# Full wwPDB EM Validation Report ⓘ

Aug 15, 2026 – 07:40 am BST

| | | |
|---|---|---|
| PDB ID | : | 9I3V / pdb_00009i3v |
| EMDB ID | : | EMD-52617 |
| Title | : | Cryo-EM structure of the human LRP2 ectodomain |
| Authors | : | Ramanadane, K.; Coscia, F. |
| Deposited on | : | 2025-01-24 |
| Resolution | : | 3.51 Å(reported) |
| Based on initial model | : | 8EM4 |

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

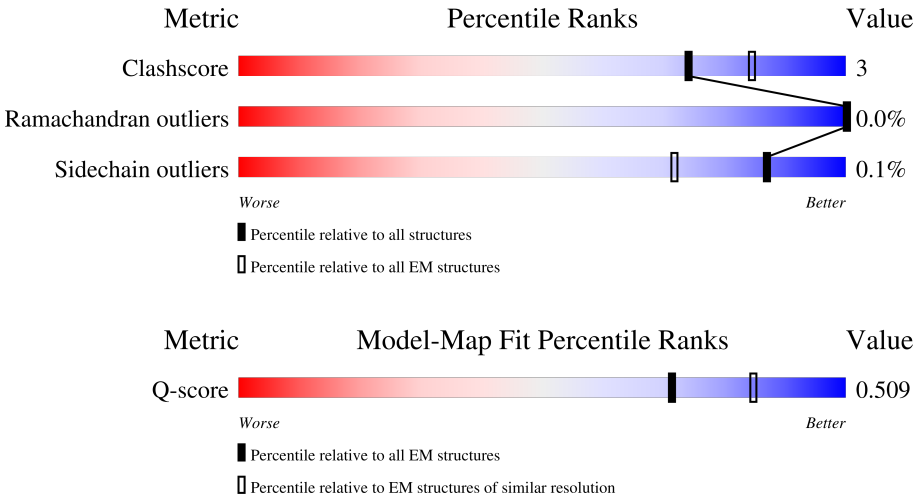
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev133 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| EM percentile statistics | : | 202505.v01 (Using data in the EMDB archive up until May 2025) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.50 |

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.51 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 (#Entries) | EM structures (#Entries) | Similar EM resolution (#Entries, resolution range(Å)) |
|---|---|---|---|
| Clashscore | 229148 | 23984 | - |
| Ramachandran outliers | 224038 | 23583 | - |
| Sidechain outliers | 223484 | 23102 | - |
| Q-score | - | 25397 | 13085 ( 3.01 - 4.01 ) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 4473 | 5% 79% 7% 15% |
| 1 | B | 4473 | 78% 7% 15% |
| 2 | D | 10 | 100% |
| 2 | E | 10 | 100% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 3 | C | 7 | 86% 14% |
| 3 | F | 7 | 100% |
| 3 | J | 7 | 100% |
| 4 | H | 12 | 25% 100% |
| 5 | I | 8 | 100% |
| 6 | G | 13 | 23% 100% |
| 7 | K | 3 | 67% 67% 33% |
| 7 | N | 3 | 33% 67% |
| 7 | O | 3 | 33% 67% |
| 7 | P | 3 | 33% 33% 67% |
| 7 | Q | 3 | 33% 100% |
| 7 | W | 3 | 100% |
| 7 | X | 3 | 33% 100% |
| 8 | L | 2 | 100% |
| 8 | M | 2 | 50% 100% |
| 8 | R | 2 | 100% |
| 8 | S | 2 | 100% 50% 50% |
| 8 | T | 2 | 50% 50% |
| 8 | U | 2 | 100% |
| 8 | V | 2 | 100% |
| 8 | Y | 2 | 100% |

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 |
|---|---|---|---|---|---|---|---|
| 10 | NGA | B | 4511 | X | - | - | - |

# 2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 118041 atoms, of which 56764 are hydrogens and 0 are deuteriums.

In the tables below, 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 Low-density lipoprotein receptor-related protein 2.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 3811 | Total | C | H | N | O | S | 0 | 0 |
| | | | 58095 | 18655 | 28064 | 5256 | 5817 | 303 | | |
| 1 | B | 3804 | Total | C | H | N | O | S | 0 | 0 |
| | | | 57947 | 18608 | 27987 | 5241 | 5808 | 303 | | |

There are 100 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 4424 | GLY | - | expression tag | UNP P98164 |
| A | 4425 | TRP | - | expression tag | UNP P98164 |
| A | 4426 | SER | - | expression tag | UNP P98164 |
| A | 4427 | HIS | - | expression tag | UNP P98164 |
| A | 4428 | PRO | - | expression tag | UNP P98164 |
| A | 4429 | GLN | - | expression tag | UNP P98164 |
| A | 4430 | PHE | - | expression tag | UNP P98164 |
| A | 4431 | GLU | - | expression tag | UNP P98164 |
| A | 4432 | LYS | - | expression tag | UNP P98164 |
| A | 4433 | ALA | - | expression tag | UNP P98164 |
| A | 4434 | GLY | - | expression tag | UNP P98164 |
| A | 4435 | GLY | - | expression tag | UNP P98164 |
| A | 4436 | GLY | - | expression tag | UNP P98164 |
| A | 4437 | SER | - | expression tag | UNP P98164 |
| A | 4438 | GLY | - | expression tag | UNP P98164 |
| A | 4439 | GLY | - | expression tag | UNP P98164 |
| A | 4440 | GLY | - | expression tag | UNP P98164 |
| A | 4441 | SER | - | expression tag | UNP P98164 |
| A | 4442 | GLY | - | expression tag | UNP P98164 |
| A | 4443 | GLY | - | expression tag | UNP P98164 |
| A | 4444 | GLY | - | expression tag | UNP P98164 |
| A | 4445 | SER | - | expression tag | UNP P98164 |
| A | 4446 | TRP | - | expression tag | UNP P98164 |
| A | 4447 | SER | - | expression tag | UNP P98164 |
| A | 4448 | HIS | - | expression tag | UNP P98164 |
| A | 4449 | PRO | - | expression tag | UNP P98164 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 4450 | GLN | - | expression tag | UNP P98164 |
| A | 4451 | PHE | - | expression tag | UNP P98164 |
| A | 4452 | GLU | - | expression tag | UNP P98164 |
| A | 4453 | LYS | - | expression tag | UNP P98164 |
| A | 4454 | GLY | - | expression tag | UNP P98164 |
| A | 4455 | GLY | - | expression tag | UNP P98164 |
| A | 4456 | GLY | - | expression tag | UNP P98164 |
| A | 4457 | SER | - | expression tag | UNP P98164 |
| A | 4458 | GLY | - | expression tag | UNP P98164 |
| A | 4459 | GLY | - | expression tag | UNP P98164 |
| A | 4460 | GLY | - | expression tag | UNP P98164 |
| A | 4461 | SER | - | expression tag | UNP P98164 |
| A | 4462 | GLY | - | expression tag | UNP P98164 |
| A | 4463 | GLY | - | expression tag | UNP P98164 |
| A | 4464 | GLY | - | expression tag | UNP P98164 |
| A | 4465 | SER | - | expression tag | UNP P98164 |
| A | 4466 | TRP | - | expression tag | UNP P98164 |
| A | 4467 | SER | - | expression tag | UNP P98164 |
| A | 4468 | HIS | - | expression tag | UNP P98164 |
| A | 4469 | PRO | - | expression tag | UNP P98164 |
| A | 4470 | GLN | - | expression tag | UNP P98164 |
| A | 4471 | PHE | - | expression tag | UNP P98164 |
| A | 4472 | GLU | - | expression tag | UNP P98164 |
| A | 4473 | LYS | - | expression tag | UNP P98164 |
| B | 4424 | GLY | - | expression tag | UNP P98164 |
| B | 4425 | TRP | - | expression tag | UNP P98164 |
| B | 4426 | SER | - | expression tag | UNP P98164 |
| B | 4427 | HIS | - | expression tag | UNP P98164 |
| B | 4428 | PRO | - | expression tag | UNP P98164 |
| B | 4429 | GLN | - | expression tag | UNP P98164 |
| B | 4430 | PHE | - | expression tag | UNP P98164 |
| B | 4431 | GLU | - | expression tag | UNP P98164 |
| B | 4432 | LYS | - | expression tag | UNP P98164 |
| B | 4433 | ALA | - | expression tag | UNP P98164 |
| B | 4434 | GLY | - | expression tag | UNP P98164 |
| B | 4435 | GLY | - | expression tag | UNP P98164 |
| B | 4436 | GLY | - | expression tag | UNP P98164 |
| B | 4437 | SER | - | expression tag | UNP P98164 |
| B | 4438 | GLY | - | expression tag | UNP P98164 |
| B | 4439 | GLY | - | expression tag | UNP P98164 |
| B | 4440 | GLY | - | expression tag | UNP P98164 |
| B | 4441 | SER | - | expression tag | UNP P98164 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | 4442 | GLY | - | expression tag | UNP P98164 |
| B | 4443 | GLY | - | expression tag | UNP P98164 |
| B | 4444 | GLY | - | expression tag | UNP P98164 |
| B | 4445 | SER | - | expression tag | UNP P98164 |
| B | 4446 | TRP | - | expression tag | UNP P98164 |
| B | 4447 | SER | - | expression tag | UNP P98164 |
| B | 4448 | HIS | - | expression tag | UNP P98164 |
| B | 4449 | PRO | - | expression tag | UNP P98164 |
| B | 4450 | GLN | - | expression tag | UNP P98164 |
| B | 4451 | PHE | - | expression tag | UNP P98164 |
| B | 4452 | GLU | - | expression tag | UNP P98164 |
| B | 4453 | LYS | - | expression tag | UNP P98164 |
| B | 4454 | GLY | - | expression tag | UNP P98164 |
| B | 4455 | GLY | - | expression tag | UNP P98164 |
| B | 4456 | GLY | - | expression tag | UNP P98164 |
| B | 4457 | SER | - | expression tag | UNP P98164 |
| B | 4458 | GLY | - | expression tag | UNP P98164 |
| B | 4459 | GLY | - | expression tag | UNP P98164 |
| B | 4460 | GLY | - | expression tag | UNP P98164 |
| B | 4461 | SER | - | expression tag | UNP P98164 |
| B | 4462 | GLY | - | expression tag | UNP P98164 |
| B | 4463 | GLY | - | expression tag | UNP P98164 |
| B | 4464 | GLY | - | expression tag | UNP P98164 |
| B | 4465 | SER | - | expression tag | UNP P98164 |
| B | 4466 | TRP | - | expression tag | UNP P98164 |
| B | 4467 | SER | - | expression tag | UNP P98164 |
| B | 4468 | HIS | - | expression tag | UNP P98164 |
| B | 4469 | PRO | - | expression tag | UNP P98164 |
| B | 4470 | GLN | - | expression tag | UNP P98164 |
| B | 4471 | PHE | - | expression tag | UNP P98164 |
| B | 4472 | GLU | - | expression tag | UNP P98164 |
| B | 4473 | LYS | - | expression tag | UNP P98164 |

- Molecule 2 is a protein called Unidentified peptide.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 2 | D | 10 | Total | C | N | O | 0 | 0 |
| | | | 50 | 30 | 10 | 10 | | |
| 2 | E | 10 | Total | C | N | O | 0 | 0 |
| | | | 50 | 30 | 10 | 10 | | |

- Molecule 3 is a protein called Unidentified peptide.

| Mol | Chain | Residues | Atoms | AltConf | Trace |
|---|---|---|---|---|---|
| 3 | C | 7 | Total C N O<br>35 21 7 7 | 0 | 0 |
| 3 | F | 7 | Total C N O<br>35 21 7 7 | 0 | 0 |
| 3 | J | 7 | Total C N O<br>35 21 7 7 | 0 | 0 |

- Molecule 4 is a protein called Unidentified peptide.

| Mol | Chain | Residues | Atoms | AltConf | Trace |
|---|---|---|---|---|---|
| 4 | H | 12 | Total C N O<br>60 36 12 12 | 0 | 0 |

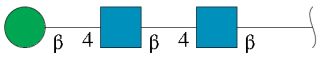
- Molecule 5 is a protein called Unidentified peptide.

| Mol | Chain | Residues | Atoms | AltConf | Trace |
|---|---|---|---|---|---|
| 5 | I | 8 | Total C N O<br>40 24 8 8 | 0 | 0 |

- Molecule 6 is a protein called Unidentified peptide.

| Mol | Chain | Residues | Atoms | AltConf | Trace |
|---|---|---|---|---|---|
| 6 | G | 13 | Total C N O<br>65 39 13 13 | 0 | 0 |

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.




| Mol | Chain | Residues | Atoms | AltConf | Trace |
|---|---|---|---|---|---|
| 7 | K | 3 | Total C H N O<br>76 22 37 2 15 | 0 | 0 |
| 7 | N | 3 | Total C H N O<br>76 22 37 2 15 | 0 | 0 |
| 7 | O | 3 | Total C H N O<br>76 22 37 2 15 | 0 | 0 |
| 7 | P | 3 | Total C H N O<br>76 22 37 2 15 | 0 | 0 |
| 7 | Q | 3 | Total C H N O<br>76 22 37 2 15 | 0 | 0 |

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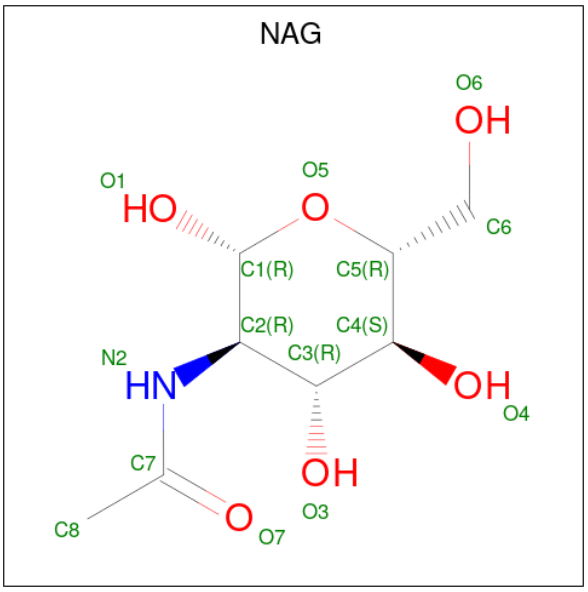
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | W | 3 | Total | C | H | N | O | 0 | 0 |
| | | | 76 | 22 | 37 | 2 | 15 | | |
| 7 | X | 3 | Total | C | H | N | O | 0 | 0 |
| | | | 76 | 22 | 37 | 2 | 15 | | |

