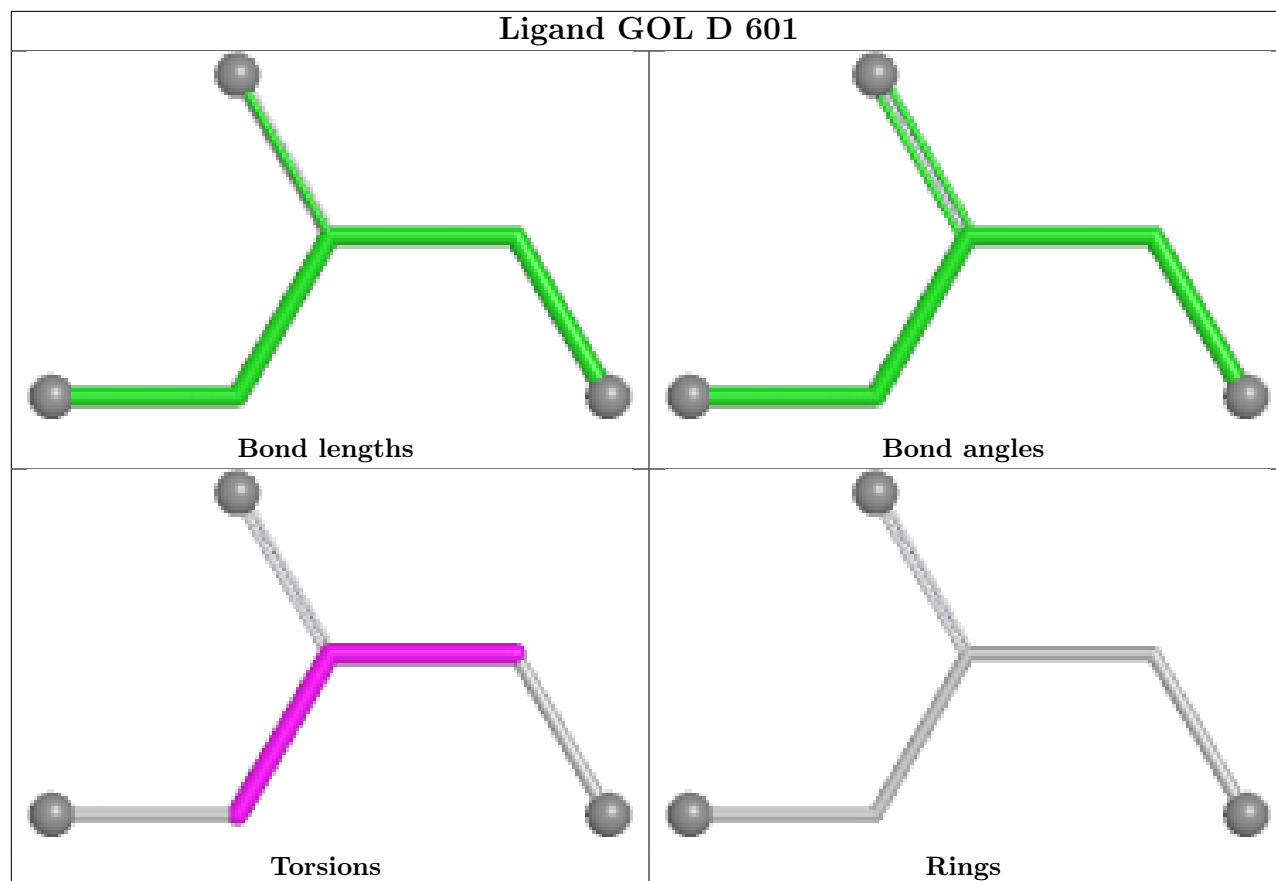
8 monomers are involved in 17 short contacts:

