



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:05 PM UTC

PDB ID : 2F2H / pdb\_00002f2h  
Title : Structure of the YicI thiosugar Michaelis complex  
Authors : Kim, Y.-W.; Lovering, A.L.; Strynadka, N.C.J.; Withers, S.G.  
Deposited on : 2005-11-16  
Resolution : 1.95 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

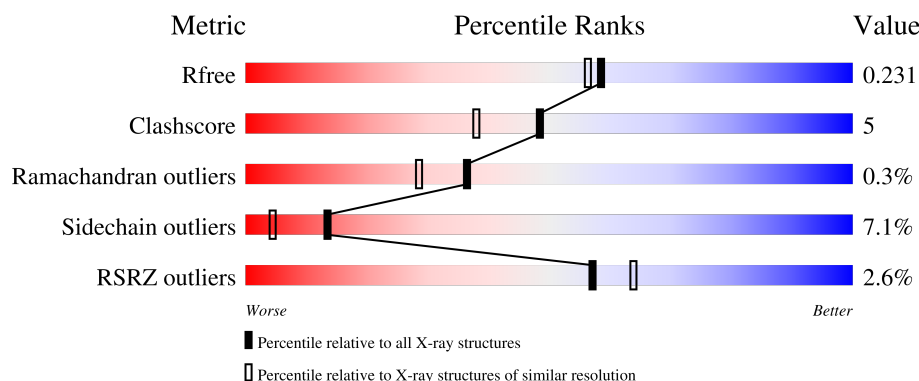
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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                      | 3494 (1.96-1.96)                                      |
| Clashscore            | 190562                      | 3612 (1.96-1.96)                                      |
| Ramachandran outliers | 187476                      | 3587 (1.96-1.96)                                      |
| Sidechain outliers    | 187428                      | 3587 (1.96-1.96)                                      |
| RSRZ outliers         | 180081                      | 3495 (1.96-1.96)                                      |

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     | 773    | <div> <div>2%</div> <div>85% 12% .</div> </div>   |
| 1   | B     | 773    | <div> <div>3%</div> <div>86% 13% .</div> </div>   |
| 1   | C     | 773    | <div> <div>%</div> <div>84% 14% .</div> </div>    |
| 1   | D     | 773    | <div> <div>3%</div> <div>85% 13% ..</div> </div>  |
| 1   | E     | 773    | <div> <div>3%</div> <div>82% 14% ...</div> </div> |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 1   | F     | 773    |  |

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   | SO4  | F     | 3001 | -         | -        | X       | -                |

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 39799 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 Putative family 31 glucosidase yicI.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1   | A     | 773      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6232  | 3981 | 1071 | 1148 | 32 |         |         |       |
| 1   | B     | 773      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6232  | 3981 | 1071 | 1148 | 32 |         |         |       |
| 1   | C     | 773      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6232  | 3981 | 1071 | 1148 | 32 |         |         |       |
| 1   | D     | 773      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6232  | 3981 | 1071 | 1148 | 32 |         |         |       |
| 1   | E     | 773      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6232  | 3981 | 1071 | 1148 | 32 |         |         |       |
| 1   | F     | 773      | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 6232  | 3981 | 1071 | 1148 | 32 |         |         |       |

There are 6 discrepancies between the modelled and reference sequences:

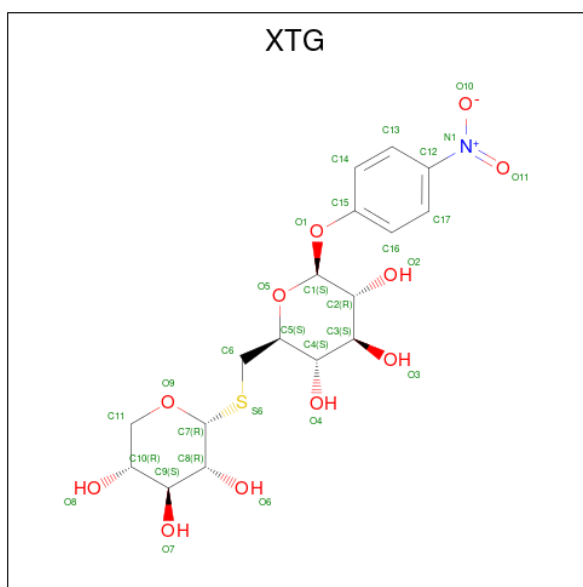
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 773     | HIS      | -      | expression tag | UNP P31434 |
| B     | 773     | HIS      | -      | expression tag | UNP P31434 |
| C     | 773     | HIS      | -      | expression tag | UNP P31434 |
| D     | 773     | HIS      | -      | expression tag | UNP P31434 |
| E     | 773     | HIS      | -      | expression tag | UNP P31434 |
| F     | 773     | HIS      | -      | expression tag | UNP P31434 |

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



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

- Molecule 3 is 4-NITROPHENYL 6-THIO-6-S-ALPHA-D-XYLOPYRANOSYL-BETA-D-G LUCOPYRANOSIDE (CCD ID: XTG) (formula: C<sub>17</sub>H<sub>23</sub>NO<sub>11</sub>S).



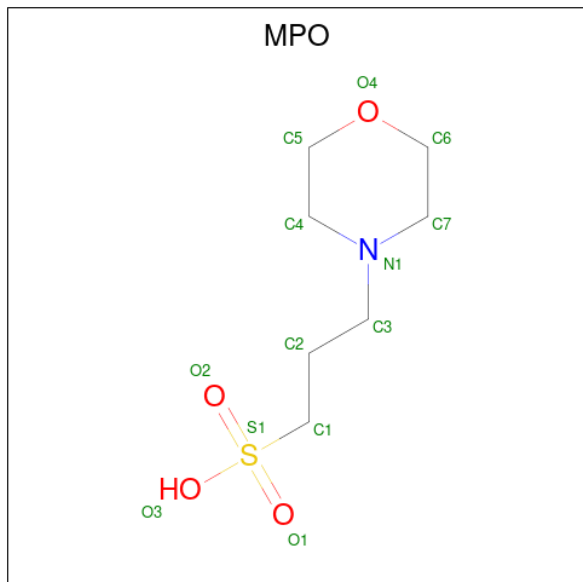
| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 3   | A     | 1        | Total | C  | N | O  | S | 0       | 0       |
|     |       |          | 30    | 17 | 1 | 11 | 1 |         |         |
| 3   | B     | 1        | Total | C  | N | O  | S | 0       | 0       |
|     |       |          | 30    | 17 | 1 | 11 | 1 |         |         |
| 3   | C     | 1        | Total | C  | N | O  | S | 0       | 0       |
|     |       |          | 30    | 17 | 1 | 11 | 1 |         |         |
| 3   | D     | 1        | Total | C  | N | O  | S | 0       | 0       |
|     |       |          | 30    | 17 | 1 | 11 | 1 |         |         |
| 3   | E     | 1        | Total | C  | N | O  | S | 0       | 0       |
|     |       |          | 30    | 17 | 1 | 11 | 1 |         |         |
| 3   | F     | 1        | Total | C  | N | O  | S | 0       | 0       |
|     |       |          | 30    | 17 | 1 | 11 | 1 |         |         |
| 3   | F     | 1        | Total | C  | N | O  | S | 0       | 0       |
|     |       |          | 30    | 17 | 1 | 11 | 1 |         |         |

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 5 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (CCD ID: MPO) (formula:  $C_7H_{15}NO_4S$ ).



| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 5   | B     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 13    | 7 | 1 | 4 | 1 |         |         |
| 5   | C     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 13    | 7 | 1 | 4 | 1 |         |         |
| 5   | D     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 13    | 7 | 1 | 4 | 1 |         |         |
| 5   | E     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 13    | 7 | 1 | 4 | 1 |         |         |
| 5   | F     | 1        | Total | C | N | O | S | 5       | 0       |
|     |       |          | 13    | 7 | 1 | 4 | 1 |         |         |

- Molecule 6 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 6   | A     | 373      | Total | O   | 0       | 0       |
|     |       |          | 373   | 373 |         |         |
| 6   | B     | 290      | Total | O   | 0       | 0       |
|     |       |          | 290   | 290 |         |         |
| 6   | C     | 344      | Total | O   | 0       | 0       |
|     |       |          | 344   | 344 |         |         |
| 6   | D     | 370      | Total | O   | 0       | 0       |
|     |       |          | 370   | 370 |         |         |
| 6   | E     | 300      | Total | O   | 0       | 0       |
|     |       |          | 300   | 300 |         |         |

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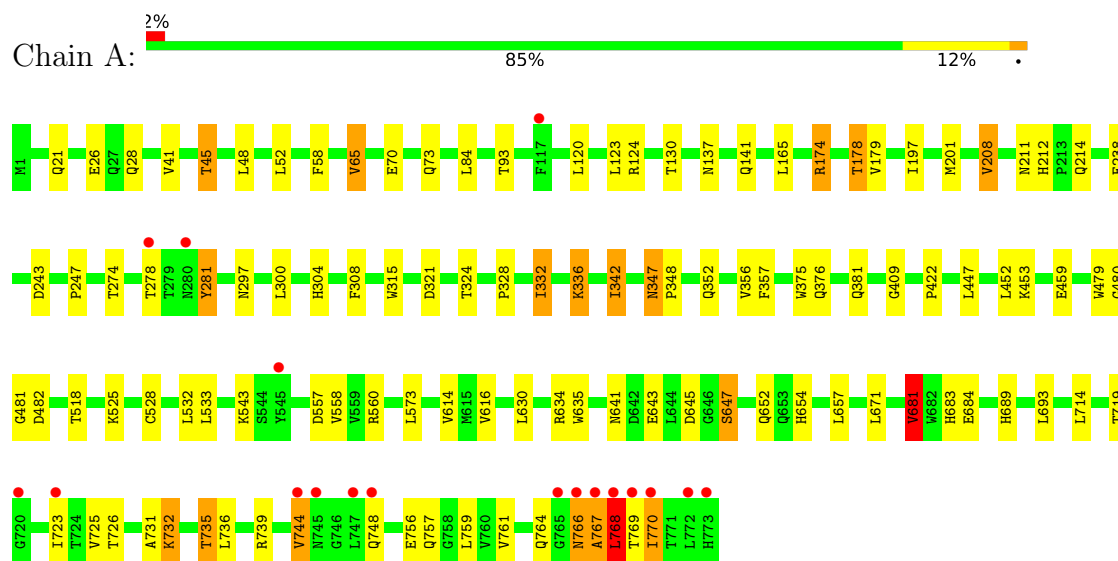
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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 6   | F     | 326      | Total<br>326 | O<br>326 | 0       | 0       |

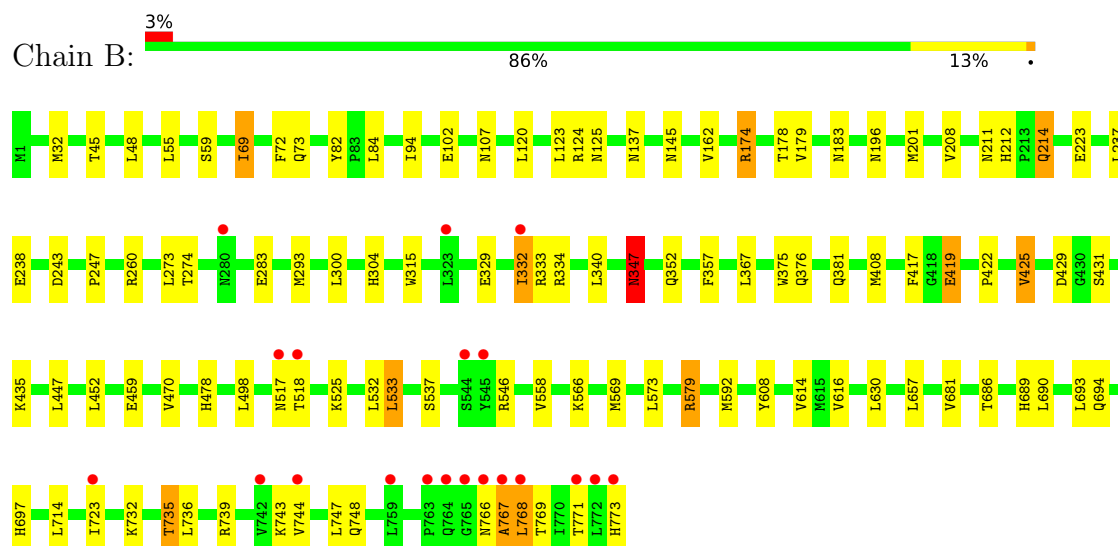
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

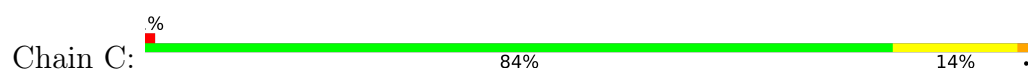
- Molecule 1: Putative family 31 glucosidase yicI

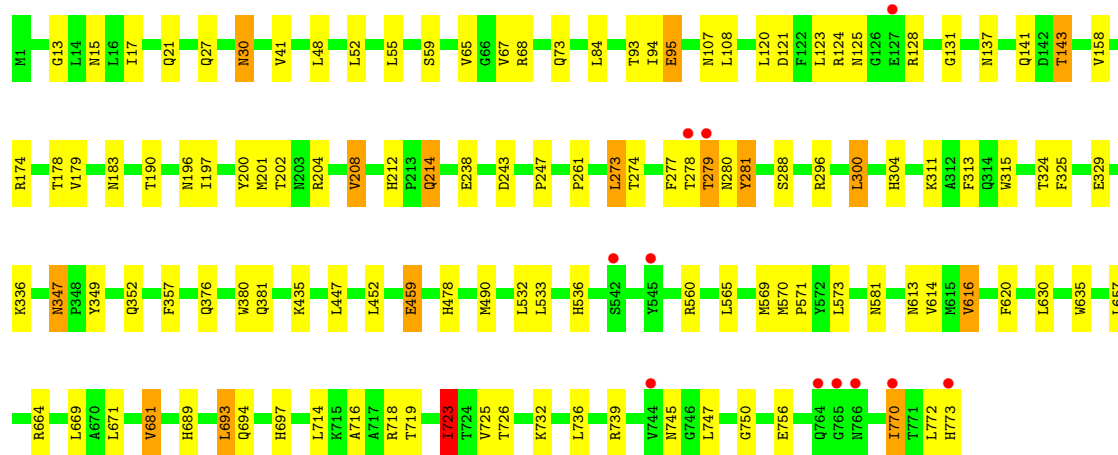


- Molecule 1: Putative family 31 glucosidase yicI

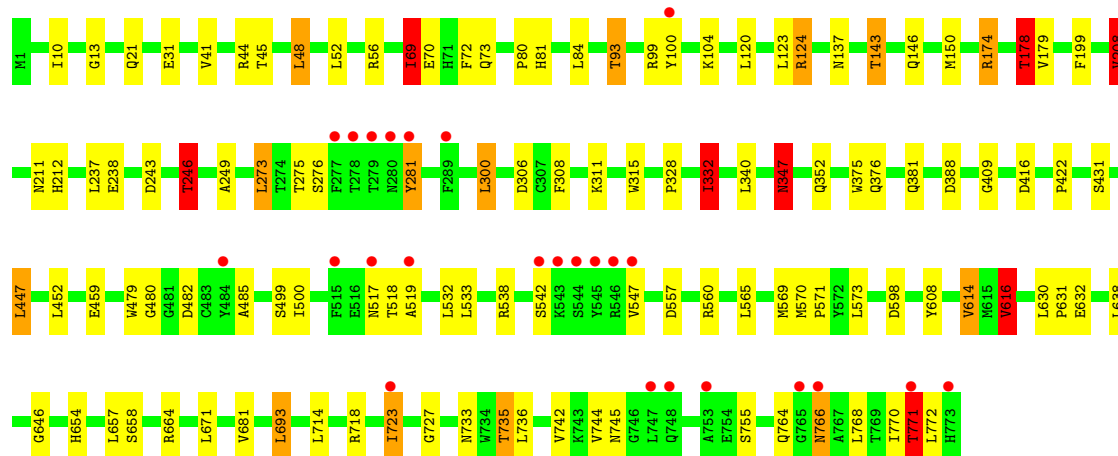
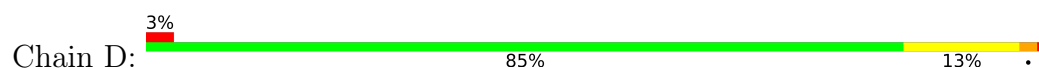


- Molecule 1: Putative family 31 glucosidase yicI

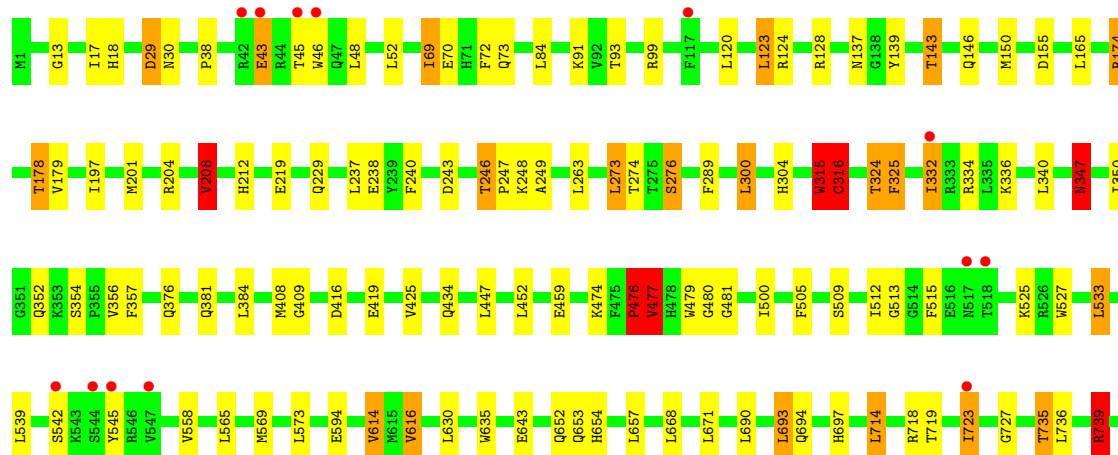
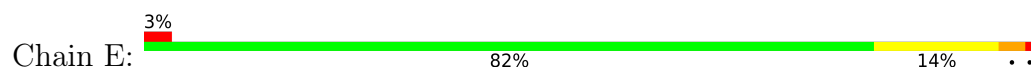


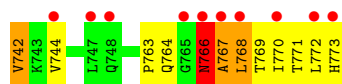


• Molecule 1: Putative family 31 glucosidase yicI

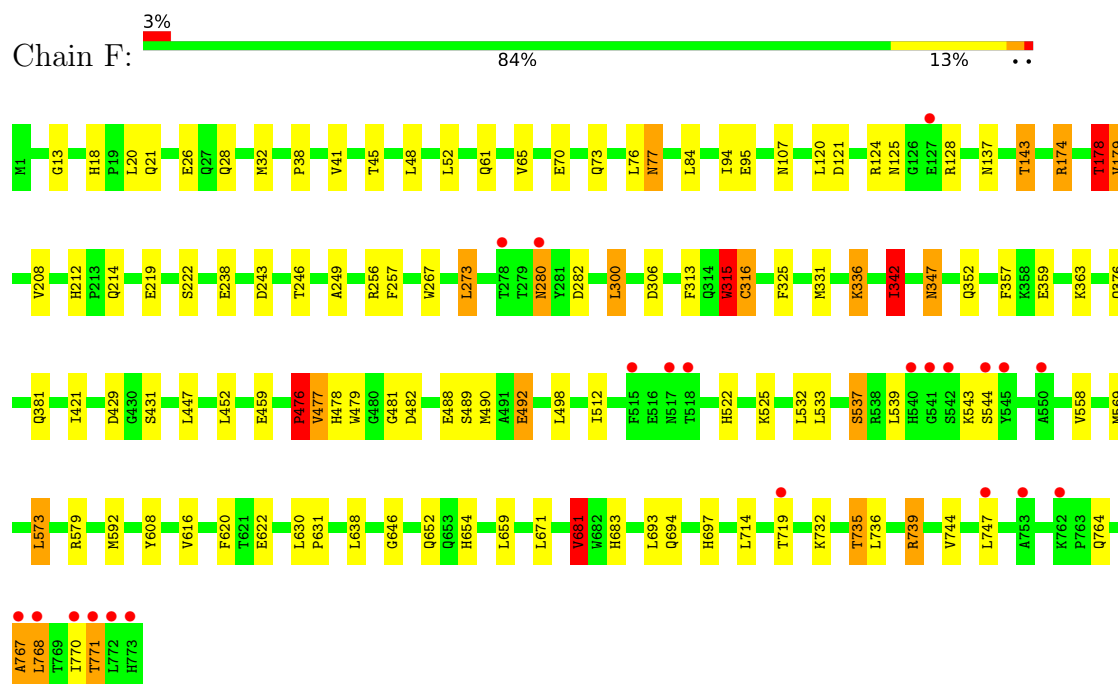


• Molecule 1: Putative family 31 glucosidase yicI





- Molecule 1: Putative family 31 glucosidase yicI



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 162.32Å 175.84Å 210.74Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 28.64 – 1.95<br>28.64 – 1.95                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 86.4 (28.64-1.95)<br>86.3 (28.64-1.95)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.10                                                        | Depositor        |
| $R_{sym}$                                                               | 0.10                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.58 (at 1.95Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC                                                      | Depositor        |
| R, $R_{free}$                                                           | 0.180 , 0.225<br>0.188 , 0.231                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 18828 reflections (4.02%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 17.2                                                        | Xtriage          |
| Anisotropy                                                              | 0.526                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.36 , 41.5                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                        | EDS              |
| Total number of atoms                                                   | 39799                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 19.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% 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: MPO, GOL, XTG, SO4

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

| Mol | Chain | Bond lengths |                 | Bond angles |                 |
|-----|-------|--------------|-----------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$     | RMSZ        | # $ Z  > 5$     |
| 1   | A     | 1.07         | 4/6416 (0.1%)   | 1.07        | 12/8719 (0.1%)  |
| 1   | B     | 0.97         | 2/6416 (0.0%)   | 1.01        | 8/8719 (0.1%)   |
| 1   | C     | 1.01         | 2/6416 (0.0%)   | 1.03        | 9/8719 (0.1%)   |
| 1   | D     | 1.04         | 4/6416 (0.1%)   | 1.06        | 16/8719 (0.2%)  |
| 1   | E     | 1.00         | 3/6416 (0.0%)   | 1.06        | 26/8719 (0.3%)  |
| 1   | F     | 1.05         | 5/6416 (0.1%)   | 1.05        | 14/8719 (0.2%)  |
| All | All   | 1.02         | 20/38496 (0.1%) | 1.05        | 85/52314 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 1   | D     | 0                   | 1                   |
| 1   | E     | 0                   | 6                   |
| 1   | F     | 0                   | 4                   |
| All | All   | 0                   | 12                  |