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.




| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | L | 2 | Total | C | H | N | O | 0 | 0 |
| | | | 55 | 16 | 27 | 2 | 10 | | |
| 8 | M | 2 | Total | C | H | N | O | 0 | 0 |
| | | | 55 | 16 | 27 | 2 | 10 | | |
| 8 | R | 2 | Total | C | H | N | O | 0 | 0 |
| | | | 55 | 16 | 27 | 2 | 10 | | |
| 8 | S | 2 | Total | C | H | N | O | 0 | 0 |
| | | | 55 | 16 | 27 | 2 | 10 | | |
| 8 | T | 2 | Total | C | H | N | O | 0 | 0 |
| | | | 55 | 16 | 27 | 2 | 10 | | |
| 8 | U | 2 | Total | C | H | N | O | 0 | 0 |
| | | | 55 | 16 | 27 | 2 | 10 | | |
| 8 | V | 2 | Total | C | H | N | O | 0 | 0 |
| | | | 55 | 16 | 27 | 2 | 10 | | |
| 8 | Y | 2 | Total | C | H | N | O | 0 | 0 |
| | | | 55 | 16 | 27 | 2 | 10 | | |

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



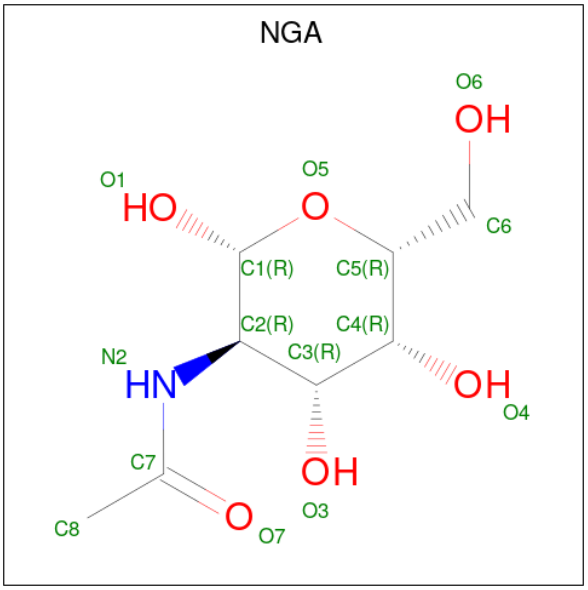

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 9 | A | 1 | Total C H N O<br>28 8 14 1 5 | 0 |
| 9 | A | 1 | Total C H N O<br>28 8 14 1 5 | 0 |
| 9 | A | 1 | Total C H N O<br>28 8 14 1 5 | 0 |
| 9 | A | 1 | Total C H N O<br>28 8 14 1 5 | 0 |
| 9 | A | 1 | Total C H N O<br>28 8 14 1 5 | 0 |
| 9 | A | 1 | Total C H N O<br>28 8 14 1 5 | 0 |
| 9 | A | 1 | Total C H N O<br>28 8 14 1 5 | 0 |
| 9 | A | 1 | Total C H N O<br>28 8 14 1 5 | 0 |
| 9 | A | 1 | Total C H N O<br>28 8 14 1 5 | 0 |
| 9 | A | 1 | Total C N O<br>14 8 1 5 | 0 |
| 9 | A | 1 | Total C N O<br>14 8 1 5 | 0 |
| 9 | B | 1 | Total C H N O<br>28 8 14 1 5 | 0 |
| 9 | B | 1 | Total C H N O<br>28 8 14 1 5 | 0 |
| 9 | B | 1 | Total C H N O<br>28 8 14 1 5 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 9 | B | 1 | Total | C | H | N | O | 0 |
| | | | 28 | 8 | 14 | 1 | 5 | |
| 9 | B | 1 | Total | C | H | N | O | 0 |
| | | | 28 | 8 | 14 | 1 | 5 | |
| 9 | B | 1 | Total | C | H | N | O | 0 |
| | | | 28 | 8 | 14 | 1 | 5 | |
| 9 | B | 1 | Total | C | H | N | O | 0 |
| | | | 28 | 8 | 14 | 1 | 5 | |
| 9 | B | 1 | Total | C | H | N | O | 0 |
| | | | 28 | 8 | 14 | 1 | 5 | |

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-galactopyranose (CCD ID: NGA) (formula: $C_8H_{15}NO_6$).




| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 10 | A | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |
| 10 | A | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |
| 10 | A | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |
| 10 | A | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |
| 10 | B | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |
| 10 | B | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |

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| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 10 | B | 1 | Total C N O<br>14 8 1 5 | 0 |
| 10 | B | 1 | Total C N O<br>14 8 1 5 | 0 |
| 10 | B | 1 | Total C N O<br>14 8 1 5 | 0 |

- Molecule 11 is CALCIUM ION (CCD ID: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 11 | A | 12 | Total Ca<br>12 12 | 0 |
| 11 | B | 13 | Total Ca<br>13 13 | 0 |

- Molecule 12 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 12 | A | 1 | Total Ni<br>1 1 | 0 |
| 12 | B | 1 | Total Ni<br>1 1 | 0 |

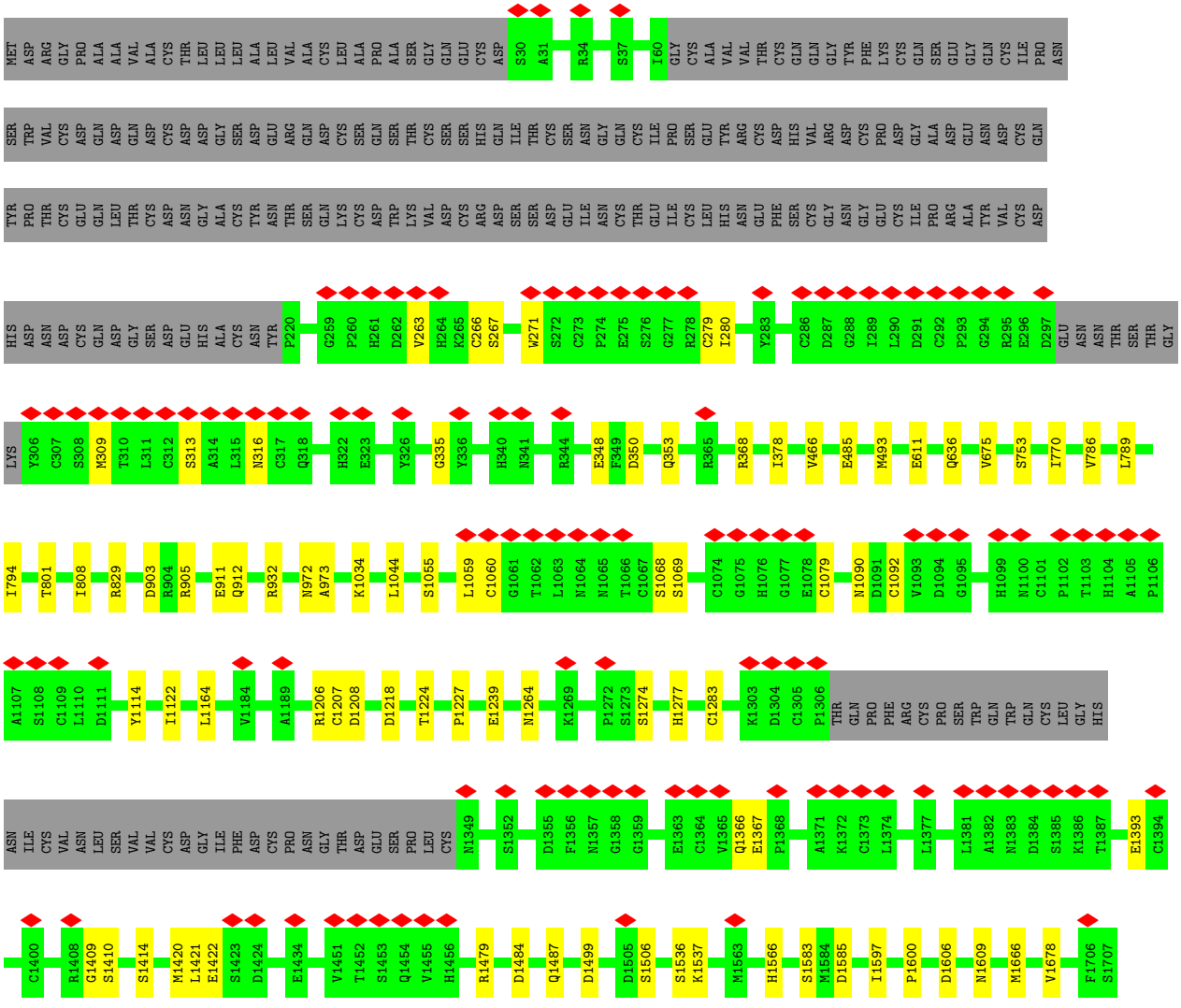
# 3 Residue-property plots (i)

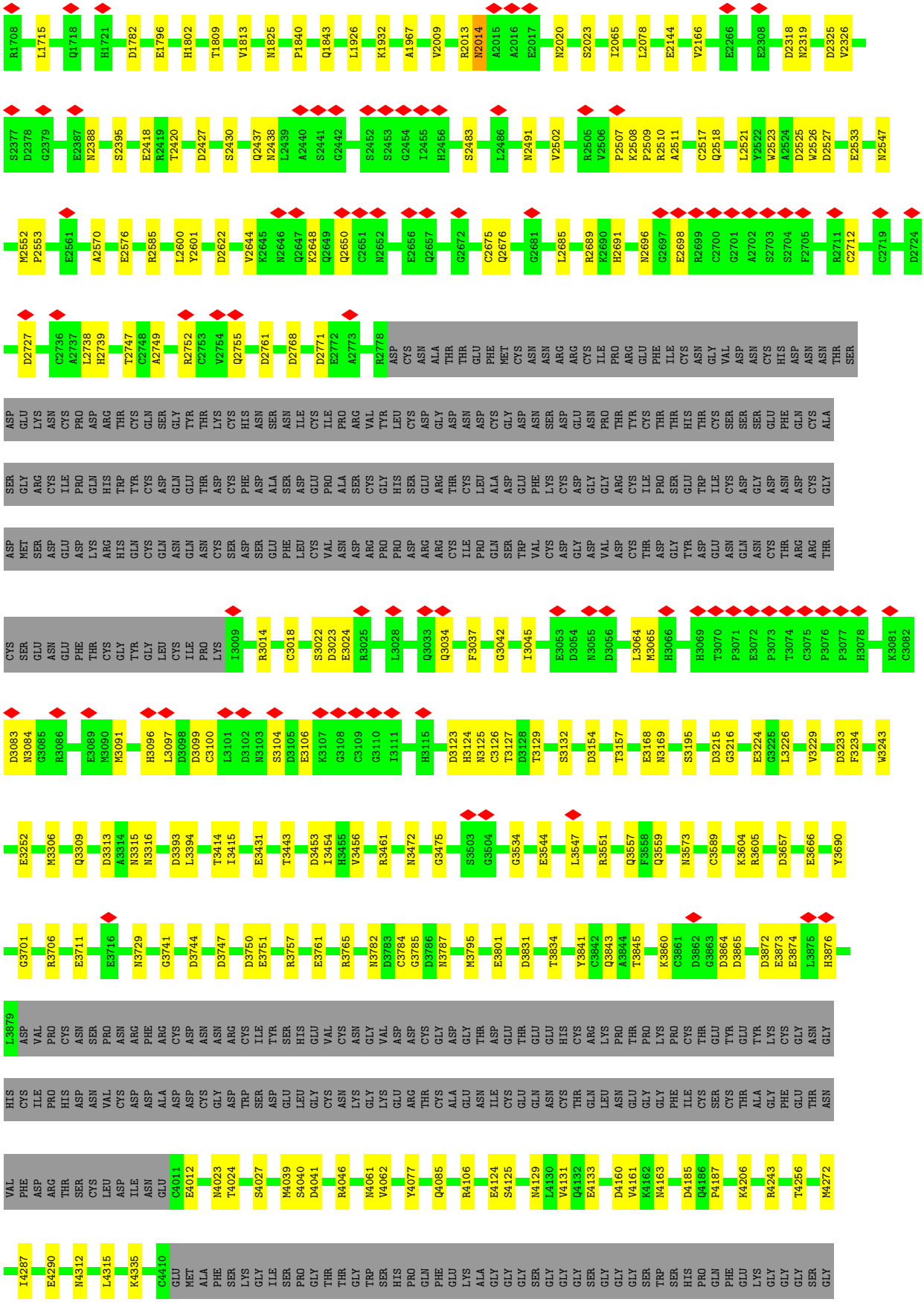
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Low-density lipoprotein receptor-related protein 2

Chain A:



