



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 11:58 pm GMT

PDB ID : 1O7A  
Title : Human beta-Hexosaminidase B  
Authors : Maier, T.; Strater, N.; Schuette, C.; Klingenstein, R.; Sandhoff, K.; Saenger, W.  
Deposited on : 2002-10-29  
Resolution : 2.25 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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

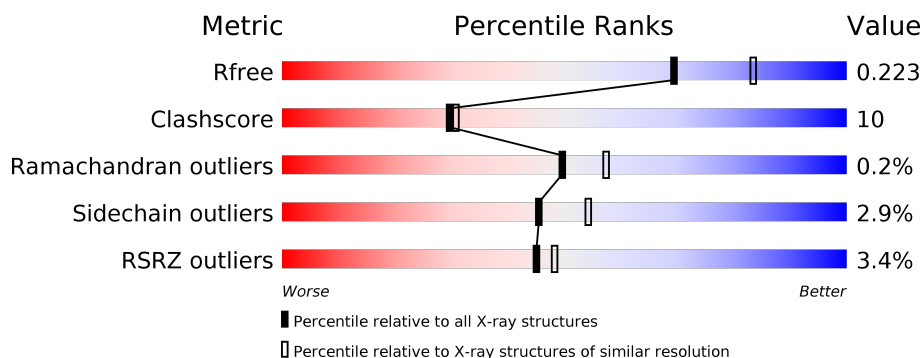
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 111664                      | 1178 (2.26-2.26)                                      |
| Clashscore            | 122126                      | 1286 (2.26-2.26)                                      |
| Ramachandran outliers | 120053                      | 1253 (2.26-2.26)                                      |
| Sidechain outliers    | 120020                      | 1254 (2.26-2.26)                                      |
| RSRZ outliers         | 108989                      | 1158 (2.26-2.26)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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     | 515    | <div> <div>3%</div> <div> <div></div> <div>72%</div> <div>20%</div> <div>6%</div> </div> </div> |
| 1   | B     | 515    | <div> <div>2%</div> <div> <div></div> <div>77%</div> <div>16%</div> <div>6%</div> </div> </div> |
| 1   | C     | 515    | <div> <div>4%</div> <div> <div></div> <div>77%</div> <div>16%</div> <div>6%</div> </div> </div> |
| 1   | D     | 515    | <div> <div>3%</div> <div> <div></div> <div>74%</div> <div>18%</div> <div>6%</div> </div> </div> |
| 1   | E     | 515    | <div> <div>3%</div> <div> <div></div> <div>74%</div> <div>18%</div> <div>6%</div> </div> </div> |
| 1   | F     | 515    | <div> <div>5%</div> <div> <div></div> <div>73%</div> <div>20%</div> <div>6%</div> </div> </div> |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3   | NAG  | A     | 701 | -         | -        | -       | X                |
| 3   | NAG  | B     | 701 | -         | -        | -       | X                |
| 3   | NAG  | C     | 701 | -         | -        | -       | X                |
| 3   | NAG  | C     | 703 | -         | -        | -       | X                |
| 3   | NAG  | D     | 701 | -         | -        | -       | X                |
| 3   | NAG  | E     | 701 | -         | -        | -       | X                |
| 3   | NAG  | E     | 702 | -         | -        | -       | X                |
| 3   | NAG  | F     | 702 | -         | -        | -       | X                |
| 3   | NAG  | F     | 703 | -         | -        | -       | X                |
| 4   | EDO  | B     | 801 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

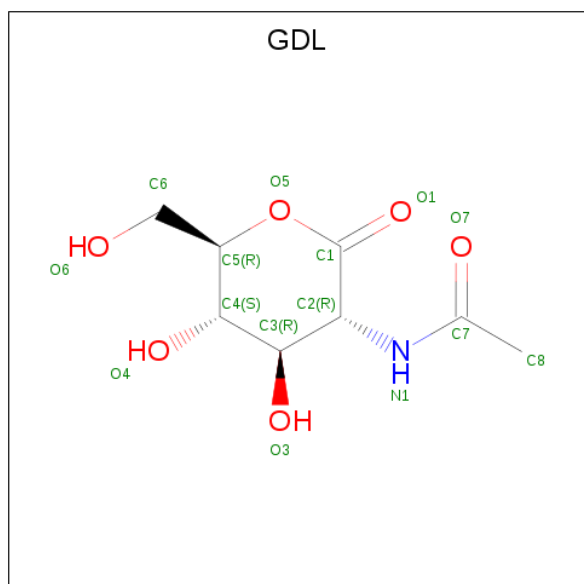
There are 5 unique types of molecules in this entry. The entry contains 26351 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BETA-HEXOSAMINIDASE BETA CHAIN.

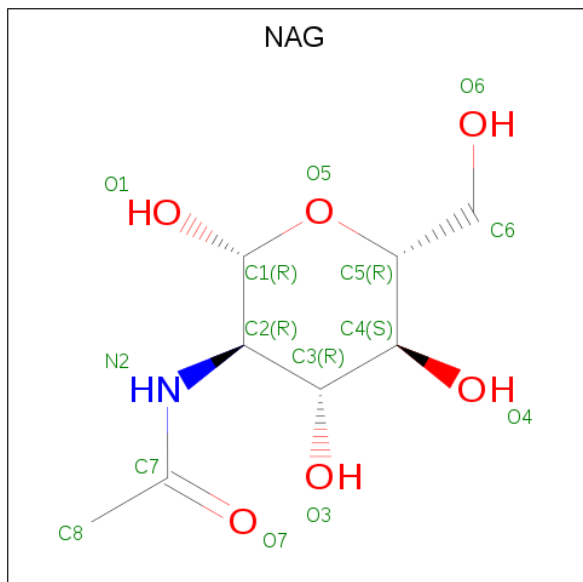
| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 484      | Total | C    | N   | O   | S  | 0       | 4       | 1     |
|     |       |          | 3933  | 2538 | 654 | 725 | 16 |         |         |       |
| 1   | B     | 484      | Total | C    | N   | O   | S  | 0       | 3       | 1     |
|     |       |          | 3927  | 2535 | 653 | 724 | 15 |         |         |       |
| 1   | C     | 484      | Total | C    | N   | O   | S  | 0       | 4       | 1     |
|     |       |          | 3935  | 2538 | 656 | 727 | 14 |         |         |       |
| 1   | D     | 483      | Total | C    | N   | O   | S  | 0       | 6       | 1     |
|     |       |          | 3939  | 2542 | 655 | 726 | 16 |         |         |       |
| 1   | E     | 484      | Total | C    | N   | O   | S  | 0       | 5       | 1     |
|     |       |          | 3941  | 2542 | 655 | 728 | 16 |         |         |       |
| 1   | F     | 484      | Total | C    | N   | O   | S  | 0       | 6       | 1     |
|     |       |          | 3948  | 2546 | 656 | 730 | 16 |         |         |       |

- Molecule 2 is 2-ACETAMIDO-2-DEOXY-D-GLUCONO-1,5-LACTONE (three-letter code: GDL) (formula:  $C_8H_{13}NO_6$ ).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 2   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 15    | 8 | 1 | 6 |         |         |
| 2   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 15    | 8 | 1 | 6 |         |         |
| 2   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 15    | 8 | 1 | 6 |         |         |
| 2   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 15    | 8 | 1 | 6 |         |         |
| 2   | E     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 15    | 8 | 1 | 6 |         |         |
| 2   | F     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 15    | 8 | 1 | 6 |         |         |

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



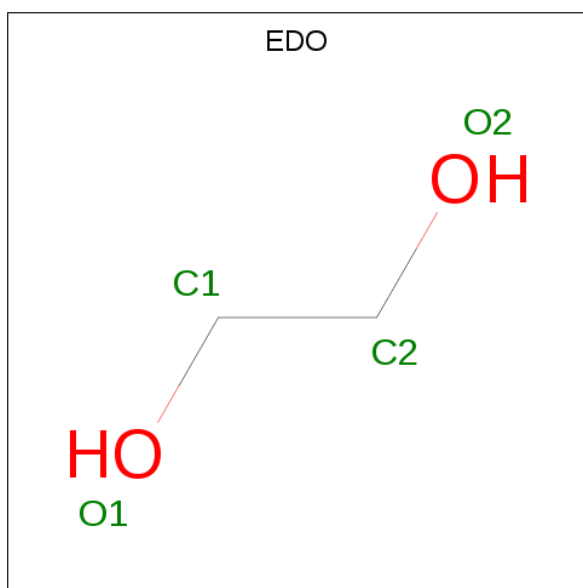
| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 3   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |

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| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 3   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | E     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | E     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | E     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | F     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | F     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | F     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 4   | A     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | A     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | A     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | B     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | B     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | B     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | C     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | C     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | C     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | E     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | E     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | E     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | F     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | F     | 1        | Total C O<br>4 2 2 | 0       | 0       |
| 4   | F     | 1        | Total C O<br>4 2 2 | 0       | 0       |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 5   | A     | 385      | Total O<br>385 385 | 0       | 0       |
| 5   | B     | 399      | Total O<br>399 399 | 0       | 0       |
| 5   | C     | 385      | Total O<br>385 385 | 0       | 0       |
| 5   | D     | 346      | Total O<br>346 346 | 0       | 0       |
| 5   | E     | 448      | Total O<br>448 448 | 0       | 0       |

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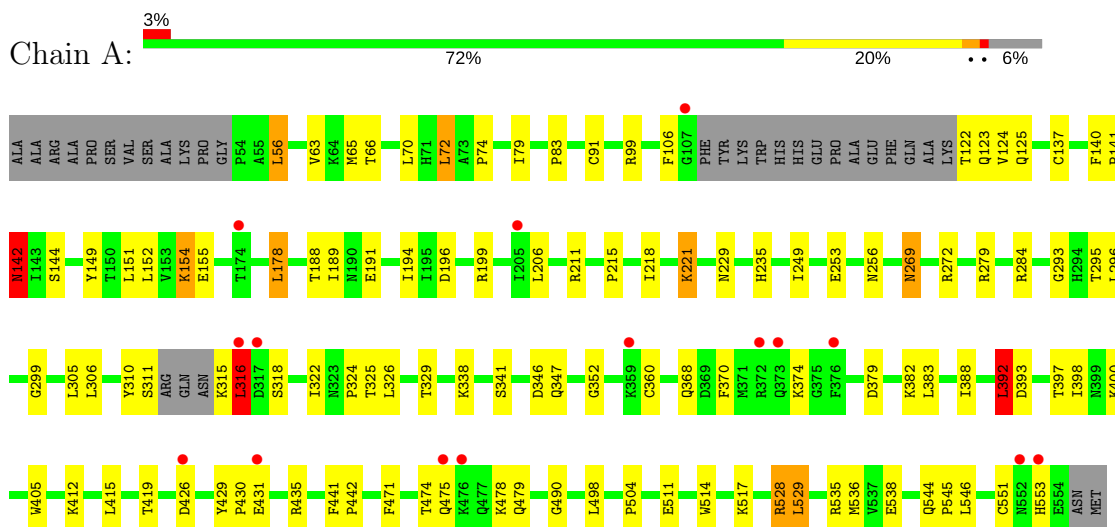
| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 5   | F     | 363      | Total<br>363 | O<br>363 | 0       | 0       |



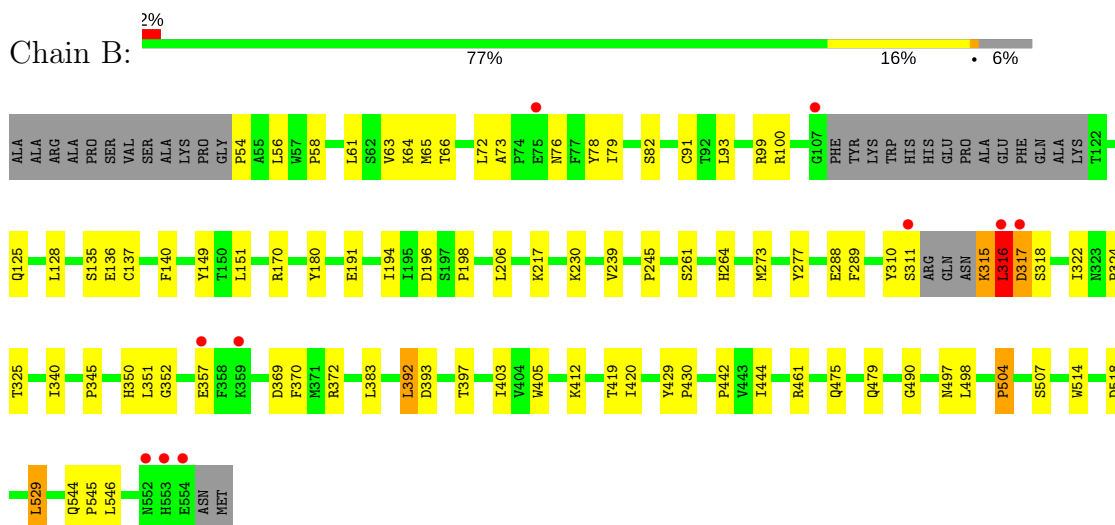
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

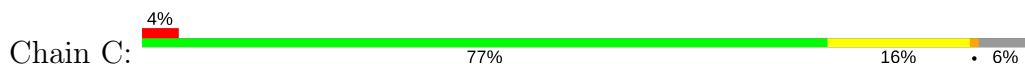
#### • Molecule 1: BETA-HEXOSAMINIDASE BETA CHAIN