All (20) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | D     | 616 | VAL  | CA-CB | 6.37  | 1.61        | 1.54     |
| 1   | F     | 178 | THR  | CA-CB | 6.10  | 1.62        | 1.53     |
| 1   | A     | 214 | GLN  | CB-CG | -5.79 | 1.35        | 1.52     |
| 1   | F     | 179 | VAL  | CA-CB | 5.71  | 1.61        | 1.54     |
| 1   | A     | 681 | VAL  | CA-CB | 5.66  | 1.59        | 1.53     |
| 1   | F     | 537 | SER  | CB-OG | 5.59  | 1.53        | 1.42     |
| 1   | E     | 276 | SER  | CA-C  | 5.53  | 1.60        | 1.52     |
| 1   | B     | 332 | ILE  | CA-CB | 5.42  | 1.60        | 1.54     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | E     | 208 | VAL  | CA-CB | 5.41  | 1.61        | 1.54     |
| 1   | D     | 208 | VAL  | CA-CB | 5.34  | 1.61        | 1.54     |
| 1   | F     | 421 | ILE  | N-CA  | -5.33 | 1.42        | 1.46     |
| 1   | A     | 130 | THR  | CA-CB | 5.29  | 1.60        | 1.53     |
| 1   | D     | 771 | THR  | CA-CB | 5.27  | 1.60        | 1.53     |
| 1   | D     | 332 | ILE  | CA-CB | 5.23  | 1.61        | 1.54     |
| 1   | C     | 723 | ILE  | CA-CB | 5.16  | 1.60        | 1.54     |
| 1   | A     | 178 | THR  | CA-CB | 5.12  | 1.60        | 1.53     |
| 1   | F     | 222 | SER  | C-O   | -5.06 | 1.17        | 1.23     |
| 1   | C     | 197 | ILE  | CA-CB | 5.03  | 1.60        | 1.54     |
| 1   | B     | 69  | ILE  | C-O   | -5.02 | 1.18        | 1.24     |
| 1   | E     | 434 | GLN  | C-O   | -5.01 | 1.18        | 1.24     |

All (85) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | F     | 316 | CYS  | N-CA-C    | 9.38  | 130.77      | 110.80   |
| 1   | E     | 316 | CYS  | N-CA-C    | 9.34  | 130.68      | 110.80   |
| 1   | E     | 477 | VAL  | N-CA-C    | 9.10  | 128.28      | 109.34   |
| 1   | F     | 477 | VAL  | N-CA-C    | 8.65  | 127.33      | 109.34   |
| 1   | A     | 767 | ALA  | N-CA-C    | -8.63 | 102.88      | 113.41   |
| 1   | E     | 476 | PRO  | CA-C-N    | 8.43  | 137.14      | 121.97   |
| 1   | E     | 476 | PRO  | C-N-CA    | 8.43  | 137.14      | 121.97   |
| 1   | E     | 174 | ARG  | NE-CZ-NH2 | -7.97 | 112.03      | 119.20   |
| 1   | D     | 480 | GLY  | N-CA-C    | 7.43  | 124.53      | 115.31   |
| 1   | A     | 174 | ARG  | NE-CZ-NH2 | -6.85 | 113.04      | 119.20   |
| 1   | D     | 664 | ARG  | N-CA-CB   | -6.80 | 100.05      | 110.04   |
| 1   | E     | 739 | ARG  | CG-CD-NE  | -6.76 | 97.13       | 112.00   |
| 1   | E     | 174 | ARG  | NE-CZ-NH1 | 6.73  | 128.23      | 121.50   |
| 1   | D     | 347 | ASN  | CB-CA-C   | 6.68  | 119.52      | 110.37   |
| 1   | F     | 476 | PRO  | CA-C-N    | 6.57  | 133.79      | 121.97   |
| 1   | F     | 476 | PRO  | C-N-CA    | 6.57  | 133.79      | 121.97   |
| 1   | E     | 155 | ASP  | N-CA-C    | 6.47  | 119.36      | 110.24   |
| 1   | D     | 547 | VAL  | N-CA-C    | 6.44  | 115.26      | 108.95   |
| 1   | D     | 517 | ASN  | N-CA-C    | 6.41  | 118.26      | 111.28   |
| 1   | E     | 315 | TRP  | CA-C-N    | 6.40  | 133.76      | 121.54   |
| 1   | E     | 315 | TRP  | C-N-CA    | 6.40  | 133.76      | 121.54   |
| 1   | E     | 70  | GLU  | N-CA-C    | 6.39  | 119.60      | 109.50   |
| 1   | C     | 613 | ASN  | N-CA-C    | 6.33  | 121.96      | 113.72   |
| 1   | A     | 647 | SER  | CB-CA-C   | 6.28  | 121.43      | 111.51   |
| 1   | D     | 598 | ASP  | CA-C-O    | 6.23  | 123.34      | 119.29   |
| 1   | E     | 263 | LEU  | CA-C-N    | -6.12 | 115.25      | 119.66   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | E     | 263 | LEU  | C-N-CA    | -6.12 | 115.25      | 119.66   |
| 1   | A     | 174 | ARG  | CB-CG-CD  | 6.10  | 125.33      | 111.30   |
| 1   | F     | 659 | LEU  | N-CA-C    | -6.05 | 102.68      | 108.07   |
| 1   | E     | 354 | SER  | CA-C-N    | 6.04  | 126.48      | 119.47   |
| 1   | E     | 354 | SER  | C-N-CA    | 6.04  | 126.48      | 119.47   |
| 1   | F     | 174 | ARG  | NE-CZ-NH2 | -6.01 | 113.79      | 119.20   |
| 1   | D     | 124 | ARG  | NE-CZ-NH2 | 6.00  | 124.60      | 119.20   |
| 1   | A     | 174 | ARG  | NE-CZ-NH1 | 5.98  | 127.48      | 121.50   |
| 1   | B     | 517 | ASN  | N-CA-C    | 5.92  | 117.54      | 111.14   |
| 1   | D     | 174 | ARG  | NE-CZ-NH2 | -5.92 | 113.87      | 119.20   |
| 1   | D     | 69  | ILE  | N-CA-C    | 5.87  | 116.31      | 107.80   |
| 1   | B     | 59  | SER  | CA-C-N    | 5.80  | 125.34      | 119.19   |
| 1   | B     | 59  | SER  | C-N-CA    | 5.80  | 125.34      | 119.19   |
| 1   | A     | 342 | ILE  | N-CA-C    | 5.76  | 116.24      | 108.17   |
| 1   | D     | 178 | THR  | CB-CA-C   | 5.76  | 119.03      | 109.53   |
| 1   | E     | 347 | ASN  | CB-CA-C   | 5.72  | 118.21      | 110.37   |
| 1   | E     | 174 | ARG  | CB-CG-CD  | 5.70  | 124.41      | 111.30   |
| 1   | F     | 315 | TRP  | CA-C-N    | 5.69  | 132.41      | 121.54   |
| 1   | F     | 315 | TRP  | C-N-CA    | 5.69  | 132.41      | 121.54   |
| 1   | A     | 214 | GLN  | CB-CA-C   | -5.67 | 98.65       | 111.30   |
| 1   | D     | 174 | ARG  | CB-CG-CD  | 5.67  | 124.35      | 111.30   |
| 1   | F     | 178 | THR  | CB-CA-C   | 5.65  | 119.07      | 109.80   |
| 1   | D     | 538 | ARG  | N-CA-C    | 5.63  | 117.96      | 109.23   |
| 1   | E     | 480 | GLY  | N-CA-C    | 5.63  | 122.29      | 115.31   |
| 1   | E     | 616 | VAL  | N-CA-C    | 5.62  | 116.67      | 108.53   |
| 1   | F     | 739 | ARG  | CG-CD-NE  | -5.60 | 99.68       | 112.00   |
| 1   | A     | 480 | GLY  | N-CA-C    | 5.60  | 120.61      | 114.40   |
| 1   | C     | 723 | ILE  | CB-CA-C   | 5.60  | 118.45      | 110.84   |
| 1   | E     | 325 | PHE  | CA-C-N    | 5.60  | 125.44      | 119.28   |
| 1   | E     | 325 | PHE  | C-N-CA    | 5.60  | 125.44      | 119.28   |
| 1   | D     | 614 | VAL  | N-CA-C    | 5.57  | 116.14      | 108.12   |
| 1   | E     | 350 | ILE  | N-CA-C    | 5.53  | 115.84      | 108.27   |
| 1   | E     | 614 | VAL  | N-CA-C    | 5.47  | 115.76      | 108.11   |
| 1   | F     | 342 | ILE  | N-CA-C    | 5.46  | 115.76      | 108.11   |
| 1   | B     | 579 | ARG  | CG-CD-NE  | -5.42 | 100.06      | 112.00   |
| 1   | F     | 681 | VAL  | CB-CA-C   | 5.38  | 118.81      | 111.88   |
| 1   | C     | 95  | GLU  | CB-CA-C   | 5.33  | 118.67      | 110.62   |
| 1   | A     | 174 | ARG  | CD-NE-CZ  | 5.32  | 131.85      | 124.40   |
| 1   | D     | 499 | SER  | N-CA-C    | 5.31  | 117.07      | 111.28   |
| 1   | F     | 70  | GLU  | N-CA-C    | 5.30  | 117.87      | 109.50   |
| 1   | A     | 528 | CYS  | N-CA-CB   | 5.29  | 117.90      | 110.12   |
| 1   | A     | 65  | VAL  | CB-CA-C   | 5.28  | 118.67      | 110.96   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 174 | ARG  | CB-CG-CD  | 5.25  | 123.38      | 111.30   |
| 1   | C     | 325 | PHE  | CA-C-N    | 5.24  | 125.05      | 119.28   |
| 1   | C     | 325 | PHE  | C-N-CA    | 5.24  | 125.05      | 119.28   |
| 1   | B     | 162 | VAL  | N-CA-C    | 5.21  | 116.09      | 108.53   |
| 1   | C     | 59  | SER  | CA-C-N    | 5.17  | 124.86      | 119.64   |
| 1   | C     | 59  | SER  | C-N-CA    | 5.17  | 124.86      | 119.64   |
| 1   | D     | 246 | THR  | N-CA-CB   | -5.14 | 100.31      | 110.70   |
| 1   | D     | 174 | ARG  | NE-CZ-NH1 | 5.13  | 126.64      | 121.50   |
| 1   | B     | 347 | ASN  | CB-CA-C   | 5.13  | 120.28      | 110.17   |
| 1   | E     | 174 | ARG  | CD-NE-CZ  | 5.12  | 131.57      | 124.40   |
| 1   | F     | 20  | LEU  | CB-CA-C   | -5.12 | 100.77      | 109.38   |
| 1   | B     | 214 | GLN  | CB-CA-C   | -5.10 | 99.92       | 111.30   |
| 1   | E     | 742 | VAL  | CB-CA-C   | -5.10 | 105.19      | 112.22   |
| 1   | A     | 208 | VAL  | CB-CA-C   | 5.07  | 117.73      | 110.33   |
| 1   | C     | 681 | VAL  | CB-CA-C   | 5.06  | 118.45      | 112.68   |
| 1   | E     | 767 | ALA  | N-CA-C    | -5.05 | 107.12      | 113.28   |
| 1   | C     | 616 | VAL  | CB-CA-C   | 5.04  | 118.10      | 110.63   |

There are no chirality outliers.

All (12) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 1   | A     | 766 | ASN  | Peptide           |
| 1   | D     | 766 | ASN  | Peptide           |
| 1   | E     | 315 | TRP  | Peptide,Mainchain |
| 1   | E     | 476 | PRO  | Peptide,Mainchain |
| 1   | E     | 763 | PRO  | Peptide           |
| 1   | E     | 766 | ASN  | Peptide           |
| 1   | F     | 315 | TRP  | Peptide,Mainchain |
| 1   | F     | 476 | PRO  | Peptide,Mainchain |

## 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     | 6232  | 0        | 5939     | 68      | 0            |
| 1   | B     | 6232  | 0        | 5939     | 64      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | C     | 6232  | 0        | 5939     | 65      | 0            |
| 1   | D     | 6232  | 0        | 5939     | 78      | 0            |
| 1   | E     | 6232  | 0        | 5939     | 75      | 0            |
| 1   | F     | 6232  | 0        | 5939     | 75      | 0            |
| 2   | A     | 5     | 0        | 0        | 0       | 0            |
| 2   | B     | 5     | 0        | 0        | 0       | 0            |
| 2   | C     | 5     | 0        | 0        | 0       | 0            |
| 2   | D     | 5     | 0        | 0        | 1       | 0            |
| 2   | E     | 10    | 0        | 0        | 1       | 0            |
| 2   | F     | 15    | 0        | 0        | 3       | 0            |
| 3   | A     | 30    | 0        | 23       | 2       | 0            |
| 3   | B     | 30    | 0        | 23       | 1       | 0            |
| 3   | C     | 30    | 0        | 23       | 0       | 0            |
| 3   | D     | 30    | 0        | 23       | 6       | 0            |
| 3   | E     | 30    | 0        | 23       | 1       | 0            |
| 3   | F     | 60    | 0        | 46       | 2       | 0            |
| 4   | A     | 18    | 0        | 24       | 5       | 0            |
| 4   | B     | 12    | 0        | 16       | 2       | 0            |
| 4   | C     | 18    | 0        | 24       | 1       | 0            |
| 4   | D     | 12    | 0        | 16       | 2       | 0            |
| 4   | E     | 12    | 0        | 16       | 0       | 0            |
| 4   | F     | 12    | 0        | 16       | 2       | 0            |
| 5   | B     | 13    | 0        | 15       | 0       | 0            |
| 5   | C     | 13    | 0        | 15       | 0       | 0            |
| 5   | D     | 13    | 0        | 15       | 0       | 0            |
| 5   | E     | 13    | 0        | 15       | 0       | 0            |
| 5   | F     | 13    | 0        | 15       | 0       | 0            |
| 6   | A     | 373   | 0        | 0        | 5       | 0            |
| 6   | B     | 290   | 0        | 0        | 4       | 0            |
| 6   | C     | 344   | 0        | 0        | 6       | 0            |
| 6   | D     | 370   | 0        | 0        | 10      | 0            |
| 6   | E     | 300   | 0        | 0        | 9       | 0            |
| 6   | F     | 326   | 0        | 0        | 6       | 0            |
| All | All   | 39799 | 0        | 35982    | 405     | 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 5.