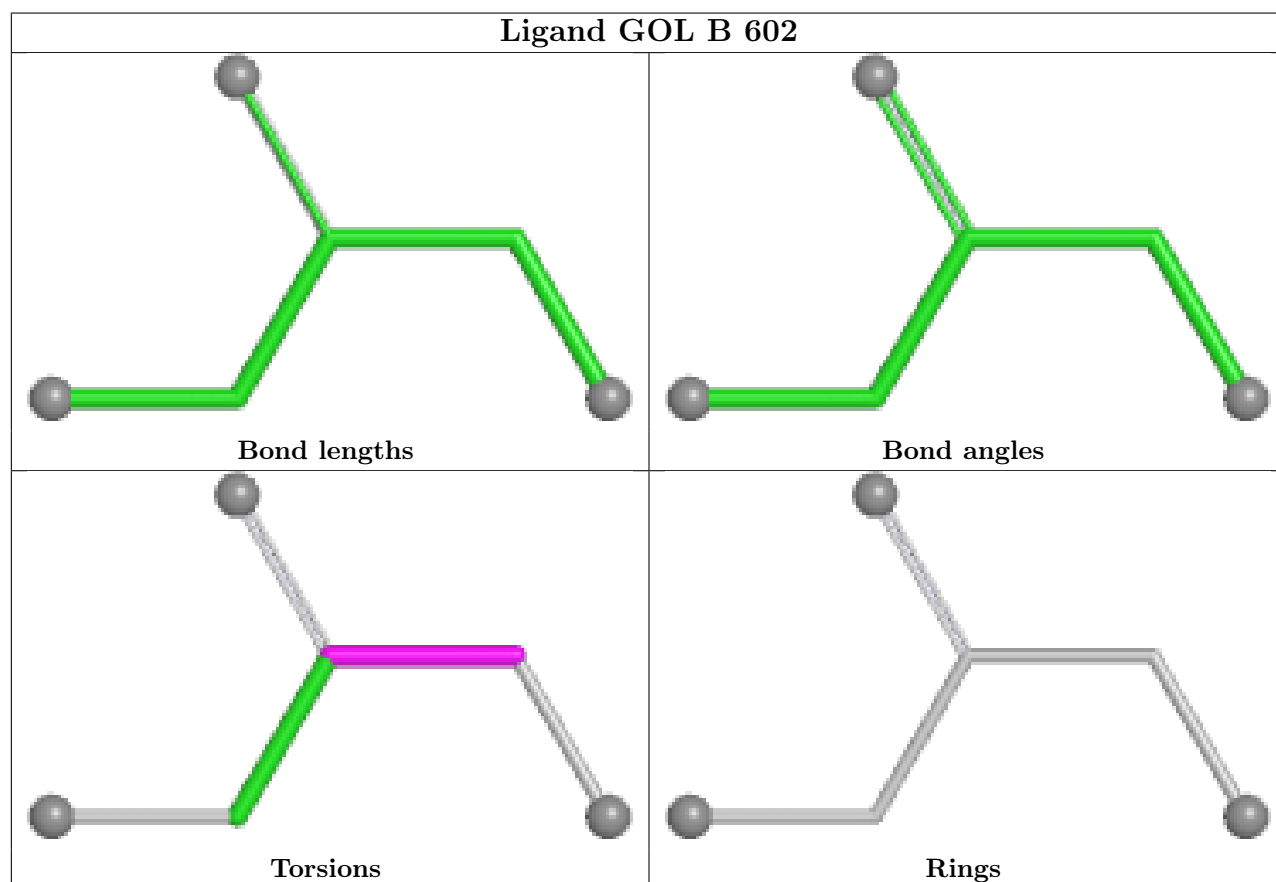
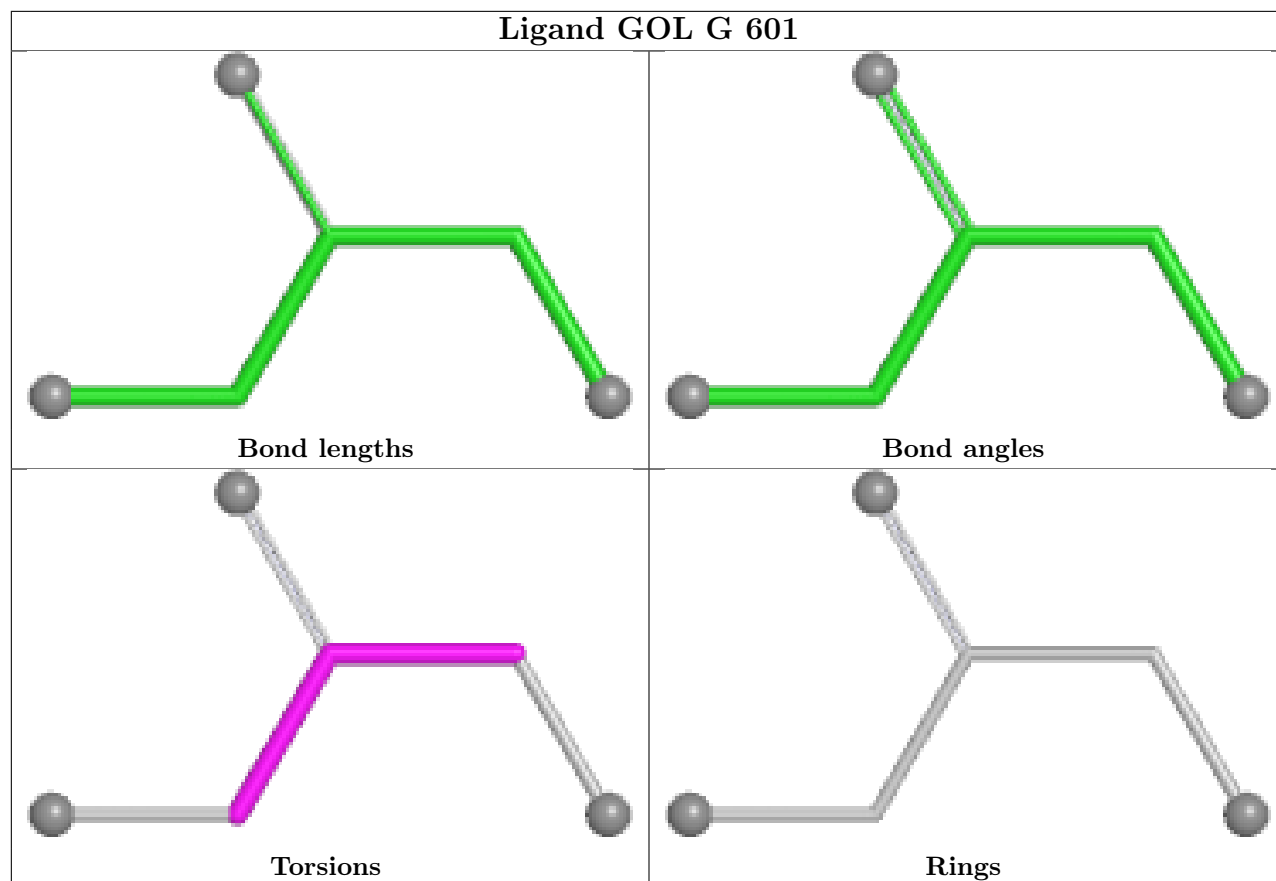
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 8   | F     | 601 | GOL  | 2       | 0            |
| 8   | E     | 601 | GOL  | 4       | 0            |
| 8   | B     | 601 | GOL  | 2       | 0            |
| 8   | H     | 601 | GOL  | 2       | 0            |
| 8   | D     | 601 | GOL  | 1       | 0            |
| 8   | C     | 601 | GOL  | 1       | 0            |
| 8   | G     | 601 | GOL  | 1       | 0            |
| 8   | B     | 602 | GOL  | 4       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9  |
|-----|-------|-----------------|--------|---------------|-----------------------|--------|
| 1   | A     | 501/501 (100%)  | -0.14  | 5 (0%) 79 81  | 35, 51, 87, 129       | 0      |
| 2   | B     | 497/498 (99%)   | -0.14  | 3 (0%) 85 86  | 35, 50, 79, 127       | 0      |
| 3   | C     | 496/497 (99%)   | -0.13  | 6 (1%) 76 78  | 30, 51, 85, 112       | 1 (0%) |
| 4   | D     | 498/499 (99%)   | -0.10  | 2 (0%) 88 89  | 30, 52, 79, 104       | 1 (0%) |
| 4   | H     | 498/499 (99%)   | 0.00   | 5 (1%) 79 81  | 36, 56, 91, 114       | 0      |
| 5   | E     | 499/500 (99%)   | 0.01   | 6 (1%) 76 78  | 34, 58, 93, 126       | 0      |
| 6   | F     | 497/497 (100%)  | -0.01  | 11 (2%) 62 64 | 36, 52, 92, 157       | 0      |
| 7   | G     | 495/496 (99%)   | 0.17   | 6 (1%) 76 78  | 38, 65, 100, 128      | 0      |
| All | All   | 3981/3987 (99%) | -0.04  | 44 (1%) 78 79 | 30, 54, 90, 157       | 2 (0%) |