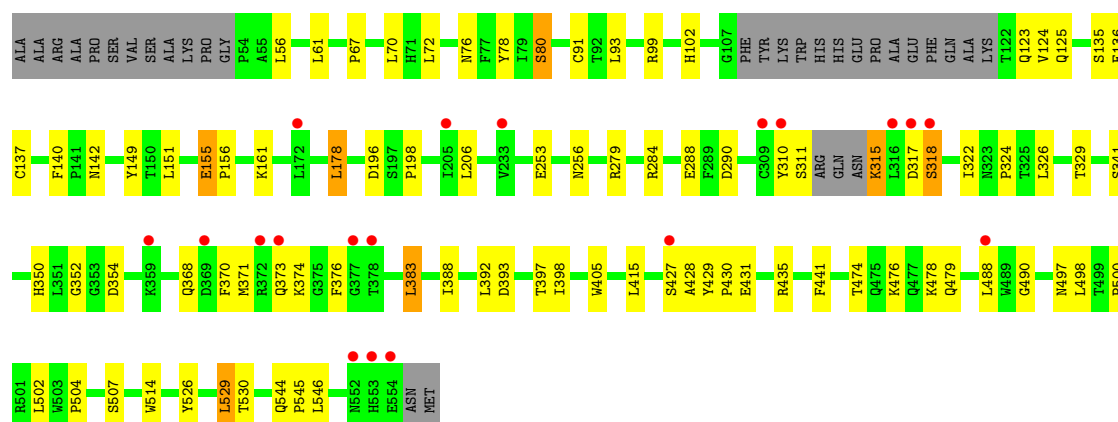


#### • Molecule 1: BETA-HEXOSAMINIDASE BETA CHAIN

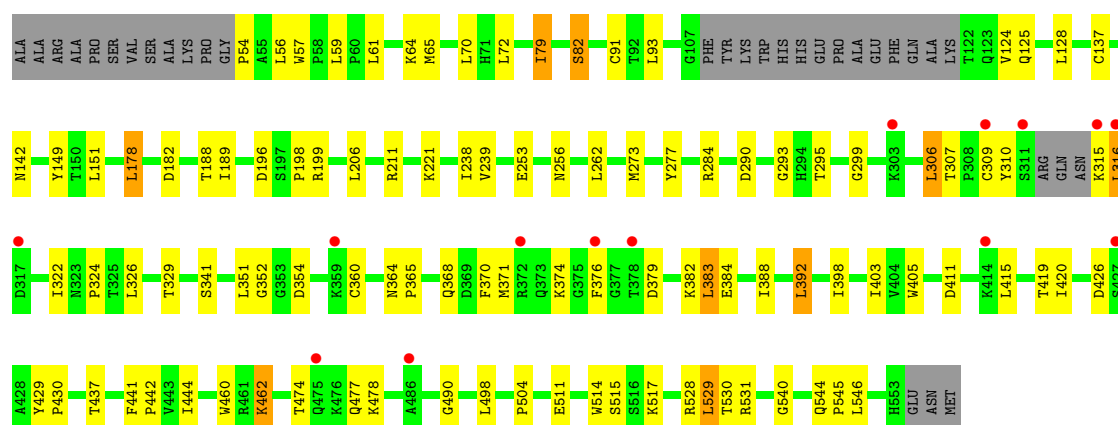


#### • Molecule 1: BETA-HEXOSAMINIDASE BETA CHAIN

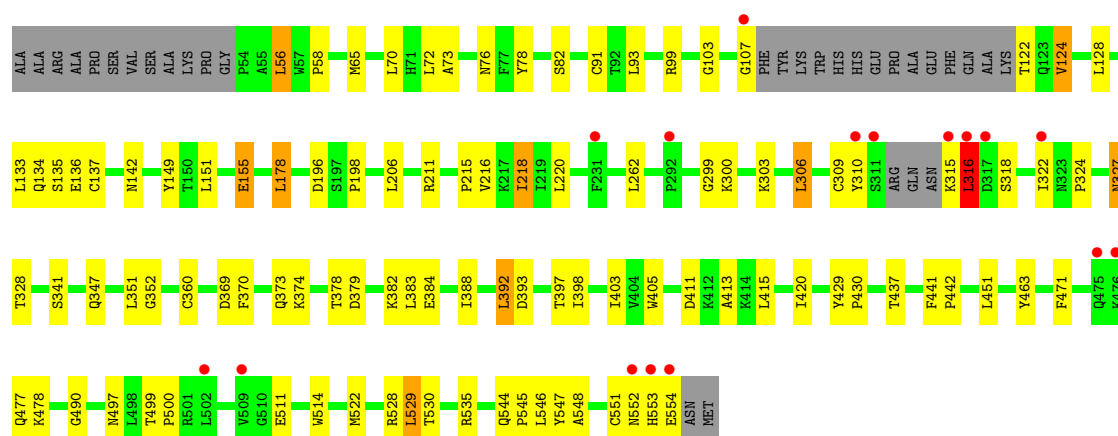
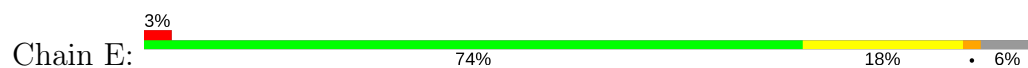




• Molecule 1: BETA-HEXOSAMINIDASE BETA CHAIN

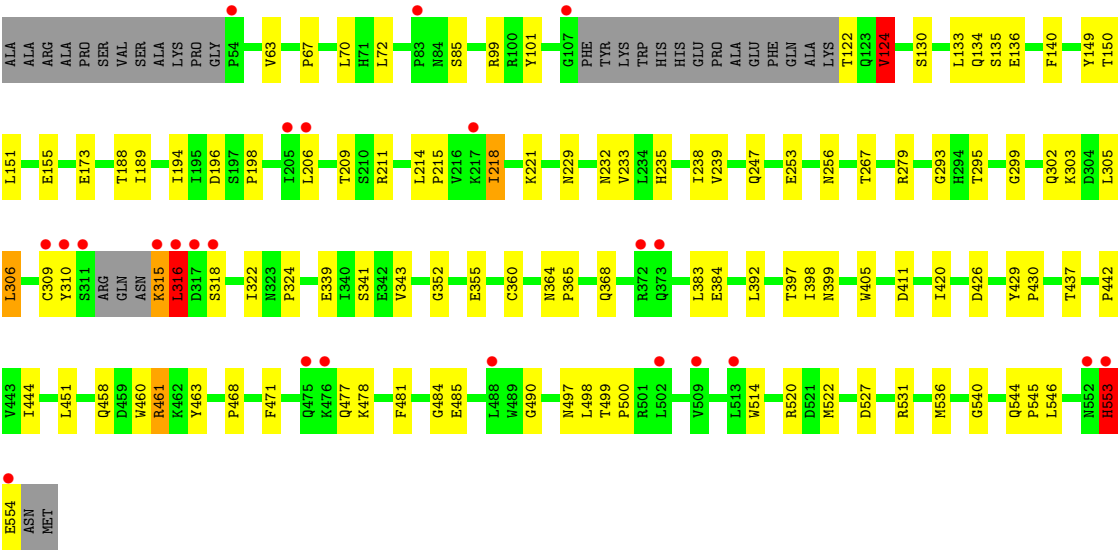


• Molecule 1: BETA-HEXOSAMINIDASE BETA CHAIN



• Molecule 1: BETA-HEXOSAMINIDASE BETA CHAIN





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 31 2 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 163.93Å 163.93Å 244.72Å<br>90.00° 90.00° 120.00°            | Depositor        |
| Resolution (Å)  | 28.12 – 2.25<br>28.12 – 2.25                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.4 (28.12-2.25)<br>97.4 (28.12-2.25)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.07  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 4.84 (at 2.24Å)   | Xtriage          |
| Refinement program  | CNS 1.0   | Depositor        |
| R, $R_{free}$   | 0.196 , 0.236<br>0.187 , 0.223                              | Depositor<br>DCC |
| $R_{free}$ test set   | 1715 reflections (0.98%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 35.3  | Xtriage          |
| Anisotropy  | 0.622   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.33 , 47.2   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$ | Xtriage          |
| Estimated twinning fraction   | 0.004 for -h,-k,l   | Xtriage          |
| $F_o, F_c$ correlation  | 0.96  | EDS              |
| Total number of atoms   | 26351   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 41.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: GDL, NAG, EDO

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$    | RMSZ        | # $ Z  > 5$     |
| 1   | A     | 0.54         | 1/4045 (0.0%)  | 0.73        | 6/5499 (0.1%)   |
| 1   | B     | 0.50         | 0/4039         | 0.71        | 1/5491 (0.0%)   |
| 1   | C     | 0.49         | 0/4047         | 0.68        | 2/5503 (0.0%)   |
| 1   | D     | 0.46         | 0/4050         | 0.69        | 2/5506 (0.0%)   |
| 1   | E     | 0.51         | 0/4053         | 0.72        | 3/5510 (0.1%)   |
| 1   | F     | 0.47         | 0/4060         | 0.70        | 3/5520 (0.1%)   |
| All | All   | 0.50         | 1/24294 (0.0%) | 0.70        | 17/33029 (0.1%) |

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                   |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 142 | ASN  | CG-ND2 | 12.73 | 1.64        | 1.32     |

All (17) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | A     | 142 | ASN  | OD1-CG-ND2 | -11.23 | 96.07       | 121.90   |
| 1   | E     | 155 | GLU  | C-N-CD     | -7.06  | 105.07      | 120.60   |
| 1   | A     | 142 | ASN  | CB-CG-ND2  | 6.98   | 133.45      | 116.70   |
| 1   | F     | 316 | LEU  | CA-CB-CG   | -6.56  | 100.20      | 115.30   |
| 1   | E     | 490 | GLY  | N-CA-C     | 5.88   | 127.81      | 113.10   |
| 1   | A     | 316 | LEU  | N-CA-C     | -5.81  | 95.33       | 111.00   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | F     | 490 | GLY  | N-CA-C    | 5.63  | 127.17      | 113.10   |
| 1   | F     | 124 | VAL  | N-CA-C    | -5.63 | 95.80       | 111.00   |
| 1   | C     | 123 | GLN  | N-CA-C    | 5.47  | 125.78      | 111.00   |
| 1   | A     | 528 | ARG  | NE-CZ-NH2 | -5.46 | 117.57      | 120.30   |
| 1   | A     | 392 | LEU  | CA-CB-CG  | 5.32  | 127.54      | 115.30   |
| 1   | B     | 490 | GLY  | N-CA-C    | 5.25  | 126.22      | 113.10   |
| 1   | A     | 490 | GLY  | N-CA-C    | 5.23  | 126.17      | 113.10   |
| 1   | C     | 490 | GLY  | N-CA-C    | 5.18  | 126.04      | 113.10   |
| 1   | D     | 490 | GLY  | N-CA-C    | 5.11  | 125.87      | 113.10   |
| 1   | D     | 79  | ILE  | N-CA-C    | -5.04 | 97.40       | 111.00   |
| 1   | E     | 535 | ARG  | NE-CZ-NH2 | -5.01 | 117.80      | 120.30   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | A     | 142 | ASN  | Sidechain |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3933  | 0        | 3832     | 91      | 0            |
| 1   | B     | 3927  | 0        | 3828     | 70      | 0            |
| 1   | C     | 3935  | 0        | 3830     | 72      | 0            |
| 1   | D     | 3939  | 0        | 3843     | 86      | 0            |
| 1   | E     | 3941  | 0        | 3835     | 79      | 0            |
| 1   | F     | 3948  | 0        | 3840     | 76      | 0            |
| 2   | A     | 15    | 0        | 13       | 0       | 0            |
| 2   | B     | 15    | 0        | 13       | 0       | 0            |
| 2   | C     | 15    | 0        | 13       | 0       | 0            |
| 2   | D     | 15    | 0        | 13       | 0       | 0            |
| 2   | E     | 15    | 0        | 13       | 0       | 0            |
| 2   | F     | 15    | 0        | 13       | 1       | 0            |
| 3   | A     | 42    | 0        | 38       | 3       | 0            |
| 3   | B     | 42    | 0        | 38       | 4       | 0            |
| 3   | C     | 42    | 0        | 38       | 4       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | D     | 28    | 0        | 25       | 2       | 0            |
| 3   | E     | 42    | 0        | 38       | 2       | 0            |
| 3   | F     | 56    | 0        | 51       | 2       | 0            |
| 4   | A     | 12    | 0        | 18       | 4       | 0            |
| 4   | B     | 12    | 0        | 18       | 4       | 0            |
| 4   | C     | 12    | 0        | 18       | 2       | 0            |
| 4   | E     | 12    | 0        | 18       | 1       | 0            |
| 4   | F     | 12    | 0        | 18       | 1       | 0            |
| 5   | A     | 385   | 0        | 0        | 17      | 0            |
| 5   | B     | 399   | 0        | 0        | 11      | 0            |
| 5   | C     | 385   | 0        | 0        | 11      | 0            |
| 5   | D     | 346   | 0        | 0        | 8       | 0            |
| 5   | E     | 448   | 0        | 0        | 14      | 0            |
| 5   | F     | 363   | 0        | 0        | 11      | 0            |
| All | All   | 26351 | 0        | 23404    | 480     | 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 10.