All (405) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:124:ARG:NH2  | 1:A:243:ASP:OD1   | 1.88                     | 1.04              |
| 1:B:32:MET:HE3   | 1:B:94:ILE:HG23   | 1.42                     | 1.02              |
| 1:B:32:MET:CE    | 1:B:94:ILE:HG23   | 2.03                     | 0.89              |
| 1:C:30:ASN:HD22  | 1:C:30:ASN:H      | 1.19                     | 0.88              |
| 1:C:352:GLN:NE2  | 1:D:73:GLN:H      | 1.72                     | 0.86              |
| 1:D:352:GLN:HE21 | 1:D:376:GLN:HE22  | 1.24                     | 0.85              |
| 1:C:352:GLN:HE22 | 1:D:73:GLN:H      | 1.23                     | 0.84              |
| 1:C:352:GLN:HE21 | 1:C:376:GLN:HE22  | 1.28                     | 0.81              |
| 1:C:158:VAL:O    | 1:C:204:ARG:NH2   | 2.13                     | 0.81              |
| 1:C:13:GLY:O     | 1:C:143:THR:HB    | 1.81                     | 0.80              |
| 1:D:70:GLU:OE1   | 6:D:3123:HOH:O    | 1.99                     | 0.79              |
| 1:F:212:HIS:HE1  | 1:F:238:GLU:H     | 1.28                     | 0.79              |
| 1:E:204:ARG:NH2  | 6:E:3297:HOH:O    | 2.15                     | 0.78              |
| 1:A:141:GLN:CD   | 6:A:3289:HOH:O    | 2.27                     | 0.75              |
| 1:F:246:THR:HG21 | 2:F:3001:SO4:O3   | 1.86                     | 0.75              |
| 3:B:3016:XTG:H14 | 1:F:48:LEU:HD11   | 1.66                     | 0.75              |
| 1:D:727:GLY:H    | 1:D:766:ASN:HD21  | 1.35                     | 0.74              |
| 1:A:352:GLN:NE2  | 1:B:73:GLN:H      | 1.85                     | 0.74              |
| 1:A:352:GLN:HE22 | 1:B:73:GLN:H      | 1.35                     | 0.74              |
| 1:D:569:MET:CE   | 1:D:638:LEU:HD21  | 2.18                     | 0.74              |
| 1:D:569:MET:CE   | 1:D:638:LEU:CD2   | 2.66                     | 0.73              |
| 1:B:352:GLN:HE21 | 1:B:376:GLN:HE22  | 1.37                     | 0.72              |
| 1:A:352:GLN:HE21 | 1:A:376:GLN:HE22  | 1.36                     | 0.72              |
| 1:A:641:ASN:HD21 | 1:A:739:ARG:HH21  | 1.36                     | 0.71              |
| 1:B:332:ILE:CD1  | 1:B:408:MET:O     | 2.39                     | 0.71              |
| 1:E:347:ASN:C    | 1:E:347:ASN:HD22  | 2.00                     | 0.70              |
| 1:B:211:ASN:ND2  | 4:B:3026:GOL:H32  | 2.07                     | 0.69              |
| 1:D:485:ALA:HB1  | 1:D:519:ALA:HB2   | 1.73                     | 0.69              |
| 1:F:306:ASP:OD1  | 6:F:3038:HOH:O    | 2.10                     | 0.69              |
| 1:A:212:HIS:HE1  | 1:A:238:GLU:H     | 1.40                     | 0.68              |
| 1:F:13:GLY:O     | 1:F:143:THR:HB    | 1.93                     | 0.68              |
| 1:F:719:THR:HG22 | 6:F:3241:HOH:O    | 1.93                     | 0.68              |
| 1:D:352:GLN:NE2  | 1:E:73:GLN:H      | 1.92                     | 0.67              |
| 1:B:332:ILE:HD12 | 1:B:333:ARG:N     | 2.10                     | 0.66              |
| 1:D:306:ASP:OD2  | 3:D:3018:XTG:H112 | 1.96                     | 0.66              |
| 1:B:211:ASN:HD21 | 4:B:3026:GOL:H32  | 1.61                     | 0.66              |
| 1:C:30:ASN:H     | 1:C:30:ASN:ND2    | 1.93                     | 0.65              |
| 1:F:767:ALA:O    | 1:F:768:LEU:C     | 2.38                     | 0.65              |
| 1:E:723:ILE:HG12 | 1:E:770:ILE:HB    | 1.79                     | 0.65              |
| 1:A:73:GLN:H     | 1:F:352:GLN:HE22  | 1.45                     | 0.65              |
| 1:B:212:HIS:HE1  | 1:B:238:GLU:H     | 1.44                     | 0.65              |
| 1:F:694:GLN:HB2  | 1:F:697:HIS:CD2   | 2.32                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:681:VAL:O    | 1:D:681:VAL:HG13 | 1.96                     | 0.65              |
| 1:E:300:LEU:HD13 | 1:E:340:LEU:HD21 | 1.77                     | 0.64              |
| 1:D:569:MET:HE2  | 1:D:638:LEU:HD21 | 1.78                     | 0.64              |
| 1:D:93:THR:HG22  | 1:D:104:LYS:HB3  | 1.78                     | 0.64              |
| 1:C:296:ARG:O    | 1:C:560:ARG:NH1  | 2.30                     | 0.64              |
| 1:D:569:MET:HE2  | 1:D:638:LEU:CD2  | 2.27                     | 0.64              |
| 1:A:45:THR:HB    | 1:F:543:LYS:HZ1  | 1.63                     | 0.63              |
| 1:E:336:LYS:HE2  | 1:E:409:GLY:O    | 1.98                     | 0.63              |
| 1:F:280:ASN:HD22 | 1:F:282:ASP:H    | 1.43                     | 0.63              |
| 1:A:73:GLN:H     | 1:F:352:GLN:NE2  | 1.95                     | 0.63              |
| 1:A:211:ASN:ND2  | 4:A:3029:GOL:H32 | 2.12                     | 0.63              |
| 1:F:212:HIS:CE1  | 1:F:238:GLU:H    | 2.14                     | 0.63              |
| 1:A:525:LYS:HG2  | 1:A:558:VAL:HG21 | 1.81                     | 0.63              |
| 1:F:347:ASN:C    | 1:F:347:ASN:HD22 | 2.07                     | 0.63              |
| 1:D:744:VAL:HG21 | 1:D:770:ILE:HG23 | 1.81                     | 0.63              |
| 1:E:212:HIS:HE1  | 1:E:238:GLU:H    | 1.47                     | 0.62              |
| 1:D:246:THR:HG22 | 1:D:249:ALA:CB   | 2.29                     | 0.62              |
| 1:E:143:THR:HG22 | 6:E:3181:HOH:O   | 1.99                     | 0.62              |
| 1:C:770:ILE:HD11 | 1:C:772:LEU:HD13 | 1.81                     | 0.62              |
| 1:D:273:LEU:HB2  | 1:D:300:LEU:HD21 | 1.82                     | 0.62              |
| 1:F:178:THR:CG2  | 6:F:3256:HOH:O   | 2.48                     | 0.62              |
| 1:D:212:HIS:HE1  | 1:D:238:GLU:H    | 1.48                     | 0.61              |
| 1:E:315:TRP:H    | 1:E:381:GLN:HE21 | 1.47                     | 0.61              |
| 1:A:281:TYR:O    | 1:A:324:THR:HG23 | 2.00                     | 0.61              |
| 1:E:13:GLY:O     | 1:E:143:THR:HB   | 2.01                     | 0.61              |
| 1:C:212:HIS:HE1  | 1:C:238:GLU:H    | 1.46                     | 0.61              |
| 1:A:641:ASN:ND2  | 1:A:739:ARG:HH21 | 1.98                     | 0.60              |
| 1:E:246:THR:HG23 | 1:E:249:ALA:H    | 1.67                     | 0.60              |
| 1:F:336:LYS:HD2  | 1:F:342:ILE:HD12 | 1.83                     | 0.60              |
| 1:A:744:VAL:HG21 | 1:A:770:ILE:HD13 | 1.83                     | 0.60              |
| 1:B:283:GLU:OE1  | 1:B:334:ARG:HD2  | 2.01                     | 0.60              |
| 1:C:347:ASN:C    | 1:C:347:ASN:HD22 | 2.10                     | 0.60              |
| 1:F:61:GLN:HE22  | 1:F:256:ARG:C    | 2.09                     | 0.60              |
| 1:B:525:LYS:HG2  | 1:B:558:VAL:HG21 | 1.83                     | 0.60              |
| 1:D:352:GLN:NE2  | 1:D:376:GLN:HE22 | 1.96                     | 0.59              |
| 1:E:352:GLN:HE21 | 1:E:376:GLN:HE22 | 1.49                     | 0.59              |
| 1:A:347:ASN:C    | 1:A:347:ASN:HD22 | 2.10                     | 0.59              |
| 1:E:332:ILE:HD11 | 1:E:409:GLY:HA3  | 1.83                     | 0.59              |
| 1:F:280:ASN:ND2  | 1:F:282:ASP:H    | 1.99                     | 0.59              |
| 1:C:716:ALA:HB1  | 1:C:723:ILE:HD13 | 1.85                     | 0.59              |
| 1:A:93:THR:HA    | 4:A:3024:GOL:H12 | 1.84                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:735:THR:CG2  | 6:F:3193:HOH:O   | 2.50                     | 0.58              |
| 1:A:681:VAL:HG23 | 1:A:683:HIS:CE1  | 2.39                     | 0.58              |
| 1:B:124:ARG:HD3  | 1:B:243:ASP:OD1  | 2.04                     | 0.58              |
| 1:C:214:GLN:HG3  | 1:C:435:LYS:HG2  | 1.86                     | 0.58              |
| 1:B:352:GLN:NE2  | 1:B:376:GLN:HE22 | 2.01                     | 0.57              |
| 1:D:211:ASN:ND2  | 4:D:3032:GOL:H32 | 2.20                     | 0.57              |
| 1:F:489:SER:HA   | 1:F:492:GLU:HG3  | 1.86                     | 0.57              |
| 1:C:124:ARG:HD3  | 1:C:243:ASP:OD1  | 2.03                     | 0.57              |
| 1:C:73:GLN:H     | 1:E:352:GLN:NE2  | 2.01                     | 0.57              |
| 1:B:735:THR:HG23 | 6:B:3294:HOH:O   | 2.04                     | 0.57              |
| 1:E:565:LEU:HG   | 1:E:569:MET:HE2  | 1.86                     | 0.57              |
| 1:C:121:ASP:OD1  | 1:C:128:ARG:NH2  | 2.37                     | 0.57              |
| 1:C:274:THR:HG22 | 1:C:304:HIS:HB3  | 1.87                     | 0.57              |
| 1:D:13:GLY:O     | 1:D:143:THR:HB   | 2.04                     | 0.57              |
| 1:F:61:GLN:NE2   | 1:F:257:PHE:HA   | 2.20                     | 0.57              |
| 1:E:124:ARG:HD3  | 1:E:243:ASP:OD1  | 2.05                     | 0.57              |
| 1:C:459:GLU:CD   | 1:C:459:GLU:H    | 2.13                     | 0.57              |
| 1:E:727:GLY:H    | 1:E:766:ASN:HD21 | 1.50                     | 0.57              |
| 1:B:690:LEU:O    | 1:B:739:ARG:HB2  | 2.05                     | 0.56              |
| 1:D:735:THR:CG2  | 6:D:3161:HOH:O   | 2.54                     | 0.56              |
| 1:E:201:MET:HE1  | 1:E:247:PRO:HB3  | 1.87                     | 0.56              |
| 1:A:201:MET:HE1  | 1:A:247:PRO:HB3  | 1.88                     | 0.56              |
| 1:B:352:GLN:NE2  | 1:F:73:GLN:H     | 2.04                     | 0.56              |
| 1:D:485:ALA:CB   | 1:D:519:ALA:HB2  | 2.34                     | 0.56              |
| 1:D:447:LEU:C    | 1:D:447:LEU:HD23 | 2.30                     | 0.56              |
| 1:A:725:VAL:HB   | 1:A:768:LEU:HB3  | 1.88                     | 0.56              |
| 1:E:315:TRP:H    | 1:E:381:GLN:NE2  | 2.04                     | 0.55              |
| 1:A:352:GLN:NE2  | 1:A:376:GLN:HE22 | 2.03                     | 0.55              |
| 1:B:447:LEU:HD23 | 1:B:447:LEU:C    | 2.31                     | 0.55              |
| 1:C:723:ILE:HD11 | 1:C:725:VAL:HG22 | 1.88                     | 0.55              |
| 1:E:18:HIS:O     | 1:E:38:PRO:HA    | 2.07                     | 0.55              |
| 1:E:246:THR:HG21 | 2:E:3004:SO4:O4  | 2.06                     | 0.55              |
| 1:E:352:GLN:NE2  | 1:E:376:GLN:HE22 | 2.05                     | 0.55              |
| 1:E:525:LYS:HG2  | 1:E:558:VAL:HG21 | 1.87                     | 0.55              |
| 1:A:744:VAL:CG2  | 1:A:770:ILE:HD13 | 2.37                     | 0.55              |
| 1:D:565:LEU:HD11 | 1:D:569:MET:HE3  | 1.89                     | 0.55              |
| 1:F:478:HIS:HD2  | 6:F:3069:HOH:O   | 1.89                     | 0.55              |
| 1:C:128:ARG:HH22 | 1:C:131:GLY:HA3  | 1.72                     | 0.54              |
| 1:A:328:PRO:O    | 1:A:332:ILE:HG23 | 2.08                     | 0.54              |
| 1:D:352:GLN:HE22 | 1:E:73:GLN:H     | 1.55                     | 0.54              |
| 1:F:488:GLU:O    | 1:F:492:GLU:HG2  | 2.08                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:124:ARG:HD3  | 1:D:243:ASP:OD1  | 2.07                     | 0.54              |
| 1:C:352:GLN:NE2  | 1:C:376:GLN:HE22 | 2.02                     | 0.54              |
| 1:B:429:ASP:OD1  | 1:B:431:SER:OG   | 2.23                     | 0.54              |
| 1:D:21:GLN:HE22  | 1:D:41:VAL:H     | 1.55                     | 0.54              |
| 1:D:178:THR:CG2  | 6:D:3276:HOH:O   | 2.54                     | 0.54              |
| 1:A:641:ASN:HD21 | 1:A:739:ARG:NH2  | 2.05                     | 0.54              |
| 1:C:447:LEU:C    | 1:C:447:LEU:HD23 | 2.33                     | 0.54              |
| 1:E:533:LEU:CD1  | 1:E:569:MET:HE1  | 2.37                     | 0.54              |
| 1:D:212:HIS:CE1  | 1:D:238:GLU:H    | 2.26                     | 0.53              |
| 1:C:347:ASN:ND2  | 1:C:349:TYR:H    | 2.06                     | 0.53              |
| 1:E:43:GLU:H     | 1:E:43:GLU:CD    | 2.16                     | 0.53              |
| 1:F:352:GLN:HE21 | 1:F:376:GLN:HE22 | 1.54                     | 0.53              |
| 1:F:681:VAL:HG23 | 1:F:683:HIS:CE1  | 2.44                     | 0.53              |
| 1:D:275:THR:O    | 1:D:276:SER:HB2  | 2.08                     | 0.53              |
| 1:C:107:ASN:ND2  | 1:C:125:ASN:HD21 | 2.07                     | 0.53              |
| 1:C:73:GLN:H     | 1:E:352:GLN:HE22 | 1.57                     | 0.52              |
| 1:C:273:LEU:HB2  | 1:C:300:LEU:HD21 | 1.90                     | 0.52              |
| 1:C:719:THR:HG22 | 6:C:3086:HOH:O   | 2.08                     | 0.52              |
| 1:E:512:ILE:HB   | 1:E:539:LEU:HD23 | 1.91                     | 0.52              |
| 1:D:246:THR:HG22 | 1:D:249:ALA:HB2  | 1.90                     | 0.52              |
| 1:B:212:HIS:CE1  | 1:B:238:GLU:H    | 2.27                     | 0.52              |
| 1:D:569:MET:HE3  | 1:D:638:LEU:HD21 | 1.90                     | 0.52              |
| 1:E:347:ASN:C    | 1:E:347:ASN:ND2  | 2.62                     | 0.52              |
| 1:D:300:LEU:HD13 | 1:D:340:LEU:HD21 | 1.90                     | 0.52              |
| 1:A:770:ILE:HD12 | 1:A:770:ILE:C    | 2.34                     | 0.52              |
| 4:A:3029:GOL:H31 | 6:A:3127:HOH:O   | 2.09                     | 0.52              |
| 1:E:332:ILE:C    | 1:E:332:ILE:HD12 | 2.35                     | 0.52              |
| 1:B:767:ALA:O    | 1:B:768:LEU:O    | 2.28                     | 0.52              |
| 1:C:329:GLU:HB2  | 6:C:3243:HOH:O   | 2.09                     | 0.52              |
| 1:F:124:ARG:HD3  | 1:F:243:ASP:OD1  | 2.10                     | 0.52              |
| 1:E:212:HIS:CE1  | 1:E:238:GLU:H    | 2.26                     | 0.52              |
| 1:F:347:ASN:C    | 1:F:347:ASN:ND2  | 2.68                     | 0.52              |
| 1:D:482:ASP:OD2  | 3:D:3018:XTG:H62 | 2.10                     | 0.51              |
| 1:B:352:GLN:HA   | 1:B:357:PHE:CD2  | 2.45                     | 0.51              |
| 1:F:48:LEU:HD12  | 1:F:48:LEU:O     | 2.10                     | 0.51              |
| 1:A:315:TRP:H    | 1:A:381:GLN:HE21 | 1.57                     | 0.51              |
| 1:B:352:GLN:HE22 | 1:F:73:GLN:H     | 1.57                     | 0.51              |
| 1:B:367:LEU:HD11 | 1:B:425:VAL:HG13 | 1.92                     | 0.51              |
| 1:F:246:THR:HG23 | 1:F:249:ALA:H    | 1.76                     | 0.51              |
| 1:E:212:HIS:HD2  | 6:E:3148:HOH:O   | 1.94                     | 0.51              |
| 1:D:93:THR:CG2   | 6:D:3217:HOH:O   | 2.58                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:45:THR:HG23  | 1:E:46:TRP:CD1   | 2.46                     | 0.51              |
| 1:B:329:GLU:HA   | 1:B:332:ILE:HG13 | 1.92                     | 0.50              |
| 1:B:375:TRP:CE2  | 1:B:422:PRO:HG3  | 2.46                     | 0.50              |
| 1:D:352:GLN:HE22 | 1:E:72:PHE:HA    | 1.76                     | 0.50              |
| 1:F:26:GLU:CD    | 1:F:28:GLN:HE21  | 2.19                     | 0.50              |
| 1:B:332:ILE:HD13 | 1:B:408:MET:O    | 2.11                     | 0.50              |
| 1:B:735:THR:CG2  | 6:B:3294:HOH:O   | 2.60                     | 0.50              |
| 1:B:55:LEU:HD12  | 1:B:55:LEU:N     | 2.27                     | 0.50              |
| 1:F:490:MET:HE2  | 1:F:620:PHE:CE1  | 2.46                     | 0.50              |
| 1:F:482:ASP:OD2  | 3:F:3020:XTG:H62 | 2.11                     | 0.50              |
| 1:B:767:ALA:O    | 1:B:768:LEU:C    | 2.54                     | 0.50              |
| 1:C:478:HIS:HE1  | 6:C:3149:HOH:O   | 1.95                     | 0.50              |
| 1:B:478:HIS:HD2  | 6:B:3236:HOH:O   | 1.93                     | 0.50              |
| 1:D:723:ILE:HG12 | 1:D:770:ILE:HB   | 1.93                     | 0.50              |
| 1:E:123:LEU:HD12 | 1:E:128:ARG:HA   | 1.92                     | 0.50              |
| 1:E:324:THR:HG23 | 1:E:325:PHE:CD2  | 2.47                     | 0.50              |
| 1:B:566:LYS:HA   | 1:B:569:MET:HE2  | 1.93                     | 0.50              |
| 1:C:723:ILE:HD11 | 1:C:725:VAL:CG2  | 2.42                     | 0.49              |
| 1:F:61:GLN:HE22  | 1:F:257:PHE:N    | 2.09                     | 0.49              |
| 1:A:278:THR:HG21 | 1:B:45:THR:HA    | 1.94                     | 0.49              |
| 1:B:201:MET:HE1  | 1:B:247:PRO:HB3  | 1.93                     | 0.49              |
| 1:C:279:THR:O    | 1:D:44:ARG:NH2   | 2.44                     | 0.49              |
| 1:A:767:ALA:C    | 1:A:769:THR:N    | 2.71                     | 0.49              |
| 1:B:201:MET:CE   | 1:B:247:PRO:HB3  | 2.42                     | 0.49              |
| 1:E:416:ASP:OD2  | 3:E:3019:XTG:H8  | 2.13                     | 0.49              |
| 1:F:638:LEU:O    | 1:F:739:ARG:NH2  | 2.44                     | 0.49              |
| 1:A:352:GLN:HA   | 1:A:357:PHE:CD2  | 2.47                     | 0.49              |
| 1:A:641:ASN:HD21 | 1:A:739:ARG:HE   | 1.60                     | 0.49              |
| 1:C:490:MET:HE2  | 1:C:620:PHE:CD1  | 2.48                     | 0.49              |
| 1:D:306:ASP:OD1  | 3:D:3018:XTG:O8  | 2.13                     | 0.49              |
| 1:D:332:ILE:HD11 | 1:D:409:GLY:HA3  | 1.95                     | 0.49              |
| 1:C:212:HIS:CE1  | 1:C:238:GLU:H    | 2.29                     | 0.48              |
| 1:E:300:LEU:HD13 | 1:E:340:LEU:CD2  | 2.43                     | 0.48              |
| 1:A:238:GLU:OE1  | 4:A:3029:GOL:H32 | 2.13                     | 0.48              |
| 1:A:212:HIS:CE1  | 1:A:238:GLU:H    | 2.26                     | 0.48              |
| 1:B:417:PHE:HA   | 1:B:419:GLU:OE2  | 2.13                     | 0.48              |
| 1:C:15:ASN:HD22  | 1:C:141:GLN:NE2  | 2.12                     | 0.48              |
| 1:F:178:THR:HB   | 1:F:219:GLU:OE1  | 2.14                     | 0.48              |
| 1:A:332:ILE:HD11 | 1:A:409:GLY:HA3  | 1.95                     | 0.48              |
| 1:D:306:ASP:OD2  | 3:D:3018:XTG:C11 | 2.61                     | 0.48              |
| 1:A:281:TYR:CZ   | 1:A:308:PHE:HB2  | 2.49                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:533:LEU:CD1  | 1:B:569:MET:HE1  | 2.44                     | 0.48              |
| 1:C:478:HIS:HD2  | 6:C:3063:HOH:O   | 1.96                     | 0.48              |
| 1:B:32:MET:HE1   | 1:B:102:GLU:C    | 2.39                     | 0.48              |
| 1:D:81:HIS:HB2   | 6:D:3206:HOH:O   | 2.14                     | 0.48              |
| 1:F:246:THR:HG21 | 2:F:3001:SO4:S   | 2.54                     | 0.48              |
| 1:A:315:TRP:H    | 1:A:381:GLN:NE2  | 2.11                     | 0.48              |
| 1:A:684:GLU:HG2  | 1:A:732:LYS:HB2  | 1.96                     | 0.48              |
| 1:E:767:ALA:O    | 1:E:768:LEU:C    | 2.57                     | 0.47              |
| 1:F:429:ASP:OD1  | 1:F:431:SER:OG   | 2.25                     | 0.47              |
| 1:F:681:VAL:HG12 | 2:F:3003:SO4:O3  | 2.14                     | 0.47              |
| 1:E:513:GLY:H    | 1:E:527:TRP:CG   | 2.32                     | 0.47              |
| 1:B:332:ILE:HG12 | 1:B:408:MET:O    | 2.14                     | 0.47              |
| 1:E:693:LEU:HD13 | 1:E:718:ARG:HB2  | 1.95                     | 0.47              |
| 1:A:58:PHE:CZ    | 4:A:3028:GOL:H12 | 2.49                     | 0.47              |
| 1:A:482:ASP:OD2  | 3:A:3015:XTG:H62 | 2.12                     | 0.47              |
| 1:C:30:ASN:HD22  | 1:C:30:ASN:N     | 1.93                     | 0.47              |
| 1:D:557:ASP:OD1  | 1:D:560:ARG:NH2  | 2.47                     | 0.47              |
| 1:E:332:ILE:CD1  | 1:E:409:GLY:HA3  | 2.44                     | 0.47              |
| 1:F:32:MET:HE3   | 1:F:94:ILE:HG23  | 1.96                     | 0.47              |
| 1:E:212:HIS:CE1  | 1:E:237:LEU:HD12 | 2.50                     | 0.47              |
| 1:B:329:GLU:O    | 1:B:332:ILE:HG13 | 2.15                     | 0.47              |
| 1:F:306:ASP:OD2  | 3:F:3020:XTG:O8  | 2.31                     | 0.47              |
| 1:F:315:TRP:H    | 1:F:381:GLN:NE2  | 2.12                     | 0.47              |
| 1:B:766:ASN:ND2  | 6:B:3171:HOH:O   | 2.47                     | 0.47              |
| 1:D:485:ALA:HB1  | 1:D:519:ALA:CB   | 2.44                     | 0.47              |
| 1:D:199:PHE:HA   | 1:D:208:VAL:O    | 2.15                     | 0.46              |
| 1:D:735:THR:HG22 | 6:D:3161:HOH:O   | 2.16                     | 0.46              |
| 1:E:17:ILE:CG1   | 1:E:139:TYR:HB3  | 2.45                     | 0.46              |
| 1:F:352:GLN:NE2  | 1:F:376:GLN:HE22 | 2.13                     | 0.46              |
| 1:A:347:ASN:C    | 1:A:347:ASN:ND2  | 2.73                     | 0.46              |
| 1:C:352:GLN:HE22 | 1:D:73:GLN:N     | 2.01                     | 0.46              |
| 1:A:274:THR:HG22 | 1:A:304:HIS:HB3  | 1.97                     | 0.46              |
| 1:B:32:MET:HE1   | 1:B:102:GLU:O    | 2.14                     | 0.46              |
| 1:C:27:GLN:HG3   | 1:C:94:ILE:HD13  | 1.97                     | 0.46              |
| 1:F:273:LEU:HB2  | 1:F:300:LEU:HD21 | 1.97                     | 0.46              |
| 1:E:735:THR:HG22 | 6:E:3178:HOH:O   | 2.15                     | 0.46              |
| 1:A:761:VAL:CG1  | 1:A:768:LEU:HD21 | 2.46                     | 0.46              |
| 1:E:143:THR:CG2  | 6:E:3181:HOH:O   | 2.61                     | 0.46              |
| 1:A:45:THR:HB    | 1:F:543:LYS:NZ   | 2.29                     | 0.46              |
| 1:A:70:GLU:HG3   | 6:A:3251:HOH:O   | 2.15                     | 0.46              |
| 1:B:766:ASN:O    | 1:B:767:ALA:HB2  | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:248:LYS:NZ   | 1:E:594:GLU:OE1  | 2.49                     | 0.46              |
| 1:A:21:GLN:NE2   | 1:A:41:VAL:H     | 2.13                     | 0.46              |
| 1:E:477:VAL:HG11 | 1:E:509:SER:HB2  | 1.97                     | 0.46              |
| 3:A:3015:XTG:C14 | 1:B:48:LEU:HD11  | 2.46                     | 0.46              |
| 1:E:500:ILE:HG12 | 1:E:505:PHE:HB2  | 1.98                     | 0.46              |
| 1:F:359:GLU:OE2  | 1:F:363:LYS:NZ   | 2.40                     | 0.46              |
| 1:B:347:ASN:C    | 1:B:347:ASN:HD22 | 2.24                     | 0.45              |
| 1:E:274:THR:HG22 | 1:E:304:HIS:HB3  | 1.98                     | 0.45              |
| 1:F:267:TRP:HD1  | 4:F:3022:GOL:HO3 | 1.63                     | 0.45              |
| 1:A:767:ALA:O    | 1:A:769:THR:N    | 2.49                     | 0.45              |
| 1:B:498:LEU:HD21 | 1:B:608:TYR:HB3  | 1.97                     | 0.45              |
| 1:D:479:TRP:HH2  | 3:D:3018:XTG:HO7 | 1.64                     | 0.45              |
| 1:A:336:LYS:HE2  | 1:A:409:GLY:O    | 2.17                     | 0.45              |
| 1:F:512:ILE:HB   | 1:F:539:LEU:HD23 | 1.99                     | 0.45              |
| 1:E:204:ARG:HG3  | 6:E:3297:HOH:O   | 2.15                     | 0.45              |
| 1:F:107:ASN:HD22 | 1:F:125:ASN:HD21 | 1.64                     | 0.45              |
| 1:C:347:ASN:C    | 1:C:347:ASN:ND2  | 2.73                     | 0.45              |
| 1:C:380:TRP:CZ3  | 1:D:48:LEU:HD13  | 2.51                     | 0.45              |
| 1:E:91:LYS:CE    | 6:E:3177:HOH:O   | 2.64                     | 0.45              |
| 1:D:93:THR:HG23  | 6:D:3217:HOH:O   | 2.15                     | 0.45              |
| 1:D:388:ASP:OD1  | 1:D:388:ASP:C    | 2.59                     | 0.45              |
| 1:A:297:ASN:O    | 1:A:560:ARG:HD3  | 2.17                     | 0.45              |
| 1:C:65:VAL:HG12  | 1:C:108:LEU:CD2  | 2.46                     | 0.45              |
| 1:F:479:TRP:CZ3  | 1:F:481:GLY:HA2  | 2.52                     | 0.45              |
| 1:A:21:GLN:HE22  | 1:A:41:VAL:H     | 1.64                     | 0.45              |
| 1:A:321:ASP:OD1  | 1:A:321:ASP:C    | 2.58                     | 0.45              |
| 1:C:67:VAL:O     | 1:C:238:GLU:HA   | 2.17                     | 0.45              |
| 1:B:214:GLN:HG3  | 1:B:435:LYS:HG2  | 1.98                     | 0.45              |
| 1:B:315:TRP:H    | 1:B:381:GLN:HE21 | 1.62                     | 0.45              |
| 1:D:238:GLU:OE1  | 4:D:3032:GOL:H32 | 2.17                     | 0.45              |
| 1:A:652:GLN:NE2  | 1:A:654:HIS:NE2  | 2.64                     | 0.44              |
| 1:B:300:LEU:HD12 | 1:B:340:LEU:HD21 | 1.99                     | 0.44              |
| 1:D:693:LEU:HD13 | 1:D:718:ARG:HB2  | 1.98                     | 0.44              |
| 1:F:267:TRP:CD1  | 4:F:3022:GOL:HO3 | 2.34                     | 0.44              |
| 1:F:315:TRP:H    | 1:F:381:GLN:HE21 | 1.64                     | 0.44              |
| 1:C:281:TYR:O    | 1:C:324:THR:CG2  | 2.66                     | 0.44              |
| 1:D:654:HIS:ND1  | 1:D:658:SER:OG   | 2.36                     | 0.44              |
| 1:E:289:PHE:HZ   | 1:E:545:TYR:CD1  | 2.34                     | 0.44              |
| 1:A:352:GLN:HE22 | 1:B:72:PHE:HA    | 1.82                     | 0.44              |
| 1:B:107:ASN:ND2  | 1:B:125:ASN:HD21 | 2.15                     | 0.44              |
| 1:E:477:VAL:CG1  | 1:E:509:SER:HB2  | 2.48                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:515:PHE:O    | 1:E:542:SER:HB2  | 2.17                     | 0.44              |
| 1:E:635:TRP:O    | 1:E:643:GLU:HA   | 2.18                     | 0.44              |
| 1:F:336:LYS:HD2  | 1:F:342:ILE:CD1  | 2.46                     | 0.44              |
| 1:B:274:THR:HG22 | 1:B:304:HIS:HB3  | 1.99                     | 0.44              |
| 1:C:201:MET:HE1  | 1:C:247:PRO:HB3  | 1.99                     | 0.44              |
| 1:F:447:LEU:C    | 1:F:447:LEU:HD23 | 2.43                     | 0.44              |
| 1:A:447:LEU:C    | 1:A:447:LEU:HD23 | 2.43                     | 0.44              |
| 1:E:668:LEU:HD21 | 1:E:714:LEU:HD13 | 1.99                     | 0.44              |
| 1:F:48:LEU:HD12  | 1:F:48:LEU:C     | 2.43                     | 0.44              |
| 1:B:183:ASN:HA   | 1:B:196:ASN:ND2  | 2.32                     | 0.44              |
| 1:D:328:PRO:O    | 1:D:332:ILE:HG23 | 2.18                     | 0.44              |
| 1:C:570:MET:N    | 1:C:571:PRO:CD   | 2.81                     | 0.44              |
| 1:E:352:GLN:HA   | 1:E:357:PHE:CD2  | 2.53                     | 0.44              |
| 1:E:479:TRP:CZ3  | 1:E:481:GLY:HA2  | 2.53                     | 0.44              |
| 1:A:748:GLN:HG2  | 1:A:769:THR:CG2  | 2.47                     | 0.43              |
| 1:C:565:LEU:O    | 1:C:569:MET:HG3  | 2.18                     | 0.43              |
| 1:C:689:HIS:ND1  | 1:C:739:ARG:HD3  | 2.33                     | 0.43              |
| 1:E:178:THR:CG2  | 6:E:3308:HOH:O   | 2.66                     | 0.43              |
| 1:A:26:GLU:CD    | 1:A:28:GLN:HE21  | 2.26                     | 0.43              |
| 1:B:212:HIS:CE1  | 1:B:237:LEU:HD12 | 2.53                     | 0.43              |
| 1:F:313:PHE:HA   | 1:F:381:GLN:NE2  | 2.33                     | 0.43              |
| 1:C:261:PRO:O    | 1:C:581:ASN:HA   | 2.18                     | 0.43              |
| 1:E:165:LEU:HA   | 1:E:197:ILE:O    | 2.18                     | 0.43              |
| 1:D:347:ASN:C    | 1:D:347:ASN:HD22 | 2.27                     | 0.43              |
| 1:D:69:ILE:HG12  | 1:D:150:MET:HE2  | 2.00                     | 0.43              |
| 1:D:123:LEU:N    | 1:D:123:LEU:HD22 | 2.34                     | 0.43              |
| 1:D:570:MET:N    | 1:D:571:PRO:CD   | 2.82                     | 0.43              |
| 1:D:744:VAL:HG22 | 1:D:771:THR:O    | 2.18                     | 0.43              |
| 1:C:315:TRP:H    | 1:C:381:GLN:NE2  | 2.17                     | 0.43              |
| 1:D:300:LEU:HD13 | 1:D:340:LEU:CD2  | 2.49                     | 0.43              |
| 1:A:635:TRP:O    | 1:A:643:GLU:HA   | 2.18                     | 0.43              |
| 1:B:32:MET:HE2   | 1:B:94:ILE:HG23  | 1.92                     | 0.43              |
| 1:C:693:LEU:HD13 | 1:C:718:ARG:HB2  | 2.01                     | 0.43              |
| 1:D:246:THR:HG21 | 2:D:3002:SO4:O2  | 2.19                     | 0.43              |
| 1:C:352:GLN:HE22 | 1:D:72:PHE:HA    | 1.84                     | 0.42              |
| 1:C:635:TRP:CH2  | 1:C:664:ARG:HG2  | 2.54                     | 0.42              |
| 1:D:31:GLU:OE1   | 1:D:56:ARG:HD3   | 2.19                     | 0.42              |
| 1:A:557:ASP:OD1  | 1:A:560:ARG:NH2  | 2.52                     | 0.42              |
| 1:D:375:TRP:CE2  | 1:D:422:PRO:HG3  | 2.54                     | 0.42              |
| 1:E:69:ILE:HG12  | 1:E:150:MET:CE   | 2.49                     | 0.42              |
| 1:F:61:GLN:NE2   | 1:F:257:PHE:CA   | 2.82                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:566:LYS:HA   | 1:B:569:MET:CE   | 2.50                     | 0.42              |
| 1:C:277:PHE:CD2  | 1:C:278:THR:HG23 | 2.55                     | 0.42              |
| 1:A:165:LEU:HA   | 1:A:197:ILE:O    | 2.20                     | 0.42              |
| 1:A:281:TYR:O    | 1:A:324:THR:CG2  | 2.67                     | 0.42              |
| 1:D:681:VAL:O    | 1:D:681:VAL:CG1  | 2.66                     | 0.42              |
| 1:B:293:MET:HE2  | 1:B:300:LEU:HD23 | 2.02                     | 0.42              |
| 4:C:3023:GOL:H12 | 6:C:3365:HOH:O   | 2.19                     | 0.42              |
| 1:D:212:HIS:CE1  | 1:D:237:LEU:HD12 | 2.55                     | 0.42              |
| 1:A:634:ARG:NH2  | 1:A:645:ASP:OD1  | 2.53                     | 0.42              |
| 1:C:536:HIS:HA   | 6:C:3099:HOH:O   | 2.19                     | 0.42              |
| 1:E:474:LYS:C    | 1:E:476:PRO:HD3  | 2.45                     | 0.42              |
| 1:F:18:HIS:O     | 1:F:38:PRO:HA    | 2.19                     | 0.42              |
| 1:F:498:LEU:HD21 | 1:F:608:TYR:HB3  | 2.00                     | 0.42              |
| 1:F:631:PRO:O    | 1:F:646:GLY:HA3  | 2.19                     | 0.42              |
| 1:F:735:THR:HG23 | 6:F:3193:HOH:O   | 2.17                     | 0.42              |
| 1:C:200:TYR:CZ   | 1:C:208:VAL:HG13 | 2.54                     | 0.42              |
| 1:F:652:GLN:NE2  | 1:F:654:HIS:NE2  | 2.68                     | 0.42              |
| 1:D:178:THR:HG23 | 6:D:3276:HOH:O   | 2.19                     | 0.42              |
| 1:C:352:GLN:HA   | 1:C:357:PHE:CD2  | 2.55                     | 0.41              |
| 1:D:143:THR:CG2  | 6:D:3311:HOH:O   | 2.68                     | 0.41              |
| 1:D:416:ASP:OD2  | 3:D:3018:XTG:H8  | 2.20                     | 0.41              |
| 1:E:219:GLU:HB2  | 1:E:229:GLN:HB3  | 2.02                     | 0.41              |
| 1:F:121:ASP:OD1  | 1:F:128:ARG:HD2  | 2.20                     | 0.41              |
| 1:B:748:GLN:O    | 1:B:768:LEU:HA   | 2.20                     | 0.41              |
| 1:C:313:PHE:CA   | 1:C:381:GLN:HE22 | 2.33                     | 0.41              |
| 1:E:273:LEU:HB2  | 1:E:300:LEU:HD21 | 2.02                     | 0.41              |
| 1:E:690:LEU:O    | 1:E:739:ARG:HB2  | 2.19                     | 0.41              |
| 1:D:99:ARG:NH2   | 1:D:100:TYR:OH   | 2.53                     | 0.41              |
| 1:E:48:LEU:HD23  | 1:E:48:LEU:N     | 2.36                     | 0.41              |
| 1:F:352:GLN:HA   | 1:F:357:PHE:CD2  | 2.55                     | 0.41              |
| 1:F:525:LYS:HG2  | 1:F:558:VAL:HG21 | 2.03                     | 0.41              |
| 1:A:731:ALA:C    | 1:A:732:LYS:HD2  | 2.46                     | 0.41              |
| 1:C:183:ASN:HA   | 1:C:196:ASN:ND2  | 2.36                     | 0.41              |
| 1:E:29:ASP:HB3   | 1:E:30:ASN:H     | 1.73                     | 0.41              |
| 1:E:447:LEU:HD23 | 1:E:447:LEU:C    | 2.46                     | 0.41              |
| 1:F:429:ASP:CG   | 1:F:431:SER:HG   | 2.25                     | 0.41              |
| 1:B:82:TYR:CD1   | 1:B:470:VAL:HB   | 2.55                     | 0.41              |
| 1:D:281:TYR:CZ   | 1:D:308:PHE:HB2  | 2.56                     | 0.41              |
| 1:F:76:LEU:O     | 1:F:77:ASN:C     | 2.62                     | 0.41              |
| 1:F:522:HIS:CB   | 1:F:622:GLU:HG3  | 2.50                     | 0.41              |
| 1:F:768:LEU:HD12 | 1:F:768:LEU:HA   | 1.82                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:747:LEU:HD22 | 1:C:750:GLY:O    | 2.20                     | 0.41              |
| 1:F:569:MET:HB2  | 1:F:573:LEU:HD22 | 2.03                     | 0.41              |
| 1:A:375:TRP:CE2  | 1:A:422:PRO:HG3  | 2.56                     | 0.41              |
| 1:A:748:GLN:HB2  | 1:A:769:THR:HG22 | 2.03                     | 0.41              |
| 1:B:223:GLU:O    | 1:C:190:THR:HA   | 2.20                     | 0.41              |
| 1:B:748:GLN:HB2  | 1:B:769:THR:HB   | 2.03                     | 0.41              |
| 1:F:21:GLN:NE2   | 1:F:41:VAL:H     | 2.19                     | 0.41              |
| 1:A:201:MET:HE3  | 6:A:3246:HOH:O   | 2.20                     | 0.41              |
| 1:A:342:ILE:N    | 1:A:342:ILE:HD12 | 2.36                     | 0.41              |
| 1:B:694:GLN:HB2  | 1:B:697:HIS:CD2  | 2.55                     | 0.41              |
| 1:C:21:GLN:NE2   | 1:C:41:VAL:H     | 2.19                     | 0.41              |
| 1:C:55:LEU:HA    | 1:C:68:ARG:O     | 2.21                     | 0.41              |
| 1:C:128:ARG:NH2  | 1:C:131:GLY:HA3  | 2.34                     | 0.41              |
| 1:C:694:GLN:HB2  | 1:C:697:HIS:CD2  | 2.56                     | 0.41              |
| 1:D:631:PRO:O    | 1:D:646:GLY:HA3  | 2.21                     | 0.41              |
| 1:A:479:TRP:CZ3  | 1:A:481:GLY:HA2  | 2.56                     | 0.41              |
| 1:B:145:ASN:OD1  | 1:B:145:ASN:C    | 2.63                     | 0.41              |
| 1:E:208:VAL:HA   | 1:E:240:PHE:O    | 2.22                     | 0.41              |
| 1:E:694:GLN:HB2  | 1:E:697:HIS:CD2  | 2.56                     | 0.41              |
| 1:A:735:THR:HG23 | 6:A:3229:HOH:O   | 2.22                     | 0.40              |
| 1:A:689:HIS:ND1  | 1:A:739:ARG:HD3  | 2.36                     | 0.40              |
| 1:D:608:TYR:CZ   | 1:D:616:VAL:HG22 | 2.56                     | 0.40              |
| 1:E:376:GLN:HA   | 1:E:384:LEU:O    | 2.21                     | 0.40              |
| 1:F:744:VAL:HG22 | 1:F:771:THR:O    | 2.21                     | 0.40              |
| 1:D:735:THR:HG23 | 6:D:3161:HOH:O   | 2.21                     | 0.40              |
| 1:C:21:GLN:HE22  | 1:C:41:VAL:H     | 1.68                     | 0.40              |
| 1:D:315:TRP:H    | 1:D:381:GLN:NE2  | 2.19                     | 0.40              |
| 1:F:107:ASN:ND2  | 1:F:125:ASN:HD21 | 2.20                     | 0.40              |
| 1:F:325:PHE:CD1  | 1:F:331:MET:HE1  | 2.57                     | 0.40              |
| 1:A:726:THR:HA   | 1:A:766:ASN:HD21 | 1.87                     | 0.40              |
| 1:B:689:HIS:HB3  | 1:B:739:ARG:HH11 | 1.86                     | 0.40              |
| 1:D:80:PRO:HD3   | 1:D:431:SER:HB3  | 2.03                     | 0.40              |
| 1:E:91:LYS:HE2   | 6:E:3177:HOH:O   | 2.22                     | 0.40              |
| 1:E:315:TRP:N    | 1:E:381:GLN:HE21 | 2.17                     | 0.40              |
| 1:E:652:GLN:NE2  | 1:E:654:HIS:NE2  | 2.70                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 1   | A     | 771/773 (100%)   | 744 (96%)  | 25 (3%)  | 2 (0%)   | 36          | 28  |
| 1   | B     | 771/773 (100%)   | 736 (96%)  | 33 (4%)  | 2 (0%)   | 36          | 28  |
| 1   | C     | 771/773 (100%)   | 740 (96%)  | 30 (4%)  | 1 (0%)   | 48          | 41  |
| 1   | D     | 771/773 (100%)   | 743 (96%)  | 28 (4%)  | 0        | 100         | 100 |
| 1   | E     | 771/773 (100%)   | 740 (96%)  | 27 (4%)  | 4 (0%)   | 24          | 16  |
| 1   | F     | 771/773 (100%)   | 737 (96%)  | 28 (4%)  | 6 (1%)   | 16          | 8   |
| All | All   | 4626/4638 (100%) | 4440 (96%) | 171 (4%) | 15 (0%)  | 36          | 28  |