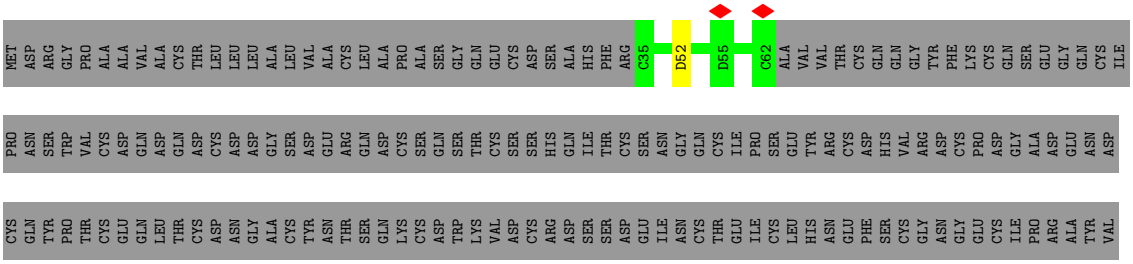

R1708 L1715 Q1718 H1721 D1782 E1796 H1802 T1809 V1813 N1825 P1840 Q1843 L1926 K1932 A1967 V2009 R2013 N2014 A2015 A2016 E2017 N2020 S2023 I2065 L2078 E2144 V2166 E2266 E2308 D2318 N2319 D2325 V2326
S2377 D2378 G2379 E2387 N2388 S2395 E2418 R2419 T2420 D2427 S2430 Q2437 N2438 L2439 A2440 S2441 G2442 S2452 S2453 G2454 I2455 H2456 S2483 L2486 N2491 V2502 R2505 V2506 P2507 K2508 P2509 R2510 A2511 C2517 Q2518 L2521 Y2522 W2523 A2524 D2525 W2526 D2527 E2533 N2547
M2552 P2553 E2561 A2570 E2576 R2585 L2600 Y2601 D2622 V2644 K2645 N2646 Q2647 K2648 Q2649 Q2650 C2651 N2652 E2656 Q2657 G2672 C2675 Q2676 G2681 L2685 R2689 K2690 H2691 N2696 C2697 E2698 R2699 C2700 C2701 A2702 S2703 S2704 F2705 R2711 C2712 C2719 D2724
D2727 C2736 A2737 L2738 H2739 T2747 C2748 A2749 R2752 C2753 V2754 Q2755 D2761 D2768 D2771 E2772 A2773 R2778 ASP CYS ASN ALA THR THR GLU PHE MET CYS ASN ASN ARG ARG CYS ILE PRO ARG GLU PHE ILE CYS ASN GLY VAL ASP ASN ASN ARG CYS ASP GLU ASN PRO THR TYR CYS THR THR HIS THR CYS SER SER SER GLU PHE GLN CYS ALA
SER GLY ARG CYS ILE PRO GLN HIS TRP TYR CYS ASP GLN GLU GLU THR ASP CYS CYS PHE ASP ALA SER ASP GLU GLU PRO ALA SER CYS GLY HIS SER GLU ARG THR CYS LEU ALA ASP GLU PHE LYS CYS ASP GLY GLY ARG CYS ILE PRO SER GLU TRP ILE CYS ASP GLY ASP ASN ASP CYS GLY
ASP MET SER ASP GLU ASP LYS ARG HIS GLN CYS GLN ASN GLN ASN CYS SER ASP SER GLU PHE LEU CYS VAL ASN ASP ARG PRO PRO ASP ARG ARG CYS ILE PRO GLN SER TRP VAL CYS ASP GLY ASP VAL ASP CYS THR ASP GLY TYR ASP GLU ASN GLN ASN CYS THR ARG ARG THR
CYS SER GLU ASN GLU PHE THR CYS GLY TYR GLY LEU CYS ILE PRO LYS I3009 R3014 C3018 S3022 D3023 E3024 R3025 L3028 Q3033 Q3034 F3037 G3042 I3045 E3053 D3054 N3055 D3056 L3064 M3065 H3066 H3069 T3070 P3071 E3072 P3073 T3074 C3075 P3076 P3077 H3078 K3081 C3082
D3083 N3084 G3085 R3086 E3089 M3090 M3091 H3096 L3097 D3098 D3099 C3100 L3101 D3102 N3103 S3104 D3105 E3106 K3107 G3108 C3109 G3110 I3111 H3115 D3123 H3124 N3125 C3126 T3127 D3128 T3129 S3132 D3154 T3157 E3168 N3169 S3195 D3215 G3216 E3224 G3225 L3226 V3229 D3233 F3234 W3243
E3252 M3306 Q3309 D3313 A3314 N3315 N3316 D3393 L3394 T3414 I3415 E3431 T3443 D3453 I3454 H3455 V3456 R3461 N3472 G3475 S3503 G3504 G3534 E3544 L3547 R3551 Q3557 F3558 Q3559 N3573 C3589 K3604 R3605 D3657 E3666 Y3690
G3701 R3706 E3711 E3716 N3729 G3741 D3744 D3747 D3750 E3751 R3757 E3761 R3765 N3782 D3783 C3784 G3785 D3786 N3787 M3795 E3801 D3831 T3834 Y3841 C3842 Q3843 A3844 T3845 K3860 C3861 D3862 G3863 D3864 D3865 D3872 E3873 E3874 L3875 H3876
L3879 ASP VAL PRO CYS ASN SER PRO ASN ARG PHE ARG CYS ASP ASN ASN ARG CYS ILE TYR SER HIS GLU VAL CYS ASN GLY VAL ASP ASP CYS GLY ASP THR ASP GLU THR GLU GLU HIS CYS ARG LYS PRO THR PRO LYS PRO CYS THR GLU TYR GLU TYR LYS CYS GLY GLY ASN
HIS CYS ILE PRO HIS ASP ASN VAL CYS ASP ASP ALA ASP ASP CYS GLY ASP TRP SER ASP GLU LEU GLU GLY CYS ASN LYS GLY VAL LYS GLU ARG THR CYS ALA GLU ASN ILE CYS GLU GLN ASN CYS THR GLN LEU ASN GLU GLY PHE GLU THR ASN
VAL PHE ASP ARG THR SER CYS LEU ASP ILE ASN GLU C4011 E4012 N4023 T4024 S4027 M4039 S4040 D4041 R4046 N4061 V4062 Y4077 Q4085 R4106 E4124 S4125 N4129 L4130 V4131 Q4132 E4133 D4160 V4161 K4162 N4163 D4185 Q4186 P4187 K4206 R4243 T4256 M4272
I4287 E4290 N4312 L4315 K4335 C4410 GLU MET ALA PHE SER LYS GLY ILE SER PRO GLY THR THR GLY TRP SER HIS PRO GLN PHE GLU LYS ALA GLY GLY GLY SER GLY GLY GLY SER GLY GLY GLY SER TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY GLY SER GLY

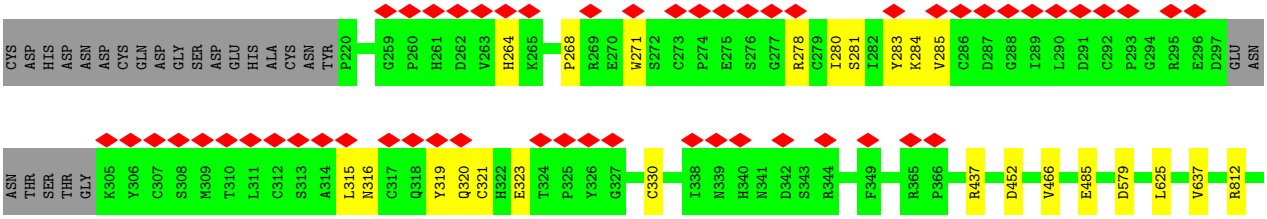



• Molecule 1: Low-density lipoprotein receptor-related protein 2

Chain B:

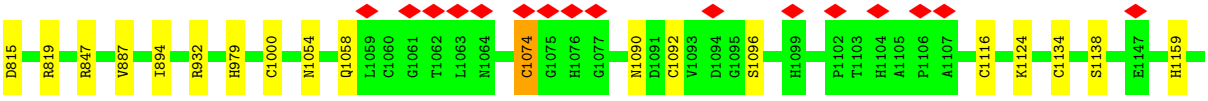


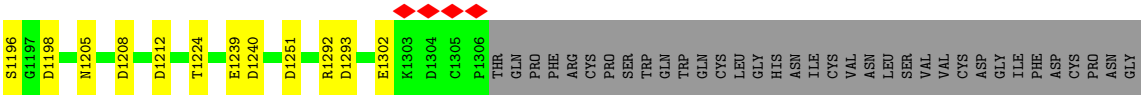



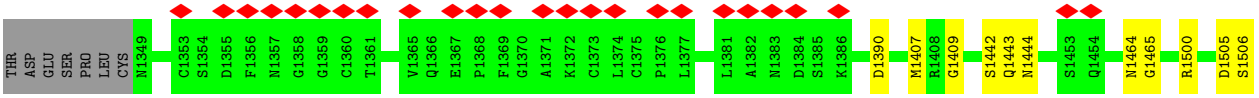



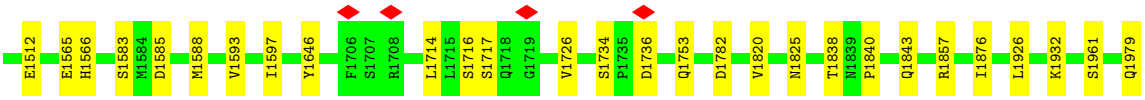


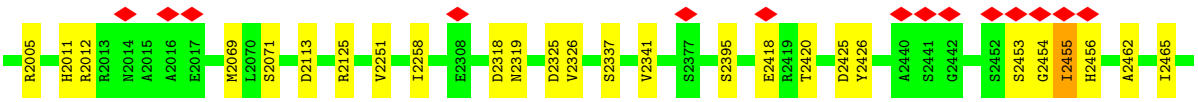


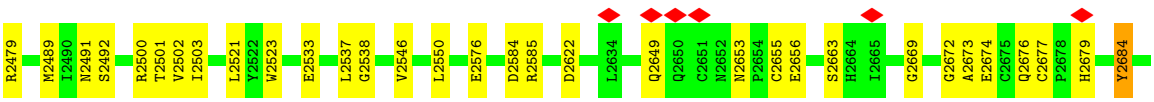


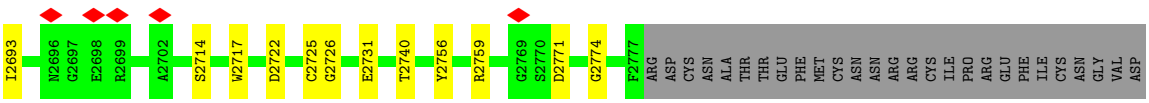



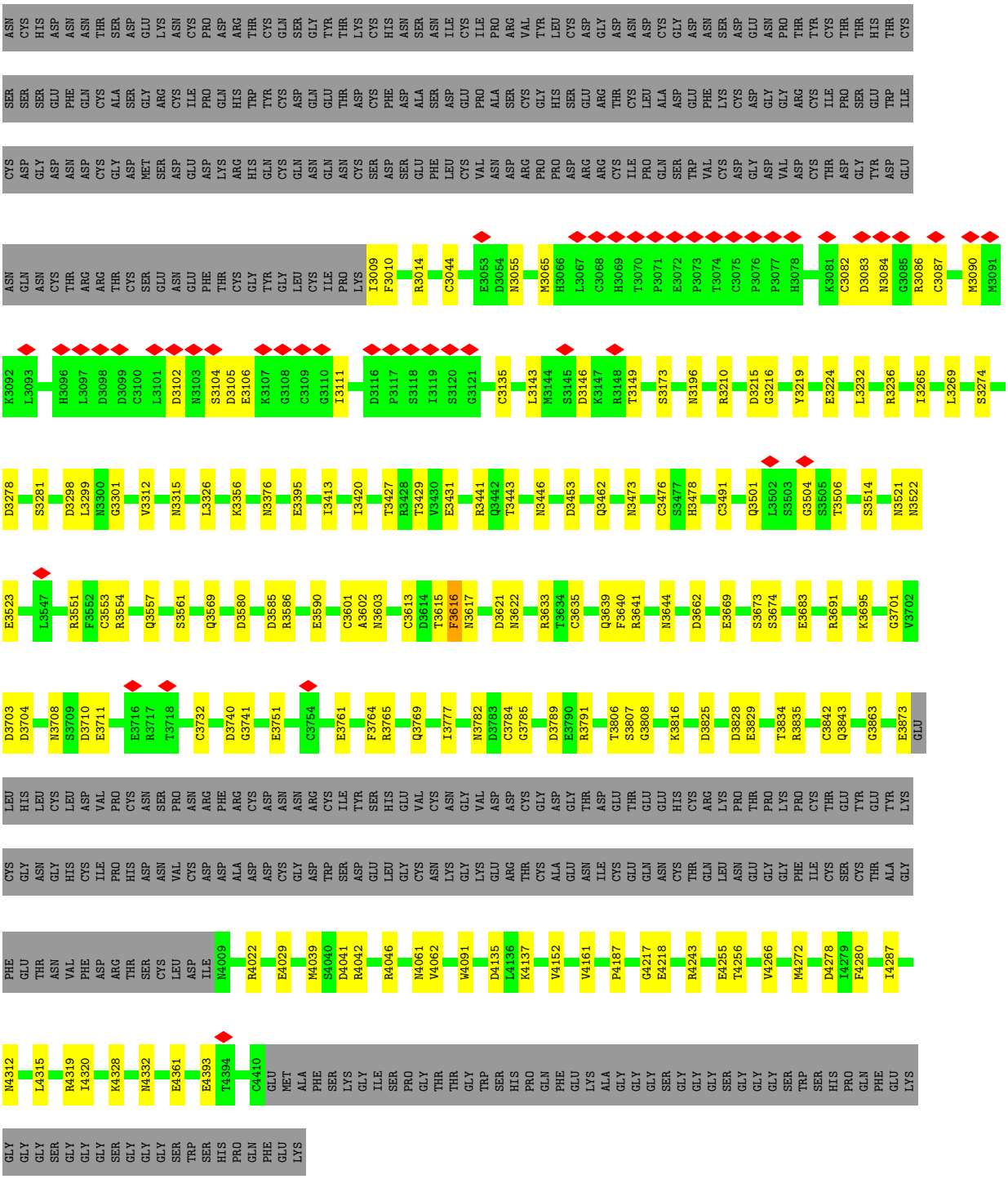



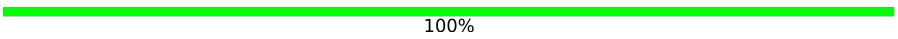





• Molecule 2: Unidentified peptide

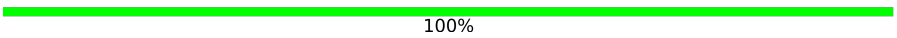
Chain D:




There are no outlier residues recorded for this chain.