All (44) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | D     | 412 | PHE  | 4.2  |
| 4   | H     | 412 | PHE  | 4.1  |
| 6   | F     | 412 | PHE  | 4.0  |
| 7   | G     | 424 | TYR  | 3.6  |
| 5   | E     | 412 | PHE  | 3.6  |
| 3   | C     | 7   | LEU  | 3.5  |
| 2   | B     | 412 | PHE  | 3.5  |
| 3   | C     | 412 | PHE  | 3.5  |
| 6   | F     | 15  | ILE  | 3.3  |
| 6   | F     | 21  | PHE  | 3.3  |
| 5   | E     | 5   | VAL  | 3.3  |
| 7   | G     | 412 | PHE  | 3.2  |
| 5   | E     | 249 | TYR  | 3.2  |
| 6   | F     | 17  | ARG  | 3.1  |
| 5   | E     | 424 | TYR  | 3.0  |
| 4   | H     | 5   | VAL  | 3.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 6   | F     | 424 | TYR  | 3.0  |
| 6   | F     | 7   | LEU  | 3.0  |
| 1   | A     | 412 | PHE  | 2.9  |
| 4   | H     | 21  | PHE  | 2.8  |
| 6   | F     | 12  | VAL  | 2.7  |
| 6   | F     | 241 | PHE  | 2.7  |
| 7   | G     | 241 | PHE  | 2.7  |
| 7   | G     | 220 | ILE  | 2.6  |
| 1   | A     | 424 | TYR  | 2.5  |
| 3   | C     | 503 | TYR  | 2.5  |
| 1   | A     | 5   | VAL  | 2.4  |
| 5   | E     | 420 | LEU  | 2.4  |
| 4   | H     | 241 | PHE  | 2.4  |
| 3   | C     | 211 | LEU  | 2.4  |
| 4   | H     | 424 | TYR  | 2.4  |
| 7   | G     | 503 | TYR  | 2.3  |
| 7   | G     | 12  | VAL  | 2.3  |
| 1   | A     | 423 | THR  | 2.3  |
| 6   | F     | 420 | LEU  | 2.2  |
| 1   | A     | 21  | PHE  | 2.2  |
| 6   | F     | 503 | TYR  | 2.2  |
| 6   | F     | 425 | GLY  | 2.1  |
| 2   | B     | 183 | LEU  | 2.1  |
| 4   | D     | 211 | LEU  | 2.1  |
| 3   | C     | 220 | ILE  | 2.1  |
| 2   | B     | 6   | ALA  | 2.1  |
| 5   | E     | 144 | PRO  | 2.1  |
| 3   | C     | 414 | ASN  | 2.0  |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 7   | ALY  | G     | 403 | 12/13 | 0.89 | 0.11 | 41,63,82,82                | 0     |
| 2   | ALY  | B     | 403 | 12/13 | 0.92 | 0.12 | 44,68,86,86                | 0     |
| 4   | ALY  | H     | 403 | 12/13 | 0.92 | 0.10 | 34,60,73,77                | 0     |
| 5   | ALY  | E     | 403 | 12/13 | 0.93 | 0.09 | 45,61,74,76                | 0     |
| 3   | ALY  | C     | 403 | 12/13 | 0.94 | 0.10 | 35,58,73,76                | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 4   | ALY  | D     | 403 | 12/13 | 0.95 | 0.08 | 40,60,73,76                 | 0     |