All (480) 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:D:56:LEU:HD21  | 1:D:178:LEU:HD13 | 1.51                     | 0.93              |
| 1:C:488:LEU:HD23 | 1:C:502:LEU:HD13 | 1.51                     | 0.92              |
| 1:C:393:ASP:O    | 1:C:397:THR:HG23 | 1.70                     | 0.92              |
| 1:C:488:LEU:HD12 | 1:C:488:LEU:O    | 1.74                     | 0.87              |
| 1:F:553:HIS:ND1  | 1:F:554:GLU:N    | 2.22                     | 0.86              |
| 1:A:63:VAL:HG22  | 1:A:194:ILE:HD12 | 1.58                     | 0.85              |
| 1:E:315:LYS:HG2  | 1:E:316:LEU:H    | 1.40                     | 0.84              |
| 1:D:56:LEU:HD21  | 1:D:178:LEU:CD1  | 2.06                     | 0.84              |
| 1:E:56:LEU:HD11  | 1:E:178:LEU:HD13 | 1.60                     | 0.84              |
| 1:D:371:MET:HE3  | 1:D:383:LEU:HG   | 1.59                     | 0.84              |
| 1:F:303:LYS:HA   | 1:F:303:LYS:HE2  | 1.60                     | 0.83              |
| 1:E:315:LYS:N    | 5:E:2243:HOH:O   | 2.11                     | 0.83              |
| 1:C:125:GLN:NE2  | 1:C:156:PRO:HB2  | 1.93                     | 0.83              |
| 1:A:310:TYR:CE1  | 1:A:315:LYS:HG2  | 2.15                     | 0.82              |
| 1:B:316:LEU:HD13 | 1:B:318:SER:HB3  | 1.62                     | 0.82              |
| 1:E:553:HIS:ND1  | 1:E:554:GLU:N    | 2.28                     | 0.81              |
| 1:C:56:LEU:HD11  | 1:C:178:LEU:HD13 | 1.60                     | 0.81              |
| 1:C:125:GLN:HE21 | 1:C:156:PRO:HB2  | 1.46                     | 0.81              |
| 1:D:315:LYS:HG2  | 5:D:2201:HOH:O   | 1.81                     | 0.79              |

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| Atom-1          | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|--------------------|--------------------------|-------------------|
| 1:E:122:THR:N   | 5:E:2057:HOH:O     | 2.15                     | 0.78              |
| 1:E:347:GLN:HB2 | 5:E:2082:HOH:O     | 1.83                     | 0.78              |
| 1:E:300:LYS:HA  | 1:E:300:LYS:HE2    | 1.66                     | 0.77              |
| 3:F:701:NAG:H82 | 5:F:2360:HOH:O     | 1.85                     | 0.77              |
| 1:C:371:MET:HE2 | 1:C:376:PHE:HD1    | 1.49                     | 0.76              |
| 1:F:99:ARG:NH1  | 5:F:2044:HOH:O     | 2.17                     | 0.76              |
| 1:F:315:LYS:O   | 1:F:316:LEU:HB2    | 1.86                     | 0.75              |
| 1:B:78:TYR:CE2  | 1:D:262:LEU:HD11   | 2.22                     | 0.74              |
| 3:A:700:NAG:H62 | 3:A:701:NAG:HN2    | 1.51                     | 0.74              |
| 1:D:309:CYS:O   | 1:D:316:LEU:HB2    | 1.87                     | 0.74              |
| 1:F:458:GLN:O   | 1:F:461:ARG:HG2    | 1.89                     | 0.73              |
| 1:C:488:LEU:CD2 | 1:C:502:LEU:HD13   | 2.18                     | 0.73              |
| 1:B:170:ARG:HD2 | 1:B:230:LYS:HD2    | 1.71                     | 0.72              |
| 1:E:56:LEU:HD11 | 1:E:178:LEU:CD1    | 2.19                     | 0.72              |
| 1:A:310:TYR:HE1 | 1:A:315:LYS:HG2    | 1.53                     | 0.72              |
| 1:A:310:TYR:CD1 | 1:A:315:LYS:HA     | 2.25                     | 0.71              |
| 1:C:91:CYS:SG   | 1:C:137[B]:CYS:HB2 | 2.31                     | 0.71              |
| 1:A:431:GLU:HG2 | 1:A:435:ARG:NH1    | 2.05                     | 0.70              |
| 1:A:346:ASP:O   | 1:A:400:LYS:HE3    | 1.91                     | 0.70              |
| 1:D:299:GLY:HA3 | 1:D:306:LEU:HD22   | 1.73                     | 0.70              |
| 1:A:91:CYS:SG   | 1:A:137[B]:CYS:HB2 | 2.31                     | 0.69              |
| 1:F:437:THR:HB  | 1:F:477:GLN:HG2    | 1.74                     | 0.69              |
| 1:E:99:ARG:NH2  | 5:E:2038:HOH:O     | 2.23                     | 0.69              |
| 1:E:315:LYS:HG2 | 1:E:316:LEU:N      | 2.07                     | 0.69              |
| 1:A:341:SER:HB3 | 1:A:398:ILE:HD12   | 1.74                     | 0.69              |
| 1:A:56:LEU:HD11 | 1:A:178:LEU:HD13   | 1.75                     | 0.68              |
| 1:E:299:GLY:HA3 | 1:E:306:LEU:HD22   | 1.75                     | 0.68              |
| 1:B:315:LYS:O   | 1:B:316:LEU:HB2    | 1.93                     | 0.68              |
| 1:C:371:MET:HE3 | 1:C:383:LEU:HB2    | 1.75                     | 0.67              |
| 1:F:67:PRO:O    | 3:F:700:NAG:H61    | 1.94                     | 0.67              |
| 1:E:310:TYR:CE2 | 1:E:315:LYS:HA     | 2.30                     | 0.67              |
| 1:C:371:MET:HE2 | 1:C:376:PHE:CD1    | 2.29                     | 0.66              |
| 1:E:478:LYS:HE2 | 5:E:2380:HOH:O     | 1.95                     | 0.66              |
| 1:C:317:ASP:O   | 1:C:318:SER:HB2    | 1.95                     | 0.66              |
| 1:D:379:ASP:OD2 | 1:D:382:LYS:HG3    | 1.94                     | 0.65              |
| 1:C:102:HIS:ND1 | 5:C:2048:HOH:O     | 2.29                     | 0.65              |
| 1:D:310:TYR:HD2 | 1:D:315:LYS:HA     | 1.62                     | 0.64              |
| 1:E:91:CYS:SG   | 1:E:137[B]:CYS:HB2 | 2.37                     | 0.64              |
| 1:B:79:ILE:H    | 4:B:801:EDO:C1     | 2.11                     | 0.64              |
| 1:A:99:ARG:HD3  | 5:C:2181:HOH:O     | 1.98                     | 0.64              |
| 1:C:67:PRO:O    | 3:C:700:NAG:H61    | 1.98                     | 0.64              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:F:316:LEU:HD23   | 1:F:318:SER:OG      | 1.97                     | 0.64              |
| 1:F:315:LYS:HD2    | 5:F:2111:HOH:O      | 1.98                     | 0.63              |
| 1:E:478:LYS:HE3    | 5:E:2372:HOH:O      | 1.98                     | 0.63              |
| 1:F:520:ARG:O      | 1:F:522:MET:HE3     | 1.98                     | 0.63              |
| 1:E:529:LEU:HB3    | 1:E:546:LEU:HD11    | 1.80                     | 0.63              |
| 3:B:700:NAG:H61    | 3:B:701:NAG:HN2     | 1.64                     | 0.63              |
| 1:D:529:LEU:HB3    | 1:D:546[A]:LEU:HD11 | 1.79                     | 0.63              |
| 1:F:229:ASN:HD21   | 1:F:536:MET:CE      | 2.12                     | 0.63              |
| 1:D:221:LYS:HE2    | 5:D:2122:HOH:O      | 2.00                     | 0.62              |
| 1:C:317:ASP:O      | 1:C:318:SER:CB      | 2.46                     | 0.62              |
| 1:B:91:CYS:SG      | 1:B:137[B]:CYS:HB2  | 2.38                     | 0.62              |
| 1:A:72:LEU:N       | 1:A:72:LEU:HD12     | 2.14                     | 0.62              |
| 1:D:310:TYR:CD2    | 1:D:315:LYS:HA      | 2.34                     | 0.62              |
| 4:C:801:EDO:H12    | 1:D:79:ILE:H        | 1.64                     | 0.61              |
| 1:A:360[B]:CYS:HB3 | 5:A:2261:HOH:O      | 1.99                     | 0.61              |
| 1:C:206:LEU:O      | 1:C:488:LEU:HG      | 2.00                     | 0.61              |
| 1:C:529:LEU:HB3    | 1:C:546:LEU:HD11    | 1.83                     | 0.61              |
| 1:A:551:CYS:HB3    | 1:A:553:HIS:HD2     | 1.66                     | 0.61              |
| 1:D:315:LYS:N      | 5:D:2201:HOH:O      | 2.34                     | 0.61              |
| 1:A:152:LEU:CD2    | 1:A:154:LYS:HE2     | 2.31                     | 0.60              |
| 1:F:299:GLY:HA3    | 1:F:306:LEU:HD22    | 1.83                     | 0.60              |
| 1:F:497:ASN:HB2    | 5:F:2322:HOH:O      | 2.01                     | 0.60              |
| 1:F:341:SER:HB3    | 1:F:398:ILE:HD12    | 1.84                     | 0.60              |
| 1:D:368:GLN:NE2    | 1:D:368:GLN:HA      | 2.16                     | 0.60              |
| 1:D:65:MET:HG2     | 3:D:700:NAG:C7      | 2.31                     | 0.60              |
| 1:D:511:GLU:OE2    | 1:D:528:ARG:NH2     | 2.34                     | 0.60              |
| 1:D:529:LEU:HB3    | 1:D:546[B]:LEU:HD21 | 1.83                     | 0.60              |
| 1:D:273[A]:MET:HE2 | 1:D:277:TYR:HB2     | 1.84                     | 0.60              |
| 1:C:125:GLN:HB2    | 5:C:2064:HOH:O      | 2.01                     | 0.60              |
| 1:A:347:GLN:HB2    | 5:A:2077:HOH:O      | 2.01                     | 0.60              |
| 1:A:475:GLN:O      | 1:A:479:GLN:HG3     | 2.02                     | 0.60              |
| 1:A:511:GLU:OE2    | 1:A:528:ARG:NH2     | 2.35                     | 0.60              |
| 1:A:65:MET:HE2     | 3:A:700:NAG:C7      | 2.32                     | 0.59              |
| 1:D:371:MET:CE     | 1:D:376:PHE:HD1     | 2.14                     | 0.59              |
| 1:A:529:LEU:HB3    | 1:A:546:LEU:HD11    | 1.84                     | 0.59              |
| 1:C:125:GLN:HE21   | 1:C:156:PRO:CB      | 2.13                     | 0.59              |
| 1:F:303:LYS:CA     | 1:F:303:LYS:HE2     | 2.33                     | 0.59              |
| 1:B:79:ILE:H       | 4:B:801:EDO:H12     | 1.66                     | 0.59              |
| 1:A:66:THR:OG1     | 1:A:191:GLU:HB3     | 2.03                     | 0.59              |
| 1:D:142:ASN:HB3    | 5:D:2062:HOH:O      | 2.02                     | 0.59              |
| 1:A:400:LYS:HE2    | 5:A:2249:HOH:O      | 2.03                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:E:215:PRO:O      | 1:E:218:ILE:HG22   | 2.03                     | 0.59              |
| 1:D:91:CYS:SG      | 1:D:137[B]:CYS:HB2 | 2.43                     | 0.58              |
| 1:E:316:LEU:C      | 1:E:318:SER:H      | 2.06                     | 0.58              |
| 1:F:215:PRO:O      | 1:F:218:ILE:HG22   | 2.03                     | 0.58              |
| 1:A:310:TYR:C      | 1:A:316:LEU:HD12   | 2.23                     | 0.58              |
| 1:A:125:GLN:HB2    | 5:A:2051:HOH:O     | 2.04                     | 0.58              |
| 1:B:100:ARG:HD3    | 5:B:2048:HOH:O     | 2.03                     | 0.58              |
| 1:A:311:SER:N      | 1:A:316:LEU:HD12   | 2.19                     | 0.57              |
| 1:F:310:TYR:CD1    | 1:F:315:LYS:N      | 2.72                     | 0.57              |
| 1:B:412:LYS:HA     | 1:B:412:LYS:HE2    | 1.85                     | 0.57              |
| 1:A:529:LEU:HD13   | 1:A:546:LEU:HD21   | 1.86                     | 0.57              |
| 1:F:63:VAL:HG22    | 1:F:194:ILE:HD12   | 1.86                     | 0.57              |
| 1:A:122:THR:HG22   | 1:A:123:GLN:H      | 1.69                     | 0.57              |
| 1:B:322:ILE:O      | 1:B:324:PRO:HD3    | 2.05                     | 0.57              |
| 1:B:351:LEU:HD12   | 1:B:392:LEU:HD13   | 1.85                     | 0.57              |
| 4:B:801:EDO:O1     | 1:D:262:LEU:HD13   | 2.04                     | 0.57              |
| 1:E:198:PRO:HB3    | 1:E:514:TRP:CE3    | 2.40                     | 0.57              |
| 1:B:206:LEU:C      | 1:B:206:LEU:HD23   | 2.25                     | 0.57              |
| 1:F:527[A]:ASP:OD2 | 1:F:531:ARG:NH1    | 2.37                     | 0.57              |
| 1:F:498:LEU:HD23   | 1:F:498:LEU:C      | 2.26                     | 0.57              |
| 1:A:56:LEU:HD11    | 1:A:178:LEU:CD1    | 2.34                     | 0.56              |
| 1:C:125:GLN:HG2    | 1:C:156:PRO:O      | 2.05                     | 0.56              |
| 1:C:310:TYR:HD2    | 1:C:315:LYS:HB3    | 1.69                     | 0.56              |
| 1:A:310:TYR:HD1    | 1:A:315:LYS:HA     | 1.70                     | 0.56              |
| 1:B:72:LEU:HD12    | 1:B:72:LEU:N       | 2.20                     | 0.56              |
| 3:C:700:NAG:H62    | 3:C:701:NAG:HN2    | 1.69                     | 0.56              |
| 1:E:370:PHE:CZ     | 1:E:374:LYS:HE3    | 2.39                     | 0.56              |
| 1:D:420:ILE:HG21   | 1:D:444:ILE:HD12   | 1.86                     | 0.56              |
| 1:D:474:THR:O      | 1:D:478:LYS:HG2    | 2.06                     | 0.56              |
| 1:F:444:ILE:HG23   | 1:F:484:GLY:HA2    | 1.88                     | 0.56              |
| 1:B:529:LEU:HB3    | 1:B:546:LEU:HD11   | 1.87                     | 0.56              |
| 1:F:399:ASN:ND2    | 5:F:2248:HOH:O     | 2.38                     | 0.56              |
| 1:F:352:GLY:HA2    | 1:F:405:TRP:CD1    | 2.41                     | 0.56              |
| 1:F:451:LEU:HD22   | 1:F:463:TYR:CE2    | 2.41                     | 0.56              |
| 1:A:379:ASP:OD2    | 1:A:382:LYS:HG3    | 2.06                     | 0.56              |
| 1:D:125:GLN:HB2    | 5:D:2046:HOH:O     | 2.06                     | 0.56              |
| 1:E:315:LYS:CG     | 1:E:316:LEU:H      | 2.14                     | 0.56              |
| 1:C:488:LEU:CD1    | 5:C:2134:HOH:O     | 2.52                     | 0.56              |
| 1:A:299:GLY:HA3    | 1:A:306:LEU:HD22   | 1.89                     | 0.55              |
| 1:D:307:THR:HG22   | 1:D:360[B]:CYS:SG  | 2.47                     | 0.55              |
| 1:D:415:LEU:HB2    | 1:D:441:PHE:CZ     | 2.40                     | 0.55              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:A:316:LEU:HD22   | 1:A:318:SER:HB3  | 1.87                     | 0.55              |
| 1:C:488:LEU:HD23   | 1:C:502:LEU:CD1  | 2.30                     | 0.55              |
| 1:B:125:GLN:HB3    | 5:B:2061:HOH:O   | 2.06                     | 0.55              |
| 1:D:61:LEU:HD23    | 1:D:61:LEU:C     | 2.27                     | 0.55              |
| 1:A:284:ARG:HD3    | 5:A:2202:HOH:O   | 2.05                     | 0.55              |
| 1:B:310:TYR:O      | 1:B:311:SER:HB2  | 2.05                     | 0.55              |
| 1:E:72:LEU:HG      | 1:E:124:VAL:HG13 | 1.88                     | 0.55              |
| 1:F:238:ILE:HG23   | 1:F:239:VAL:HG13 | 1.87                     | 0.54              |
| 1:C:371:MET:CE     | 1:C:376:PHE:HD1  | 2.20                     | 0.54              |
| 1:F:499:THR:HB     | 1:F:500:PRO:HD3  | 1.89                     | 0.54              |
| 1:E:70:LEU:HD22    | 1:E:155:GLU:HB3  | 1.90                     | 0.54              |
| 1:B:273[B]:MET:HE2 | 1:B:277:TYR:HB2  | 1.90                     | 0.54              |
| 1:D:419:THR:O      | 1:D:442:PRO:HD2  | 2.07                     | 0.54              |
| 1:B:429:TYR:N      | 1:B:430:PRO:CD   | 2.70                     | 0.54              |
| 1:B:461:ARG:NH2    | 5:B:2329:HOH:O   | 2.40                     | 0.54              |
| 1:C:488:LEU:HD12   | 5:C:2134:HOH:O   | 2.07                     | 0.54              |
| 1:E:499:THR:HB     | 1:E:500:PRO:HD3  | 1.90                     | 0.54              |
| 1:D:72:LEU:HD12    | 1:D:72:LEU:N     | 2.24                     | 0.53              |
| 1:E:216:VAL:O      | 1:E:220:LEU:HG   | 2.09                     | 0.53              |
| 1:F:364:ASN:O      | 1:F:368:GLN:HG2  | 2.08                     | 0.53              |
| 1:F:72:LEU:HD12    | 1:F:72:LEU:N     | 2.23                     | 0.53              |
| 1:C:370:PHE:CZ     | 1:C:374:LYS:HE3  | 2.44                     | 0.53              |
| 1:E:378:THR:HA     | 5:E:2297:HOH:O   | 2.08                     | 0.53              |
| 1:F:471:PHE:O      | 1:F:478:LYS:HE2  | 2.09                     | 0.53              |
| 1:B:544:GLN:HB2    | 1:B:545:PRO:HD2  | 1.91                     | 0.53              |
| 1:B:99:ARG:HD3     | 5:B:2043:HOH:O   | 2.09                     | 0.53              |
| 1:B:315:LYS:O      | 1:B:316:LEU:CB   | 2.56                     | 0.52              |
| 1:C:341:SER:HB3    | 1:C:398:ILE:HD12 | 1.91                     | 0.52              |
| 1:C:530:THR:HG22   | 1:C:546:LEU:HD12 | 1.92                     | 0.52              |
| 1:C:529:LEU:HD13   | 1:C:546:LEU:HD21 | 1.90                     | 0.52              |
| 1:C:311:SER:N      | 1:C:315:LYS:O    | 2.37                     | 0.52              |
| 1:E:388:ILE:O      | 1:E:392:LEU:HD22 | 2.10                     | 0.52              |
| 1:D:206:LEU:HD23   | 1:D:206:LEU:C    | 2.29                     | 0.52              |
| 1:A:249:ILE:HD12   | 5:A:2092:HOH:O   | 2.09                     | 0.52              |
| 1:D:59:LEU:HB2     | 1:D:528:ARG:NH2  | 2.25                     | 0.52              |
| 1:B:56:LEU:HD12    | 1:B:56:LEU:N     | 2.25                     | 0.52              |
| 1:B:497:ASN:HB2    | 5:B:2352:HOH:O   | 2.10                     | 0.52              |
| 1:D:82:SER:HA      | 1:D:128:LEU:HD22 | 1.91                     | 0.52              |
| 1:D:64:LYS:HD2     | 5:D:2011:HOH:O   | 2.10                     | 0.52              |
| 1:E:65:MET:HG2     | 3:E:700:NAG:C7   | 2.40                     | 0.51              |
| 1:A:293:GLY:O      | 1:A:295:THR:HG23 | 2.09                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:54:PRO:HD3   | 1:B:180:TYR:CD2   | 2.45                     | 0.51              |
| 1:B:63:VAL:HG13  | 1:B:194:ILE:CD1   | 2.40                     | 0.51              |
| 1:B:78:TYR:CD2   | 1:D:262:LEU:HD11  | 2.45                     | 0.51              |
| 1:A:142:ASN:ND2  | 5:A:2079:HOH:O    | 2.40                     | 0.51              |
| 1:E:206:LEU:HD23 | 1:E:206:LEU:C     | 2.31                     | 0.51              |
| 1:E:300:LYS:HE2  | 1:E:300:LYS:CA    | 2.39                     | 0.51              |
| 1:E:352:GLY:HA2  | 1:E:405:TRP:CD1   | 2.46                     | 0.51              |
| 1:A:74:PRO:HG3   | 1:A:106:PHE:CD2   | 2.45                     | 0.51              |
| 1:A:388:ILE:HG13 | 1:A:392:LEU:HD22  | 1.93                     | 0.51              |
| 1:E:309:CYS:SG   | 1:E:360[B]:CYS:SG | 3.06                     | 0.51              |
| 1:E:437:THR:OG1  | 1:E:477:GLN:HG2   | 2.11                     | 0.51              |
| 1:A:498:LEU:HD23 | 1:A:498:LEU:C     | 2.30                     | 0.50              |
| 1:B:66:THR:OG1   | 1:B:191:GLU:HB3   | 2.11                     | 0.50              |
| 1:F:221:LYS:HD2  | 5:F:2138:HOH:O    | 2.11                     | 0.50              |
| 1:C:125:GLN:NE2  | 1:C:156:PRO:CB    | 2.71                     | 0.50              |
| 1:C:142:ASN:HB3  | 5:C:2083:HOH:O    | 2.09                     | 0.50              |
| 1:D:54:PRO:HD2   | 1:D:531:ARG:NH2   | 2.26                     | 0.50              |
| 1:E:511:GLU:OE2  | 1:E:528:ARG:NH2   | 2.39                     | 0.50              |
| 1:C:530:THR:CG2  | 1:C:546:LEU:HD12  | 2.41                     | 0.50              |
| 1:E:529:LEU:HD13 | 1:E:546:LEU:HD11  | 1.93                     | 0.50              |
| 1:A:431:GLU:HG2  | 1:A:435:ARG:HH11  | 1.77                     | 0.50              |
| 1:E:522:MET:HE3  | 5:E:2409:HOH:O    | 2.11                     | 0.50              |
| 1:A:370:PHE:CZ   | 1:A:374:LYS:HE3   | 2.46                     | 0.50              |
| 3:C:700:NAG:H62  | 3:C:701:NAG:C1    | 2.42                     | 0.50              |
| 1:F:309:CYS:O    | 1:F:316:LEU:HB3   | 2.11                     | 0.50              |
| 1:C:504:PRO:O    | 1:C:507:SER:HB2   | 2.12                     | 0.50              |
| 1:C:322:ILE:O    | 1:C:324:PRO:HD3   | 2.12                     | 0.50              |
| 5:B:2014:HOH:O   | 1:D:262:LEU:HD12  | 2.10                     | 0.50              |
| 1:A:141:PRO:HB2  | 5:A:2199:HOH:O    | 2.11                     | 0.50              |
| 1:A:83:PRO:HD2   | 3:A:702:NAG:H82   | 1.93                     | 0.50              |
| 1:C:70:LEU:HD22  | 1:C:155:GLU:HB3   | 1.93                     | 0.50              |
| 1:D:326:LEU:O    | 1:D:329:THR:HB    | 2.12                     | 0.50              |
| 1:D:370:PHE:CZ   | 1:D:374:LYS:HE3   | 2.46                     | 0.50              |
| 1:D:70:LEU:HB3   | 1:D:124:VAL:HG23  | 1.94                     | 0.49              |
| 1:B:58:PRO:HD2   | 1:B:230:LYS:HG3   | 1.94                     | 0.49              |
| 1:D:352:GLY:HA2  | 1:D:405:TRP:CD1   | 2.47                     | 0.49              |
| 1:A:70:LEU:HD22  | 1:A:155:GLU:HB3   | 1.94                     | 0.49              |
| 1:F:293:GLY:O    | 1:F:295:THR:HG23  | 2.11                     | 0.49              |
| 1:B:529:LEU:HD13 | 1:B:546:LEU:HD21  | 1.95                     | 0.49              |
| 1:E:327:ASN:HD22 | 1:E:328:THR:N     | 2.10                     | 0.49              |
| 1:A:352:GLY:HA2  | 1:A:405:TRP:CD1   | 2.47                     | 0.49              |