• Molecule 2: Unidentified peptide

Chain E:



There are no outlier residues recorded for this chain.

• Molecule 3: Unidentified peptide

Chain C:

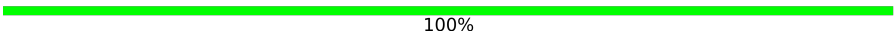






• Molecule 3: Unidentified peptide

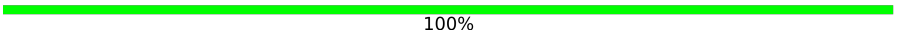
Chain F:




There are no outlier residues recorded for this chain.

• Molecule 3: Unidentified peptide

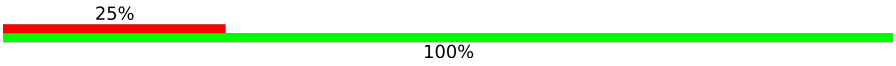
Chain J:

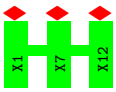



There are no outlier residues recorded for this chain.

• Molecule 4: Unidentified peptide

Chain H:




• Molecule 5: Unidentified peptide

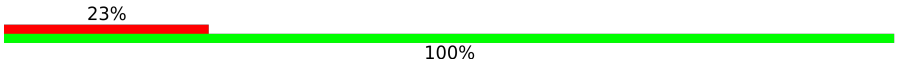
Chain I:

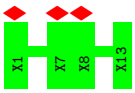



There are no outlier residues recorded for this chain.

• Molecule 6: Unidentified peptide

Chain G:




• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:






• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:







• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:







• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

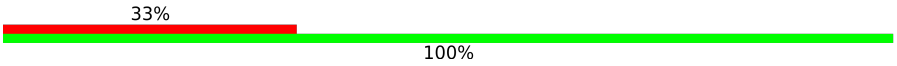






• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:







• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:

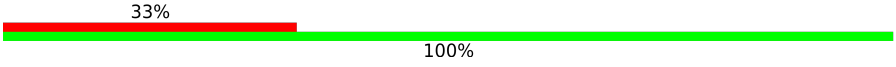






• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

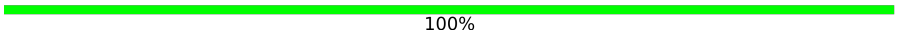
Chain X:






• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

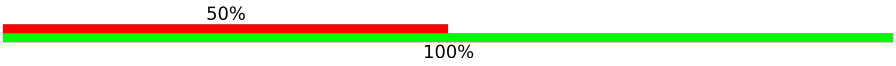






• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:







• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

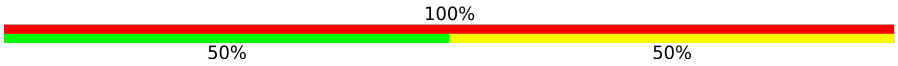






• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:







• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

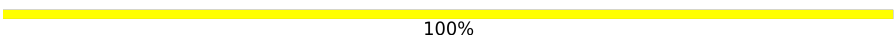






• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:







• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

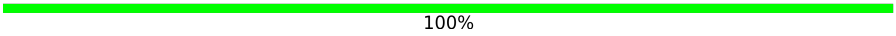






• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:






# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 300645 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | TFS KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 50 | Depositor |
| Minimum defocus (nm) | 750 | Depositor |
| Maximum defocus (nm) | 2000 | Depositor |
| Magnification | Not provided | |
| Image detector | TFS FALCON 4i (4k x 4k) | Depositor |
| Maximum map value | 1.330 | Depositor |
| Minimum map value | -0.312 | Depositor |
| Average map value | 0.001 | Depositor |
| Map value standard deviation | 0.041 | Depositor |
| Recommended contour level | 0.318 | Depositor |
| Map size (Å) | 534.8, 534.8, 534.8 | wwPDB |
| Map dimensions | 560, 560, 560 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.955, 0.955, 0.955 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, CA, NI, NGA

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 | 0.15 | 0/30775 | 0.35 | 2/41803 (0.0%) |
| 1 | B | 0.16 | 0/30701 | 0.37 | 6/41703 (0.0%) |
| All | All | 0.16 | 0/61476 | 0.36 | 8/83506 (0.0%) |

There are no bond length outliers.

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 1224 | THR | CA-C-N | 7.71 | 131.13 | 120.65 |
| 1 | B | 1224 | THR | C-N-CA | 7.71 | 131.13 | 120.65 |
| 1 | A | 2014 | ASN | CA-C-N | 5.89 | 132.30 | 121.70 |
| 1 | A | 2014 | ASN | C-N-CA | 5.89 | 132.30 | 121.70 |
| 1 | B | 2649 | GLN | CA-C-N | 5.71 | 131.97 | 121.70 |
| 1 | B | 2649 | GLN | C-N-CA | 5.71 | 131.97 | 121.70 |
| 1 | B | 3616 | PHE | CA-C-N | 5.71 | 131.97 | 121.70 |
| 1 | B | 3616 | PHE | C-N-CA | 5.71 | 131.97 | 121.70 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 30031 | 28064 | 28143 | 190 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | B | 29960 | 27987 | 28060 | 191 | 0 |
| 2 | D | 50 | 0 | 12 | 0 | 0 |
| 2 | E | 50 | 0 | 13 | 0 | 0 |
| 3 | C | 35 | 0 | 9 | 1 | 0 |
| 3 | F | 35 | 0 | 9 | 0 | 0 |
| 3 | J | 35 | 0 | 10 | 0 | 0 |
| 4 | H | 60 | 0 | 15 | 0 | 0 |
| 5 | I | 40 | 0 | 11 | 0 | 0 |
| 6 | G | 65 | 0 | 16 | 0 | 0 |
| 7 | K | 39 | 37 | 34 | 1 | 0 |
| 7 | N | 39 | 37 | 34 | 1 | 0 |
| 7 | O | 39 | 37 | 34 | 0 | 0 |
| 7 | P | 39 | 37 | 34 | 1 | 0 |
| 7 | Q | 39 | 37 | 34 | 0 | 0 |
| 7 | W | 39 | 37 | 34 | 0 | 0 |
| 7 | X | 39 | 37 | 34 | 0 | 0 |
| 8 | L | 28 | 27 | 25 | 0 | 0 |
| 8 | M | 28 | 27 | 25 | 0 | 0 |
| 8 | R | 28 | 27 | 25 | 0 | 0 |
| 8 | S | 28 | 27 | 25 | 0 | 0 |
| 8 | T | 28 | 27 | 25 | 0 | 0 |
| 8 | U | 28 | 27 | 25 | 1 | 0 |
| 8 | V | 28 | 27 | 25 | 0 | 0 |
| 8 | Y | 28 | 27 | 25 | 0 | 0 |
| 9 | A | 154 | 126 | 143 | 6 | 0 |
| 9 | B | 112 | 112 | 104 | 0 | 0 |
| 10 | A | 56 | 0 | 52 | 4 | 0 |
| 10 | B | 70 | 0 | 65 | 3 | 0 |
| 11 | A | 12 | 0 | 0 | 0 | 0 |
| 11 | B | 13 | 0 | 0 | 0 | 0 |
| 12 | A | 1 | 0 | 0 | 0 | 0 |
| 12 | B | 1 | 0 | 0 | 0 | 0 |
| All | All | 61277 | 56764 | 57100 | 379 | 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 3.