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

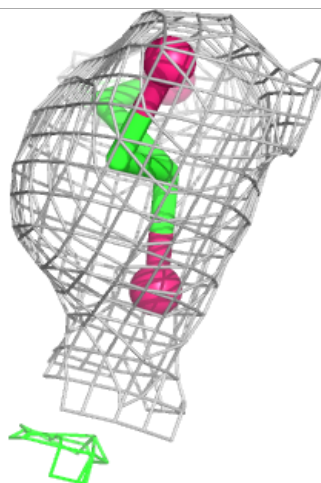
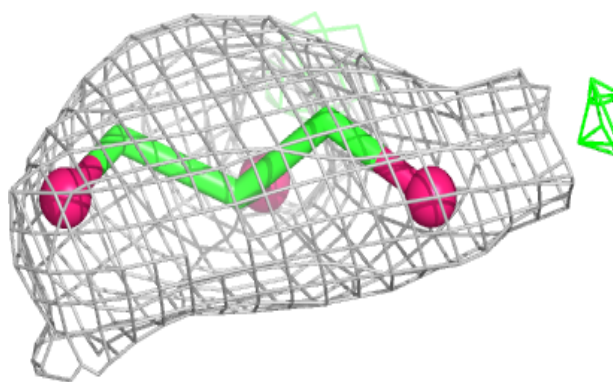
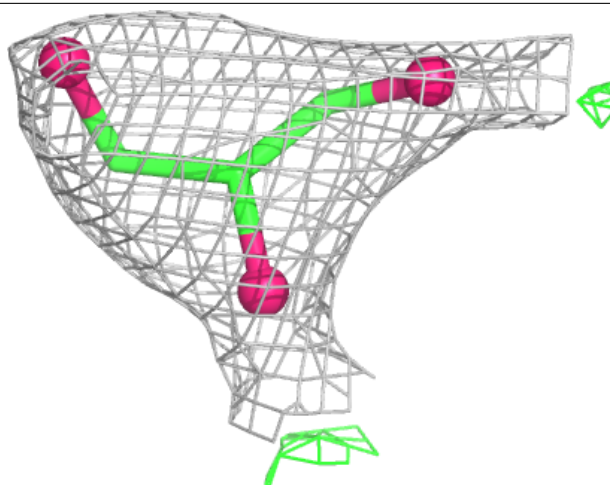
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 8   | GOL  | H     | 601 | 6/6   | 0.85 | 0.13 | 56,68,71,72                 | 0     |
| 9   | CU   | J     | 1   | 1/1   | 0.85 | 0.14 | 124,124,124,124             | 0     |
| 8   | GOL  | B     | 602 | 6/6   | 0.89 | 0.11 | 52,76,81,84                 | 0     |
| 8   | GOL  | F     | 601 | 6/6   | 0.90 | 0.12 | 56,62,68,75                 | 0     |
| 8   | GOL  | C     | 601 | 6/6   | 0.91 | 0.15 | 41,45,66,70                 | 0     |
| 8   | GOL  | B     | 601 | 6/6   | 0.91 | 0.12 | 45,59,72,76                 | 0     |
| 8   | GOL  | D     | 601 | 6/6   | 0.92 | 0.09 | 52,68,71,80                 | 0     |
| 8   | GOL  | E     | 601 | 6/6   | 0.93 | 0.10 | 61,74,88,94                 | 0     |
| 8   | GOL  | G     | 601 | 6/6   | 0.93 | 0.13 | 44,48,53,60                 | 0     |