All (15) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 768 | LEU  |
| 1   | B     | 768 | LEU  |
| 1   | E     | 316 | CYS  |
| 1   | E     | 477 | VAL  |
| 1   | F     | 316 | CYS  |
| 1   | B     | 767 | ALA  |
| 1   | E     | 766 | ASN  |
| 1   | F     | 768 | LEU  |
| 1   | C     | 279 | THR  |
| 1   | E     | 768 | LEU  |
| 1   | F     | 77  | ASN  |
| 1   | F     | 477 | VAL  |
| 1   | F     | 767 | ALA  |
| 1   | A     | 348 | PRO  |
| 1   | F     | 476 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |   |
|-----|-------|------------------|------------|----------|-------------|---|
| 1   | A     | 660/660 (100%)   | 613 (93%)  | 47 (7%)  | 13          | 4 |
| 1   | B     | 660/660 (100%)   | 619 (94%)  | 41 (6%)  | 16          | 6 |
| 1   | C     | 660/660 (100%)   | 613 (93%)  | 47 (7%)  | 13          | 4 |
| 1   | D     | 660/660 (100%)   | 610 (92%)  | 50 (8%)  | 12          | 4 |
| 1   | E     | 660/660 (100%)   | 606 (92%)  | 54 (8%)  | 10          | 3 |
| 1   | F     | 660/660 (100%)   | 618 (94%)  | 42 (6%)  | 16          | 6 |
| All | All   | 3960/3960 (100%) | 3679 (93%) | 281 (7%) | 13          | 4 |