All (379) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:335:GLY:O | 1:A:368:ARG:NH1 | 2.19 | 0.74 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:3278:ASP:OD2 | 1:B:3281:SER:OG | 2.05 | 0.74 |
| 1:A:4163:ASN:OD1 | 1:B:3791:ARG:NH1 | 2.21 | 0.73 |
| 1:B:1961:SER:OG | 1:B:1979:GLN:OE1 | 2.08 | 0.72 |
| 1:A:313:SER:O | 1:A:316:ASN:ND2 | 2.23 | 0.71 |
| 1:B:1782:ASP:OD2 | 1:B:1825:ASN:ND2 | 2.24 | 0.70 |
| 1:B:3842:CYS:SG | 1:B:3843:GLN:N | 2.65 | 0.70 |
| 1:A:3589:CYS:O | 1:A:3604:LYS:NZ | 2.24 | 0.69 |
| 1:A:829:ARG:NH2 | 3:C:4:UNK:O | 2.25 | 0.69 |
| 1:B:3491:CYS:SG | 1:B:3506:THR:OG1 | 2.49 | 0.69 |
| 1:A:3472:ASN:OD1 | 1:A:3475:GLY:N | 2.26 | 0.68 |
| 1:A:4024:THR:O | 1:A:4027:SER:OG | 2.06 | 0.68 |
| 1:A:3551:ARG:NH2 | 1:A:3557:GLN:O | 2.27 | 0.68 |
| 1:A:4160:ASP:OD2 | 1:A:4163:ASN:ND2 | 2.26 | 0.68 |
| 1:B:3829:GLU:OE2 | 1:B:3835:ARG:NH2 | 2.27 | 0.68 |
| 9:A:4510:NAG:H83 | 9:A:4510:NAG:H3 | 1.76 | 0.67 |
| 1:B:1442:SER:OG | 1:B:1443:GLN:OE1 | 2.12 | 0.67 |
| 1:B:316:ASN:OD1 | 1:B:320:GLN:NE2 | 2.28 | 0.67 |
| 1:B:1512:GLU:OE2 | 1:B:1646:TYR:OH | 2.11 | 0.67 |
| 1:A:2675:CYS:SG | 1:A:2676:GLN:N | 2.67 | 0.66 |
| 1:B:3491:CYS:HG | 1:B:3506:THR:HG1 | 1.40 | 0.66 |
| 1:B:3639:GLN:NE2 | 1:B:3640:PHE:O | 2.29 | 0.65 |
| 1:B:4393:GLU:N | 1:B:4393:GLU:OE1 | 2.30 | 0.65 |
| 1:B:3086:ARG:NH1 | 1:B:3087:CYS:O | 2.29 | 0.65 |
| 1:B:2453:SER:O | 1:B:2456:HIS:NE2 | 2.29 | 0.65 |
| 1:A:3224:GLU:OE2 | 1:A:3224:GLU:N | 2.31 | 0.64 |
| 1:B:1205:ASN:ND2 | 1:B:1212:ASP:OD2 | 2.30 | 0.64 |
| 1:B:1565:GLU:OE1 | 1:B:1565:GLU:N | 2.31 | 0.64 |
| 1:A:1274:SER:O | 1:A:1274:SER:OG | 2.16 | 0.64 |
| 1:A:1606:ASP:OD2 | 1:A:1609:ASN:ND2 | 2.32 | 0.63 |
| 1:B:3601:CYS:SG | 1:B:3602:ALA:N | 2.71 | 0.63 |
| 1:A:4312:ASN:ND2 | 1:B:4312:ASN:OD1 | 2.31 | 0.62 |
| 1:B:1566:HIS:ND1 | 1:B:1716:SER:O | 2.32 | 0.62 |
| 1:A:2768:ASP:N | 1:A:2771:ASP:OD1 | 2.32 | 0.62 |
| 1:A:3226:LEU:HD13 | 1:A:3229:VAL:HG11 | 1.82 | 0.62 |
| 1:A:1090:ASN:ND2 | 1:A:1092:CYS:O | 2.33 | 0.61 |
| 1:A:3415:ILE:O | 1:A:3461:ARG:NH1 | 2.33 | 0.61 |
| 1:B:2676:GLN:N | 1:B:2676:GLN:OE1 | 2.34 | 0.61 |
| 1:B:1444:ASN:ND2 | 1:B:1465:GLY:O | 2.33 | 0.61 |
| 1:A:3083:ASP:OD2 | 1:A:3104:SER:OG | 2.18 | 0.61 |
| 1:A:903:ASP:OD2 | 1:A:905:ARG:NH2 | 2.34 | 0.60 |
| 1:A:2418:GLU:OE2 | 1:A:2437:GLN:NE2 | 2.32 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1840:PRO:O | 1:A:1843:GLN:NE2 | 2.33 | 0.60 |
| 1:A:3014:ARG:NE | 1:A:3042:GLY:O | 2.34 | 0.60 |
| 1:A:2648:LYS:O | 1:A:2650:GLN:NE2 | 2.34 | 0.60 |
| 1:A:2013:ARG:O | 1:A:2014:ASN:ND2 | 2.35 | 0.60 |
| 1:A:3657:ASP:OD2 | 1:A:3706:ARG:NH2 | 2.35 | 0.60 |
| 1:A:3091:MET:HE1 | 1:B:3111:ILE:HD11 | 1.84 | 0.59 |
| 1:A:1409:GLY:O | 10:A:4514:NGA:O6 | 2.21 | 0.59 |
| 1:A:3037:PHE:N | 1:A:3045:ILE:O | 2.36 | 0.59 |
| 1:B:1054:ASN:O | 1:B:1058:GLN:N | 2.36 | 0.59 |
| 1:A:4012:GLU:OE2 | 1:A:4023:ASN:ND2 | 2.35 | 0.59 |
| 1:A:2576:GLU:OE2 | 1:A:2585:ARG:NH1 | 2.36 | 0.59 |
| 1:B:3084:ASN:ND2 | 1:B:3102:ASP:OD1 | 2.36 | 0.59 |
| 1:A:1479:ARG:NH2 | 1:A:1499:ASP:OD2 | 2.36 | 0.59 |
| 1:A:4125:SER:OG | 1:A:4129:ASN:OD1 | 2.20 | 0.59 |
| 1:A:3729:ASN:N | 1:A:3747:ASP:OD2 | 2.35 | 0.58 |
| 1:B:1840:PRO:O | 1:B:1843:GLN:NE2 | 2.36 | 0.58 |
| 1:B:3633:ARG:NH2 | 1:B:3635:CYS:SG | 2.76 | 0.58 |
| 1:B:3741:GLY:N | 1:B:3751:GLU:OE1 | 2.37 | 0.58 |
| 1:A:2552:MET:HE3 | 1:A:2552:MET:HA | 1.85 | 0.57 |
| 1:A:4133:GLU:OE1 | 1:A:4133:GLU:N | 2.37 | 0.57 |
| 1:A:1206:ARG:NH1 | 1:A:1218:ASP:O | 2.37 | 0.57 |
| 1:A:2685:LEU:HD13 | 1:A:2696:ASN:OD1 | 2.04 | 0.57 |
| 1:A:3084:ASN:ND2 | 1:A:3100:CYS:O | 2.38 | 0.57 |
| 1:B:3014:ARG:NH2 | 1:B:3044:CYS:SG | 2.78 | 0.57 |
| 1:A:1506:SER:OG | 1:A:1809:THR:O | 2.10 | 0.57 |
| 1:A:2552:MET:HE3 | 1:A:2553:PRO:HD2 | 1.86 | 0.57 |
| 1:A:801:THR:HG22 | 1:A:808:ILE:HG12 | 1.85 | 0.57 |
| 1:A:2738:LEU:O | 1:A:2739:HIS:ND1 | 2.36 | 0.57 |
| 1:B:2501:THR:OG1 | 1:B:2677:CYS:O | 2.23 | 0.56 |
| 1:A:2395:SER:O | 1:A:2420:THR:N | 2.38 | 0.56 |
| 1:A:2420:THR:OG1 | 1:A:2438:ASN:O | 2.22 | 0.56 |
| 1:A:3129:THR:OG1 | 1:A:3132:SER:N | 2.38 | 0.56 |
| 1:B:1116:CYS:SG | 1:B:1138:SER:OG | 2.59 | 0.56 |
| 1:B:1407:MET:N | 1:B:1407:MET:SD | 2.78 | 0.56 |
| 1:A:3831:ASP:OD1 | 1:A:3831:ASP:N | 2.36 | 0.56 |
| 1:A:4039:MET:O | 1:A:4046:ARG:NH1 | 2.38 | 0.56 |
| 1:B:437:ARG:NH1 | 1:B:452:ASP:OD1 | 2.38 | 0.56 |
| 1:A:2689:ARG:O | 1:A:2691:HIS:ND1 | 2.38 | 0.56 |
| 1:B:3673:SER:OG | 1:B:3674:SER:N | 2.38 | 0.56 |
| 1:A:1410:SER:HA | 10:A:4514:NGA:O5 | 2.03 | 0.56 |
| 1:A:2508:LYS:NZ | 1:A:2533:GLU:OE2 | 2.25 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3795:MET:N | 1:A:3795:MET:HE2 | 2.22 | 0.55 |
| 1:A:3573:ASN:O | 1:A:3605:ARG:NH2 | 2.40 | 0.55 |
| 1:B:2454:GLY:O | 1:B:2456:HIS:N | 2.40 | 0.55 |
| 1:B:2546:VAL:HG12 | 1:B:2550:LEU:HD11 | 1.89 | 0.55 |
| 1:B:3764:PHE:HB2 | 1:B:3777:ILE:HD11 | 1.87 | 0.55 |
| 1:B:2722:ASP:N | 1:B:2731:GLU:OE2 | 2.38 | 0.55 |
| 1:A:3125:ASN:HA | 9:A:4528:NAG:O7 | 2.07 | 0.55 |
| 1:A:3782:ASN:OD1 | 1:A:3787:ASN:ND2 | 2.40 | 0.55 |
| 1:B:3173:SER:HA | 10:B:4509:NGA:O5 | 2.03 | 0.55 |
| 1:A:1796:GLU:OE2 | 1:A:1802:HIS:NE2 | 2.40 | 0.55 |
| 1:A:4243:ARG:NH1 | 1:A:4256:THR:OG1 | 2.40 | 0.55 |
| 1:A:1224:THR:HG21 | 10:A:4512:NGA:O7 | 2.07 | 0.55 |
| 1:B:1716:SER:OG | 1:B:1717:SER:N | 2.40 | 0.54 |
| 1:A:1239:GLU:N | 1:A:1239:GLU:OE1 | 2.40 | 0.54 |
| 1:B:3521:ASN:ND2 | 1:B:3523:GLU:OE2 | 2.40 | 0.54 |
| 1:A:3123:ASP:OD1 | 1:A:3124:HIS:N | 2.40 | 0.54 |
| 1:B:3551:ARG:NH2 | 1:B:3557:GLN:O | 2.40 | 0.54 |
| 1:A:4024:THR:N | 1:A:4027:SER:O | 2.40 | 0.54 |
| 1:A:1227:PRO:O | 1:A:3195:SER:OG | 2.24 | 0.54 |
| 1:A:3168:GLU:OE1 | 1:A:3169:ASN:N | 2.40 | 0.54 |
| 1:A:3782:ASN:ND2 | 1:A:3784:CYS:O | 2.41 | 0.54 |
| 7:P:1:NAG:O3 | 7:P:2:NAG:O5 | 2.22 | 0.54 |
| 1:A:2622:ASP:N | 1:A:2622:ASP:OD1 | 2.39 | 0.54 |
| 1:A:4272:MET:SD | 1:A:4272:MET:N | 2.81 | 0.54 |
| 1:A:3666:GLU:OE1 | 1:A:3690:TYR:OH | 2.14 | 0.54 |
| 1:B:2318:ASP:OD1 | 1:B:2319:ASN:N | 2.41 | 0.53 |
| 1:B:3146:ASP:OD2 | 1:B:3149:THR:OG1 | 2.16 | 0.53 |
| 1:A:2526:TRP:CZ2 | 1:A:2552:MET:HE1 | 2.44 | 0.53 |
| 1:A:3018:CYS:SG | 1:A:3022:SER:N | 2.82 | 0.53 |
| 1:B:264:HIS:O | 1:B:278:ARG:NE | 2.42 | 0.53 |
| 1:B:1464:ASN:OD1 | 1:B:1500:ARG:NH1 | 2.40 | 0.53 |
| 1:A:4085:GLN:OE1 | 1:A:4106:ARG:NH2 | 2.42 | 0.53 |
| 1:B:2622:ASP:OD1 | 1:B:2622:ASP:N | 2.40 | 0.53 |
| 1:A:309:MET:HE2 | 1:A:309:MET:HA | 1.91 | 0.53 |
| 1:A:2698:GLU:N | 1:A:2698:GLU:OE1 | 2.42 | 0.53 |
| 1:A:4124:GLU:OE1 | 1:A:4125:SER:N | 2.42 | 0.53 |
| 1:B:1390:ASP:OD1 | 1:B:1409:GLY:N | 2.41 | 0.53 |
| 1:B:2677:CYS:O | 1:B:2679:HIS:ND1 | 2.42 | 0.52 |
| 1:B:2489:MET:SD | 1:B:2491:ASN:ND2 | 2.82 | 0.52 |
| 1:B:3761:GLU:N | 1:B:3761:GLU:OE1 | 2.42 | 0.52 |
| 1:A:1366:GLN:NE2 | 1:A:1367:GLU:O | 2.42 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3761:GLU:N | 1:A:3761:GLU:OE1 | 2.42 | 0.52 |
| 1:B:3633:ARG:O | 1:B:3641:ARG:NH2 | 2.43 | 0.52 |
| 1:A:3034:GLN:OE1 | 1:A:3034:GLN:N | 2.42 | 0.52 |
| 1:A:3860:LYS:N | 1:A:3864:ASP:OD2 | 2.43 | 0.52 |
| 8:U:1:NAG:O3 | 8:U:2:NAG:O5 | 2.25 | 0.52 |
| 1:A:3551:ARG:O | 1:A:3559:GLN:NE2 | 2.41 | 0.52 |
| 1:A:3233:ASP:OD1 | 1:A:3234:PHE:N | 2.42 | 0.52 |
| 1:A:1059:LEU:HD23 | 1:A:1060:CYS:O | 2.09 | 0.52 |
| 1:B:3215:ASP:OD1 | 1:B:3216:GLY:N | 2.43 | 0.52 |
| 1:B:1293:ASP:N | 1:B:1302:GLU:OE2 | 2.41 | 0.51 |
| 1:B:1734:SER:OG | 1:B:1736:ASP:OD1 | 2.23 | 0.51 |
| 1:B:3082:CYS:N | 1:B:3086:ARG:O | 2.43 | 0.51 |
| 1:B:4255:GLU:HG2 | 1:B:4266:VAL:HG22 | 1.91 | 0.51 |
| 1:B:2337:SER:O | 1:B:2341:VAL:HG22 | 2.11 | 0.51 |
| 1:B:3603:ASN:ND2 | 1:B:3622:ASN:OD1 | 2.43 | 0.51 |
| 1:A:2491:ASN:OD1 | 1:A:2502:VAL:HG22 | 2.11 | 0.51 |
| 1:B:1588:MET:HE3 | 1:B:1588:MET:HA | 1.93 | 0.51 |
| 1:B:1714:LEU:HD12 | 1:B:1726:VAL:HG11 | 1.92 | 0.51 |
| 1:B:2425:ASP:OD1 | 1:B:2426:TYR:N | 2.43 | 0.51 |
| 1:B:812:ARG:NH1 | 1:B:815:ASP:OD2 | 2.44 | 0.51 |
| 1:B:3429:THR:HG22 | 1:B:3446:ASN:HB3 | 1.93 | 0.51 |
| 1:A:1583:SER:OG | 1:A:1585:ASP:OD1 | 2.24 | 0.51 |
| 1:A:1926:LEU:HD12 | 1:A:1932:LYS:O | 2.11 | 0.51 |
| 1:B:2653:ASN:ND2 | 1:B:2656:GLU:OE1 | 2.43 | 0.51 |
| 1:B:3621:ASP:OD1 | 1:B:3621:ASP:N | 2.44 | 0.51 |
| 1:B:932:ARG:NH2 | 1:B:1208:ASP:OD2 | 2.44 | 0.51 |
| 1:B:3765:ARG:NH1 | 1:B:3769:GLN:OE1 | 2.44 | 0.51 |
| 1:A:1666:MET:SD | 1:A:1678:VAL:HG22 | 2.51 | 0.51 |
| 1:B:1443:GLN:OE1 | 1:B:1443:GLN:N | 2.44 | 0.50 |
| 1:B:2395:SER:O | 1:B:2420:THR:N | 2.43 | 0.50 |
| 1:B:2523:TRP:NE1 | 1:B:2533:GLU:OE2 | 2.44 | 0.50 |
| 1:B:3196:ASN:OD1 | 1:B:3196:ASN:N | 2.45 | 0.50 |
| 1:B:3478:HIS:NE2 | 1:B:3522:ASN:O | 2.44 | 0.50 |
| 1:A:2318:ASP:OD1 | 1:A:2319:ASN:N | 2.45 | 0.50 |
| 1:B:2714:SER:HG | 1:B:2717:TRP:CD1 | 2.30 | 0.50 |
| 1:A:493:MET:HE1 | 1:A:675:VAL:HG12 | 1.94 | 0.50 |
| 1:B:3616:PHE:HB3 | 1:B:3617:ASN:HA | 1.94 | 0.50 |
| 1:B:3807:SER:OG | 1:B:3808:GLY:N | 2.44 | 0.50 |
| 1:A:911:GLU:OE1 | 1:A:912:GLN:N | 2.45 | 0.49 |
| 1:A:266:CYS:SG | 1:A:267:SER:N | 2.86 | 0.49 |
| 1:A:753:SER:HB3 | 1:A:770:ILE:HD12 | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:285:VAL:HG21 | 1:B:321:CYS:SG | 2.52 | 0.49 |
| 1:B:466:VAL:HG12 | 1:B:485:GLU:OE2 | 2.13 | 0.49 |
| 1:B:3501:GLN:NE2 | 1:B:3504:GLY:O | 2.43 | 0.49 |
| 1:B:3644:ASN:ND2 | 1:B:3662:ASP:OD1 | 2.45 | 0.49 |
| 1:B:2663:SER:O | 1:B:2663:SER:OG | 2.22 | 0.49 |
| 1:A:1277:HIS:ND1 | 1:A:1283:CYS:SG | 2.74 | 0.49 |
| 1:B:3784:CYS:N | 1:B:3789:ASP:OD1 | 2.41 | 0.49 |
| 1:A:3744:ASP:N | 1:A:3750:ASP:OD2 | 2.44 | 0.49 |
| 1:A:3125:ASN:CG | 9:A:4528:NAG:H2 | 2.38 | 0.49 |
| 1:B:3265:ILE:HD11 | 1:B:3301:GLY:HA2 | 1.94 | 0.49 |
| 1:B:1583:SER:OG | 1:B:1585:ASP:OD1 | 2.26 | 0.49 |
| 1:B:3701:GLY:N | 1:B:3711:GLU:OE1 | 2.43 | 0.49 |
| 1:A:2600:LEU:HD23 | 1:A:2601:TYR:N | 2.28 | 0.48 |
| 1:B:2418:GLU:OE1 | 1:B:2418:GLU:N | 2.45 | 0.48 |
| 1:B:3691:ARG:NH1 | 1:B:3704:ASP:O | 2.46 | 0.48 |
| 1:A:3154:ASP:OD2 | 1:A:3157:THR:OG1 | 2.23 | 0.48 |
| 1:A:3843:GLN:OE1 | 1:A:3845:THR:OG1 | 2.31 | 0.48 |
| 1:B:3224:GLU:OE1 | 1:B:3224:GLU:N | 2.46 | 0.48 |
| 1:A:2427:ASP:OD2 | 1:A:2430:SER:OG | 2.31 | 0.48 |
| 1:A:3065:MET:HE2 | 1:A:3065:MET:N | 2.28 | 0.48 |
| 1:A:786:VAL:HG11 | 1:A:789:LEU:HD21 | 1.95 | 0.48 |
| 1:A:1484:ASP:OD2 | 1:A:1487:GLN:NE2 | 2.47 | 0.48 |
| 1:A:2510:ARG:HB2 | 1:A:2526:TRP:H | 1.79 | 0.48 |
| 1:B:3553:CYS:SG | 1:B:3554:ARG:N | 2.86 | 0.48 |
| 1:A:1206:ARG:NH1 | 1:A:1207:CYS:SG | 2.87 | 0.48 |
| 1:A:3701:GLY:N | 1:A:3711:GLU:OE1 | 2.46 | 0.48 |
| 1:B:2113:ASP:OD2 | 1:B:2125:ARG:NH1 | 2.47 | 0.48 |
| 1:B:4091:TRP:O | 1:B:4328:LYS:NZ | 2.43 | 0.48 |