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

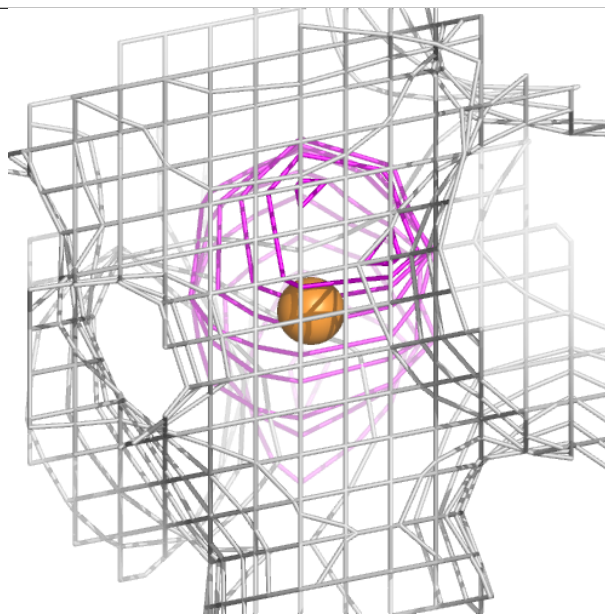
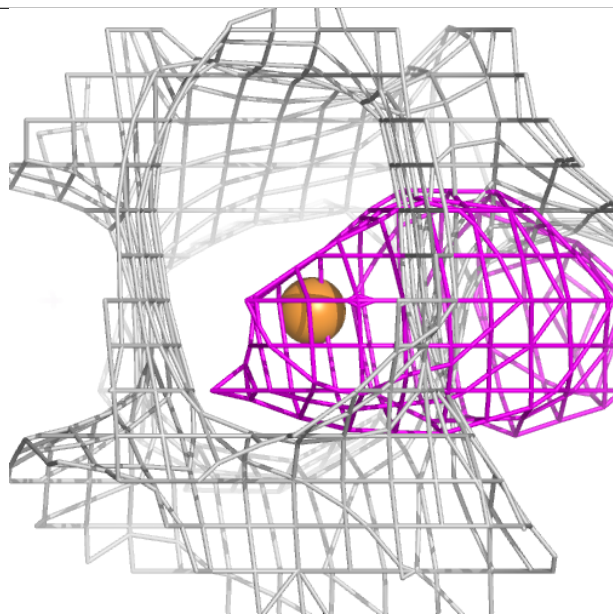
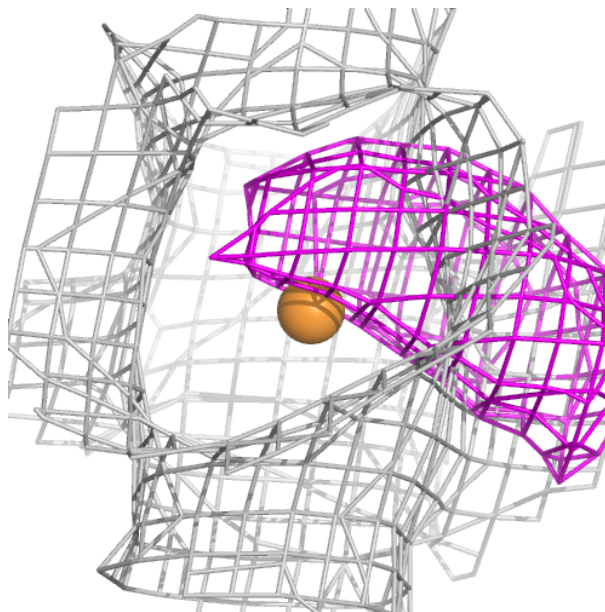
**Electron density around GOL H 601:**