All (281) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 45  | THR  |
| 1   | A     | 48  | LEU  |
| 1   | A     | 52  | LEU  |
| 1   | A     | 65  | VAL  |
| 1   | A     | 84  | LEU  |
| 1   | A     | 120 | LEU  |
| 1   | A     | 123 | LEU  |
| 1   | A     | 137 | ASN  |
| 1   | A     | 174 | ARG  |
| 1   | A     | 178 | THR  |
| 1   | A     | 179 | VAL  |
| 1   | A     | 208 | VAL  |
| 1   | A     | 281 | TYR  |
| 1   | A     | 300 | LEU  |
| 1   | A     | 332 | ILE  |
| 1   | A     | 336 | LYS  |
| 1   | A     | 347 | ASN  |
| 1   | A     | 356 | VAL  |
| 1   | A     | 452 | LEU  |
| 1   | A     | 453 | LYS  |
| 1   | A     | 459 | GLU  |
| 1   | A     | 518 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 532 | LEU  |
| 1   | A     | 533 | LEU  |
| 1   | A     | 543 | LYS  |
| 1   | A     | 573 | LEU  |
| 1   | A     | 614 | VAL  |
| 1   | A     | 616 | VAL  |
| 1   | A     | 630 | LEU  |
| 1   | A     | 647 | SER  |
| 1   | A     | 657 | LEU  |
| 1   | A     | 671 | LEU  |
| 1   | A     | 681 | VAL  |
| 1   | A     | 693 | LEU  |
| 1   | A     | 714 | LEU  |
| 1   | A     | 719 | THR  |
| 1   | A     | 723 | ILE  |
| 1   | A     | 732 | LYS  |
| 1   | A     | 735 | THR  |
| 1   | A     | 736 | LEU  |
| 1   | A     | 744 | VAL  |
| 1   | A     | 756 | GLU  |
| 1   | A     | 757 | GLN  |
| 1   | A     | 759 | LEU  |
| 1   | A     | 764 | GLN  |
| 1   | A     | 768 | LEU  |
| 1   | A     | 770 | ILE  |
| 1   | B     | 69  | ILE  |
| 1   | B     | 84  | LEU  |
| 1   | B     | 120 | LEU  |
| 1   | B     | 123 | LEU  |
| 1   | B     | 137 | ASN  |
| 1   | B     | 174 | ARG  |
| 1   | B     | 178 | THR  |
| 1   | B     | 179 | VAL  |
| 1   | B     | 208 | VAL  |
| 1   | B     | 260 | ARG  |
| 1   | B     | 273 | LEU  |
| 1   | B     | 347 | ASN  |
| 1   | B     | 419 | GLU  |
| 1   | B     | 425 | VAL  |
| 1   | B     | 452 | LEU  |
| 1   | B     | 459 | GLU  |
| 1   | B     | 518 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 532 | LEU  |
| 1   | B     | 533 | LEU  |
| 1   | B     | 537 | SER  |
| 1   | B     | 546 | ARG  |
| 1   | B     | 573 | LEU  |
| 1   | B     | 579 | ARG  |
| 1   | B     | 592 | MET  |
| 1   | B     | 614 | VAL  |
| 1   | B     | 616 | VAL  |
| 1   | B     | 630 | LEU  |
| 1   | B     | 657 | LEU  |
| 1   | B     | 681 | VAL  |
| 1   | B     | 686 | THR  |
| 1   | B     | 693 | LEU  |
| 1   | B     | 714 | LEU  |
| 1   | B     | 723 | ILE  |
| 1   | B     | 732 | LYS  |
| 1   | B     | 735 | THR  |
| 1   | B     | 736 | LEU  |
| 1   | B     | 743 | LYS  |
| 1   | B     | 744 | VAL  |
| 1   | B     | 747 | LEU  |
| 1   | B     | 771 | THR  |
| 1   | B     | 773 | HIS  |
| 1   | C     | 17  | ILE  |
| 1   | C     | 30  | ASN  |
| 1   | C     | 48  | LEU  |
| 1   | C     | 52  | LEU  |
| 1   | C     | 84  | LEU  |
| 1   | C     | 93  | THR  |
| 1   | C     | 95  | GLU  |
| 1   | C     | 120 | LEU  |
| 1   | C     | 123 | LEU  |
| 1   | C     | 137 | ASN  |
| 1   | C     | 143 | THR  |
| 1   | C     | 174 | ARG  |
| 1   | C     | 178 | THR  |
| 1   | C     | 179 | VAL  |
| 1   | C     | 202 | THR  |
| 1   | C     | 208 | VAL  |
| 1   | C     | 214 | GLN  |
| 1   | C     | 273 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 280 | ASN  |
| 1   | C     | 281 | TYR  |
| 1   | C     | 288 | SER  |
| 1   | C     | 300 | LEU  |
| 1   | C     | 311 | LYS  |
| 1   | C     | 336 | LYS  |
| 1   | C     | 347 | ASN  |
| 1   | C     | 452 | LEU  |
| 1   | C     | 459 | GLU  |
| 1   | C     | 532 | LEU  |
| 1   | C     | 533 | LEU  |
| 1   | C     | 573 | LEU  |
| 1   | C     | 614 | VAL  |
| 1   | C     | 616 | VAL  |
| 1   | C     | 630 | LEU  |
| 1   | C     | 657 | LEU  |
| 1   | C     | 669 | LEU  |
| 1   | C     | 671 | LEU  |
| 1   | C     | 681 | VAL  |
| 1   | C     | 693 | LEU  |
| 1   | C     | 714 | LEU  |
| 1   | C     | 723 | ILE  |
| 1   | C     | 726 | THR  |
| 1   | C     | 732 | LYS  |
| 1   | C     | 736 | LEU  |
| 1   | C     | 745 | ASN  |
| 1   | C     | 756 | GLU  |
| 1   | C     | 770 | ILE  |
| 1   | C     | 773 | HIS  |
| 1   | D     | 10  | ILE  |
| 1   | D     | 45  | THR  |
| 1   | D     | 48  | LEU  |
| 1   | D     | 52  | LEU  |
| 1   | D     | 69  | ILE  |
| 1   | D     | 84  | LEU  |
| 1   | D     | 93  | THR  |
| 1   | D     | 120 | LEU  |
| 1   | D     | 137 | ASN  |
| 1   | D     | 143 | THR  |
| 1   | D     | 146 | GLN  |
| 1   | D     | 174 | ARG  |
| 1   | D     | 178 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 179 | VAL  |
| 1   | D     | 208 | VAL  |
| 1   | D     | 246 | THR  |
| 1   | D     | 273 | LEU  |
| 1   | D     | 281 | TYR  |
| 1   | D     | 300 | LEU  |
| 1   | D     | 311 | LYS  |
| 1   | D     | 332 | ILE  |
| 1   | D     | 347 | ASN  |
| 1   | D     | 447 | LEU  |
| 1   | D     | 452 | LEU  |
| 1   | D     | 459 | GLU  |
| 1   | D     | 500 | ILE  |
| 1   | D     | 518 | THR  |
| 1   | D     | 532 | LEU  |
| 1   | D     | 533 | LEU  |
| 1   | D     | 542 | SER  |
| 1   | D     | 573 | LEU  |
| 1   | D     | 614 | VAL  |
| 1   | D     | 616 | VAL  |
| 1   | D     | 630 | LEU  |
| 1   | D     | 632 | GLU  |
| 1   | D     | 657 | LEU  |
| 1   | D     | 671 | LEU  |
| 1   | D     | 693 | LEU  |
| 1   | D     | 714 | LEU  |
| 1   | D     | 723 | ILE  |
| 1   | D     | 733 | ASN  |
| 1   | D     | 735 | THR  |
| 1   | D     | 736 | LEU  |
| 1   | D     | 742 | VAL  |
| 1   | D     | 745 | ASN  |
| 1   | D     | 755 | SER  |
| 1   | D     | 764 | GLN  |
| 1   | D     | 768 | LEU  |
| 1   | D     | 771 | THR  |
| 1   | D     | 772 | LEU  |
| 1   | E     | 29  | ASP  |
| 1   | E     | 43  | GLU  |
| 1   | E     | 52  | LEU  |
| 1   | E     | 69  | ILE  |
| 1   | E     | 84  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 93  | THR  |
| 1   | E     | 99  | ARG  |
| 1   | E     | 120 | LEU  |
| 1   | E     | 123 | LEU  |
| 1   | E     | 137 | ASN  |
| 1   | E     | 143 | THR  |
| 1   | E     | 146 | GLN  |
| 1   | E     | 174 | ARG  |
| 1   | E     | 178 | THR  |
| 1   | E     | 179 | VAL  |
| 1   | E     | 208 | VAL  |
| 1   | E     | 246 | THR  |
| 1   | E     | 273 | LEU  |
| 1   | E     | 276 | SER  |
| 1   | E     | 300 | LEU  |
| 1   | E     | 316 | CYS  |
| 1   | E     | 324 | THR  |
| 1   | E     | 332 | ILE  |
| 1   | E     | 334 | ARG  |
| 1   | E     | 347 | ASN  |
| 1   | E     | 356 | VAL  |
| 1   | E     | 408 | MET  |
| 1   | E     | 419 | GLU  |
| 1   | E     | 425 | VAL  |
| 1   | E     | 452 | LEU  |
| 1   | E     | 459 | GLU  |
| 1   | E     | 477 | VAL  |
| 1   | E     | 533 | LEU  |
| 1   | E     | 573 | LEU  |
| 1   | E     | 614 | VAL  |
| 1   | E     | 616 | VAL  |
| 1   | E     | 630 | LEU  |
| 1   | E     | 653 | GLN  |
| 1   | E     | 657 | LEU  |
| 1   | E     | 671 | LEU  |
| 1   | E     | 693 | LEU  |
| 1   | E     | 714 | LEU  |
| 1   | E     | 719 | THR  |
| 1   | E     | 723 | ILE  |
| 1   | E     | 735 | THR  |
| 1   | E     | 736 | LEU  |
| 1   | E     | 739 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 742 | VAL  |
| 1   | E     | 744 | VAL  |
| 1   | E     | 764 | GLN  |
| 1   | E     | 769 | THR  |
| 1   | E     | 771 | THR  |
| 1   | E     | 772 | LEU  |
| 1   | E     | 773 | HIS  |
| 1   | F     | 45  | THR  |
| 1   | F     | 52  | LEU  |
| 1   | F     | 65  | VAL  |
| 1   | F     | 84  | LEU  |
| 1   | F     | 95  | GLU  |
| 1   | F     | 120 | LEU  |
| 1   | F     | 137 | ASN  |
| 1   | F     | 143 | THR  |
| 1   | F     | 174 | ARG  |
| 1   | F     | 178 | THR  |
| 1   | F     | 179 | VAL  |
| 1   | F     | 208 | VAL  |
| 1   | F     | 214 | GLN  |
| 1   | F     | 273 | LEU  |
| 1   | F     | 280 | ASN  |
| 1   | F     | 300 | LEU  |
| 1   | F     | 336 | LYS  |
| 1   | F     | 342 | ILE  |
| 1   | F     | 347 | ASN  |
| 1   | F     | 452 | LEU  |
| 1   | F     | 459 | GLU  |
| 1   | F     | 492 | GLU  |
| 1   | F     | 532 | LEU  |
| 1   | F     | 533 | LEU  |
| 1   | F     | 537 | SER  |
| 1   | F     | 544 | SER  |
| 1   | F     | 573 | LEU  |
| 1   | F     | 579 | ARG  |
| 1   | F     | 592 | MET  |
| 1   | F     | 616 | VAL  |
| 1   | F     | 630 | LEU  |
| 1   | F     | 671 | LEU  |
| 1   | F     | 681 | VAL  |
| 1   | F     | 693 | LEU  |
| 1   | F     | 714 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 732 | LYS  |
| 1   | F     | 735 | THR  |
| 1   | F     | 736 | LEU  |
| 1   | F     | 747 | LEU  |
| 1   | F     | 764 | GLN  |
| 1   | F     | 770 | ILE  |
| 1   | F     | 771 | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 11  | GLN  |
| 1   | A     | 21  | GLN  |
| 1   | A     | 27  | GLN  |
| 1   | A     | 73  | GLN  |
| 1   | A     | 107 | ASN  |
| 1   | A     | 137 | ASN  |
| 1   | A     | 141 | GLN  |
| 1   | A     | 177 | GLN  |
| 1   | A     | 211 | ASN  |
| 1   | A     | 212 | HIS  |
| 1   | A     | 347 | ASN  |
| 1   | A     | 352 | GLN  |
| 1   | A     | 381 | GLN  |
| 1   | A     | 434 | GLN  |
| 1   | A     | 564 | GLN  |
| 1   | A     | 641 | ASN  |
| 1   | A     | 652 | GLN  |
| 1   | A     | 653 | GLN  |
| 1   | A     | 692 | ASN  |
| 1   | A     | 721 | ASN  |
| 1   | A     | 766 | ASN  |
| 1   | B     | 21  | GLN  |
| 1   | B     | 47  | GLN  |
| 1   | B     | 73  | GLN  |
| 1   | B     | 107 | ASN  |
| 1   | B     | 133 | GLN  |
| 1   | B     | 137 | ASN  |
| 1   | B     | 144 | ASN  |
| 1   | B     | 146 | GLN  |
| 1   | B     | 177 | GLN  |
| 1   | B     | 211 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 212 | HIS  |
| 1   | B     | 347 | ASN  |
| 1   | B     | 352 | GLN  |
| 1   | B     | 381 | GLN  |
| 1   | B     | 478 | HIS  |
| 1   | B     | 613 | ASN  |
| 1   | B     | 652 | GLN  |
| 1   | B     | 692 | ASN  |
| 1   | B     | 721 | ASN  |
| 1   | B     | 733 | ASN  |
| 1   | B     | 745 | ASN  |
| 1   | B     | 773 | HIS  |
| 1   | C     | 21  | GLN  |
| 1   | C     | 27  | GLN  |
| 1   | C     | 30  | ASN  |
| 1   | C     | 47  | GLN  |
| 1   | C     | 73  | GLN  |
| 1   | C     | 107 | ASN  |
| 1   | C     | 125 | ASN  |
| 1   | C     | 137 | ASN  |
| 1   | C     | 141 | GLN  |
| 1   | C     | 212 | HIS  |
| 1   | C     | 347 | ASN  |
| 1   | C     | 352 | GLN  |
| 1   | C     | 381 | GLN  |
| 1   | C     | 426 | GLN  |
| 1   | C     | 478 | HIS  |
| 1   | C     | 652 | GLN  |
| 1   | C     | 692 | ASN  |
| 1   | C     | 733 | ASN  |
| 1   | C     | 748 | GLN  |
| 1   | C     | 764 | GLN  |
| 1   | C     | 773 | HIS  |
| 1   | D     | 21  | GLN  |
| 1   | D     | 27  | GLN  |
| 1   | D     | 47  | GLN  |
| 1   | D     | 73  | GLN  |
| 1   | D     | 77  | ASN  |
| 1   | D     | 125 | ASN  |
| 1   | D     | 133 | GLN  |
| 1   | D     | 137 | ASN  |
| 1   | D     | 141 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 146 | GLN  |
| 1   | D     | 177 | GLN  |
| 1   | D     | 212 | HIS  |
| 1   | D     | 347 | ASN  |
| 1   | D     | 352 | GLN  |
| 1   | D     | 381 | GLN  |
| 1   | D     | 426 | GLN  |
| 1   | D     | 613 | ASN  |
| 1   | D     | 652 | GLN  |
| 1   | D     | 692 | ASN  |
| 1   | D     | 766 | ASN  |
| 1   | E     | 27  | GLN  |
| 1   | E     | 81  | HIS  |
| 1   | E     | 137 | ASN  |
| 1   | E     | 177 | GLN  |
| 1   | E     | 212 | HIS  |
| 1   | E     | 347 | ASN  |
| 1   | E     | 352 | GLN  |
| 1   | E     | 381 | GLN  |
| 1   | E     | 517 | ASN  |
| 1   | E     | 564 | GLN  |
| 1   | E     | 613 | ASN  |
| 1   | E     | 652 | GLN  |
| 1   | E     | 697 | HIS  |
| 1   | E     | 745 | ASN  |
| 1   | E     | 766 | ASN  |
| 1   | F     | 21  | GLN  |
| 1   | F     | 27  | GLN  |
| 1   | F     | 61  | GLN  |
| 1   | F     | 73  | GLN  |
| 1   | F     | 81  | HIS  |
| 1   | F     | 107 | ASN  |
| 1   | F     | 133 | GLN  |
| 1   | F     | 137 | ASN  |
| 1   | F     | 177 | GLN  |
| 1   | F     | 212 | HIS  |
| 1   | F     | 280 | ASN  |
| 1   | F     | 347 | ASN  |
| 1   | F     | 352 | GLN  |
| 1   | F     | 381 | GLN  |
| 1   | F     | 478 | HIS  |
| 1   | F     | 564 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 613 | ASN  |
| 1   | F     | 652 | GLN  |
| 1   | F     | 692 | ASN  |
| 1   | F     | 697 | HIS  |
| 1   | F     | 733 | ASN  |
| 1   | F     | 748 | GLN  |
| 1   | F     | 752 | GLN  |
| 1   | F     | 757 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

35 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | XTG  | F     | 3020 | -    | 32,32,32     | 2.64 | 10 (31%)    | 43,46,46    | 2.72 | 14 (32%)    |
| 4   | GOL  | D     | 3031 | -    | 5,5,5        | 0.45 | 0           | 5,5,5       | 0.59 | 0           |
| 3   | XTG  | F     | 3021 | -    | 32,32,32     | 2.78 | 6 (18%)     | 43,46,46    | 2.10 | 7 (16%)     |
| 4   | GOL  | E     | 3033 | -    | 5,5,5        | 0.45 | 0           | 5,5,5       | 0.64 | 0           |
| 3   | XTG  | A     | 3015 | -    | 32,32,32     | 2.88 | 4 (12%)     | 43,46,46    | 2.57 | 17 (39%)    |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | GOL  | A     | 3029 | -    | 5,5,5        | 0.54 | 0        | 5,5,5       | 1.23 | 1 (20%)  |
| 5   | MPO  | B     | 3010 | -    | 13,13,13     | 2.09 | 1 (7%)   | 17,17,17    | 1.13 | 1 (5%)   |
| 5   | MPO  | F     | 3014 | -    | 13,13,13     | 8.22 | 2 (15%)  | 17,17,17    | 8.54 | 6 (35%)  |
| 4   | GOL  | C     | 3030 | -    | 5,5,5        | 0.48 | 0        | 5,5,5       | 0.54 | 0        |
| 4   | GOL  | D     | 3032 | -    | 5,5,5        | 0.47 | 0        | 5,5,5       | 0.98 | 0        |
| 4   | GOL  | F     | 3022 | -    | 5,5,5        | 0.61 | 0        | 5,5,5       | 0.86 | 0        |
| 3   | XTG  | E     | 3019 | -    | 32,32,32     | 2.48 | 6 (18%)  | 43,46,46    | 2.16 | 11 (25%) |
| 5   | MPO  | D     | 3012 | -    | 13,13,13     | 2.12 | 1 (7%)   | 17,17,17    | 1.30 | 3 (17%)  |
| 2   | SO4  | D     | 3002 | -    | 4,4,4        | 0.33 | 0        | 6,6,6       | 0.50 | 0        |
| 4   | GOL  | A     | 3028 | -    | 5,5,5        | 0.37 | 0        | 5,5,5       | 0.68 | 0        |
| 5   | MPO  | E     | 3013 | -    | 13,13,13     | 2.01 | 1 (7%)   | 17,17,17    | 1.52 | 3 (17%)  |
| 4   | GOL  | B     | 3026 | -    | 5,5,5        | 0.32 | 0        | 5,5,5       | 0.83 | 0        |
| 2   | SO4  | F     | 3003 | -    | 4,4,4        | 0.34 | 0        | 6,6,6       | 0.39 | 0        |
| 3   | XTG  | B     | 3016 | -    | 32,32,32     | 3.07 | 7 (21%)  | 43,46,46    | 2.76 | 13 (30%) |
| 2   | SO4  | E     | 3004 | -    | 4,4,4        | 0.37 | 0        | 6,6,6       | 0.55 | 0        |
| 2   | SO4  | C     | 3005 | -    | 4,4,4        | 0.17 | 0        | 6,6,6       | 0.72 | 0        |
| 2   | SO4  | E     | 3009 | -    | 4,4,4        | 0.24 | 0        | 6,6,6       | 0.51 | 0        |
| 4   | GOL  | C     | 3023 | -    | 5,5,5        | 0.59 | 0        | 5,5,5       | 1.51 | 1 (20%)  |
| 5   | MPO  | C     | 3011 | -    | 13,13,13     | 1.97 | 1 (7%)   | 17,17,17    | 1.37 | 4 (23%)  |
| 3   | XTG  | C     | 3017 | -    | 32,32,32     | 2.91 | 4 (12%)  | 43,46,46    | 1.93 | 7 (16%)  |
| 4   | GOL  | E     | 3035 | -    | 5,5,5        | 0.67 | 0        | 5,5,5       | 0.82 | 0        |
| 4   | GOL  | C     | 3027 | -    | 5,5,5        | 0.60 | 0        | 5,5,5       | 0.79 | 0        |
| 4   | GOL  | F     | 3034 | -    | 5,5,5        | 0.45 | 0        | 5,5,5       | 0.48 | 0        |
| 4   | GOL  | B     | 3025 | -    | 5,5,5        | 0.42 | 0        | 5,5,5       | 1.12 | 0        |
| 2   | SO4  | F     | 3007 | -    | 4,4,4        | 0.22 | 0        | 6,6,6       | 0.25 | 0        |
| 2   | SO4  | F     | 3001 | -    | 4,4,4        | 0.32 | 0        | 6,6,6       | 0.74 | 0        |
| 3   | XTG  | D     | 3018 | -    | 32,32,32     | 3.87 | 10 (31%) | 43,46,46    | 3.13 | 16 (37%) |
| 2   | SO4  | A     | 3008 | -    | 4,4,4        | 0.38 | 0        | 6,6,6       | 0.50 | 0        |
| 2   | SO4  | B     | 3006 | -    | 4,4,4        | 0.28 | 0        | 6,6,6       | 0.32 | 0        |
| 4   | GOL  | A     | 3024 | -    | 5,5,5        | 0.44 | 0        | 5,5,5       | 0.88 | 0        |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 3   | XTG  | F     | 3020 | -    | -       | 6/11/50/50 | 0/3/3/3 |
| 4   | GOL  | D     | 3031 | -    | -       | 4/4/4/4    | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 3   | XTG  | F     | 3021 | -    | -       | 2/11/50/50 | 0/3/3/3 |
| 4   | GOL  | E     | 3033 | -    | -       | 3/4/4/4    | -       |
| 3   | XTG  | A     | 3015 | -    | -       | 5/11/50/50 | 0/3/3/3 |
| 4   | GOL  | A     | 3029 | -    | -       | 1/4/4/4    | -       |
| 5   | MPO  | B     | 3010 | -    | -       | 0/7/15/15  | 0/1/1/1 |
| 5   | MPO  | F     | 3014 | -    | -       | 3/7/15/15  | 0/1/1/1 |
| 4   | GOL  | C     | 3030 | -    | -       | 2/4/4/4    | -       |
| 4   | GOL  | D     | 3032 | -    | -       | 0/4/4/4    | -       |
| 4   | GOL  | F     | 3022 | -    | -       | 4/4/4/4    | -       |
| 3   | XTG  | E     | 3019 | -    | -       | 5/11/50/50 | 0/3/3/3 |
| 5   | MPO  | D     | 3012 | -    | -       | 3/7/15/15  | 0/1/1/1 |
| 4   | GOL  | A     | 3028 | -    | -       | 3/4/4/4    | -       |
| 5   | MPO  | E     | 3013 | -    | -       | 5/7/15/15  | 0/1/1/1 |
| 4   | GOL  | B     | 3026 | -    | -       | 2/4/4/4    | -       |
| 3   | XTG  | B     | 3016 | -    | -       | 7/11/50/50 | 0/3/3/3 |
| 4   | GOL  | C     | 3023 | -    | -       | 0/4/4/4    | -       |
| 5   | MPO  | C     | 3011 | -    | -       | 0/7/15/15  | 0/1/1/1 |
| 3   | XTG  | C     | 3017 | -    | -       | 7/11/50/50 | 0/3/3/3 |
| 4   | GOL  | E     | 3035 | -    | -       | 1/4/4/4    | -       |
| 4   | GOL  | C     | 3027 | -    | -       | 1/4/4/4    | -       |
| 4   | GOL  | F     | 3034 | -    | -       | 4/4/4/4    | -       |
| 4   | GOL  | B     | 3025 | -    | -       | 3/4/4/4    | -       |
| 3   | XTG  | D     | 3018 | -    | -       | 6/11/50/50 | 0/3/3/3 |
| 4   | GOL  | A     | 3024 | -    | -       | 4/4/4/4    | -       |

All (53) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 5   | F     | 3014 | MPO  | C4-N1  | 28.66 | 2.24        | 1.46     |
| 3   | D     | 3018 | XTG  | O11-N1 | 15.17 | 1.48        | 1.22     |
| 3   | C     | 3017 | XTG  | O11-N1 | 14.64 | 1.48        | 1.22     |
| 3   | A     | 3015 | XTG  | O11-N1 | 13.52 | 1.46        | 1.22     |
| 3   | B     | 3016 | XTG  | O11-N1 | 12.99 | 1.45        | 1.22     |
| 3   | F     | 3021 | XTG  | O11-N1 | 12.28 | 1.44        | 1.22     |
| 3   | F     | 3020 | XTG  | O11-N1 | 11.26 | 1.42        | 1.22     |
| 3   | E     | 3019 | XTG  | O11-N1 | 10.49 | 1.40        | 1.22     |
| 3   | D     | 3018 | XTG  | O9-C11 | 7.13  | 1.55        | 1.43     |
| 5   | D     | 3012 | MPO  | C1-S1  | -7.01 | 1.67        | 1.77     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5   | F     | 3014 | MPO  | C1-S1   | -6.94 | 1.67        | 1.77     |
| 5   | B     | 3010 | MPO  | C1-S1   | -6.93 | 1.67        | 1.77     |
| 5   | E     | 3013 | MPO  | C1-S1   | -6.89 | 1.67        | 1.77     |
| 5   | C     | 3011 | MPO  | C1-S1   | -6.47 | 1.68        | 1.77     |
| 3   | B     | 3016 | XTG  | O1-C1   | 6.30  | 1.50        | 1.41     |
| 3   | D     | 3018 | XTG  | O9-C7   | 6.08  | 1.54        | 1.41     |
| 3   | D     | 3018 | XTG  | O8-C10  | 5.87  | 1.55        | 1.43     |
| 3   | D     | 3018 | XTG  | C7-S6   | 5.75  | 1.90        | 1.80     |
| 3   | F     | 3020 | XTG  | C7-S6   | 4.97  | 1.89        | 1.80     |
| 3   | D     | 3018 | XTG  | C7-C8   | 4.97  | 1.61        | 1.53     |
| 3   | D     | 3018 | XTG  | C12-N1  | -4.87 | 1.33        | 1.45     |
| 3   | F     | 3021 | XTG  | O9-C11  | 4.84  | 1.51        | 1.43     |
| 3   | A     | 3015 | XTG  | O1-C1   | 4.65  | 1.48        | 1.41     |
| 3   | C     | 3017 | XTG  | C12-N1  | -4.57 | 1.34        | 1.45     |
| 3   | F     | 3021 | XTG  | O9-C7   | 4.52  | 1.51        | 1.41     |
| 3   | E     | 3019 | XTG  | C7-S6   | 4.40  | 1.88        | 1.80     |
| 3   | A     | 3015 | XTG  | C7-S6   | 4.12  | 1.87        | 1.80     |
| 3   | B     | 3016 | XTG  | C12-N1  | -4.11 | 1.35        | 1.45     |
| 3   | B     | 3016 | XTG  | C10-C9  | 4.07  | 1.58        | 1.52     |
| 3   | D     | 3018 | XTG  | C8-C9   | 3.91  | 1.62        | 1.52     |
| 3   | F     | 3021 | XTG  | C12-N1  | -3.91 | 1.35        | 1.45     |
| 3   | B     | 3016 | XTG  | C7-S6   | 3.90  | 1.87        | 1.80     |
| 3   | A     | 3015 | XTG  | C12-N1  | -3.83 | 1.36        | 1.45     |
| 3   | E     | 3019 | XTG  | C12-N1  | -3.56 | 1.36        | 1.45     |
| 3   | F     | 3020 | XTG  | C10-C9  | 3.47  | 1.57        | 1.52     |
| 3   | E     | 3019 | XTG  | O1-C1   | 3.43  | 1.46        | 1.41     |
| 3   | F     | 3020 | XTG  | C12-N1  | -3.38 | 1.37        | 1.45     |
| 3   | B     | 3016 | XTG  | C8-C9   | 3.13  | 1.60        | 1.52     |
| 3   | E     | 3019 | XTG  | C10-C9  | 3.05  | 1.57        | 1.52     |
| 3   | F     | 3021 | XTG  | C11-C10 | 2.94  | 1.59        | 1.52     |
| 3   | F     | 3020 | XTG  | O6-C8   | 2.80  | 1.49        | 1.43     |
| 3   | C     | 3017 | XTG  | C7-S6   | 2.77  | 1.85        | 1.80     |
| 3   | F     | 3021 | XTG  | C7-S6   | 2.65  | 1.85        | 1.80     |
| 3   | F     | 3020 | XTG  | C8-C9   | 2.55  | 1.59        | 1.52     |
| 3   | F     | 3020 | XTG  | O5-C1   | 2.46  | 1.48        | 1.41     |
| 3   | F     | 3020 | XTG  | O9-C7   | 2.35  | 1.46        | 1.41     |
| 3   | B     | 3016 | XTG  | O9-C11  | 2.35  | 1.47        | 1.43     |
| 3   | E     | 3019 | XTG  | C7-C8   | 2.22  | 1.57        | 1.53     |
| 3   | C     | 3017 | XTG  | C8-C9   | 2.19  | 1.58        | 1.52     |
| 3   | D     | 3018 | XTG  | O6-C8   | 2.19  | 1.48        | 1.43     |
| 3   | F     | 3020 | XTG  | O7-C9   | 2.16  | 1.48        | 1.43     |
| 3   | F     | 3020 | XTG  | C7-C8   | 2.12  | 1.57        | 1.53     |