| 7:N:1:NAG:O3 | 7:N:2:NAG:O5 | 2.26 | 0.48 |
| 1:A:3315:ASN:ND2 | 9:A:4510:NAG:H2 | 2.29 | 0.48 |
| 1:A:4077:TYR:O | 1:A:4131:VAL:HG21 | 2.13 | 0.48 |
| 1:A:3023:ASP:OD1 | 1:A:3024:GLU:N | 2.47 | 0.48 |
| 1:B:2491:ASN:OD1 | 1:B:2500:ARG:NH1 | 2.47 | 0.48 |
| 1:B:3585:ASP:OD1 | 1:B:3586:ARG:N | 2.46 | 0.48 |
| 1:A:4290:GLU:OE1 | 1:A:4290:GLU:N | 2.46 | 0.47 |
| 1:A:3215:ASP:OD1 | 1:A:3216:GLY:N | 2.46 | 0.47 |
| 1:A:3872:ASP:OD1 | 1:A:3873:GLU:N | 2.47 | 0.47 |
| 1:B:3828:ASP:OD1 | 1:B:3829:GLU:N | 2.46 | 0.47 |
| 1:A:1034:LYS:HG2 | 1:A:1055:SER:HB3 | 1.96 | 0.47 |
| 1:A:4335:LYS:NZ | 1:B:52:ASP:OD1 | 2.28 | 0.47 |
| 1:B:1240:ASP:OD1 | 1:B:1240:ASP:N | 2.44 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:3683:GLU:O | 1:B:3695:LYS:NZ | 2.46 | 0.47 |
| 1:B:2455:ILE:HG13 | 1:B:2456:HIS:H | 1.80 | 0.47 |
| 1:A:1164:LEU:O | 1:A:1164:LEU:HD23 | 2.14 | 0.47 |
| 1:A:3313:ASP:OD2 | 1:A:3316:ASN:N | 2.48 | 0.47 |
| 1:B:2011:HIS:ND1 | 1:B:2012:ARG:O | 2.46 | 0.47 |
| 1:A:1802:HIS:CE1 | 1:A:1813:VAL:HG22 | 2.50 | 0.47 |
| 1:A:3018:CYS:N | 1:A:3023:ASP:OD2 | 2.48 | 0.47 |
| 1:A:3534:GLY:N | 1:A:3544:GLU:OE1 | 2.46 | 0.47 |
| 1:B:2759:ARG:NH1 | 1:B:2771:ASP:O | 2.47 | 0.47 |
| 1:B:1292:ARG:N | 1:B:1302:GLU:OE2 | 2.47 | 0.47 |
| 1:B:1505:ASP:OD1 | 1:B:1506:SER:N | 2.48 | 0.46 |
| 1:B:4022:ARG:NH1 | 1:B:4029:GLU:OE2 | 2.48 | 0.46 |
| 1:B:4243:ARG:NH1 | 1:B:4256:THR:OG1 | 2.48 | 0.46 |
| 1:B:4152:VAL:O | 1:B:4332:ASN:ND2 | 2.48 | 0.46 |
| 1:A:3801:GLU:OE1 | 1:A:3801:GLU:N | 2.46 | 0.46 |
| 1:A:4023:ASN:OD1 | 1:A:4024:THR:N | 2.48 | 0.46 |
| 1:A:279:CYS:SG | 1:A:280:ILE:N | 2.88 | 0.46 |
| 1:B:3395:GLU:N | 1:B:3395:GLU:OE1 | 2.48 | 0.46 |
| 1:A:1393:GLU:OE2 | 10:A:4514:NGA:O6 | 2.34 | 0.46 |
| 1:A:2388:ASN:ND2 | 1:A:2644:VAL:HG13 | 2.31 | 0.46 |
| 1:A:2508:LYS:HD3 | 1:A:2525:ASP:OD2 | 2.16 | 0.46 |
| 1:A:3315:ASN:CG | 9:A:4510:NAG:H2 | 2.41 | 0.46 |
| 1:B:1239:GLU:OE1 | 1:B:1239:GLU:N | 2.48 | 0.46 |
| 1:B:3376:ASN:OD1 | 1:B:3376:ASN:N | 2.48 | 0.46 |
| 1:B:3312:VAL:HG23 | 1:B:3356:LYS:HB3 | 1.96 | 0.46 |
| 1:A:2517:CYS:SG | 1:A:2518:GLN:N | 2.85 | 0.46 |
| 1:B:2489:MET:HE2 | 1:B:2502:VAL:HG13 | 1.98 | 0.46 |
| 1:B:3009:ILE:HD12 | 1:B:3010:PHE:CZ | 2.50 | 0.46 |
| 1:B:3835:ARG:O | 10:B:4510:NGA:H5 | 2.15 | 0.46 |
| 1:A:1277:HIS:HD1 | 1:A:1283:CYS:HG | 1.49 | 0.46 |
| 1:B:819:ARG:NE | 1:B:1000:CYS:O | 2.44 | 0.46 |
| 1:B:3055:ASN:O | 1:B:3055:ASN:ND2 | 2.49 | 0.46 |
| 1:A:4024:THR:OG1 | 1:A:4027:SER:O | 2.14 | 0.46 |
| 1:B:2479:ARG:NH2 | 1:B:2492:SER:OG | 2.49 | 0.46 |
| 1:A:2521:LEU:HD23 | 1:A:2523:TRP:CE3 | 2.52 | 0.45 |
| 1:B:847:ARG:NH2 | 1:B:1251:ASP:OD2 | 2.49 | 0.45 |
| 1:B:2492:SER:HB3 | 1:B:2503:ILE:HD11 | 1.98 | 0.45 |
| 1:A:2065:ILE:HD11 | 1:A:2078:LEU:CD2 | 2.46 | 0.45 |
| 1:A:3097:LEU:HD23 | 1:A:3099:ASP:N | 2.32 | 0.45 |
| 1:A:2325:ASP:OD1 | 1:A:2326:VAL:N | 2.46 | 0.45 |
| 1:A:3453:ASP:OD1 | 1:A:3454:ILE:N | 2.49 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:2576:GLU:OE1 | 1:B:2585:ARG:NH2 | 2.48 | 0.45 |
| 1:A:1566:HIS:ND1 | 1:A:1715:LEU:HD23 | 2.32 | 0.45 |
| 1:B:3863:GLY:N | 1:B:3873:GLU:OE1 | 2.46 | 0.45 |
| 1:A:3243:TRP:NE1 | 1:A:3252:GLU:OE1 | 2.47 | 0.45 |
| 1:A:3226:LEU:CD1 | 1:A:3229:VAL:HG11 | 2.46 | 0.45 |
| 1:B:3274:SER:O | 1:B:3326:LEU:HD22 | 2.17 | 0.45 |
| 1:A:3306:MET:HE3 | 1:A:3309:GLN:HB3 | 1.99 | 0.45 |
| 1:B:887:VAL:HG22 | 1:B:894:ILE:HG12 | 1.99 | 0.45 |
| 1:A:2507:PRO:HD2 | 1:A:2508:LYS:HZ2 | 1.80 | 0.45 |
| 1:B:3669:GLU:OE1 | 1:B:3669:GLU:N | 2.45 | 0.45 |
| 1:B:4287:ILE:HD12 | 1:B:4315:LEU:HD23 | 1.99 | 0.45 |
| 1:B:3105:ASP:OD1 | 1:B:3106:GLU:N | 2.50 | 0.45 |
| 1:A:3393:ASP:OD1 | 1:A:3394:LEU:N | 2.49 | 0.44 |
| 1:B:2725:CYS:SG | 1:B:2726:GLY:N | 2.90 | 0.44 |
| 1:A:1420:MET:HE1 | 1:A:1422:GLU:OE1 | 2.18 | 0.44 |
| 1:B:2655:CYS:SG | 1:B:2673:ALA:HB1 | 2.57 | 0.44 |
| 1:B:3740:ASP:N | 1:B:3751:GLU:OE1 | 2.51 | 0.44 |
| 1:B:1753:GLN:OE1 | 1:B:2005:ARG:NH2 | 2.51 | 0.44 |
| 1:B:4278:ASP:OD2 | 1:B:4319:ARG:NH1 | 2.50 | 0.44 |
| 1:B:4280:PHE:HB2 | 1:B:4320:ILE:HD13 | 2.00 | 0.44 |
| 1:B:2669:GLY:N | 1:B:2672:GLY:O | 2.49 | 0.44 |
| 1:B:3806:THR:OG1 | 1:B:3825:ASP:OD2 | 2.33 | 0.44 |
| 1:B:4135:ASP:O | 1:B:4137:LYS:NZ | 2.43 | 0.44 |
| 1:A:1782:ASP:OD2 | 1:A:1825:ASN:ND2 | 2.50 | 0.44 |
| 1:B:1593:VAL:CG1 | 1:B:1597:ILE:HD11 | 2.47 | 0.44 |
| 1:A:493:MET:HE1 | 1:A:675:VAL:CG1 | 2.48 | 0.44 |
| 1:A:3414:THR:HG21 | 1:A:3456:VAL:HG23 | 2.00 | 0.44 |
| 1:B:2462:ALA:HB1 | 1:B:2465:ILE:HD11 | 1.99 | 0.44 |
| 1:B:2584:ASP:OD1 | 1:B:2584:ASP:N | 2.51 | 0.44 |
| 1:B:3265:ILE:HG22 | 1:B:3269:LEU:HD11 | 2.00 | 0.44 |
| 1:B:3561:SER:OG | 1:B:3580:ASP:OD2 | 2.36 | 0.44 |
| 1:B:4217:GLY:O | 1:B:4218:GLU:HG3 | 2.17 | 0.44 |
| 1:A:4185:ASP:OD2 | 1:A:4206:LYS:N | 2.50 | 0.44 |
| 1:B:3083:ASP:OD1 | 1:B:3104:SER:OG | 2.28 | 0.44 |
| 1:B:4041:ASP:OD1 | 1:B:4042:ARG:N | 2.51 | 0.44 |
| 1:A:1414:SER:HA | 1:A:1421:LEU:HD21 | 2.00 | 0.44 |
| 1:A:973:ALA:HB1 | 1:B:2756:TYR:OH | 2.17 | 0.43 |
| 1:A:3125:ASN:HA | 9:A:4528:NAG:C7 | 2.47 | 0.43 |
| 1:A:4061:ASN:OD1 | 1:A:4062:VAL:HG23 | 2.18 | 0.43 |
| 1:B:2325:ASP:OD1 | 1:B:2326:VAL:N | 2.46 | 0.43 |
| 1:B:2740:THR:OG1 | 10:B:4513:NGA:H4 | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2527:ASP:OD1 | 1:A:2527:ASP:N | 2.52 | 0.43 |
| 1:A:3757:ARG:O | 1:A:3765:ARG:NH2 | 2.51 | 0.43 |
| 1:B:625:LEU:CD2 | 1:B:637:VAL:HG22 | 2.47 | 0.43 |
| 1:B:3431:GLU:HG2 | 1:B:3443:THR:HG22 | 1.99 | 0.43 |
| 1:A:2552:MET:HG3 | 1:A:2570:ALA:HB3 | 1.99 | 0.43 |
| 1:B:2069:MET:O | 1:B:2071:SER:N | 2.50 | 0.43 |
| 1:A:794:ILE:HG21 | 1:A:972:ASN:OD1 | 2.18 | 0.43 |
| 1:A:2747:THR:HG21 | 1:A:2755:GLN:O | 2.18 | 0.43 |
| 1:A:3126:CYS:SG | 1:A:3127:THR:N | 2.91 | 0.43 |
| 1:B:1838:THR:HG23 | 1:B:1876:ILE:HD12 | 2.01 | 0.43 |
| 1:A:3547:LEU:HD12 | 1:A:3547:LEU:O | 2.17 | 0.43 |
| 1:A:4040:SER:OG | 1:A:4041:ASP:N | 2.52 | 0.43 |
| 1:B:2251:VAL:HG12 | 1:B:2258:ILE:HG12 | 2.00 | 0.43 |
| 1:B:3710:ASP:N | 1:B:3710:ASP:OD1 | 2.52 | 0.43 |
| 1:A:466:VAL:HG12 | 1:A:485:GLU:OE2 | 2.18 | 0.43 |
| 1:B:3065:MET:HE2 | 1:B:3065:MET:C | 2.43 | 0.43 |
| 1:B:3298:ASP:OD1 | 1:B:3299:LEU:N | 2.47 | 0.43 |
| 1:B:3473:ASN:ND2 | 1:B:3476:CYS:O | 2.50 | 0.43 |
| 1:B:4272:MET:SD | 1:B:4272:MET:N | 2.85 | 0.43 |
| 1:A:636:GLN:OE1 | 1:A:636:GLN:N | 2.51 | 0.43 |
| 1:A:2483:SER:OG | 1:A:2511:ALA:O | 2.31 | 0.43 |
| 1:A:2749:ALA:O | 1:A:2752:ARG:N | 2.52 | 0.43 |
| 1:A:3864:ASP:N | 1:A:3873:GLU:OE2 | 2.52 | 0.43 |
| 1:B:3135:CYS:SG | 1:B:3143:LEU:HD11 | 2.59 | 0.43 |
| 1:B:4039:MET:O | 1:B:4046:ARG:NH2 | 2.52 | 0.43 |
| 1:B:284:LYS:NZ | 1:B:323:GLU:OE1 | 2.46 | 0.43 |
| 1:B:2759:ARG:NH2 | 1:B:2774:GLY:O | 2.52 | 0.43 |
| 1:B:3413:ILE:CG2 | 1:B:3420:ILE:HD11 | 2.48 | 0.43 |
| 1:A:348:GLU:OE1 | 1:A:348:GLU:N | 2.49 | 0.43 |
| 1:A:1114:TYR:N | 1:A:1122:ILE:O | 2.49 | 0.43 |
| 1:B:1074:CYS:O | 1:B:1096:SER:OG | 2.30 | 0.43 |
| 1:B:4361:GLU:N | 1:B:4361:GLU:OE1 | 2.51 | 0.43 |
| 1:A:2509:PRO:O | 1:A:2510:ARG:HD3 | 2.19 | 0.42 |
| 1:A:2510:ARG:HG3 | 1:A:2527:ASP:HA | 2.00 | 0.42 |
| 1:B:1926:LEU:HD12 | 1:B:1932:LYS:O | 2.19 | 0.42 |
| 1:B:1090:ASN:ND2 | 1:B:1092:CYS:O | 2.52 | 0.42 |
| 1:B:2538:GLY:N | 1:B:2674:GLU:OE2 | 2.52 | 0.42 |
| 1:B:3427:THR:O | 1:B:3429:THR:HG23 | 2.19 | 0.42 |
| 1:A:3834:THR:HG22 | 1:A:3841:TYR:CZ | 2.54 | 0.42 |
| 1:B:1820:VAL:O | 1:B:1857:ARG:NH1 | 2.53 | 0.42 |
| 1:A:1597:ILE:HD11 | 1:A:1600:PRO:HB3 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:3622:ASN:OD1 | 1:B:3622:ASN:N | 2.51 | 0.42 |
| 1:A:3064:LEU:HA | 1:A:3065:MET:HE2 | 2.00 | 0.42 |
| 1:A:3096:HIS:N | 1:A:3106:GLU:OE1 | 2.49 | 0.42 |
| 1:B:3090:MET:N | 1:B:3090:MET:SD | 2.92 | 0.42 |
| 1:A:932:ARG:NH2 | 1:A:1208:ASP:OD2 | 2.53 | 0.42 |
| 1:A:1068:SER:OG | 1:A:1069:SER:N | 2.52 | 0.42 |
| 1:A:1536:SER:OG | 1:A:1537:LYS:N | 2.53 | 0.42 |
| 1:A:4287:ILE:HD12 | 1:A:4315:LEU:HD23 | 2.02 | 0.42 |
| 1:B:3703:ASP:OD1 | 1:B:3708:ASN:N | 2.52 | 0.42 |
| 1:A:4161:VAL:HG22 | 1:A:4187:PRO:O | 2.19 | 0.42 |
| 1:B:3232:LEU:N | 1:B:3453:ASP:OD2 | 2.46 | 0.42 |
| 1:B:280:ILE:HD12 | 1:B:283:TYR:CZ | 2.55 | 0.42 |
| 1:B:3236:ARG:NH1 | 1:B:3462:GLN:O | 2.53 | 0.42 |
| 1:A:378:ILE:HD11 | 7:K:1:NAG:H82 | 2.02 | 0.42 |
| 1:A:3431:GLU:CG | 1:A:3443:THR:HG22 | 2.50 | 0.42 |
| 1:B:3413:ILE:HG21 | 1:B:3420:ILE:HD11 | 2.02 | 0.42 |
| 1:A:3784:CYS:SG | 1:A:3785:GLY:N | 2.93 | 0.41 |
| 1:B:268:PRO:O | 1:B:281:SER:N | 2.51 | 0.41 |
| 1:A:1044:LEU:HD21 | 1:A:1059:LEU:HD13 | 2.01 | 0.41 |
| 1:A:3741:GLY:N | 1:A:3751:GLU:OE1 | 2.44 | 0.41 |
| 1:A:2526:TRP:CH2 | 1:A:2552:MET:HE1 | 2.54 | 0.41 |
| 1:B:3569:GLN:N | 1:B:3569:GLN:OE1 | 2.54 | 0.41 |
| 1:A:2020:ASN:H | 1:A:2023:SER:HG | 1.67 | 0.41 |
| 1:B:316:ASN:ND2 | 1:B:319:TYR:O | 2.48 | 0.41 |
| 1:B:579:ASP:OD2 | 1:B:1159:HIS:NE2 | 2.49 | 0.41 |
| 1:B:1196:SER:OG | 1:B:1198:ASP:OD1 | 2.35 | 0.41 |
| 1:B:2503:ILE:HG21 | 1:B:2521:LEU:CD1 | 2.50 | 0.41 |
| 1:A:1967:ALA:HB1 | 1:A:2009:VAL:HG23 | 2.03 | 0.41 |
| 1:B:3431:GLU:OE2 | 1:B:3441:ARG:NH2 | 2.54 | 0.41 |
| 1:B:3613:CYS:O | 1:B:3615:THR:HG23 | 2.20 | 0.41 |
| 1:B:3514:SER:OG | 1:B:3590:GLU:O | 2.29 | 0.41 |
| 1:A:1420:MET:HE2 | 1:A:1420:MET:C | 2.45 | 0.41 |
| 1:B:2684:TYR:N | 1:B:2693:ILE:O | 2.51 | 0.41 |
| 1:B:3210:ARG:NE | 1:B:3219:TYR:OH | 2.53 | 0.41 |
| 1:A:263:VAL:HG13 | 1:A:271:TRP:HZ2 | 1.85 | 0.41 |
| 1:A:2523:TRP:NE1 | 1:A:2533:GLU:OE1 | 2.53 | 0.41 |
| 1:A:3874:GLU:OE1 | 1:A:3876:HIS:NE2 | 2.52 | 0.41 |
| 1:B:3782:ASN:ND2 | 1:B:3785:GLY:O | 2.49 | 0.41 |
| 1:A:350:ASP:OD2 | 1:A:353:GLN:NE2 | 2.54 | 0.41 |
| 1:A:2761:ASP:OD2 | 1:B:979:HIS:ND1 | 2.51 | 0.40 |
| 1:A:1264:ASN:OD1 | 1:A:1264:ASN:N | 2.53 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2144:GLU:CD | 1:A:2166:VAL:HG23 | 2.45 | 0.40 |
| 1:A:2547:ASN:OD1 | 1:A:2547:ASN:N | 2.54 | 0.40 |
| 1:B:4161:VAL:HG22 | 1:B:4187:PRO:O | 2.21 | 0.40 |
| 1:A:2712:CYS:SG | 1:A:2727:ASP:N | 2.92 | 0.40 |
| 1:B:316:ASN:ND2 | 1:B:330:CYS:O | 2.54 | 0.40 |
| 1:B:3315:ASN:OD1 | 1:B:3315:ASN:N | 2.54 | 0.40 |
| 1:B:4061:ASN:OD1 | 1:B:4062:VAL:HG23 | 2.22 | 0.40 |
| 1:A:3865:ASP:N | 1:A:3873:GLU:OE2 | 2.53 | 0.40 |
| 1:B:2503:ILE:HG23 | 1:B:2537:LEU:O | 2.21 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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 | 3799/4473 (85%) | 3498 (92%) | 300 (8%) | 1 (0%) | 100 | 100 |
| 1 | B | 3792/4473 (85%) | 3455 (91%) | 335 (9%) | 2 (0%) | 48 | 79 |
| All | All | 7591/8946 (85%) | 6953 (92%) | 635 (8%) | 3 (0%) | 100 | 100 |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 3816 | LYS |
| 1 | B | 2455 | ILE |
| 1 | A | 611 | GLU |