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| Atom-1          | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-------------------|--------------------------|-------------------|
| 1:A:535:ARG:HA  | 1:A:538:GLU:HG2   | 1.95                     | 0.49              |
| 1:D:322:ILE:O   | 1:D:324:PRO:HD3   | 2.13                     | 0.49              |
| 1:D:429:TYR:N   | 1:D:430:PRO:CD    | 2.75                     | 0.49              |
| 1:D:198:PRO:HB3 | 1:D:514:TRP:CE3   | 2.48                     | 0.49              |
| 1:A:426:ASP:HB2 | 4:A:800:EDO:H12   | 1.94                     | 0.49              |
| 1:A:429:TYR:N   | 1:A:430:PRO:CD    | 2.76                     | 0.49              |
| 1:B:351:LEU:CD1 | 1:B:392:LEU:HD13  | 2.43                     | 0.49              |
| 1:F:397:THR:HB  | 5:F:2245:HOH:O    | 2.11                     | 0.49              |
| 1:A:412:LYS:HE2 | 1:A:412:LYS:HA    | 1.94                     | 0.48              |
| 1:B:261:SER:OG  | 1:B:264:HIS:ND1   | 2.39                     | 0.48              |
| 1:C:288:GLU:HG3 | 1:C:350:HIS:HB3   | 1.95                     | 0.48              |
| 1:E:262:LEU:HA  | 5:E:2202:HOH:O    | 2.13                     | 0.48              |
| 1:F:426:ASP:HB2 | 4:F:800:EDO:H12   | 1.95                     | 0.48              |
| 1:A:152:LEU:HG  | 1:A:154:LYS:HG2   | 1.95                     | 0.48              |
| 1:A:322:ILE:O   | 1:A:324:PRO:HD3   | 2.14                     | 0.48              |
| 1:C:56:LEU:HD11 | 1:C:178:LEU:CD1   | 2.39                     | 0.48              |
| 1:D:253:GLU:HA  | 1:D:256:ASN:HB2   | 1.96                     | 0.48              |
| 1:E:149:TYR:CZ  | 1:E:196:ASP:HB3   | 2.48                     | 0.48              |
| 1:E:471:PHE:O   | 1:E:478:LYS:NZ    | 2.45                     | 0.48              |
| 1:F:198:PRO:HB3 | 1:F:514:TRP:CE3   | 2.47                     | 0.48              |
| 1:C:488:LEU:CD2 | 1:C:502:LEU:HD22  | 2.43                     | 0.48              |
| 1:D:284:ARG:HD3 | 5:D:2181:HOH:O    | 2.13                     | 0.48              |
| 1:A:311:SER:HB2 | 5:A:2228:HOH:O    | 2.13                     | 0.48              |
| 1:B:64:LYS:HD2  | 5:B:2010:HOH:O    | 2.14                     | 0.48              |
| 1:C:91:CYS:SG   | 1:C:137[B]:CYS:CB | 2.99                     | 0.48              |
| 1:B:289:PHE:CE2 | 1:B:340:ILE:HD12  | 2.49                     | 0.48              |
| 1:B:393:ASP:O   | 1:B:397:THR:HG23  | 2.14                     | 0.48              |
| 1:D:514:TRP:CD1 | 1:D:514:TRP:C     | 2.87                     | 0.48              |
| 1:E:310:TYR:CD2 | 1:E:315:LYS:HA    | 2.48                     | 0.48              |
| 1:F:310:TYR:HD1 | 1:F:315:LYS:N     | 2.10                     | 0.48              |
| 1:A:142:ASN:OD1 | 1:A:144:SER:HB2   | 2.13                     | 0.48              |
| 1:F:322:ILE:O   | 1:F:324:PRO:HD3   | 2.13                     | 0.48              |
| 1:D:498:LEU:C   | 1:D:498:LEU:HD23  | 2.34                     | 0.48              |
| 1:E:73:ALA:HB3  | 1:E:76:ASN:HB3    | 1.95                     | 0.48              |
| 3:B:700:NAG:H61 | 3:B:701:NAG:N2    | 2.29                     | 0.47              |
| 1:E:341:SER:HB3 | 1:E:398:ILE:HD12  | 1.95                     | 0.47              |
| 1:C:498:LEU:C   | 1:C:498:LEU:HD23  | 2.34                     | 0.47              |
| 1:F:429:TYR:N   | 1:F:430:PRO:CD    | 2.77                     | 0.47              |
| 1:A:253:GLU:HA  | 1:A:256:ASN:HB2   | 1.97                     | 0.47              |
| 1:A:368:GLN:HG3 | 5:A:2265:HOH:O    | 2.14                     | 0.47              |
| 1:B:65:MET:HG2  | 3:B:700:NAG:C7    | 2.44                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:544:GLN:HB2  | 1:D:545:PRO:HD2   | 1.96                     | 0.47              |
| 1:B:91:CYS:SG    | 1:B:137[B]:CYS:CB | 3.00                     | 0.47              |
| 1:C:526:TYR:O    | 1:C:530:THR:HG23  | 2.14                     | 0.47              |
| 1:D:290:ASP:OD2  | 1:D:354:ASP:OD1   | 2.32                     | 0.47              |
| 1:F:140:PHE:CE2  | 1:F:279:ARG:HD3   | 2.50                     | 0.47              |
| 1:E:553:HIS:CG   | 1:E:554:GLU:N     | 2.82                     | 0.47              |
| 1:B:317:ASP:N    | 1:B:317:ASP:OD1   | 2.45                     | 0.47              |
| 1:B:419:THR:O    | 1:B:442:PRO:HD2   | 2.15                     | 0.47              |
| 1:C:135:SER:O    | 1:C:136:GLU:HB2   | 2.15                     | 0.47              |
| 1:D:315:LYS:HB2  | 1:D:316:LEU:H     | 1.25                     | 0.47              |
| 1:A:63:VAL:HG13  | 1:A:194:ILE:HD11  | 1.97                     | 0.47              |
| 1:C:284:ARG:HD3  | 5:C:2199:HOH:O    | 2.13                     | 0.47              |
| 1:D:315:LYS:O    | 1:D:316:LEU:HG    | 2.15                     | 0.47              |
| 1:E:91:CYS:SG    | 1:E:137[B]:CYS:CB | 3.02                     | 0.47              |
| 1:C:80:SER:HB3   | 5:C:2018:HOH:O    | 2.15                     | 0.46              |
| 1:A:229:ASN:HD21 | 1:A:536:MET:CE    | 2.28                     | 0.46              |
| 1:A:325:THR:HG22 | 1:A:370:PHE:CD2   | 2.51                     | 0.46              |
| 1:A:415:LEU:HB2  | 1:A:441:PHE:CZ    | 2.50                     | 0.46              |
| 1:E:429:TYR:N    | 1:E:430:PRO:CD    | 2.77                     | 0.46              |
| 1:A:419:THR:O    | 1:A:442:PRO:HD2   | 2.16                     | 0.46              |
| 1:E:351:LEU:HD12 | 1:E:392:LEU:HD13  | 1.96                     | 0.46              |
| 1:A:63:VAL:HG22  | 1:A:194:ILE:CD1   | 2.39                     | 0.46              |
| 1:F:221:LYS:HE3  | 1:F:540:GLY:O     | 2.16                     | 0.46              |
| 1:D:182:ASP:C    | 1:D:182:ASP:OD1   | 2.54                     | 0.46              |
| 1:E:379:ASP:HB3  | 1:E:382:LYS:HD2   | 1.98                     | 0.46              |
| 1:A:99:ARG:HB2   | 5:A:2036:HOH:O    | 2.16                     | 0.46              |
| 1:A:99:ARG:HD3   | 5:A:2036:HOH:O    | 2.15                     | 0.46              |
| 1:D:511:GLU:CD   | 1:D:528:ARG:HH22  | 2.18                     | 0.46              |
| 1:C:206:LEU:HD23 | 1:C:206:LEU:C     | 2.36                     | 0.45              |
| 1:F:514:TRP:CD1  | 1:F:514:TRP:C     | 2.89                     | 0.45              |
| 1:A:140:PHE:CE2  | 1:A:279:ARG:HD3   | 2.50                     | 0.45              |
| 1:B:54:PRO:HD3   | 1:B:180:TYR:HB3   | 1.98                     | 0.45              |
| 1:C:72:LEU:HD12  | 1:C:72:LEU:N      | 2.31                     | 0.45              |
| 1:D:61:LEU:HD23  | 1:D:61:LEU:O      | 2.16                     | 0.45              |
| 1:C:415:LEU:HB2  | 1:C:441:PHE:CZ    | 2.51                     | 0.45              |
| 1:D:199:ARG:CZ   | 1:D:517:LYS:HB2   | 2.47                     | 0.45              |
| 1:E:451:LEU:HD22 | 1:E:463:TYR:CE2   | 2.51                     | 0.45              |
| 1:F:364:ASN:HA   | 1:F:365:PRO:HD3   | 1.80                     | 0.45              |
| 1:F:553:HIS:CG   | 1:F:554:GLU:N     | 2.84                     | 0.45              |
| 1:B:79:ILE:H     | 4:B:801:EDO:H11   | 1.78                     | 0.45              |
| 1:C:368:GLN:HA   | 1:C:368:GLN:OE1   | 2.15                     | 0.45              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:C:544:GLN:HB2    | 1:C:545:PRO:HD2     | 1.97                     | 0.45              |
| 1:D:368:GLN:HE21   | 1:D:368:GLN:HA      | 1.82                     | 0.45              |
| 1:D:65:MET:HG2     | 3:D:700:NAG:O7      | 2.16                     | 0.45              |
| 1:A:63:VAL:HG13    | 1:A:194:ILE:CD1     | 2.47                     | 0.45              |
| 1:B:316:LEU:HD13   | 1:B:318:SER:CB      | 2.41                     | 0.45              |
| 1:B:65:MET:HG2     | 3:B:700:NAG:O7      | 2.17                     | 0.45              |
| 1:A:206:LEU:HD12   | 1:A:235:HIS:CE1     | 2.52                     | 0.45              |
| 1:D:403:ILE:HG12   | 1:D:420:ILE:HB      | 1.99                     | 0.45              |
| 1:E:351:LEU:CD1    | 1:E:392:LEU:HD13    | 2.47                     | 0.45              |
| 1:C:161:LYS:HB2    | 1:C:161:LYS:HE3     | 1.88                     | 0.45              |
| 1:D:460:TRP:CD1    | 1:D:546[A]:LEU:HD22 | 2.51                     | 0.45              |
| 1:F:135:SER:O      | 1:F:136:GLU:HB2     | 2.16                     | 0.45              |
| 1:B:412:LYS:HE2    | 1:B:412:LYS:CA      | 2.46                     | 0.45              |
| 1:C:352:GLY:HA2    | 1:C:405:TRP:CD1     | 2.52                     | 0.45              |
| 1:C:429:TYR:N      | 1:C:430:PRO:CD      | 2.80                     | 0.45              |
| 1:E:149:TYR:CE2    | 1:E:196:ASP:HB3     | 2.51                     | 0.45              |
| 1:E:544:GLN:HB2    | 1:E:545:PRO:HD2     | 1.99                     | 0.45              |
| 3:E:700:NAG:H62    | 3:E:701:NAG:C1      | 2.47                     | 0.45              |
| 1:B:420:ILE:HG21   | 1:B:444:ILE:HD12    | 1.99                     | 0.45              |
| 1:C:497:ASN:HB2    | 5:C:2341:HOH:O      | 2.17                     | 0.45              |
| 1:F:360[B]:CYS:HB3 | 5:F:2233:HOH:O      | 2.17                     | 0.45              |
| 1:A:152:LEU:HD23   | 1:A:154:LYS:HE2     | 1.97                     | 0.45              |
| 1:D:93:LEU:C       | 1:D:93:LEU:HD23     | 2.38                     | 0.45              |
| 1:E:78:TYR:HA      | 4:E:801:EDO:O1      | 2.17                     | 0.44              |
| 1:C:370:PHE:CE2    | 1:C:374:LYS:HG3     | 2.52                     | 0.44              |
| 1:E:178:LEU:HG     | 5:E:2127:HOH:O      | 2.17                     | 0.44              |
| 1:E:393:ASP:O      | 1:E:397:THR:HG23    | 2.17                     | 0.44              |
| 1:F:70:LEU:HD22    | 1:F:155:GLU:HB3     | 1.99                     | 0.44              |
| 1:A:188:THR:HG22   | 1:A:189:ILE:N       | 2.32                     | 0.44              |
| 1:B:420:ILE:HG12   | 1:B:442:PRO:HB2     | 1.99                     | 0.44              |
| 1:D:462:LYS:HD2    | 5:D:2274:HOH:O      | 2.17                     | 0.44              |
| 1:E:82:SER:HA      | 1:E:128:LEU:HD22    | 2.00                     | 0.44              |
| 1:A:326:LEU:O      | 1:A:329:THR:HB      | 2.17                     | 0.44              |
| 1:B:239:VAL:HG12   | 1:B:245:PRO:HD2     | 1.98                     | 0.44              |
| 1:A:272:ARG:NH2    | 5:A:2191:HOH:O      | 2.50                     | 0.44              |
| 1:A:471:PHE:O      | 1:A:478:LYS:HE2     | 2.17                     | 0.44              |
| 1:B:315:LYS:NZ     | 5:B:2219:HOH:O      | 2.51                     | 0.44              |
| 1:C:198:PRO:HB3    | 1:C:514:TRP:CE3     | 2.52                     | 0.44              |
| 1:F:339:GLU:O      | 1:F:343:VAL:HG23    | 2.18                     | 0.44              |
| 1:A:310:TYR:CE1    | 1:A:315:LYS:HA      | 2.52                     | 0.44              |
| 1:F:149:TYR:CE2    | 1:F:196:ASP:HB3     | 2.53                     | 0.44              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:B:518[A]:ASP:N | 1:B:518[A]:ASP:OD1 | 2.50                     | 0.44              |
| 1:C:428:ALA:HB1  | 1:C:431:GLU:OE1    | 2.18                     | 0.44              |
| 1:E:262:LEU:HD12 | 5:E:2202:HOH:O     | 2.16                     | 0.44              |
| 1:D:371:MET:HE2  | 1:D:376:PHE:HD1    | 1.83                     | 0.43              |
| 1:F:247:GLN:OE1  | 1:F:267:THR:HG22   | 2.18                     | 0.43              |
| 1:B:498:LEU:HD23 | 1:B:498:LEU:C      | 2.38                     | 0.43              |
| 1:E:93:LEU:HD23  | 1:E:93:LEU:C       | 2.39                     | 0.43              |
| 1:F:63:VAL:HG13  | 1:F:194:ILE:CD1    | 2.48                     | 0.43              |
| 1:F:209:THR:HG22 | 1:F:214:LEU:HD12   | 1.99                     | 0.43              |
| 1:B:352:GLY:HA2  | 1:B:405:TRP:CD1    | 2.54                     | 0.43              |
| 1:B:403:ILE:HG12 | 1:B:420:ILE:HB     | 2.00                     | 0.43              |
| 1:D:351:LEU:HD12 | 1:D:392:LEU:HD13   | 2.01                     | 0.43              |
| 1:F:229:ASN:HD21 | 1:F:536:MET:HE3    | 1.79                     | 0.43              |
| 1:A:393:ASP:O    | 1:A:397:THR:HG23   | 2.18                     | 0.43              |
| 1:A:544:GLN:HB2  | 1:A:545:PRO:HD2    | 2.00                     | 0.43              |
| 1:E:72:LEU:N     | 1:E:72:LEU:HD12    | 2.33                     | 0.43              |
| 1:A:284:ARG:HG3  | 5:A:2199:HOH:O     | 2.18                     | 0.43              |
| 1:F:232:ASN:OD1  | 1:F:233:VAL:HG23   | 2.18                     | 0.43              |
| 1:C:529:LEU:HD13 | 1:C:546:LEU:HD11   | 1.99                     | 0.43              |
| 1:F:188:THR:HG22 | 1:F:189:ILE:N      | 2.33                     | 0.43              |
| 1:C:497:ASN:O    | 1:C:500:PRO:HD2    | 2.18                     | 0.43              |
| 4:A:800:EDO:H22  | 5:A:2303:HOH:O     | 2.18                     | 0.43              |
| 1:D:91:CYS:SG    | 1:D:137[B]:CYS:CB  | 3.04                     | 0.43              |
| 1:D:188:THR:HG22 | 1:D:189:ILE:N      | 2.33                     | 0.43              |
| 1:E:303:LYS:HA   | 1:E:303:LYS:HD3    | 1.75                     | 0.43              |
| 1:F:72:LEU:HG    | 1:F:124:VAL:HG13   | 2.00                     | 0.43              |
| 1:A:206:LEU:HD23 | 1:A:206:LEU:C      | 2.39                     | 0.43              |
| 1:B:73:ALA:HB3   | 1:B:76:ASN:HB3     | 2.01                     | 0.43              |
| 1:D:57:TRP:CH2   | 1:D:529:LEU:HG     | 2.54                     | 0.43              |
| 1:F:149:TYR:CZ   | 1:F:196:ASP:HB3    | 2.54                     | 0.43              |
| 1:B:504:PRO:O    | 1:B:507:SER:HB2    | 2.19                     | 0.43              |
| 1:D:371:MET:HE2  | 1:D:376:PHE:CD1    | 2.54                     | 0.43              |
| 1:D:341:SER:HB3  | 1:D:398:ILE:HD12   | 2.01                     | 0.43              |
| 1:D:437:THR:HB   | 1:D:477:GLN:HG2    | 2.01                     | 0.42              |
| 1:E:514:TRP:CD1  | 1:E:514:TRP:C      | 2.92                     | 0.42              |
| 1:F:206:LEU:C    | 1:F:206:LEU:HD23   | 2.39                     | 0.42              |
| 1:B:325:THR:HB   | 1:B:370:PHE:CD1    | 2.54                     | 0.42              |
| 1:C:431:GLU:HB3  | 1:C:435:ARG:HH12   | 1.84                     | 0.42              |
| 1:F:85:SER:HB2   | 1:F:130:SER:HA     | 2.01                     | 0.42              |
| 1:D:384:GLU:OE1  | 1:D:411:ASP:OD2    | 2.37                     | 0.42              |
| 1:F:460:TRP:CD1  | 1:F:546:LEU:HD22   | 2.54                     | 0.42              |