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| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 3   | D     | 3018 | XTG  | C10-C9 | 2.08 | 1.55        | 1.52     |

All (104) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 5   | F     | 3014 | MPO  | C6-C7-N1   | 28.59  | 153.57      | 110.12   |
| 5   | F     | 3014 | MPO  | C7-N1-C4   | -14.52 | 77.56       | 108.84   |
| 5   | F     | 3014 | MPO  | C5-C4-N1   | 11.43  | 127.48      | 110.12   |
| 3   | B     | 3016 | XTG  | O5-C5-C6   | 10.65  | 124.33      | 106.49   |
| 3   | D     | 3018 | XTG  | C11-O9-C7  | 9.46   | 126.83      | 111.19   |
| 3   | A     | 3015 | XTG  | O5-C5-C6   | 9.01   | 121.59      | 106.49   |
| 3   | D     | 3018 | XTG  | O5-C5-C6   | 8.94   | 121.47      | 106.49   |
| 3   | C     | 3017 | XTG  | C6-S6-C7   | 8.27   | 115.45      | 100.12   |
| 3   | D     | 3018 | XTG  | C6-S6-C7   | 8.13   | 115.19      | 100.12   |
| 3   | F     | 3020 | XTG  | O5-C5-C6   | 8.05   | 119.97      | 106.49   |
| 3   | E     | 3019 | XTG  | C6-S6-C7   | 7.79   | 114.58      | 100.12   |
| 3   | B     | 3016 | XTG  | C6-S6-C7   | 7.75   | 114.49      | 100.12   |
| 3   | A     | 3015 | XTG  | C6-S6-C7   | 7.56   | 114.15      | 100.12   |
| 3   | F     | 3021 | XTG  | C6-S6-C7   | 7.54   | 114.11      | 100.12   |
| 3   | F     | 3020 | XTG  | C1-O5-C5   | -7.14  | 99.77       | 113.72   |
| 3   | F     | 3020 | XTG  | C6-S6-C7   | 6.57   | 112.31      | 100.12   |
| 3   | E     | 3019 | XTG  | O9-C7-C8   | -6.46  | 102.04      | 109.47   |
| 3   | B     | 3016 | XTG  | C15-O1-C1  | -6.23  | 109.04      | 117.82   |
| 3   | F     | 3021 | XTG  | O9-C7-C8   | 5.94   | 116.29      | 109.47   |
| 3   | F     | 3020 | XTG  | C6-C5-C4   | -5.92  | 98.07       | 112.86   |
| 3   | D     | 3018 | XTG  | O8-C10-C11 | 5.79   | 122.47      | 109.22   |
| 5   | F     | 3014 | MPO  | C3-N1-C7   | 5.71   | 126.46      | 111.24   |
| 3   | D     | 3018 | XTG  | C11-C10-C9 | -5.70  | 101.35      | 109.64   |
| 5   | F     | 3014 | MPO  | O2-S1-C1   | 5.59   | 115.18      | 106.73   |
| 3   | A     | 3015 | XTG  | C1-O5-C5   | -5.35  | 103.27      | 113.72   |
| 3   | C     | 3017 | XTG  | O5-C5-C6   | 4.93   | 114.75      | 106.49   |
| 3   | F     | 3020 | XTG  | O9-C7-C8   | 4.51   | 114.65      | 109.47   |
| 3   | F     | 3021 | XTG  | O9-C11-C10 | 4.49   | 121.50      | 110.79   |
| 3   | B     | 3016 | XTG  | O5-C1-O1   | 4.49   | 119.92      | 108.42   |
| 3   | B     | 3016 | XTG  | O1-C1-C2   | 4.45   | 113.65      | 107.16   |
| 3   | F     | 3021 | XTG  | O5-C5-C6   | -4.28  | 99.32       | 106.49   |
| 3   | D     | 3018 | XTG  | C6-C5-C4   | -4.02  | 102.83      | 112.86   |
| 3   | D     | 3018 | XTG  | O8-C10-C9  | 3.89   | 118.21      | 110.15   |
| 3   | A     | 3015 | XTG  | O11-N1-C12 | 3.76   | 123.99      | 118.82   |
| 5   | E     | 3013 | MPO  | O1-S1-C1   | 3.68   | 112.29      | 106.73   |
| 3   | F     | 3020 | XTG  | C15-O1-C1  | -3.55  | 112.81      | 117.82   |
| 3   | F     | 3021 | XTG  | C6-C5-C4   | 3.53   | 121.69      | 112.86   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3   | D     | 3018 | XTG  | O6-C8-C9   | 3.44  | 118.49      | 110.38   |
| 3   | C     | 3017 | XTG  | C1-O5-C5   | -3.42 | 107.05      | 113.72   |
| 3   | A     | 3015 | XTG  | O6-C8-C9   | 3.41  | 118.41      | 110.38   |
| 3   | E     | 3019 | XTG  | C1-O5-C5   | -3.37 | 107.14      | 113.72   |
| 3   | A     | 3015 | XTG  | O5-C1-O1   | 3.36  | 117.03      | 108.42   |
| 3   | F     | 3020 | XTG  | O1-C1-C2   | 3.35  | 112.05      | 107.16   |
| 3   | C     | 3017 | XTG  | C3-C4-C5   | -3.35 | 104.17      | 110.23   |
| 3   | E     | 3019 | XTG  | O5-C5-C6   | 3.31  | 112.04      | 106.49   |
| 3   | F     | 3020 | XTG  | O6-C8-C9   | 3.25  | 118.03      | 110.38   |
| 3   | D     | 3018 | XTG  | O9-C11-C10 | 3.14  | 118.28      | 110.79   |
| 3   | D     | 3018 | XTG  | O9-C7-C8   | -3.13 | 105.86      | 109.47   |
| 5   | E     | 3013 | MPO  | O2-S1-C1   | 3.07  | 111.36      | 106.73   |
| 3   | B     | 3016 | XTG  | O6-C8-C9   | 3.03  | 117.52      | 110.38   |
| 3   | B     | 3016 | XTG  | C3-C4-C5   | -2.97 | 104.85      | 110.23   |
| 3   | B     | 3016 | XTG  | O9-C7-C8   | -2.95 | 106.08      | 109.47   |
| 3   | E     | 3019 | XTG  | C17-C12-N1 | 2.94  | 121.91      | 119.34   |
| 3   | B     | 3016 | XTG  | C1-O5-C5   | -2.91 | 108.04      | 113.72   |
| 3   | D     | 3018 | XTG  | O6-C8-C7   | 2.91  | 115.46      | 110.30   |
| 3   | F     | 3020 | XTG  | C11-O9-C7  | -2.82 | 106.53      | 111.19   |
| 3   | E     | 3019 | XTG  | O1-C1-C2   | 2.80  | 111.23      | 107.16   |
| 3   | D     | 3018 | XTG  | O7-C9-C8   | 2.75  | 116.86      | 110.38   |
| 5   | D     | 3012 | MPO  | O1-S1-C1   | 2.72  | 110.84      | 106.73   |
| 3   | A     | 3015 | XTG  | O5-C5-C4   | -2.62 | 104.97      | 109.70   |
| 3   | A     | 3015 | XTG  | C3-C4-C5   | -2.62 | 105.49      | 110.23   |
| 5   | C     | 3011 | MPO  | O1-S1-C1   | 2.60  | 110.66      | 106.73   |
| 3   | F     | 3020 | XTG  | O7-C9-C8   | 2.58  | 116.45      | 110.38   |
| 3   | A     | 3015 | XTG  | C6-C5-C4   | -2.57 | 106.44      | 112.86   |
| 5   | D     | 3012 | MPO  | O3-S1-C1   | 2.56  | 111.01      | 106.00   |
| 3   | A     | 3015 | XTG  | C13-C12-N1 | 2.55  | 121.57      | 119.34   |
| 5   | F     | 3014 | MPO  | O2-S1-O1   | -2.54 | 105.58      | 113.82   |
| 3   | F     | 3021 | XTG  | O9-C7-S6   | 2.53  | 116.74      | 109.92   |
| 3   | D     | 3018 | XTG  | O5-C1-O1   | 2.52  | 114.87      | 108.42   |
| 3   | A     | 3015 | XTG  | O1-C1-C2   | 2.50  | 110.81      | 107.16   |
| 3   | A     | 3015 | XTG  | C4-C3-C2   | -2.48 | 106.47      | 110.83   |
| 3   | B     | 3016 | XTG  | C11-O9-C7  | -2.47 | 107.11      | 111.19   |
| 3   | A     | 3015 | XTG  | O7-C9-C8   | 2.44  | 116.14      | 110.38   |
| 3   | C     | 3017 | XTG  | O9-C11-C10 | 2.40  | 116.50      | 110.79   |
| 5   | C     | 3011 | MPO  | O2-S1-O1   | -2.36 | 106.14      | 113.82   |
| 3   | A     | 3015 | XTG  | O6-C8-C7   | -2.36 | 106.10      | 110.30   |
| 3   | D     | 3018 | XTG  | O9-C7-S6   | 2.33  | 116.21      | 109.92   |
| 3   | B     | 3016 | XTG  | C13-C12-N1 | 2.32  | 121.36      | 119.34   |
| 3   | A     | 3015 | XTG  | O9-C7-C8   | -2.31 | 106.81      | 109.47   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 3   | D     | 3018 | XTG  | C10-C9-C8  | -2.31 | 106.79      | 110.86   |
| 3   | E     | 3019 | XTG  | C15-O1-C1  | 2.29  | 121.05      | 117.82   |
| 3   | E     | 3019 | XTG  | C11-C10-C9 | 2.28  | 112.96      | 109.64   |
| 4   | C     | 3023 | GOL  | O2-C2-C3   | 2.27  | 118.56      | 109.18   |
| 3   | F     | 3020 | XTG  | C3-C4-C5   | -2.26 | 106.14      | 110.23   |
| 5   | E     | 3013 | MPO  | O2-S1-O1   | -2.26 | 106.48      | 113.82   |
| 3   | F     | 3020 | XTG  | O3-C3-C2   | -2.25 | 105.07      | 110.38   |
| 3   | E     | 3019 | XTG  | O5-C1-O1   | 2.24  | 114.16      | 108.42   |
| 3   | F     | 3020 | XTG  | C17-C12-N1 | 2.24  | 121.29      | 119.34   |
| 5   | D     | 3012 | MPO  | O3-S1-O2   | -2.22 | 105.85      | 111.40   |
| 3   | A     | 3015 | XTG  | O9-C11-C10 | 2.22  | 116.07      | 110.79   |
| 3   | E     | 3019 | XTG  | O6-C8-C7   | 2.21  | 114.23      | 110.30   |
| 5   | B     | 3010 | MPO  | O3-S1-C1   | 2.21  | 110.33      | 106.00   |
| 5   | C     | 3011 | MPO  | O3-S1-O2   | -2.20 | 105.89      | 111.40   |
| 3   | F     | 3020 | XTG  | C4-C3-C2   | -2.19 | 106.98      | 110.83   |
| 3   | C     | 3017 | XTG  | O2-C2-C1   | -2.18 | 104.89      | 110.08   |
| 3   | A     | 3015 | XTG  | O5-C1-C2   | -2.16 | 105.93      | 110.37   |
| 3   | B     | 3016 | XTG  | O8-C10-C9  | 2.15  | 114.60      | 110.15   |
| 3   | C     | 3017 | XTG  | C11-O9-C7  | 2.13  | 114.72      | 111.19   |
| 4   | A     | 3029 | GOL  | O2-C2-C1   | 2.12  | 117.97      | 109.18   |
| 3   | B     | 3016 | XTG  | O5-C1-C2   | -2.12 | 106.02      | 110.37   |
| 3   | D     | 3018 | XTG  | O11-N1-C12 | -2.11 | 115.92      | 118.82   |
| 3   | E     | 3019 | XTG  | C3-C4-C5   | -2.10 | 106.42      | 110.23   |
| 5   | C     | 3011 | MPO  | O3-S1-C1   | 2.09  | 110.10      | 106.00   |
| 3   | F     | 3021 | XTG  | C1-O5-C5   | -2.04 | 109.74      | 113.72   |

There are no chirality outliers.

All (81) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 3   | A     | 3015 | XTG  | O5-C5-C6-S6    |
| 3   | A     | 3015 | XTG  | C4-C5-C6-S6    |
| 3   | A     | 3015 | XTG  | O9-C7-S6-C6    |
| 3   | B     | 3016 | XTG  | O5-C5-C6-S6    |
| 3   | B     | 3016 | XTG  | C4-C5-C6-S6    |
| 3   | B     | 3016 | XTG  | O9-C7-S6-C6    |
| 3   | C     | 3017 | XTG  | C13-C12-N1-O11 |
| 3   | C     | 3017 | XTG  | C17-C12-N1-O11 |
| 3   | C     | 3017 | XTG  | C4-C5-C6-S6    |
| 3   | C     | 3017 | XTG  | O9-C7-S6-C6    |
| 3   | D     | 3018 | XTG  | C13-C12-N1-O11 |
| 3   | D     | 3018 | XTG  | C17-C12-N1-O11 |

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| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 3   | D     | 3018 | XTG  | O5-C5-C6-S6    |
| 3   | D     | 3018 | XTG  | C4-C5-C6-S6    |
| 3   | D     | 3018 | XTG  | O9-C7-S6-C6    |
| 3   | E     | 3019 | XTG  | C13-C12-N1-O11 |
| 3   | E     | 3019 | XTG  | C17-C12-N1-O11 |
| 3   | E     | 3019 | XTG  | O5-C1-O1-C15   |
| 3   | E     | 3019 | XTG  | O9-C7-S6-C6    |
| 3   | F     | 3020 | XTG  | C13-C12-N1-O11 |
| 3   | F     | 3020 | XTG  | C17-C12-N1-O11 |
| 3   | F     | 3020 | XTG  | O5-C5-C6-S6    |
| 3   | F     | 3020 | XTG  | C4-C5-C6-S6    |
| 3   | F     | 3020 | XTG  | O9-C7-S6-C6    |
| 3   | F     | 3021 | XTG  | O9-C7-S6-C6    |
| 4   | A     | 3024 | GOL  | O1-C1-C2-C3    |
| 4   | A     | 3028 | GOL  | O1-C1-C2-C3    |
| 4   | B     | 3025 | GOL  | O1-C1-C2-C3    |
| 4   | C     | 3030 | GOL  | O1-C1-C2-C3    |
| 4   | D     | 3031 | GOL  | O1-C1-C2-C3    |
| 4   | E     | 3033 | GOL  | O1-C1-C2-C3    |
| 4   | F     | 3022 | GOL  | O1-C1-C2-C3    |
| 4   | F     | 3022 | GOL  | C1-C2-C3-O3    |
| 4   | F     | 3034 | GOL  | O1-C1-C2-C3    |
| 4   | F     | 3034 | GOL  | C1-C2-C3-O3    |
| 5   | E     | 3013 | MPO  | C2-C1-S1-O2    |
| 5   | F     | 3014 | MPO  | C1-C2-C3-N1    |
| 5   | F     | 3014 | MPO  | C2-C3-N1-C4    |
| 3   | A     | 3015 | XTG  | O5-C1-O1-C15   |
| 5   | F     | 3014 | MPO  | C2-C3-N1-C7    |
| 3   | B     | 3016 | XTG  | C17-C12-N1-O11 |
| 4   | A     | 3024 | GOL  | C1-C2-C3-O3    |
| 4   | A     | 3024 | GOL  | O1-C1-C2-O2    |
| 4   | F     | 3022 | GOL  | O1-C1-C2-O2    |
| 4   | F     | 3022 | GOL  | O2-C2-C3-O3    |
| 4   | B     | 3025 | GOL  | O1-C1-C2-O2    |
| 4   | C     | 3030 | GOL  | O1-C1-C2-O2    |
| 4   | D     | 3031 | GOL  | O1-C1-C2-O2    |
| 4   | D     | 3031 | GOL  | O2-C2-C3-O3    |
| 4   | E     | 3033 | GOL  | O1-C1-C2-O2    |
| 4   | F     | 3034 | GOL  | O1-C1-C2-O2    |
| 4   | F     | 3034 | GOL  | O2-C2-C3-O3    |
| 5   | D     | 3012 | MPO  | C2-C3-N1-C7    |
| 3   | B     | 3016 | XTG  | O5-C1-O1-C15   |

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| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 3   | C     | 3017 | XTG  | O5-C1-O1-C15   |
| 4   | A     | 3028 | GOL  | O1-C1-C2-O2    |
| 4   | C     | 3027 | GOL  | O2-C2-C3-O3    |
| 4   | E     | 3035 | GOL  | O2-C2-C3-O3    |
| 5   | E     | 3013 | MPO  | C2-C1-S1-O3    |
| 4   | A     | 3028 | GOL  | O2-C2-C3-O3    |
| 4   | B     | 3025 | GOL  | O2-C2-C3-O3    |
| 4   | E     | 3033 | GOL  | O2-C2-C3-O3    |
| 3   | A     | 3015 | XTG  | C8-C7-S6-C6    |
| 3   | B     | 3016 | XTG  | C8-C7-S6-C6    |
| 3   | C     | 3017 | XTG  | C8-C7-S6-C6    |
| 3   | F     | 3020 | XTG  | C8-C7-S6-C6    |
| 3   | F     | 3021 | XTG  | C8-C7-S6-C6    |
| 3   | B     | 3016 | XTG  | C13-C12-N1-O11 |
| 5   | E     | 3013 | MPO  | C2-C1-S1-O1    |
| 3   | C     | 3017 | XTG  | O5-C5-C6-S6    |
| 4   | A     | 3024 | GOL  | O2-C2-C3-O3    |
| 3   | E     | 3019 | XTG  | C4-C5-C6-S6    |
| 5   | D     | 3012 | MPO  | C2-C3-N1-C4    |
| 4   | B     | 3026 | GOL  | C1-C2-C3-O3    |
| 4   | B     | 3026 | GOL  | O2-C2-C3-O3    |
| 4   | D     | 3031 | GOL  | C1-C2-C3-O3    |
| 5   | E     | 3013 | MPO  | C2-C3-N1-C7    |
| 3   | D     | 3018 | XTG  | C5-C6-S6-C7    |
| 5   | E     | 3013 | MPO  | C2-C3-N1-C4    |
| 4   | A     | 3029 | GOL  | O2-C2-C3-O3    |
| 5   | D     | 3012 | MPO  | C2-C1-S1-O3    |

There are no ring outliers.