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



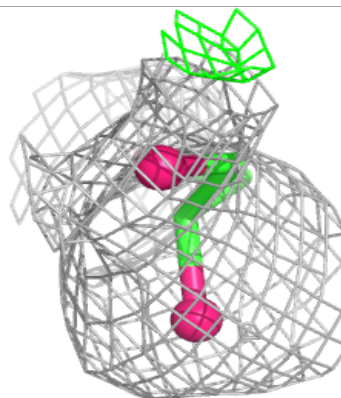
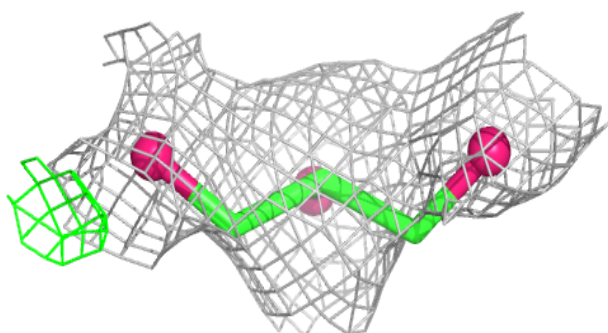
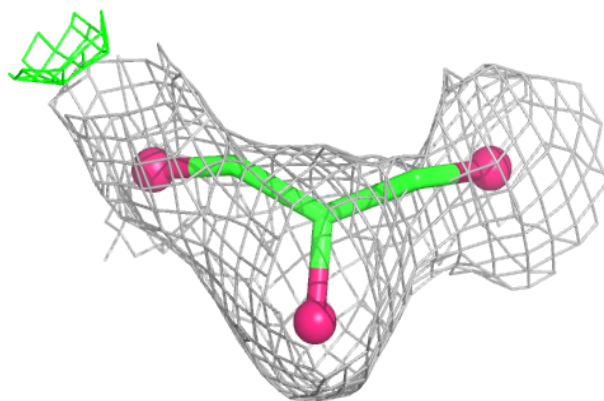
**Electron density around CU J 1:**

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

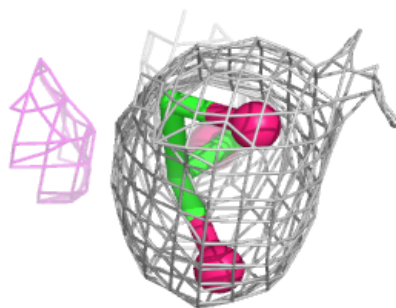
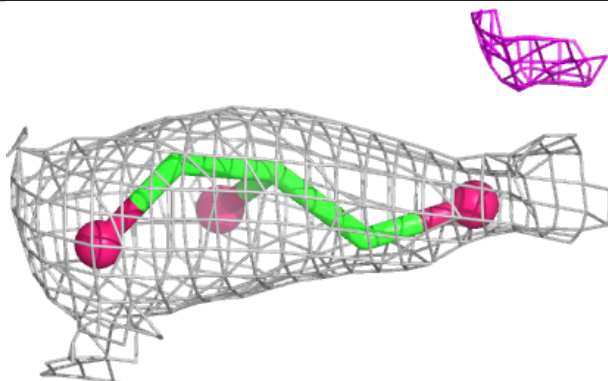
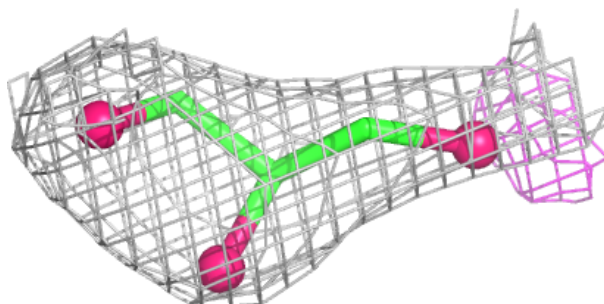


**Electron density around GOL B 602:**

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

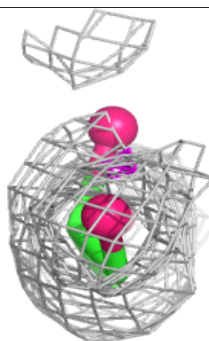
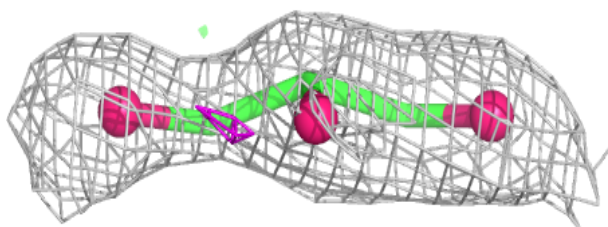
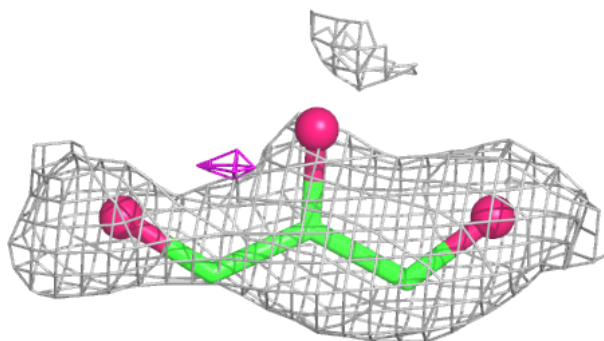
**Electron density around GOL F 601:**