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| Atom-1              | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|------------------|--------------------------|-------------------|
| 1:B:419:THR:HA      | 5:B:2293:HOH:O   | 2.18                     | 0.42              |
| 1:D:364:ASN:HA      | 1:D:365:PRO:HD3  | 1.93                     | 0.42              |
| 1:D:383:LEU:HA      | 1:D:383:LEU:HD23 | 1.83                     | 0.42              |
| 1:A:72:LEU:HG       | 1:A:124:VAL:HG13 | 2.02                     | 0.42              |
| 1:B:140:PHE:CE2     | 1:B:345:PRO:HG3  | 2.55                     | 0.42              |
| 3:C:700:NAG:C6      | 3:C:701:NAG:HN2  | 2.32                     | 0.42              |
| 1:E:420:ILE:HA      | 1:E:442:PRO:HG2  | 2.01                     | 0.42              |
| 1:E:529:LEU:HD13    | 1:E:546:LEU:HD21 | 2.02                     | 0.42              |
| 1:E:551:CYS:O       | 1:E:553:HIS:N    | 2.41                     | 0.42              |
| 1:F:253:GLU:HA      | 1:F:256:ASN:HB2  | 2.01                     | 0.42              |
| 1:B:135:SER:O       | 1:B:136:GLU:HB2  | 2.19                     | 0.42              |
| 1:C:253:GLU:HA      | 1:C:256:ASN:HB2  | 2.02                     | 0.42              |
| 1:E:142:ASN:HB2     | 5:E:2080:HOH:O   | 2.20                     | 0.42              |
| 1:E:415:LEU:HB2     | 1:E:441:PHE:CZ   | 2.54                     | 0.42              |
| 1:F:302:GLN:HG3     | 1:F:305:LEU:HB2  | 2.01                     | 0.42              |
| 1:C:149:TYR:CE2     | 1:C:196:ASP:HB3  | 2.54                     | 0.42              |
| 1:A:529:LEU:HD13    | 1:A:546:LEU:HD11 | 2.02                     | 0.42              |
| 1:A:79:ILE:H        | 4:A:801:EDO:C1   | 2.33                     | 0.42              |
| 1:B:149:TYR:CZ      | 1:B:196:ASP:HB3  | 2.54                     | 0.42              |
| 1:D:149:TYR:CZ      | 1:D:196:ASP:HB3  | 2.55                     | 0.42              |
| 1:D:371:MET:CE      | 1:D:376:PHE:CD1  | 3.01                     | 0.42              |
| 1:D:511:GLU:O       | 1:D:515:SER:HB2  | 2.20                     | 0.42              |
| 1:E:547:TYR:CG      | 1:E:548:ALA:N    | 2.88                     | 0.42              |
| 1:A:269:ASN:HB2     | 5:C:2038:HOH:O   | 2.20                     | 0.41              |
| 1:A:305:LEU:HG      | 1:A:322:ILE:HG12 | 2.02                     | 0.41              |
| 1:B:99:ARG:HG3      | 5:B:2045:HOH:O   | 2.18                     | 0.41              |
| 1:E:413:ALA:HB2     | 5:E:2302:HOH:O   | 2.20                     | 0.41              |
| 1:F:150[A]:THR:HG23 | 5:F:2093:HOH:O   | 2.20                     | 0.41              |
| 1:A:514:TRP:CD1     | 1:A:514:TRP:C    | 2.93                     | 0.41              |
| 1:B:514:TRP:CD1     | 1:B:514:TRP:C    | 2.93                     | 0.41              |
| 1:C:476:LYS:O       | 1:C:479:GLN:HB2  | 2.20                     | 0.41              |
| 1:E:103:GLY:O       | 1:E:107:GLY:N    | 2.50                     | 0.41              |
| 1:E:369:ASP:O       | 1:E:373:GLN:HG3  | 2.20                     | 0.41              |
| 1:F:384:GLU:OE1     | 1:F:411:ASP:OD2  | 2.37                     | 0.41              |
| 1:F:461:ARG:NH2     | 5:F:2296:HOH:O   | 2.47                     | 0.41              |
| 1:F:527[B]:ASP:O    | 1:F:531:ARG:HG3  | 2.20                     | 0.41              |
| 1:A:149:TYR:CE2     | 1:A:196:ASP:HB3  | 2.55                     | 0.41              |
| 1:A:221:LYS:NZ      | 5:A:2145:HOH:O   | 2.52                     | 0.41              |
| 1:B:475:GLN:O       | 1:B:479:GLN:HG3  | 2.20                     | 0.41              |
| 1:F:544:GLN:HB2     | 1:F:545:PRO:HD2  | 2.01                     | 0.41              |
| 1:E:135:SER:O       | 1:E:136:GLU:HB2  | 2.21                     | 0.41              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:C:427:SER:HB2  | 5:C:2289:HOH:O     | 2.19                     | 0.41              |
| 1:D:238:ILE:HG23 | 1:D:239:VAL:HG13   | 2.02                     | 0.41              |
| 1:E:58:PRO:HB3   | 1:E:511:GLU:HA     | 2.01                     | 0.41              |
| 1:F:235:HIS:ND1  | 1:F:485:GLU:OE1    | 2.53                     | 0.41              |
| 1:F:309:CYS:O    | 1:F:316:LEU:CB     | 2.68                     | 0.41              |
| 1:C:76:ASN:ND2   | 1:C:78:TYR:HE1     | 2.19                     | 0.41              |
| 1:D:307:THR:CG2  | 1:D:360[B]:CYS:SG  | 3.07                     | 0.41              |
| 1:B:288:GLU:HG3  | 1:B:350:HIS:HB3    | 2.03                     | 0.41              |
| 1:C:290:ASP:OD2  | 1:C:354:ASP:OD1    | 2.38                     | 0.41              |
| 1:A:79:ILE:HB    | 4:A:801:EDO:H12    | 2.02                     | 0.41              |
| 1:E:497:ASN:HB2  | 5:E:2398:HOH:O     | 2.20                     | 0.41              |
| 1:F:310:TYR:CE1  | 1:F:315:LYS:N      | 2.89                     | 0.41              |
| 1:F:355:GLU:OE1  | 2:F:600:GDL:H2     | 2.21                     | 0.41              |
| 1:D:293:GLY:O    | 1:D:295:THR:HG23   | 2.21                     | 0.41              |
| 1:E:384:GLU:OE1  | 1:E:411:ASP:OD2    | 2.39                     | 0.41              |
| 1:B:217:LYS:HG3  | 5:B:2134:HOH:O     | 2.21                     | 0.41              |
| 1:B:93:LEU:C     | 1:B:93:LEU:HD23    | 2.41                     | 0.41              |
| 1:D:371:MET:HE2  | 1:D:376:PHE:HB2    | 2.02                     | 0.41              |
| 1:E:403:ILE:HG12 | 1:E:420:ILE:HB     | 2.02                     | 0.41              |
| 1:F:437:THR:CB   | 1:F:477:GLN:HG2    | 2.48                     | 0.41              |
| 1:D:149:TYR:CE2  | 1:D:196:ASP:HB3    | 2.55                     | 0.41              |
| 1:F:461:ARG:NH2  | 5:F:2295:HOH:O     | 2.49                     | 0.41              |
| 1:B:369:ASP:O    | 1:B:372:ARG:HB3    | 2.21                     | 0.40              |
| 1:C:140:PHE:CE2  | 1:C:279:ARG:HD3    | 2.56                     | 0.40              |
| 1:E:322:ILE:O    | 1:E:324:PRO:HD3    | 2.20                     | 0.40              |
| 1:F:133:LEU:O    | 1:F:134:GLN:C      | 2.60                     | 0.40              |
| 1:F:420:ILE:HG12 | 1:F:442:PRO:HB2    | 2.04                     | 0.40              |
| 1:F:468:PRO:HB3  | 1:F:481:PHE:CZ     | 2.56                     | 0.40              |
| 1:A:199:ARG:CZ   | 1:A:517:LYS:HB2    | 2.51                     | 0.40              |
| 1:A:221:LYS:HE2  | 5:A:2147:HOH:O     | 2.21                     | 0.40              |
| 1:B:198:PRO:HB3  | 1:B:514:TRP:CE3    | 2.56                     | 0.40              |
| 4:C:801:EDO:H12  | 1:D:79:ILE:N       | 2.35                     | 0.40              |
| 1:E:309:CYS:SG   | 1:E:360[B]:CYS:HB2 | 2.62                     | 0.40              |
| 1:A:474:THR:O    | 1:A:478:LYS:HG2    | 2.21                     | 0.40              |
| 1:C:93:LEU:C     | 1:C:93:LEU:HD23    | 2.41                     | 0.40              |
| 1:D:221:LYS:NZ   | 1:D:540:GLY:O      | 2.43                     | 0.40              |
| 1:E:316:LEU:C    | 1:E:318:SER:N      | 2.73                     | 0.40              |
| 1:B:82:SER:HA    | 1:B:128:LEU:HD22   | 2.02                     | 0.40              |
| 1:B:54:PRO:HD3   | 1:B:180:TYR:CG     | 2.56                     | 0.40              |
| 1:C:326:LEU:O    | 1:C:329:THR:HB     | 2.21                     | 0.40              |
| 1:C:488:LEU:O    | 1:C:488:LEU:CD1    | 2.58                     | 0.40              |