16 monomers are involved in 29 short contacts:

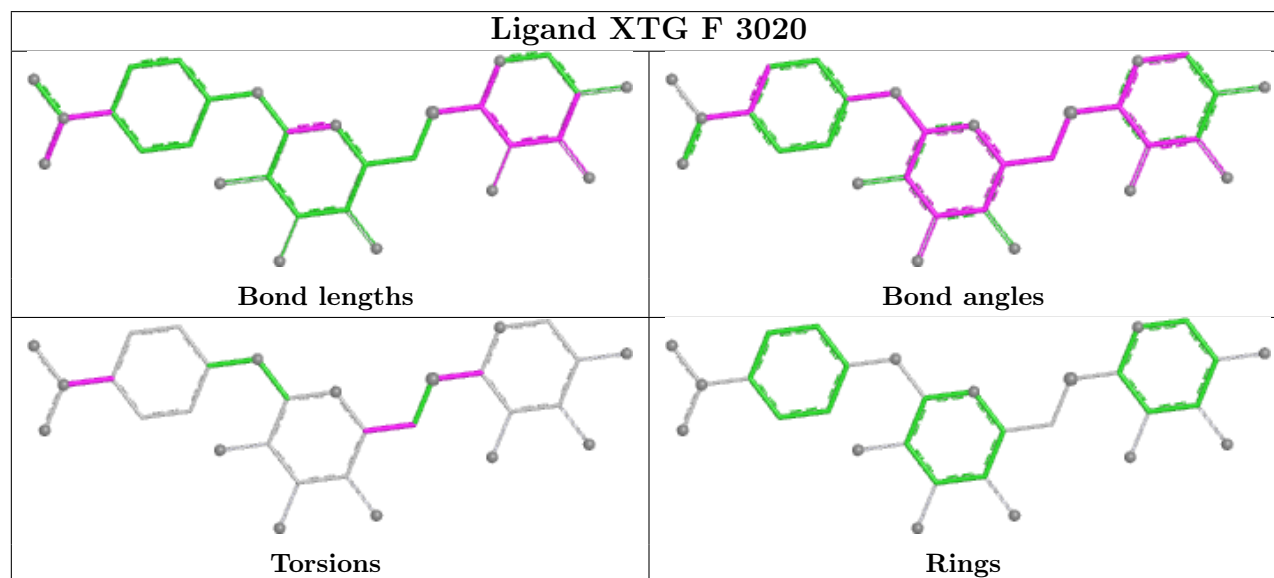
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | F     | 3020 | XTG  | 2       | 0            |
| 3   | A     | 3015 | XTG  | 2       | 0            |
| 4   | A     | 3029 | GOL  | 3       | 0            |
| 4   | D     | 3032 | GOL  | 2       | 0            |
| 4   | F     | 3022 | GOL  | 2       | 0            |
| 3   | E     | 3019 | XTG  | 1       | 0            |
| 2   | D     | 3002 | SO4  | 1       | 0            |
| 4   | A     | 3028 | GOL  | 1       | 0            |
| 4   | B     | 3026 | GOL  | 2       | 0            |
| 2   | F     | 3003 | SO4  | 1       | 0            |

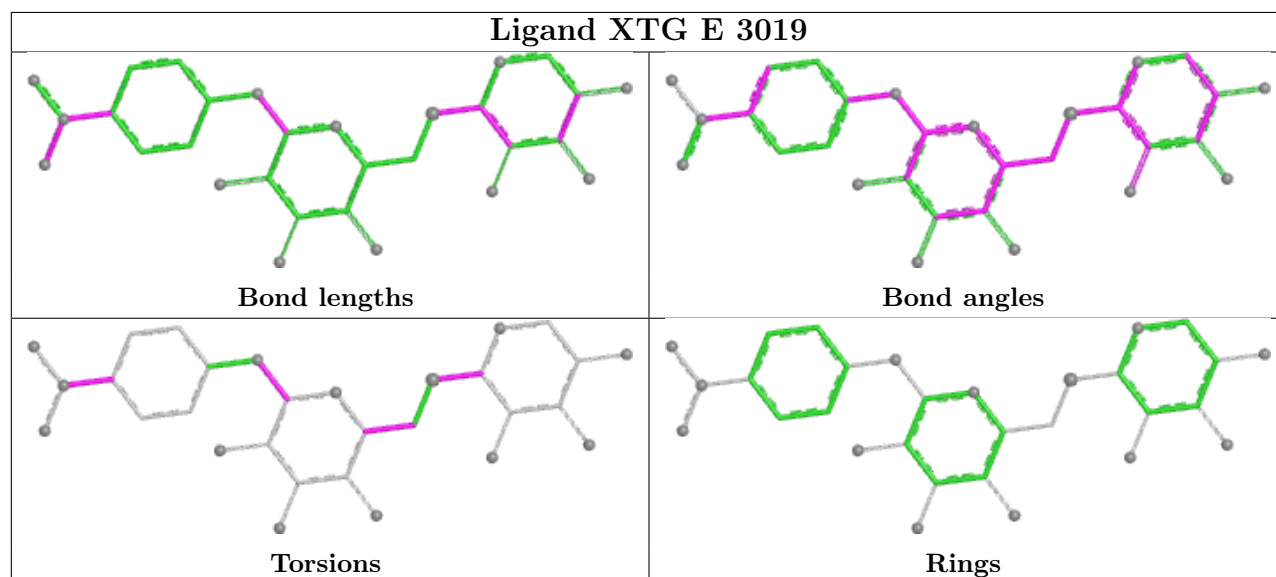
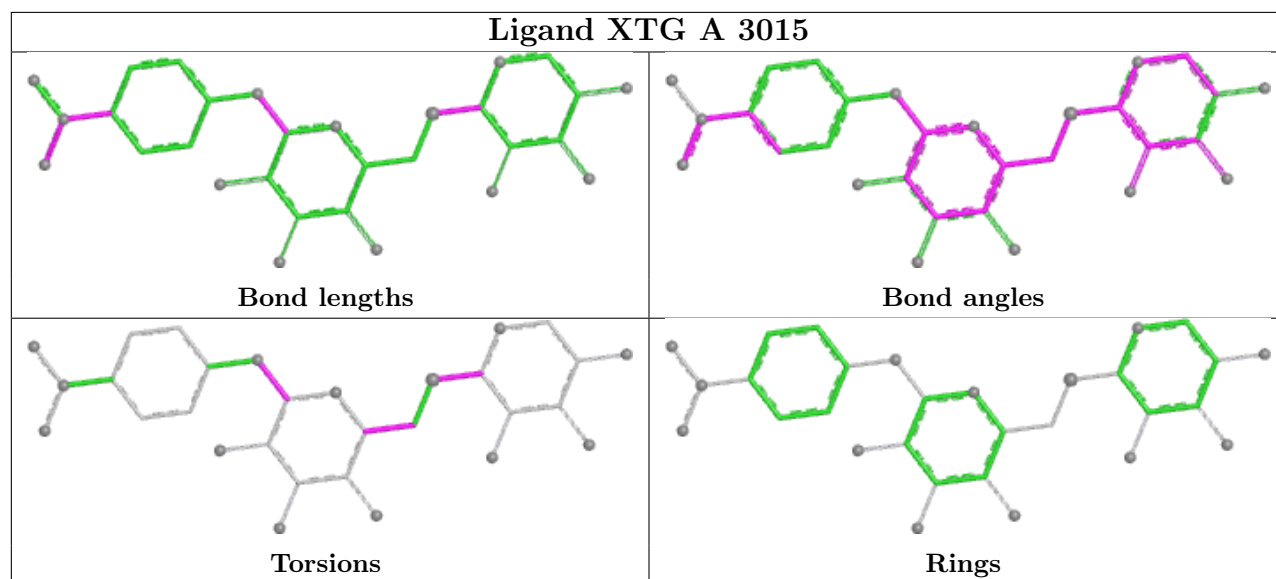
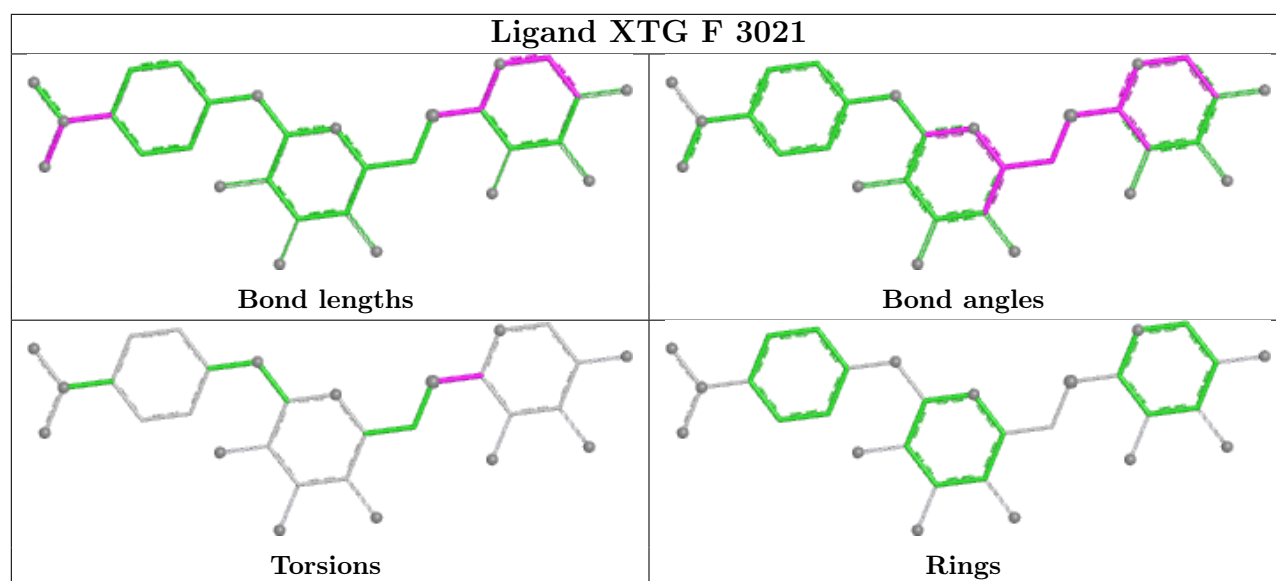
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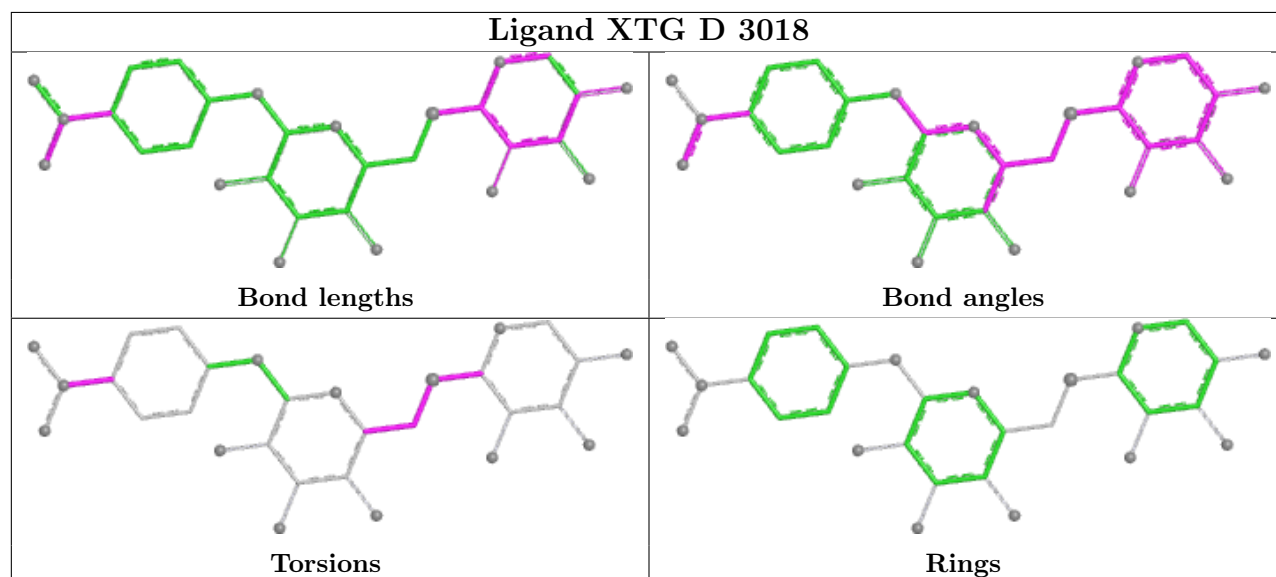
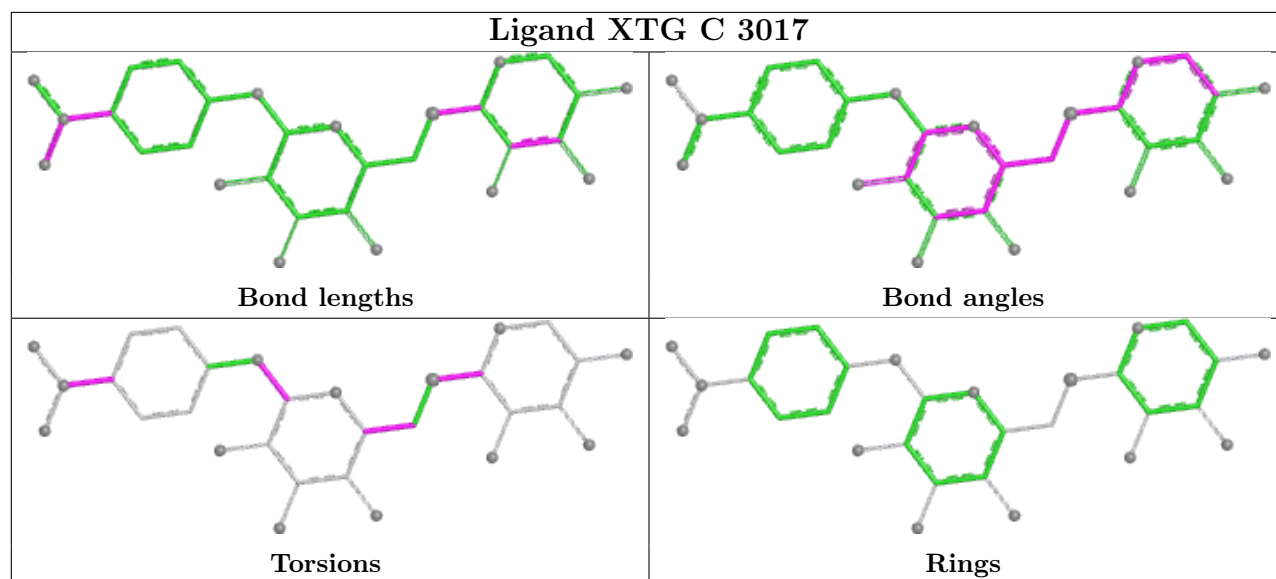
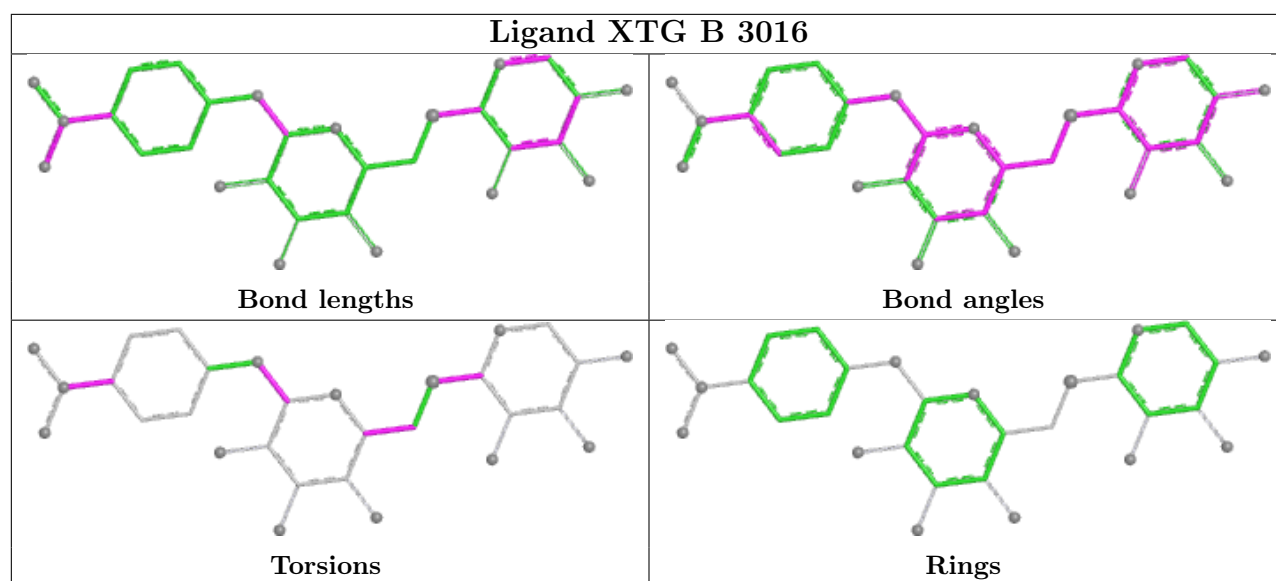
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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | B     | 3016 | XTG  | 1       | 0            |
| 2   | E     | 3004 | SO4  | 1       | 0            |
| 4   | C     | 3023 | GOL  | 1       | 0            |
| 2   | F     | 3001 | SO4  | 2       | 0            |
| 3   | D     | 3018 | XTG  | 6       | 0            |
| 4   | A     | 3024 | GOL  | 1       | 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|------------------|--------|----------------|-----------------------|-------|
| 1   | A     | 773/773 (100%)   | -0.26  | 18 (2%) 61 68  | 8, 14, 35, 53         | 0     |
| 1   | B     | 773/773 (100%)   | -0.05  | 20 (2%) 57 64  | 11, 20, 38, 58        | 0     |
| 1   | C     | 773/773 (100%)   | -0.17  | 11 (1%) 73 79  | 9, 18, 35, 50         | 0     |
| 1   | D     | 773/773 (100%)   | -0.14  | 25 (3%) 50 56  | 8, 17, 41, 55         | 0     |
| 1   | E     | 773/773 (100%)   | 0.01   | 23 (2%) 52 59  | 10, 20, 39, 55        | 0     |
| 1   | F     | 773/773 (100%)   | -0.13  | 22 (2%) 55 62  | 9, 17, 37, 54         | 0     |
| All | All   | 4638/4638 (100%) | -0.12  | 119 (2%) 57 64 | 8, 18, 38, 58         | 0     |

All (119) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 545 | TYR  | 7.8  |
| 1   | B     | 767 | ALA  | 7.2  |
| 1   | A     | 767 | ALA  | 5.8  |
| 1   | E     | 767 | ALA  | 5.8  |
| 1   | A     | 768 | LEU  | 5.0  |
| 1   | E     | 766 | ASN  | 4.8  |
| 1   | B     | 773 | HIS  | 4.8  |
| 1   | B     | 766 | ASN  | 4.4  |
| 1   | F     | 768 | LEU  | 4.3  |
| 1   | A     | 770 | ILE  | 4.2  |
| 1   | D     | 773 | HIS  | 4.1  |
| 1   | A     | 766 | ASN  | 4.1  |
| 1   | C     | 773 | HIS  | 4.1  |
| 1   | B     | 332 | ILE  | 3.8  |
| 1   | D     | 517 | ASN  | 3.8  |
| 1   | A     | 773 | HIS  | 3.8  |
| 1   | F     | 772 | LEU  | 3.7  |
| 1   | E     | 46  | TRP  | 3.7  |
| 1   | F     | 767 | ALA  | 3.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 278 | THR  | 3.6  |
| 1   | D     | 281 | TYR  | 3.6  |
| 1   | B     | 765 | GLY  | 3.5  |
| 1   | F     | 773 | HIS  | 3.5  |
| 1   | D     | 542 | SER  | 3.5  |
| 1   | E     | 773 | HIS  | 3.4  |
| 1   | D     | 277 | PHE  | 3.3  |
| 1   | D     | 544 | SER  | 3.2  |
| 1   | F     | 771 | THR  | 3.2  |
| 1   | F     | 515 | PHE  | 3.2  |
| 1   | D     | 546 | ARG  | 3.2  |
| 1   | D     | 547 | VAL  | 3.1  |
| 1   | E     | 517 | ASN  | 3.1  |
| 1   | D     | 766 | ASN  | 3.1  |
| 1   | E     | 332 | ILE  | 3.1  |
| 1   | E     | 545 | TYR  | 3.0  |
| 1   | A     | 747 | LEU  | 3.0  |
| 1   | A     | 772 | LEU  | 3.0  |
| 1   | C     | 744 | VAL  | 3.0  |
| 1   | C     | 765 | GLY  | 3.0  |
| 1   | E     | 723 | ILE  | 3.0  |
| 1   | F     | 544 | SER  | 2.9  |
| 1   | D     | 515 | PHE  | 2.9  |
| 1   | F     | 770 | ILE  | 2.9  |
| 1   | D     | 100 | TYR  | 2.8  |
| 1   | B     | 764 | GLN  | 2.8  |
| 1   | E     | 768 | LEU  | 2.8  |
| 1   | B     | 517 | ASN  | 2.8  |
| 1   | B     | 323 | LEU  | 2.8  |
| 1   | B     | 772 | LEU  | 2.8  |
| 1   | F     | 719 | THR  | 2.8  |
| 1   | E     | 43  | GLU  | 2.8  |
| 1   | E     | 45  | THR  | 2.8  |
| 1   | D     | 748 | GLN  | 2.7  |
| 1   | E     | 747 | LEU  | 2.7  |
| 1   | E     | 765 | GLY  | 2.7  |
| 1   | F     | 517 | ASN  | 2.7  |
| 1   | D     | 279 | THR  | 2.6  |
| 1   | B     | 545 | TYR  | 2.6  |
| 1   | D     | 543 | LYS  | 2.6  |
| 1   | C     | 542 | SER  | 2.6  |
| 1   | F     | 545 | TYR  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 747 | LEU  | 2.6  |
| 1   | A     | 723 | ILE  | 2.6  |
| 1   | D     | 765 | GLY  | 2.6  |
| 1   | F     | 541 | GLY  | 2.6  |
| 1   | E     | 772 | LEU  | 2.5  |
| 1   | C     | 770 | ILE  | 2.5  |
| 1   | F     | 518 | THR  | 2.5  |
| 1   | D     | 484 | TYR  | 2.5  |
| 1   | E     | 117 | PHE  | 2.5  |
| 1   | D     | 771 | THR  | 2.5  |
| 1   | A     | 744 | VAL  | 2.5  |
| 1   | E     | 547 | VAL  | 2.5  |
| 1   | A     | 720 | GLY  | 2.4  |
| 1   | D     | 723 | ILE  | 2.4  |
| 1   | D     | 278 | THR  | 2.4  |
| 1   | F     | 762 | LYS  | 2.4  |
| 1   | B     | 742 | VAL  | 2.4  |
| 1   | B     | 768 | LEU  | 2.4  |
| 1   | D     | 747 | LEU  | 2.4  |
| 1   | A     | 769 | THR  | 2.4  |
| 1   | B     | 771 | THR  | 2.4  |
| 1   | E     | 518 | THR  | 2.3  |
| 1   | B     | 723 | ILE  | 2.3  |
| 1   | E     | 770 | ILE  | 2.3  |
| 1   | E     | 542 | SER  | 2.3  |
| 1   | F     | 127 | GLU  | 2.2  |
| 1   | F     | 753 | ALA  | 2.2  |
| 1   | D     | 519 | ALA  | 2.2  |
| 1   | B     | 518 | THR  | 2.2  |
| 1   | A     | 748 | GLN  | 2.2  |
| 1   | D     | 289 | PHE  | 2.2  |
| 1   | A     | 280 | ASN  | 2.2  |
| 1   | B     | 280 | ASN  | 2.2  |
| 1   | F     | 540 | HIS  | 2.2  |
| 1   | E     | 544 | SER  | 2.2  |
| 1   | F     | 550 | ALA  | 2.2  |
| 1   | E     | 42  | ARG  | 2.2  |
| 1   | F     | 280 | ASN  | 2.1  |
| 1   | C     | 127 | GLU  | 2.1  |
| 1   | C     | 545 | TYR  | 2.1  |
| 1   | C     | 764 | GLN  | 2.1  |
| 1   | F     | 278 | THR  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 544 | SER  | 2.1  |
| 1   | B     | 759 | LEU  | 2.1  |
| 1   | B     | 763 | PRO  | 2.1  |
| 1   | B     | 744 | VAL  | 2.1  |
| 1   | D     | 280 | ASN  | 2.1  |
| 1   | D     | 753 | ALA  | 2.1  |
| 1   | E     | 748 | GLN  | 2.1  |
| 1   | F     | 542 | SER  | 2.1  |
| 1   | C     | 278 | THR  | 2.1  |
| 1   | E     | 744 | VAL  | 2.1  |
| 1   | A     | 117 | PHE  | 2.0  |
| 1   | A     | 765 | GLY  | 2.0  |
| 1   | C     | 279 | THR  | 2.0  |
| 1   | A     | 545 | TYR  | 2.0  |
| 1   | A     | 745 | ASN  | 2.0  |
| 1   | C     | 766 | ASN  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 5   | MPO  | F     | 3014 | 13/13 | 0.65 | 0.23 | 41,62,71,72                 | 5     |
| 4   | GOL  | E     | 3035 | 6/6   | 0.82 | 0.20 | 54,55,56,56                 | 0     |
| 3   | XTG  | D     | 3018 | 30/30 | 0.82 | 0.16 | 24,45,53,56                 | 0     |
| 4   | GOL  | B     | 3026 | 6/6   | 0.84 | 0.17 | 34,39,40,41                 | 0     |
| 4   | GOL  | C     | 3027 | 6/6   | 0.86 | 0.15 | 41,44,45,45                 | 0     |
| 4   | GOL  | E     | 3033 | 6/6   | 0.86 | 0.12 | 29,34,35,37                 | 0     |
| 4   | GOL  | A     | 3029 | 6/6   | 0.86 | 0.15 | 30,39,39,39                 | 0     |