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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 | 3356/3934 (85%) | 3355 (100%) | 1 (0%) | 100 100 |
| 1 | B | 3348/3934 (85%) | 3340 (100%) | 8 (0%) | 87 85 |
| All | All | 6704/7868 (85%) | 6695 (100%) | 9 (0%) | 87 87 |

All (9) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1079 | CYS |
| 1 | B | 271 | TRP |
| 1 | B | 315 | LEU |
| 1 | B | 1074 | CYS |
| 1 | B | 1124 | LYS |
| 1 | B | 1134 | CYS |
| 1 | B | 2684 | TYR |
| 1 | B | 3732 | CYS |
| 1 | B | 3834 | THR |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 238 | ASN |
| 1 | A | 678 | HIS |
| 1 | A | 912 | GLN |
| 1 | A | 925 | HIS |
| 1 | A | 1090 | ASN |
| 1 | A | 1142 | ASN |
| 1 | A | 1150 | GLN |
| 1 | A | 1263 | HIS |
| 1 | A | 1522 | ASN |
| 1 | A | 1697 | GLN |
| 1 | A | 1711 | HIS |
| 1 | A | 2211 | GLN |
| 1 | A | 2376 | GLN |
| 1 | A | 3078 | HIS |
| 1 | A | 3577 | ASN |
| 1 | A | 3738 | GLN |
| 1 | A | 3787 | ASN |
| 1 | A | 4273 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 4283 | GLN |
| 1 | B | 264 | HIS |
| 1 | B | 320 | GLN |
| 1 | B | 410 | HIS |
| 1 | B | 508 | ASN |
| 1 | B | 656 | GLN |
| 1 | B | 1010 | HIS |
| 1 | B | 1076 | HIS |
| 1 | B | 1264 | ASN |
| 1 | B | 1456 | HIS |
| 1 | B | 1825 | ASN |
| 1 | B | 1843 | GLN |
| 1 | B | 2211 | GLN |
| 1 | B | 2438 | ASN |
| 1 | B | 3342 | HIS |
| 1 | B | 3557 | GLN |
| 1 | B | 3799 | HIS |
| 1 | B | 4013 | GLN |
| 1 | B | 4273 | ASN |
| 1 | B | 4388 | ASN |

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates (i)