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| Atom-1          | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|---------------------|--------------------------|-------------------|
| 1:B:78:TYR:HE2  | 1:D:262:LEU:HD11    | 1.80                     | 0.40              |
| 1:D:530:THR:CG2 | 1:D:546[A]:LEU:HD12 | 2.51                     | 0.40              |
| 1:F:101:TYR:CE2 | 1:F:173:GLU:HA      | 2.57                     | 0.40              |
| 1:A:149:TYR:CZ  | 1:A:196:ASP:HB3     | 2.56                     | 0.40              |
| 1:A:215:PRO:O   | 1:A:218:ILE:HG22    | 2.21                     | 0.40              |
| 1:A:338:LYS:HD2 | 1:A:338:LYS:HA      | 1.87                     | 0.40              |
| 1:A:431:GLU:CG  | 1:A:435:ARG:NH1     | 2.79                     | 0.40              |
| 1:C:149:TYR:CZ  | 1:C:196:ASP:HB3     | 2.55                     | 0.40              |
| 1:C:474:THR:O   | 1:C:478:LYS:HG2     | 2.21                     | 0.40              |
| 1:E:133:LEU:O   | 1:E:134:GLN:C       | 2.60                     | 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     | 482/515 (94%)   | 466 (97%)  | 16 (3%)  | 0        | 100         | 100 |
| 1   | B     | 481/515 (93%)   | 462 (96%)  | 18 (4%)  | 1 (0%)   | 49          | 57  |
| 1   | C     | 482/515 (94%)   | 467 (97%)  | 14 (3%)  | 1 (0%)   | 49          | 57  |
| 1   | D     | 483/515 (94%)   | 462 (96%)  | 20 (4%)  | 1 (0%)   | 49          | 57  |
| 1   | E     | 483/515 (94%)   | 463 (96%)  | 18 (4%)  | 2 (0%)   | 36          | 39  |
| 1   | F     | 484/515 (94%)   | 463 (96%)  | 19 (4%)  | 2 (0%)   | 36          | 39  |
| All | All   | 2895/3090 (94%) | 2783 (96%) | 105 (4%) | 7 (0%)   | 49          | 57  |

All (7) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 316 | LEU  |
| 1   | C     | 318 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 316 | LEU  |
| 1   | E     | 552 | ASN  |
| 1   | F     | 316 | LEU  |
| 1   | E     | 316 | LEU  |
| 1   | F     | 553 | HIS  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 433/454 (95%)   | 418 (96%)  | 15 (4%)  | 39          | 47 |
| 1   | B     | 432/454 (95%)   | 422 (98%)  | 10 (2%)  | 53          | 62 |
| 1   | C     | 433/454 (95%)   | 420 (97%)  | 13 (3%)  | 44          | 53 |
| 1   | D     | 434/454 (96%)   | 422 (97%)  | 12 (3%)  | 47          | 55 |
| 1   | E     | 434/454 (96%)   | 421 (97%)  | 13 (3%)  | 44          | 53 |
| 1   | F     | 435/454 (96%)   | 423 (97%)  | 12 (3%)  | 47          | 55 |
| All | All   | 2601/2724 (96%) | 2526 (97%) | 75 (3%)  | 45          | 54 |

All (75) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 56  | LEU  |
| 1   | A     | 72  | LEU  |
| 1   | A     | 142 | ASN  |
| 1   | A     | 151 | LEU  |
| 1   | A     | 154 | LYS  |
| 1   | A     | 178 | LEU  |
| 1   | A     | 211 | ARG  |
| 1   | A     | 221 | LYS  |
| 1   | A     | 269 | ASN  |
| 1   | A     | 296 | LEU  |
| 1   | A     | 316 | LEU  |
| 1   | A     | 383 | LEU  |
| 1   | A     | 392 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 504 | PRO  |
| 1   | A     | 529 | LEU  |
| 1   | B     | 61  | LEU  |
| 1   | B     | 151 | LEU  |
| 1   | B     | 315 | LYS  |
| 1   | B     | 316 | LEU  |
| 1   | B     | 317 | ASP  |
| 1   | B     | 357 | GLU  |
| 1   | B     | 383 | LEU  |
| 1   | B     | 392 | LEU  |
| 1   | B     | 504 | PRO  |
| 1   | B     | 529 | LEU  |
| 1   | C     | 61  | LEU  |
| 1   | C     | 80  | SER  |
| 1   | C     | 99  | ARG  |
| 1   | C     | 124 | VAL  |
| 1   | C     | 151 | LEU  |
| 1   | C     | 155 | GLU  |
| 1   | C     | 178 | LEU  |
| 1   | C     | 315 | LYS  |
| 1   | C     | 373 | GLN  |
| 1   | C     | 383 | LEU  |
| 1   | C     | 388 | ILE  |
| 1   | C     | 392 | LEU  |
| 1   | C     | 529 | LEU  |
| 1   | D     | 82  | SER  |
| 1   | D     | 151 | LEU  |
| 1   | D     | 178 | LEU  |
| 1   | D     | 211 | ARG  |
| 1   | D     | 306 | LEU  |
| 1   | D     | 383 | LEU  |
| 1   | D     | 388 | ILE  |
| 1   | D     | 392 | LEU  |
| 1   | D     | 426 | ASP  |
| 1   | D     | 462 | LYS  |
| 1   | D     | 504 | PRO  |
| 1   | D     | 529 | LEU  |
| 1   | E     | 56  | LEU  |
| 1   | E     | 124 | VAL  |
| 1   | E     | 151 | LEU  |
| 1   | E     | 178 | LEU  |
| 1   | E     | 211 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 218 | ILE  |
| 1   | E     | 306 | LEU  |
| 1   | E     | 316 | LEU  |
| 1   | E     | 327 | ASN  |
| 1   | E     | 383 | LEU  |
| 1   | E     | 392 | LEU  |
| 1   | E     | 529 | LEU  |
| 1   | E     | 530 | THR  |
| 1   | F     | 122 | THR  |
| 1   | F     | 124 | VAL  |
| 1   | F     | 151 | LEU  |
| 1   | F     | 211 | ARG  |
| 1   | F     | 218 | ILE  |
| 1   | F     | 306 | LEU  |
| 1   | F     | 315 | LYS  |
| 1   | F     | 316 | LEU  |
| 1   | F     | 383 | LEU  |
| 1   | F     | 392 | LEU  |
| 1   | F     | 461 | ARG  |
| 1   | F     | 553 | HIS  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 76  | ASN  |
| 1   | A     | 553 | HIS  |
| 1   | B     | 76  | ASN  |
| 1   | B     | 134 | GLN  |
| 1   | B     | 373 | GLN  |
| 1   | C     | 71  | HIS  |
| 1   | C     | 76  | ASN  |
| 1   | C     | 125 | GLN  |
| 1   | D     | 68  | ASN  |
| 1   | D     | 76  | ASN  |
| 1   | D     | 125 | GLN  |
| 1   | D     | 126 | GLN  |
| 1   | D     | 368 | GLN  |
| 1   | D     | 373 | GLN  |
| 1   | D     | 479 | GLN  |
| 1   | E     | 71  | HIS  |
| 1   | E     | 76  | ASN  |
| 1   | E     | 327 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 102 | HIS  |
| 1   | F     | 125 | GLN  |
| 1   | F     | 142 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