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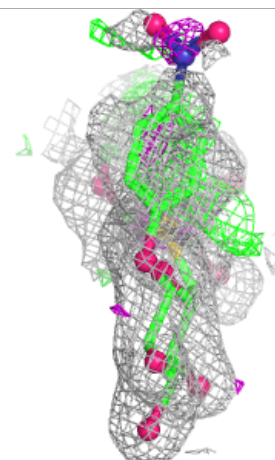
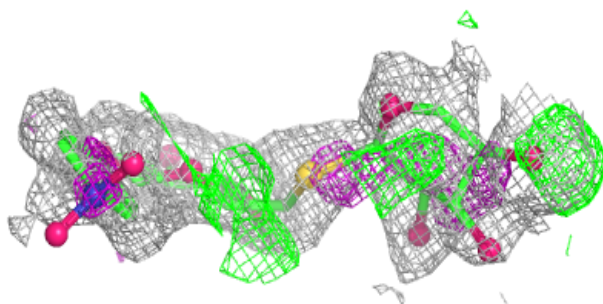
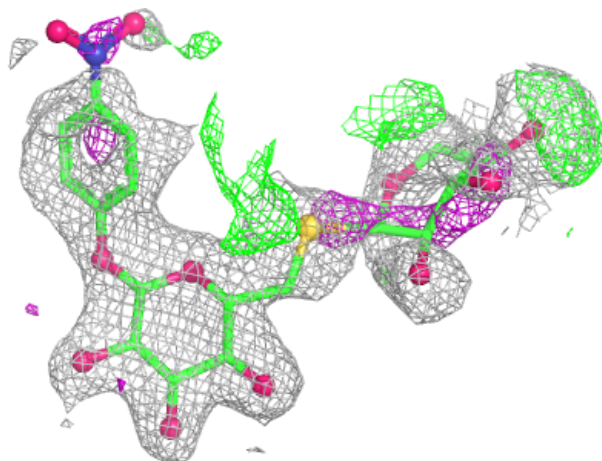
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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 2   | SO4  | E     | 3004 | 5/5   | 0.86 | 0.20 | 45,47,48,49                 | 0     |
| 5   | MPO  | E     | 3013 | 13/13 | 0.87 | 0.16 | 43,49,55,56                 | 0     |
| 2   | SO4  | E     | 3009 | 5/5   | 0.87 | 0.11 | 68,68,69,69                 | 0     |
| 4   | GOL  | A     | 3028 | 6/6   | 0.88 | 0.14 | 29,35,37,39                 | 0     |
| 4   | GOL  | B     | 3025 | 6/6   | 0.89 | 0.10 | 26,31,31,32                 | 0     |
| 2   | SO4  | D     | 3002 | 5/5   | 0.89 | 0.16 | 51,52,53,54                 | 0     |
| 4   | GOL  | F     | 3034 | 6/6   | 0.89 | 0.11 | 32,37,38,38                 | 0     |
| 4   | GOL  | A     | 3024 | 6/6   | 0.89 | 0.12 | 37,40,40,40                 | 0     |
| 4   | GOL  | C     | 3030 | 6/6   | 0.89 | 0.11 | 25,28,30,30                 | 0     |
| 2   | SO4  | F     | 3007 | 5/5   | 0.90 | 0.11 | 48,49,50,50                 | 0     |
| 4   | GOL  | C     | 3023 | 6/6   | 0.90 | 0.11 | 25,29,29,30                 | 0     |
| 2   | SO4  | B     | 3006 | 5/5   | 0.90 | 0.16 | 45,47,49,50                 | 0     |
| 2   | SO4  | F     | 3001 | 5/5   | 0.90 | 0.15 | 37,39,41,44                 | 0     |
| 4   | GOL  | D     | 3031 | 6/6   | 0.90 | 0.10 | 23,28,30,32                 | 0     |
| 4   | GOL  | D     | 3032 | 6/6   | 0.91 | 0.12 | 31,37,40,41                 | 0     |
| 2   | SO4  | A     | 3008 | 5/5   | 0.92 | 0.18 | 45,46,48,49                 | 0     |
| 2   | SO4  | C     | 3005 | 5/5   | 0.93 | 0.15 | 46,48,49,50                 | 0     |
| 5   | MPO  | B     | 3010 | 13/13 | 0.93 | 0.12 | 29,36,43,43                 | 0     |
| 5   | MPO  | C     | 3011 | 13/13 | 0.93 | 0.11 | 29,34,37,38                 | 0     |
| 3   | XTG  | F     | 3020 | 30/30 | 0.93 | 0.10 | 12,38,41,44                 | 0     |
| 3   | XTG  | F     | 3021 | 30/30 | 0.93 | 0.10 | 12,18,54,56                 | 0     |
| 3   | XTG  | E     | 3019 | 30/30 | 0.94 | 0.08 | 17,28,42,47                 | 0     |
| 5   | MPO  | D     | 3012 | 13/13 | 0.95 | 0.10 | 20,34,40,40                 | 0     |
| 4   | GOL  | F     | 3022 | 6/6   | 0.95 | 0.07 | 16,18,20,22                 | 0     |
| 3   | XTG  | B     | 3016 | 30/30 | 0.95 | 0.09 | 12,32,41,44                 | 0     |
| 3   | XTG  | C     | 3017 | 30/30 | 0.96 | 0.08 | 12,26,39,43                 | 0     |
| 3   | XTG  | A     | 3015 | 30/30 | 0.96 | 0.08 | 12,28,37,40                 | 0     |
| 2   | SO4  | F     | 3003 | 5/5   | 0.99 | 0.06 | 14,16,20,20                 | 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.

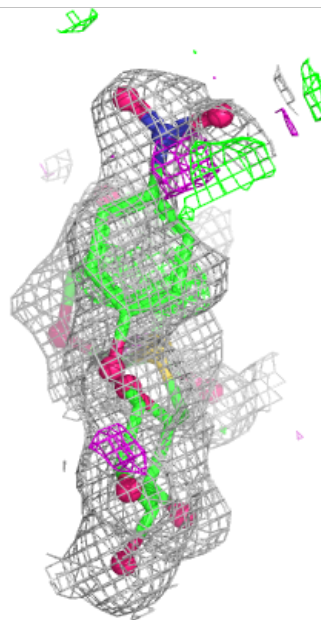
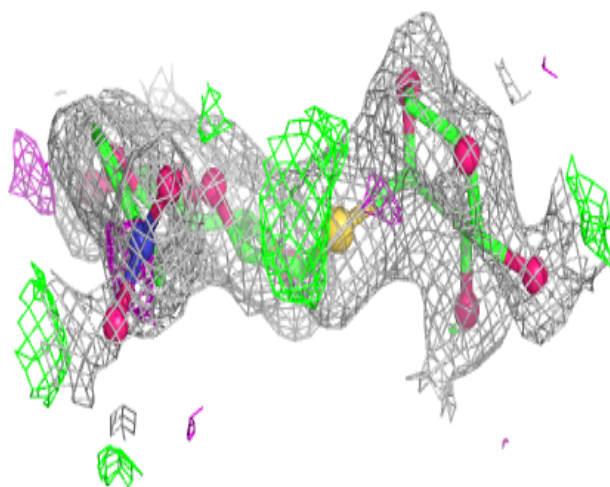
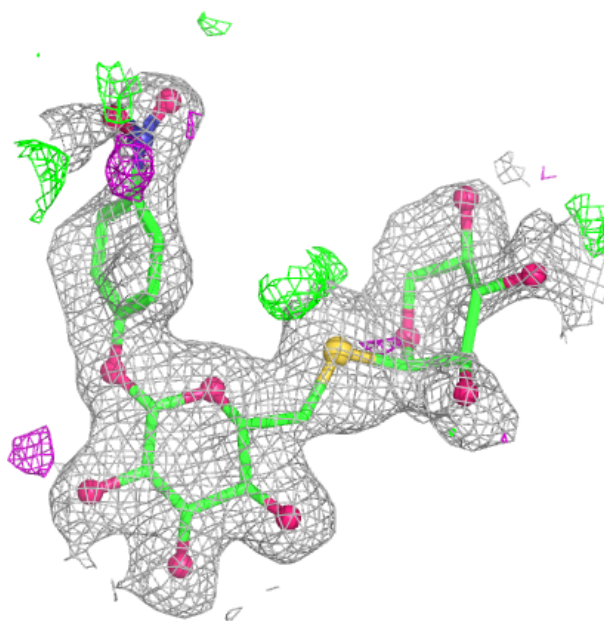
**Electron density around XTG D 3018:**

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



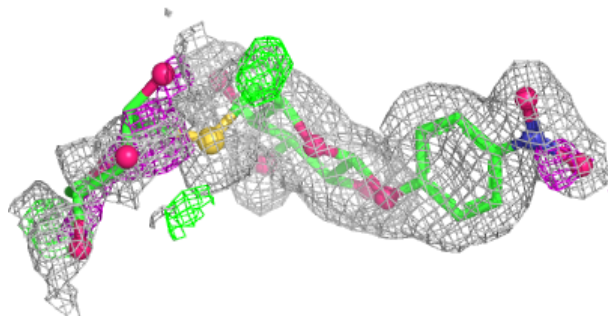
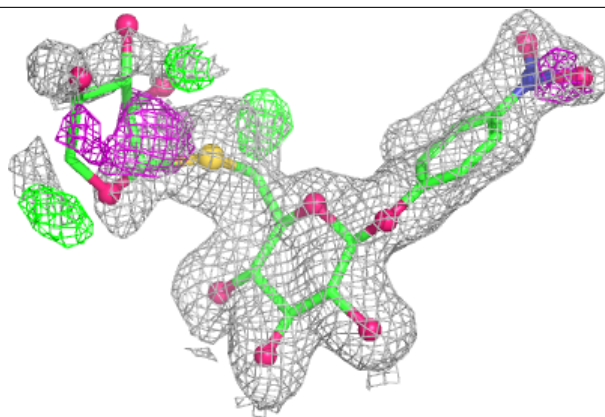
**Electron density around XTG F 3020:**

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



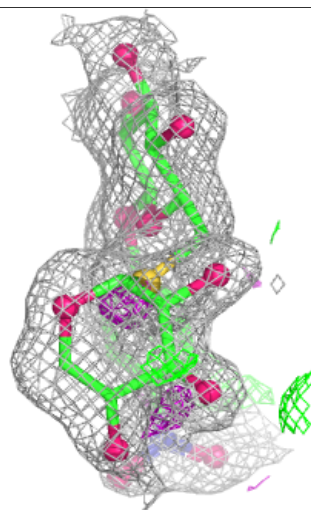
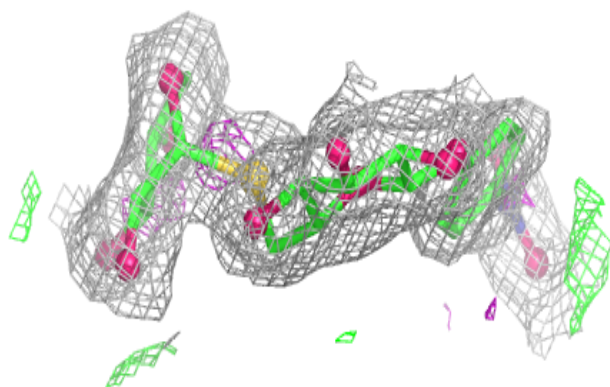
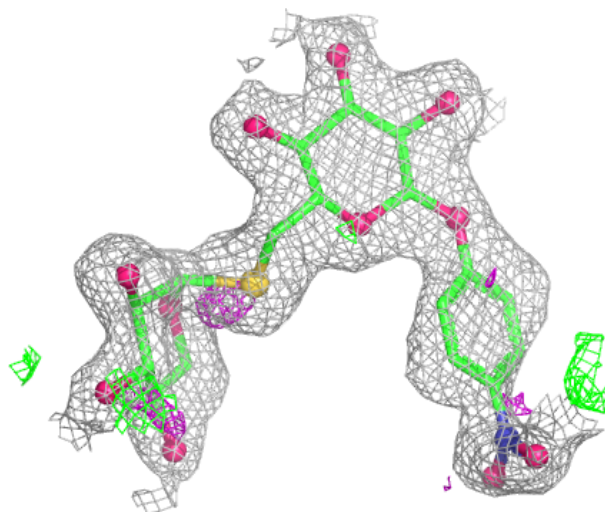
**Electron density around XTG F 3021:**

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



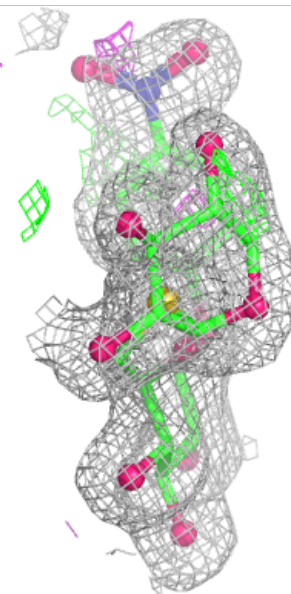
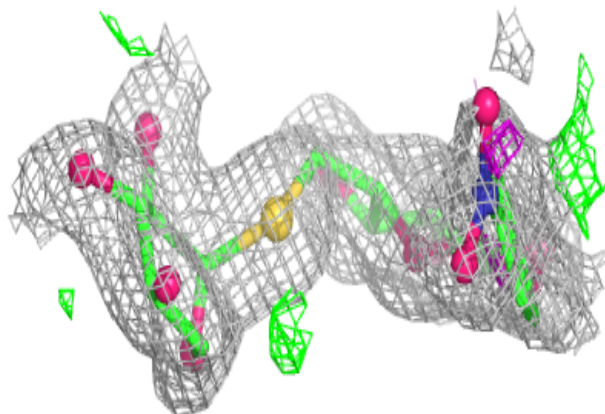
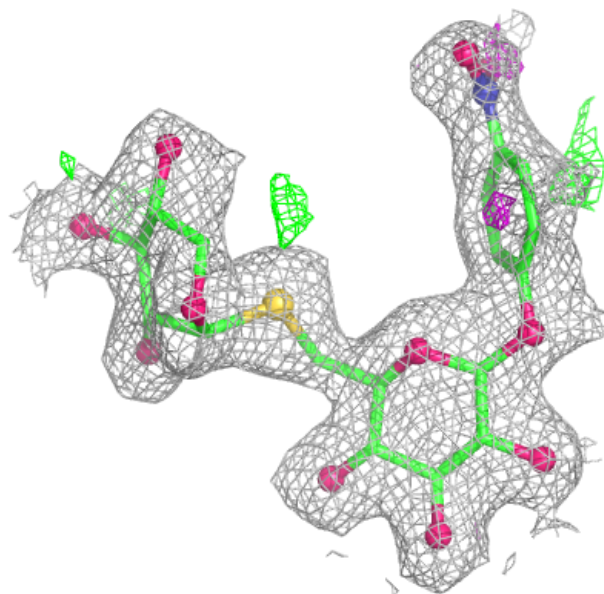
**Electron density around XTG E 3019:**

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



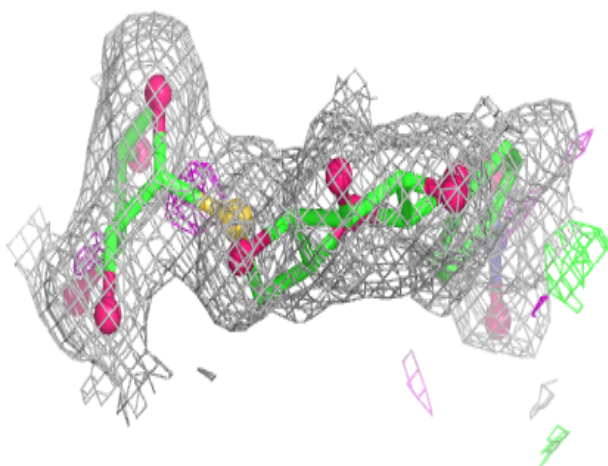
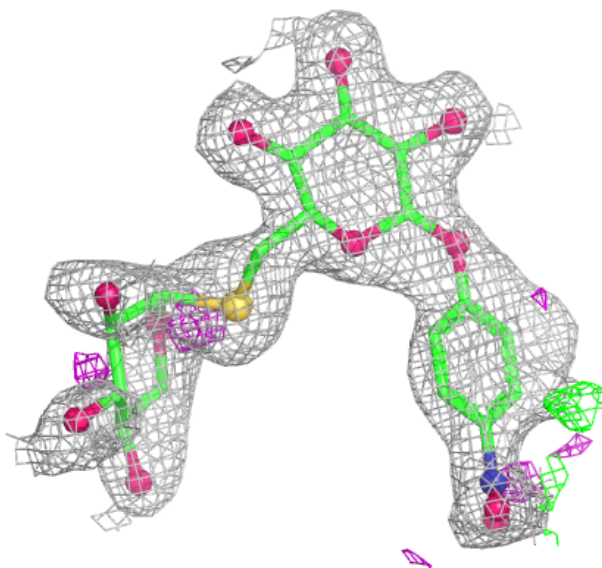
**Electron density around XTG B 3016:**

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



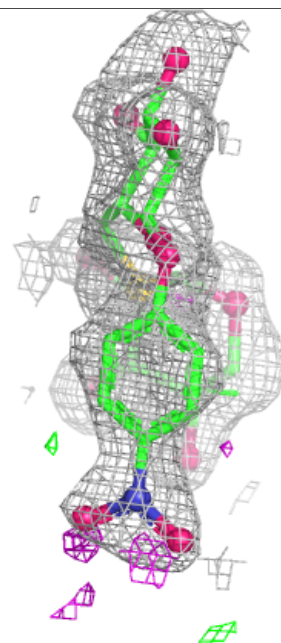
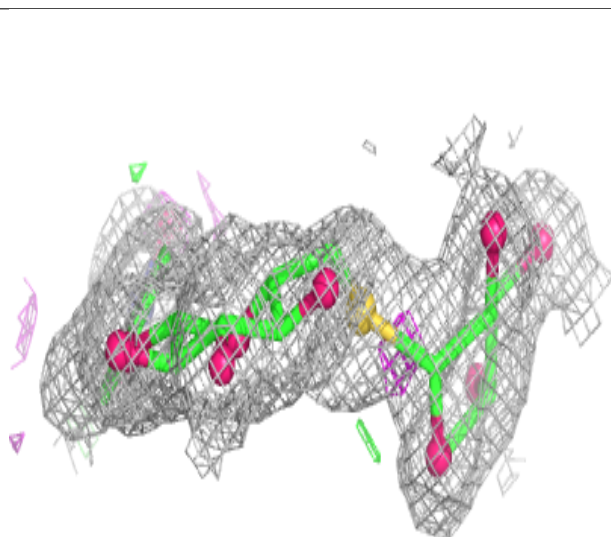
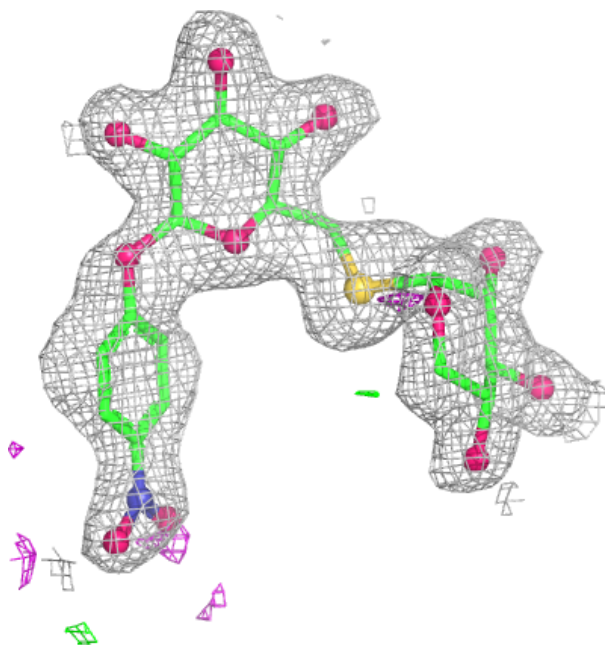
**Electron density around XTG C 3017:**

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



**Electron density around XTG A 3015:**

$2mF_o-DF_c$  (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.