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



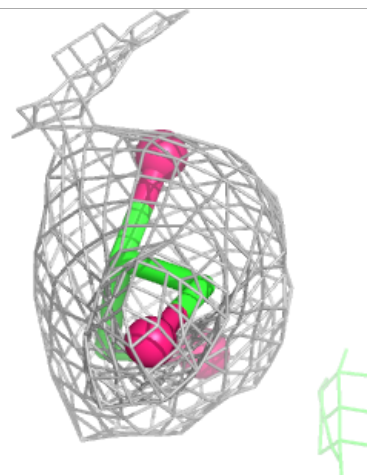
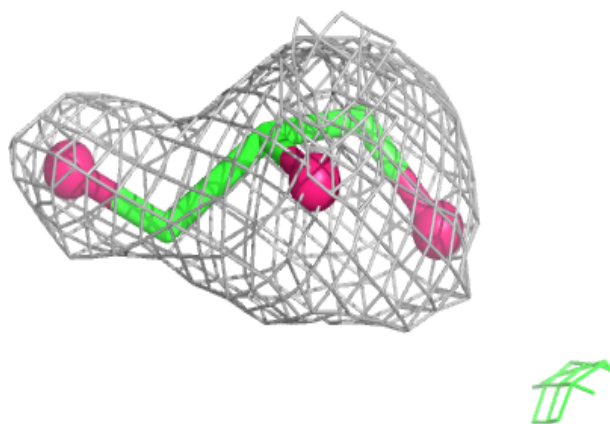
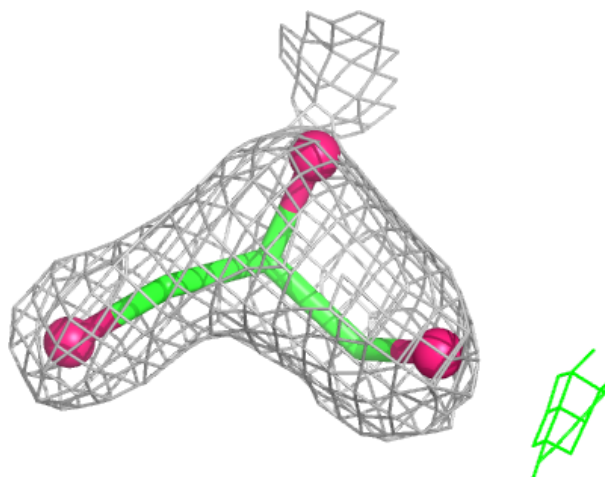
**Electron density around GOL C 601:**

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



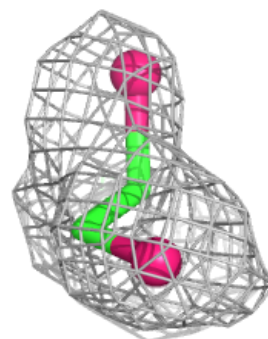
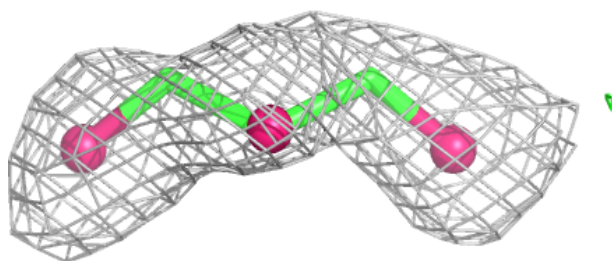
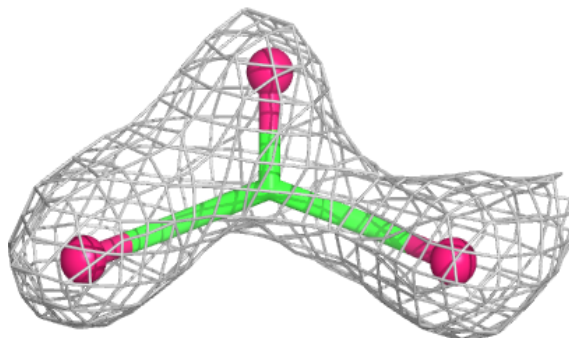
**Electron density around GOL B 601:**