39 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 2   | GDL  | A     | 600 | -    | 14,15,15     | 3.08 | 3 (21%)     | 17,21,21    | 1.81 | 4 (23%)     |
| 3   | NAG  | A     | 700 | 1,3  | 14,14,15     | 0.49 | 0           | 17,19,21    | 0.94 | 0           |
| 3   | NAG  | A     | 701 | 3    | 14,14,15     | 0.53 | 0           | 17,19,21    | 0.73 | 0           |
| 3   | NAG  | A     | 702 | 1    | 14,14,15     | 0.68 | 0           | 17,19,21    | 0.69 | 0           |
| 4   | EDO  | A     | 800 | -    | 3,3,3        | 0.57 | 0           | 2,2,2       | 0.52 | 0           |
| 4   | EDO  | A     | 801 | -    | 3,3,3        | 0.60 | 0           | 2,2,2       | 0.44 | 0           |
| 4   | EDO  | A     | 802 | -    | 3,3,3        | 0.49 | 0           | 2,2,2       | 0.41 | 0           |
| 2   | GDL  | B     | 600 | -    | 14,15,15     | 3.29 | 2 (14%)     | 17,21,21    | 1.76 | 4 (23%)     |
| 3   | NAG  | B     | 700 | 1,3  | 14,14,15     | 0.41 | 0           | 17,19,21    | 0.69 | 0           |
| 3   | NAG  | B     | 701 | 3    | 14,14,15     | 0.51 | 0           | 17,19,21    | 0.67 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | NAG  | B     | 702 | 1    | 14,14,15     | 0.61 | 0        | 17,19,21    | 0.66 | 0        |
| 4   | EDO  | B     | 800 | -    | 3,3,3        | 0.58 | 0        | 2,2,2       | 0.48 | 0        |
| 4   | EDO  | B     | 801 | -    | 3,3,3        | 0.52 | 0        | 2,2,2       | 0.38 | 0        |
| 4   | EDO  | B     | 802 | -    | 3,3,3        | 0.57 | 0        | 2,2,2       | 0.45 | 0        |
| 2   | GDL  | C     | 600 | -    | 14,15,15     | 3.24 | 3 (21%)  | 17,21,21    | 1.70 | 4 (23%)  |
| 3   | NAG  | C     | 700 | 1,3  | 14,14,15     | 0.42 | 0        | 17,19,21    | 0.90 | 0        |
| 3   | NAG  | C     | 701 | 3    | 14,14,15     | 0.55 | 0        | 17,19,21    | 0.67 | 0        |
| 3   | NAG  | C     | 703 | 1    | 14,14,15     | 0.60 | 0        | 17,19,21    | 0.71 | 0        |
| 4   | EDO  | C     | 800 | -    | 3,3,3        | 0.56 | 0        | 2,2,2       | 0.47 | 0        |
| 4   | EDO  | C     | 801 | -    | 3,3,3        | 0.59 | 0        | 2,2,2       | 0.43 | 0        |
| 4   | EDO  | C     | 802 | -    | 3,3,3        | 0.58 | 0        | 2,2,2       | 0.45 | 0        |
| 2   | GDL  | D     | 600 | -    | 14,15,15     | 3.21 | 4 (28%)  | 17,21,21    | 1.70 | 4 (23%)  |
| 3   | NAG  | D     | 700 | 1,3  | 14,14,15     | 0.48 | 0        | 17,19,21    | 0.95 | 1 (5%)   |
| 3   | NAG  | D     | 701 | 3    | 14,14,15     | 0.53 | 0        | 17,19,21    | 0.79 | 1 (5%)   |
| 2   | GDL  | E     | 600 | -    | 14,15,15     | 3.37 | 2 (14%)  | 17,21,21    | 1.68 | 4 (23%)  |
| 3   | NAG  | E     | 700 | 1,3  | 14,14,15     | 0.46 | 0        | 17,19,21    | 1.13 | 2 (11%)  |
| 3   | NAG  | E     | 701 | 3    | 14,14,15     | 0.51 | 0        | 17,19,21    | 0.68 | 0        |
| 3   | NAG  | E     | 702 | 1    | 14,14,15     | 0.58 | 0        | 17,19,21    | 0.68 | 0        |
| 4   | EDO  | E     | 800 | -    | 3,3,3        | 0.60 | 0        | 2,2,2       | 0.45 | 0        |
| 4   | EDO  | E     | 801 | -    | 3,3,3        | 0.58 | 0        | 2,2,2       | 0.39 | 0        |
| 4   | EDO  | E     | 802 | -    | 3,3,3        | 0.69 | 0        | 2,2,2       | 0.40 | 0        |
| 2   | GDL  | F     | 600 | -    | 14,15,15     | 3.08 | 2 (14%)  | 17,21,21    | 1.76 | 4 (23%)  |
| 3   | NAG  | F     | 700 | 1,3  | 14,14,15     | 0.51 | 0        | 17,19,21    | 0.82 | 1 (5%)   |
| 3   | NAG  | F     | 701 | 3    | 14,14,15     | 0.63 | 0        | 17,19,21    | 0.63 | 0        |
| 3   | NAG  | F     | 702 | 1    | 14,14,15     | 0.60 | 0        | 17,19,21    | 0.78 | 1 (5%)   |
| 3   | NAG  | F     | 703 | 1    | 14,14,15     | 0.58 | 0        | 17,19,21    | 0.61 | 0        |
| 4   | EDO  | F     | 800 | -    | 3,3,3        | 0.52 | 0        | 2,2,2       | 0.42 | 0        |
| 4   | EDO  | F     | 801 | -    | 3,3,3        | 0.59 | 0        | 2,2,2       | 0.45 | 0        |
| 4   | EDO  | F     | 802 | -    | 3,3,3        | 0.50 | 0        | 2,2,2       | 0.41 | 0        |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2   | GDL  | A     | 600 | -    | -       | 0/6/26/26 | 0/1/1/1 |
| 3   | NAG  | A     | 700 | 1,3  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | A     | 701 | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | A     | 702 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | EDO  | A     | 800 | -    | -       | 0/1/1/1   | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 4   | EDO  | A     | 801 | -    | -       | 0/1/1/1   | 0/0/0/0 |
| 4   | EDO  | A     | 802 | -    | -       | 0/1/1/1   | 0/0/0/0 |
| 2   | GDL  | B     | 600 | -    | -       | 0/6/26/26 | 0/1/1/1 |
| 3   | NAG  | B     | 700 | 1,3  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | B     | 701 | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | B     | 702 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | EDO  | B     | 800 | -    | -       | 0/1/1/1   | 0/0/0/0 |
| 4   | EDO  | B     | 801 | -    | -       | 0/1/1/1   | 0/0/0/0 |
| 4   | EDO  | B     | 802 | -    | -       | 0/1/1/1   | 0/0/0/0 |
| 2   | GDL  | C     | 600 | -    | -       | 0/6/26/26 | 0/1/1/1 |
| 3   | NAG  | C     | 700 | 1,3  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | C     | 701 | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | C     | 703 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | EDO  | C     | 800 | -    | -       | 0/1/1/1   | 0/0/0/0 |
| 4   | EDO  | C     | 801 | -    | -       | 0/1/1/1   | 0/0/0/0 |
| 4   | EDO  | C     | 802 | -    | -       | 0/1/1/1   | 0/0/0/0 |
| 2   | GDL  | D     | 600 | -    | -       | 0/6/26/26 | 0/1/1/1 |
| 3   | NAG  | D     | 700 | 1,3  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | D     | 701 | 3    | -       | 1/6/23/26 | 0/1/1/1 |
| 2   | GDL  | E     | 600 | -    | -       | 0/6/26/26 | 0/1/1/1 |
| 3   | NAG  | E     | 700 | 1,3  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | E     | 701 | 3    | -       | 1/6/23/26 | 0/1/1/1 |
| 3   | NAG  | E     | 702 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | EDO  | E     | 800 | -    | -       | 0/1/1/1   | 0/0/0/0 |
| 4   | EDO  | E     | 801 | -    | -       | 0/1/1/1   | 0/0/0/0 |
| 4   | EDO  | E     | 802 | -    | -       | 0/1/1/1   | 0/0/0/0 |
| 2   | GDL  | F     | 600 | -    | -       | 0/6/26/26 | 0/1/1/1 |
| 3   | NAG  | F     | 700 | 1,3  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | F     | 701 | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | F     | 702 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | F     | 703 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | EDO  | F     | 800 | -    | -       | 0/1/1/1   | 0/0/0/0 |
| 4   | EDO  | F     | 801 | -    | -       | 0/1/1/1   | 0/0/0/0 |
| 4   | EDO  | F     | 802 | -    | -       | 0/1/1/1   | 0/0/0/0 |

All (16) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | B     | 600 | GDL  | O5-C1 | -4.96 | 1.27        | 1.34     |
| 2   | E     | 600 | GDL  | O5-C1 | -4.94 | 1.27        | 1.34     |
| 2   | F     | 600 | GDL  | O5-C1 | -4.65 | 1.27        | 1.34     |
| 2   | C     | 600 | GDL  | O5-C1 | -4.65 | 1.27        | 1.34     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | D     | 600 | GDL  | O5-C1 | -4.37 | 1.28        | 1.34     |
| 2   | A     | 600 | GDL  | O5-C1 | -4.16 | 1.28        | 1.34     |
| 2   | A     | 600 | GDL  | C8-C7 | 2.14  | 1.55        | 1.50     |
| 2   | D     | 600 | GDL  | C8-C7 | 2.15  | 1.55        | 1.50     |
| 2   | D     | 600 | GDL  | C2-N1 | 2.26  | 1.50        | 1.45     |
| 2   | C     | 600 | GDL  | C2-N1 | 2.27  | 1.50        | 1.45     |
| 2   | F     | 600 | GDL  | C2-C1 | 9.68  | 1.64        | 1.51     |
| 2   | A     | 600 | GDL  | C2-C1 | 9.84  | 1.65        | 1.51     |
| 2   | D     | 600 | GDL  | C2-C1 | 10.18 | 1.65        | 1.51     |
| 2   | C     | 600 | GDL  | C2-C1 | 10.29 | 1.65        | 1.51     |
| 2   | B     | 600 | GDL  | C2-C1 | 10.44 | 1.65        | 1.51     |
| 2   | E     | 600 | GDL  | C2-C1 | 11.00 | 1.66        | 1.51     |

All (30) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | A     | 600 | GDL  | O1-C1-C2 | -3.92 | 113.78      | 124.24   |
| 2   | D     | 600 | GDL  | O1-C1-C2 | -3.88 | 113.89      | 124.24   |
| 2   | C     | 600 | GDL  | O1-C1-C2 | -3.80 | 114.10      | 124.24   |
| 2   | F     | 600 | GDL  | O1-C1-C2 | -3.63 | 114.56      | 124.24   |
| 2   | B     | 600 | GDL  | O1-C1-C2 | -3.59 | 114.68      | 124.24   |
| 2   | E     | 600 | GDL  | O1-C1-C2 | -3.41 | 115.14      | 124.24   |
| 2   | F     | 600 | GDL  | C3-C2-N1 | -2.58 | 108.11      | 112.29   |
| 3   | D     | 700 | NAG  | C2-N2-C7 | -2.55 | 119.23      | 122.94   |
| 3   | F     | 700 | NAG  | C2-N2-C7 | -2.21 | 119.72      | 122.94   |
| 3   | F     | 702 | NAG  | C2-N2-C7 | -2.20 | 119.73      | 122.94   |
| 3   | D     | 701 | NAG  | C2-N2-C7 | -2.17 | 119.78      | 122.94   |
| 2   | A     | 600 | GDL  | C3-C2-N1 | -2.16 | 108.79      | 112.29   |
| 2   | E     | 600 | GDL  | C3-C2-N1 | -2.11 | 108.87      | 112.29   |
| 3   | E     | 700 | NAG  | C2-N2-C7 | -2.08 | 119.91      | 122.94   |
| 2   | D     | 600 | GDL  | C3-C2-N1 | -2.07 | 108.93      | 112.29   |
| 2   | C     | 600 | GDL  | C3-C2-N1 | -2.02 | 109.01      | 112.29   |
| 2   | B     | 600 | GDL  | C2-N1-C7 | 2.05  | 124.86      | 122.04   |
| 2   | F     | 600 | GDL  | O5-C5-C4 | 2.08  | 113.45      | 109.72   |
| 2   | C     | 600 | GDL  | O5-C5-C4 | 2.21  | 113.69      | 109.72   |
| 2   | D     | 600 | GDL  | O5-C5-C4 | 2.21  | 113.69      | 109.72   |
| 3   | E     | 700 | NAG  | C3-C4-C5 | 2.59  | 114.88      | 110.24   |
| 2   | A     | 600 | GDL  | O5-C5-C4 | 2.76  | 114.68      | 109.72   |
| 2   | B     | 600 | GDL  | O5-C5-C4 | 2.88  | 114.90      | 109.72   |
| 2   | E     | 600 | GDL  | O5-C5-C4 | 2.98  | 115.08      | 109.72   |
| 2   | E     | 600 | GDL  | O5-C1-O1 | 3.40  | 123.55      | 118.49   |
| 2   | D     | 600 | GDL  | O5-C1-O1 | 3.70  | 123.98      | 118.49   |

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| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 2   | C     | 600 | GDL  | O5-C1-O1 | 3.70 | 123.98      | 118.49   |
| 2   | F     | 600 | GDL  | O5-C1-O1 | 3.74 | 124.06      | 118.49   |
| 2   | B     | 600 | GDL  | O5-C1-O1 | 3.81 | 124.16      | 118.49   |
| 2   | A     | 600 | GDL  | O5-C1-O1 | 3.88 | 124.26      | 118.49   |

There are no chirality outliers.

All (2) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 3   | E     | 701 | NAG  | O7-C7-N2-C2 |
| 3   | D     | 701 | NAG  | O7-C7-N2-C2 |

There are no ring outliers.

19 monomers are involved in 30 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | A     | 700 | NAG  | 2       | 0            |
| 3   | A     | 701 | NAG  | 1       | 0            |
| 3   | A     | 702 | NAG  | 1       | 0            |
| 4   | A     | 800 | EDO  | 2       | 0            |
| 4   | A     | 801 | EDO  | 2       | 0            |
| 3   | B     | 700 | NAG  | 4       | 0            |
| 3   | B     | 701 | NAG  | 2       | 0            |
| 4   | B     | 801 | EDO  | 4       | 0            |
| 3   | C     | 700 | NAG  | 4       | 0            |
| 3   | C     | 701 | NAG  | 3       | 0            |
| 4   | C     | 801 | EDO  | 2       | 0            |
| 3   | D     | 700 | NAG  | 2       | 0            |
| 3   | E     | 700 | NAG  | 2       | 0            |
| 3   | E     | 701 | NAG  | 1       | 0            |
| 4   | E     | 801 | EDO  | 1       | 0            |
| 2   | F     | 600 | GDL  | 1       | 0            |
| 3   | F     | 700 | NAG  | 1       | 0            |
| 3   | F     | 701 | NAG  | 1       | 0            |
| 4   | F     | 800 | EDO  | 1       | 0            |

## 5.7 Other polymers [i](#)

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     | 484/515 (93%)   | -0.04  | 15 (3%) 49 53 | 27, 38, 58, 85        | 0     |
| 1   | B     | 484/515 (93%)   | -0.15  | 10 (2%) 63 67 | 24, 37, 57, 85        | 0     |
| 1   | C     | 484/515 (93%)   | -0.05  | 19 (3%) 39 43 | 27, 38, 67, 88        | 0     |
| 1   | D     | 483/515 (93%)   | -0.03  | 14 (2%) 51 56 | 27, 39, 64, 93        | 0     |
| 1   | E     | 484/515 (93%)   | -0.11  | 16 (3%) 46 49 | 25, 36, 54, 86        | 0     |
| 1   | F     | 484/515 (93%)   | -0.05  | 24 (4%) 29 32 | 28, 39, 66, 90        | 0     |
| All | All   | 2903/3090 (93%) | -0.07  | 98 (3%) 45 48 | 24, 38, 62, 93        | 0     |

All (98) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 554 | GLU  | 13.6 |
| 1   | C     | 554 | GLU  | 10.2 |
| 1   | B     | 554 | GLU  | 9.1  |
| 1   | D     | 317 | ASP  | 7.8  |
| 1   | E     | 315 | LYS  | 7.5  |
| 1   | F     | 317 | ASP  | 7.3  |
| 1   | A     | 317 | ASP  | 6.2  |
| 1   | E     | 317 | ASP  | 6.2  |
| 1   | A     | 553 | HIS  | 5.7  |
| 1   | B     | 317 | ASP  | 5.7  |
| 1   | D     | 315 | LYS  | 4.8  |
| 1   | E     | 316 | LEU  | 4.7  |
| 1   | C     | 553 | HIS  | 4.6  |
| 1   | A     | 316 | LEU  | 4.4  |
| 1   | F     | 554 | GLU  | 4.4  |
| 1   | F     | 553 | HIS  | 4.3  |
| 1   | C     | 317 | ASP  | 4.0  |
| 1   | B     | 316 | LEU  | 3.9  |
| 1   | E     | 553 | HIS  | 3.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 553 | HIS  | 3.8  |
| 1   | D     | 378 | THR  | 3.7  |
| 1   | A     | 107 | GLY  | 3.7  |
| 1   | F     | 372 | ARG  | 3.6  |
| 1   | E     | 311 | SER  | 3.6  |
| 1   | D     | 376 | PHE  | 3.6  |
| 1   | B     | 359 | LYS  | 3.6  |
| 1   | A     | 372 | ARG  | 3.6  |
| 1   | F     | 316 | LEU  | 3.4  |
| 1   | D     | 309 | CYS  | 3.2  |
| 1   | C     | 318 | SER  | 3.2  |
| 1   | A     | 431 | GLU  | 3.2  |
| 1   | C     | 488 | LEU  | 3.2  |
| 1   | F     | 502 | LEU  | 3.2  |
| 1   | E     | 107 | GLY  | 3.2  |
| 1   | C     | 316 | LEU  | 3.0  |
| 1   | D     | 316 | LEU  | 3.0  |
| 1   | E     | 476 | LYS  | 3.0  |
| 1   | A     | 552 | ASN  | 2.9  |
| 1   | E     | 502 | LEU  | 2.9  |
| 1   | C     | 310 | TYR  | 2.9  |
| 1   | B     | 357 | GLU  | 2.8  |
| 1   | D     | 427 | SER  | 2.8  |
| 1   | F     | 509 | VAL  | 2.8  |
| 1   | A     | 359 | LYS  | 2.8  |
| 1   | A     | 376 | PHE  | 2.8  |
| 1   | B     | 311 | SER  | 2.8  |
| 1   | D     | 359 | LYS  | 2.8  |
| 1   | D     | 372 | ARG  | 2.8  |
| 1   | C     | 378 | THR  | 2.7  |
| 1   | F     | 310 | TYR  | 2.7  |
| 1   | F     | 373 | GLN  | 2.6  |
| 1   | E     | 509 | VAL  | 2.6  |
| 1   | F     | 488 | LEU  | 2.6  |
| 1   | A     | 373 | GLN  | 2.6  |
| 1   | C     | 172 | LEU  | 2.6  |
| 1   | F     | 309 | CYS  | 2.5  |
| 1   | B     | 552 | ASN  | 2.5  |
| 1   | C     | 359 | LYS  | 2.5  |
| 1   | F     | 217 | LYS  | 2.5  |
| 1   | E     | 552 | ASN  | 2.5  |
| 1   | F     | 475 | GLN  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 318 | SER  | 2.4  |
| 1   | C     | 369 | ASP  | 2.4  |
| 1   | C     | 233 | VAL  | 2.4  |
| 1   | A     | 426 | ASP  | 2.4  |
| 1   | D     | 303 | LYS  | 2.3  |
| 1   | C     | 427 | SER  | 2.3  |
| 1   | F     | 205 | ILE  | 2.3  |
| 1   | F     | 311 | SER  | 2.3  |
| 1   | F     | 476 | LYS  | 2.3  |
| 1   | D     | 486 | ALA  | 2.3  |
| 1   | F     | 315 | LYS  | 2.3  |
| 1   | B     | 75  | GLU  | 2.3  |
| 1   | E     | 475 | GLN  | 2.3  |
| 1   | A     | 205 | ILE  | 2.3  |
| 1   | B     | 107 | GLY  | 2.2  |
| 1   | C     | 372 | ARG  | 2.2  |
| 1   | D     | 311 | SER  | 2.2  |
| 1   | F     | 107 | GLY  | 2.2  |
| 1   | C     | 205 | ILE  | 2.2  |
| 1   | C     | 309 | CYS  | 2.2  |
| 1   | F     | 54  | PRO  | 2.2  |
| 1   | E     | 310 | TYR  | 2.2  |
| 1   | A     | 174 | THR  | 2.2  |
| 1   | F     | 206 | LEU  | 2.2  |
| 1   | C     | 552 | ASN  | 2.1  |
| 1   | E     | 292 | PRO  | 2.1  |
| 1   | A     | 475 | GLN  | 2.1  |
| 1   | D     | 475 | GLN  | 2.1  |
| 1   | E     | 322 | ILE  | 2.1  |
| 1   | C     | 373 | GLN  | 2.1  |
| 1   | A     | 476 | LYS  | 2.0  |
| 1   | D     | 414 | LYS  | 2.0  |
| 1   | F     | 513 | LEU  | 2.0  |
| 1   | C     | 377 | GLY  | 2.0  |
| 1   | F     | 83  | PRO  | 2.0  |
| 1   | E     | 231 | PHE  | 2.0  |
| 1   | F     | 552 | ASN  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3   | NAG  | B     | 701 | 14/15 | 0.60 | 0.47 | 80,84,87,90                | 0     |
| 3   | NAG  | B     | 702 | 14/15 | 0.67 | 0.40 | 70,72,75,76                | 0     |
| 3   | NAG  | E     | 702 | 14/15 | 0.68 | 0.48 | 77,81,82,83                | 0     |
| 3   | NAG  | C     | 703 | 14/15 | 0.69 | 0.54 | 84,88,90,90                | 0     |
| 3   | NAG  | F     | 702 | 14/15 | 0.70 | 0.52 | 83,88,90,91                | 0     |
| 3   | NAG  | A     | 702 | 14/15 | 0.70 | 0.34 | 64,71,75,78                | 0     |
| 3   | NAG  | A     | 701 | 14/15 | 0.71 | 0.56 | 89,93,95,96                | 0     |
| 3   | NAG  | C     | 701 | 14/15 | 0.72 | 0.56 | 85,88,90,91                | 0     |
| 3   | NAG  | D     | 701 | 14/15 | 0.76 | 0.42 | 81,83,86,88                | 0     |
| 4   | EDO  | C     | 801 | 4/4   | 0.77 | 0.30 | 65,66,67,67                | 0     |
| 3   | NAG  | E     | 701 | 14/15 | 0.78 | 0.46 | 81,84,86,87                | 0     |
| 3   | NAG  | F     | 703 | 14/15 | 0.80 | 0.45 | 79,82,84,84                | 0     |
| 3   | NAG  | F     | 701 | 14/15 | 0.82 | 0.54 | 80,85,88,90                | 0     |
| 3   | NAG  | F     | 700 | 14/15 | 0.84 | 0.25 | 57,60,66,74                | 0     |
| 4   | EDO  | B     | 801 | 4/4   | 0.84 | 0.31 | 61,62,63,65                | 0     |
| 4   | EDO  | A     | 801 | 4/4   | 0.84 | 0.35 | 76,76,76,77                | 0     |
| 3   | NAG  | E     | 700 | 14/15 | 0.85 | 0.26 | 64,67,70,76                | 0     |
| 3   | NAG  | D     | 700 | 14/15 | 0.85 | 0.21 | 64,68,72,77                | 0     |
| 3   | NAG  | B     | 700 | 14/15 | 0.86 | 0.18 | 62,65,69,75                | 0     |
| 3   | NAG  | A     | 700 | 14/15 | 0.88 | 0.17 | 66,70,74,82                | 0     |
| 4   | EDO  | E     | 801 | 4/4   | 0.89 | 0.27 | 65,66,66,67                | 0     |
| 3   | NAG  | C     | 700 | 14/15 | 0.89 | 0.24 | 66,69,74,80                | 0     |
| 2   | GDL  | F     | 600 | 15/15 | 0.90 | 0.10 | 33,38,40,41                | 0     |
| 4   | EDO  | E     | 802 | 4/4   | 0.91 | 0.16 | 30,31,34,38                | 0     |
| 4   | EDO  | C     | 800 | 4/4   | 0.91 | 0.19 | 59,59,59,61                | 0     |
| 4   | EDO  | F     | 801 | 4/4   | 0.91 | 0.31 | 66,67,67,69                | 0     |
| 4   | EDO  | F     | 800 | 4/4   | 0.91 | 0.17 | 48,51,52,56                | 0     |
| 4   | EDO  | E     | 800 | 4/4   | 0.92 | 0.13 | 49,49,49,51                | 0     |
| 2   | GDL  | C     | 600 | 15/15 | 0.93 | 0.10 | 30,34,38,38                | 0     |
| 4   | EDO  | B     | 802 | 4/4   | 0.93 | 0.17 | 30,35,36,38                | 0     |
| 2   | GDL  | E     | 600 | 15/15 | 0.93 | 0.12 | 29,33,34,36                | 0     |
| 2   | GDL  | D     | 600 | 15/15 | 0.94 | 0.11 | 32,34,37,40                | 0     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | GDL  | A     | 600 | 15/15 | 0.94 | 0.10 | 30,32,34,35                 | 0     |
| 2   | GDL  | B     | 600 | 15/15 | 0.95 | 0.10 | 30,33,34,35                 | 0     |
| 4   | EDO  | F     | 802 | 4/4   | 0.95 | 0.17 | 37,38,39,39                 | 0     |
| 4   | EDO  | A     | 802 | 4/4   | 0.96 | 0.17 | 31,38,40,40                 | 0     |
| 4   | EDO  | A     | 800 | 4/4   | 0.97 | 0.11 | 56,57,57,61                 | 0     |
| 4   | EDO  | B     | 800 | 4/4   | 0.97 | 0.12 | 38,38,38,41                 | 0     |
| 4   | EDO  | C     | 802 | 4/4   | 0.98 | 0.08 | 35,36,37,38                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.