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

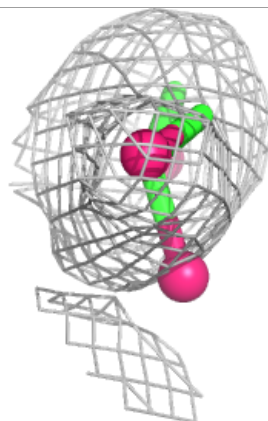
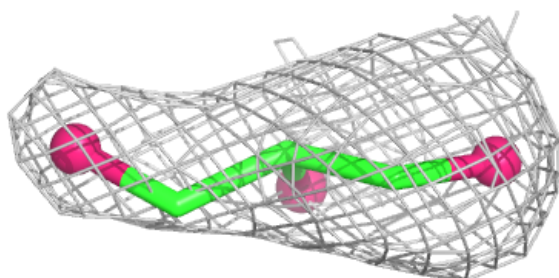
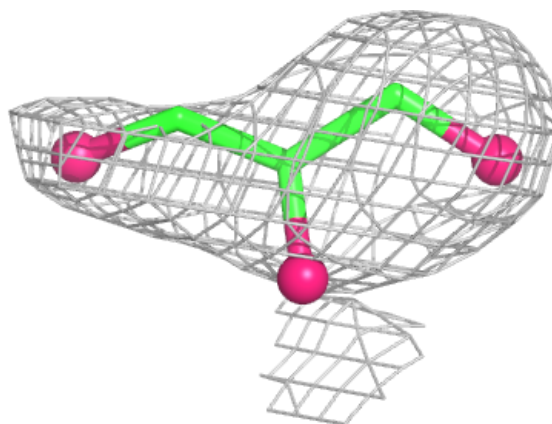


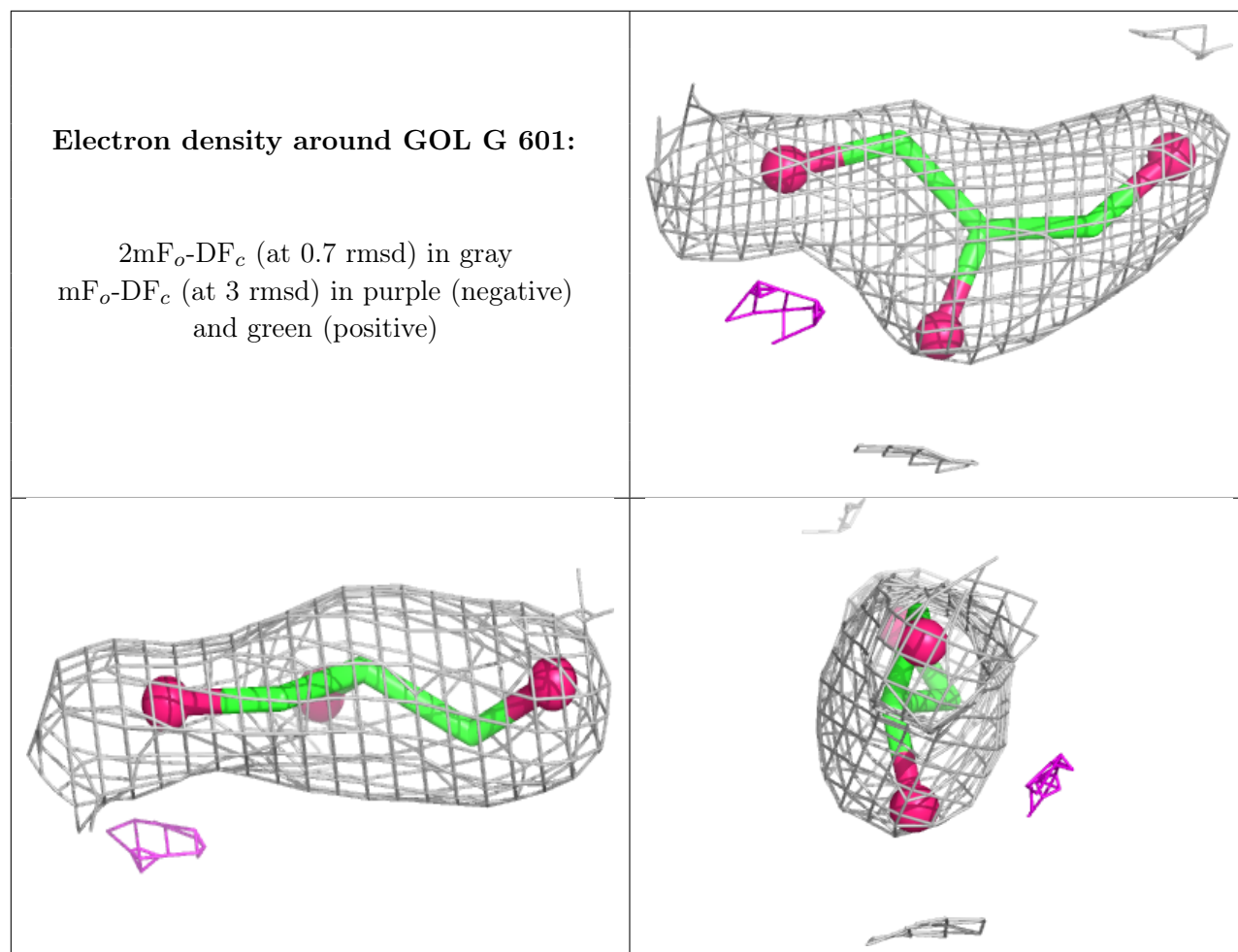
**Electron density around GOL D 601:**

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

**Electron density around GOL E 601:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.