37 monosaccharides 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 | $\#\|Z\|>2$ |
| 7 | NAG | K | 1 | 1,7 | 14,14,15 | 0.26 | 0 | 17,19,21 | 0.68 | 0 |
| 7 | NAG | K | 2 | 7 | 14,14,15 | 0.43 | 0 | 17,19,21 | 0.70 | 0 |
| 7 | BMA | K | 3 | 7 | 11,11,12 | 0.64 | 0 | 15,15,17 | 0.77 | 0 |
| 8 | NAG | L | 1 | 1,8 | 14,14,15 | 0.27 | 0 | 17,19,21 | 0.42 | 0 |
| 8 | NAG | L | 2 | 8 | 14,14,15 | 0.18 | 0 | 17,19,21 | 0.40 | 0 |
| 8 | NAG | M | 1 | 1,8 | 14,14,15 | 0.33 | 0 | 17,19,21 | 0.75 | 0 |
| 8 | NAG | M | 2 | 8 | 14,14,15 | 0.25 | 0 | 17,19,21 | 0.41 | 0 |
| 7 | NAG | N | 1 | 1,7 | 14,14,15 | 0.22 | 0 | 17,19,21 | 0.59 | 0 |
| 7 | NAG | N | 2 | 7 | 14,14,15 | 0.22 | 0 | 17,19,21 | 0.42 | 0 |
| 7 | BMA | N | 3 | 7 | 11,11,12 | 0.54 | 0 | 15,15,17 | 0.72 | 0 |
| 7 | NAG | O | 1 | 1,7 | 14,14,15 | 0.41 | 0 | 17,19,21 | 0.63 | 0 |
| 7 | NAG | O | 2 | 7 | 14,14,15 | 0.28 | 0 | 17,19,21 | 0.83 | 1 (5%) |
| 7 | BMA | O | 3 | 7 | 11,11,12 | 0.71 | 0 | 15,15,17 | 1.21 | 2 (13%) |
| 7 | NAG | P | 1 | 1,7 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.59 | 0 |
| 7 | NAG | P | 2 | 7 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.49 | 0 |
| 7 | BMA | P | 3 | 7 | 11,11,12 | 0.53 | 0 | 15,15,17 | 0.78 | 0 |
| 7 | NAG | Q | 1 | 1,7 | 14,14,15 | 0.43 | 0 | 17,19,21 | 0.47 | 0 |
| 7 | NAG | Q | 2 | 7 | 14,14,15 | 0.20 | 0 | 17,19,21 | 0.67 | 0 |
| 7 | BMA | Q | 3 | 7 | 11,11,12 | 0.58 | 0 | 15,15,17 | 0.73 | 0 |
| 8 | NAG | R | 1 | 1,8 | 14,14,15 | 0.44 | 0 | 17,19,21 | 0.62 | 0 |
| 8 | NAG | R | 2 | 8 | 14,14,15 | 0.33 | 0 | 17,19,21 | 0.52 | 0 |
| 8 | NAG | S | 1 | 1,8 | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.53 | 0 |
| 8 | NAG | S | 2 | 8 | 14,14,15 | 0.35 | 0 | 17,19,21 | 0.66 | 1 (5%) |
| 8 | NAG | T | 1 | 1,8 | 14,14,15 | 0.16 | 0 | 17,19,21 | 0.75 | 1 (5%) |
| 8 | NAG | T | 2 | 8 | 14,14,15 | 0.22 | 0 | 17,19,21 | 0.51 | 0 |
| 8 | NAG | U | 1 | 1,8 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.39 | 0 |
| 8 | NAG | U | 2 | 8 | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.50 | 0 |
| 8 | NAG | V | 1 | 1,8 | 14,14,15 | 0.27 | 0 | 17,19,21 | 0.40 | 0 |
| 8 | NAG | V | 2 | 8 | 14,14,15 | 0.19 | 0 | 17,19,21 | 0.39 | 0 |
| 7 | NAG | W | 1 | 1,7 | 14,14,15 | 0.22 | 0 | 17,19,21 | 0.56 | 0 |
| 7 | NAG | W | 2 | 7 | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.44 | 0 |
| 7 | BMA | W | 3 | 7 | 11,11,12 | 0.53 | 0 | 15,15,17 | 0.71 | 0 |
| 7 | NAG | X | 1 | 1,7 | 14,14,15 | 0.35 | 0 | 17,19,21 | 0.45 | 0 |
| 7 | NAG | X | 2 | 7 | 14,14,15 | 0.26 | 0 | 17,19,21 | 0.51 | 0 |
| 7 | BMA | X | 3 | 7 | 11,11,12 | 0.53 | 0 | 15,15,17 | 0.71 | 0 |
| 8 | NAG | Y | 1 | 1,8 | 14,14,15 | 0.54 | 0 | 17,19,21 | 0.59 | 0 |
| 8 | NAG | Y | 2 | 8 | 14,14,15 | 0.23 | 0 | 17,19,21 | 0.49 | 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 |
|---|---|---|---|---|---|---|---|
| 7 | NAG | K | 1 | 1,7 | - | 2/6/23/26 | 0/1/1/1 |
| 7 | NAG | K | 2 | 7 | - | 2/6/23/26 | 0/1/1/1 |
| 7 | BMA | K | 3 | 7 | - | 0/2/19/22 | 0/1/1/1 |
| 8 | NAG | L | 1 | 1,8 | - | 2/6/23/26 | 0/1/1/1 |
| 8 | NAG | L | 2 | 8 | - | 0/6/23/26 | 0/1/1/1 |
| 8 | NAG | M | 1 | 1,8 | - | 3/6/23/26 | 0/1/1/1 |
| 8 | NAG | M | 2 | 8 | - | 0/6/23/26 | 0/1/1/1 |
| 7 | NAG | N | 1 | 1,7 | - | 3/6/23/26 | 0/1/1/1 |
| 7 | NAG | N | 2 | 7 | - | 2/6/23/26 | 0/1/1/1 |
| 7 | BMA | N | 3 | 7 | - | 1/2/19/22 | 0/1/1/1 |
| 7 | NAG | O | 1 | 1,7 | - | 3/6/23/26 | 0/1/1/1 |
| 7 | NAG | O | 2 | 7 | - | 1/6/23/26 | 0/1/1/1 |
| 7 | BMA | O | 3 | 7 | - | 0/2/19/22 | 0/1/1/1 |
| 7 | NAG | P | 1 | 1,7 | - | 1/6/23/26 | 0/1/1/1 |
| 7 | NAG | P | 2 | 7 | - | 3/6/23/26 | 0/1/1/1 |
| 7 | BMA | P | 3 | 7 | - | 0/2/19/22 | 0/1/1/1 |
| 7 | NAG | Q | 1 | 1,7 | - | 1/6/23/26 | 0/1/1/1 |
| 7 | NAG | Q | 2 | 7 | - | 0/6/23/26 | 0/1/1/1 |
| 7 | BMA | Q | 3 | 7 | - | 0/2/19/22 | 0/1/1/1 |
| 8 | NAG | R | 1 | 1,8 | - | 0/6/23/26 | 0/1/1/1 |
| 8 | NAG | R | 2 | 8 | - | 0/6/23/26 | 0/1/1/1 |
| 8 | NAG | S | 1 | 1,8 | - | 1/6/23/26 | 0/1/1/1 |
| 8 | NAG | S | 2 | 8 | - | 3/6/23/26 | 0/1/1/1 |
| 8 | NAG | T | 1 | 1,8 | - | 3/6/23/26 | 0/1/1/1 |
| 8 | NAG | T | 2 | 8 | - | 3/6/23/26 | 0/1/1/1 |
| 8 | NAG | U | 1 | 1,8 | - | 2/6/23/26 | 0/1/1/1 |
| 8 | NAG | U | 2 | 8 | - | 3/6/23/26 | 0/1/1/1 |
| 8 | NAG | V | 1 | 1,8 | - | 0/6/23/26 | 0/1/1/1 |
| 8 | NAG | V | 2 | 8 | - | 2/6/23/26 | 0/1/1/1 |
| 7 | NAG | W | 1 | 1,7 | - | 3/6/23/26 | 0/1/1/1 |
| 7 | NAG | W | 2 | 7 | - | 2/6/23/26 | 0/1/1/1 |
| 7 | BMA | W | 3 | 7 | - | 0/2/19/22 | 0/1/1/1 |
| 7 | NAG | X | 1 | 1,7 | - | 0/6/23/26 | 0/1/1/1 |
| 7 | NAG | X | 2 | 7 | - | 3/6/23/26 | 0/1/1/1 |
| 7 | BMA | X | 3 | 7 | - | 0/2/19/22 | 0/1/1/1 |
| 8 | NAG | Y | 1 | 1,8 | - | 2/6/23/26 | 0/1/1/1 |
| 8 | NAG | Y | 2 | 8 | - | 1/6/23/26 | 0/1/1/1 |

There are no bond length outliers.

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | T | 1 | NAG | C1-O5-C5 | 2.40 | 115.45 | 112.19 |
| 7 | O | 3 | BMA | C1-C2-C3 | 2.21 | 112.39 | 109.67 |
| 8 | S | 2 | NAG | C1-O5-C5 | 2.06 | 114.98 | 112.19 |
| 7 | O | 3 | BMA | O5-C1-C2 | 2.05 | 113.93 | 110.77 |
| 7 | O | 2 | NAG | C1-O5-C5 | 2.01 | 114.91 | 112.19 |

There are no chirality outliers.

All (52) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 8 | L | 1 | NAG | C4-C5-C6-O6 |
| 8 | M | 1 | NAG | C4-C5-C6-O6 |
| 7 | N | 2 | NAG | C4-C5-C6-O6 |
| 7 | O | 1 | NAG | C4-C5-C6-O6 |
| 7 | K | 2 | NAG | O5-C5-C6-O6 |
| 7 | W | 2 | NAG | O5-C5-C6-O6 |
| 7 | P | 2 | NAG | C4-C5-C6-O6 |
| 8 | U | 2 | NAG | C4-C5-C6-O6 |
| 8 | V | 2 | NAG | O5-C5-C6-O6 |
| 8 | Y | 1 | NAG | O5-C5-C6-O6 |
| 7 | X | 2 | NAG | O5-C5-C6-O6 |
| 7 | O | 1 | NAG | O5-C5-C6-O6 |
| 7 | W | 2 | NAG | C4-C5-C6-O6 |
| 8 | T | 1 | NAG | O5-C5-C6-O6 |
| 8 | T | 2 | NAG | O5-C5-C6-O6 |
| 8 | L | 1 | NAG | O5-C5-C6-O6 |
| 8 | M | 1 | NAG | O5-C5-C6-O6 |
| 8 | U | 2 | NAG | O5-C5-C6-O6 |
| 7 | N | 2 | NAG | O5-C5-C6-O6 |
| 7 | P | 2 | NAG | O5-C5-C6-O6 |
| 8 | S | 2 | NAG | O5-C5-C6-O6 |
| 8 | S | 2 | NAG | C4-C5-C6-O6 |
| 7 | K | 2 | NAG | C4-C5-C6-O6 |
| 8 | T | 1 | NAG | C4-C5-C6-O6 |
| 8 | V | 2 | NAG | C4-C5-C6-O6 |
| 7 | W | 1 | NAG | O5-C5-C6-O6 |
| 8 | U | 1 | NAG | O5-C5-C6-O6 |
| 8 | T | 2 | NAG | C4-C5-C6-O6 |
| 7 | X | 2 | NAG | C4-C5-C6-O6 |
| 8 | Y | 1 | NAG | C4-C5-C6-O6 |
| 7 | N | 1 | NAG | O5-C5-C6-O6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 7 | K | 1 | NAG | O5-C5-C6-O6 |
| 7 | K | 1 | NAG | C4-C5-C6-O6 |
| 7 | W | 1 | NAG | C4-C5-C6-O6 |
| 8 | U | 1 | NAG | C4-C5-C6-O6 |
| 7 | N | 3 | BMA | O5-C5-C6-O6 |
| 7 | Q | 1 | NAG | O5-C5-C6-O6 |
| 7 | N | 1 | NAG | C4-C5-C6-O6 |
| 7 | N | 1 | NAG | C3-C2-N2-C7 |
| 7 | O | 1 | NAG | C3-C2-N2-C7 |
| 7 | P | 1 | NAG | C3-C2-N2-C7 |
| 7 | P | 2 | NAG | C3-C2-N2-C7 |
| 7 | W | 1 | NAG | C3-C2-N2-C7 |
| 7 | X | 2 | NAG | C3-C2-N2-C7 |
| 8 | S | 1 | NAG | C3-C2-N2-C7 |
| 8 | S | 2 | NAG | C3-C2-N2-C7 |
| 8 | T | 1 | NAG | C3-C2-N2-C7 |
| 8 | T | 2 | NAG | C3-C2-N2-C7 |
| 8 | U | 2 | NAG | C3-C2-N2-C7 |
| 8 | Y | 2 | NAG | C3-C2-N2-C7 |
| 7 | O | 2 | NAG | C4-C5-C6-O6 |
| 8 | M | 1 | NAG | C3-C2-N2-C7 |

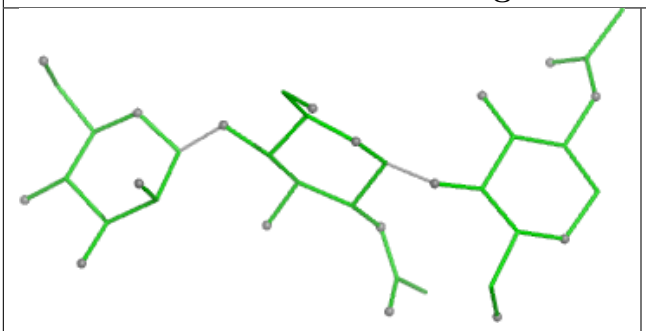
There are no ring outliers.

7 monomers are involved in 4 short contacts:

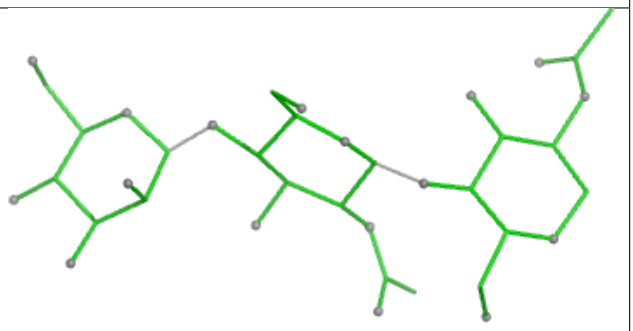
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 8 | U | 2 | NAG | 1 | 0 |
| 7 | N | 2 | NAG | 1 | 0 |
| 7 | N | 1 | NAG | 1 | 0 |
| 7 | K | 1 | NAG | 1 | 0 |
| 8 | U | 1 | NAG | 1 | 0 |
| 7 | P | 2 | NAG | 1 | 0 |
| 7 | P | 1 | NAG | 1 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

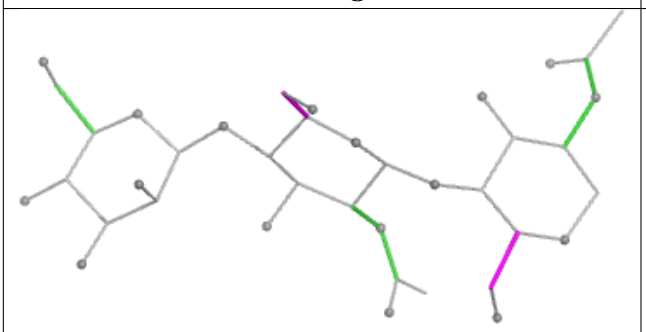
## Oligosaccharide Chain K



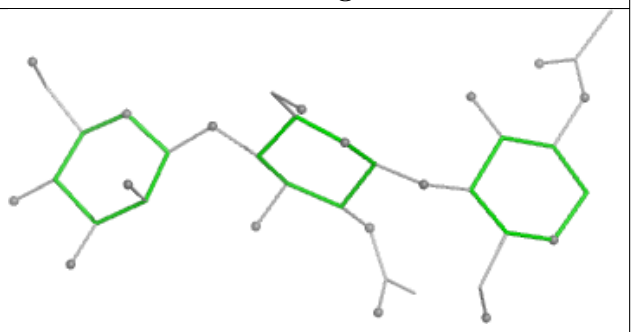
Bond lengths



Bond angles

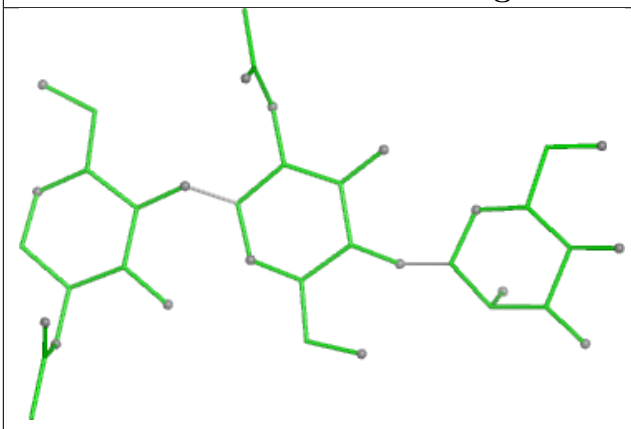


Torsions

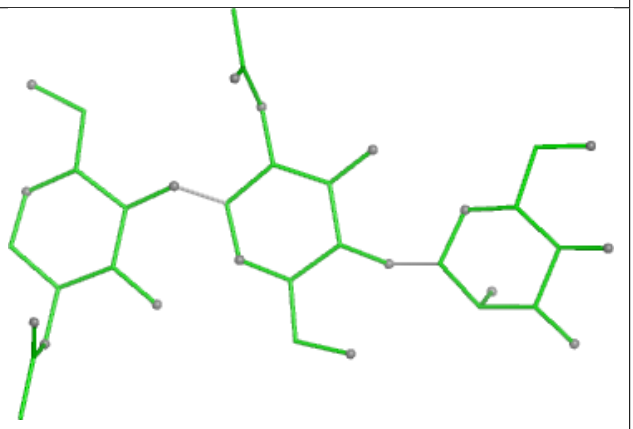


Rings

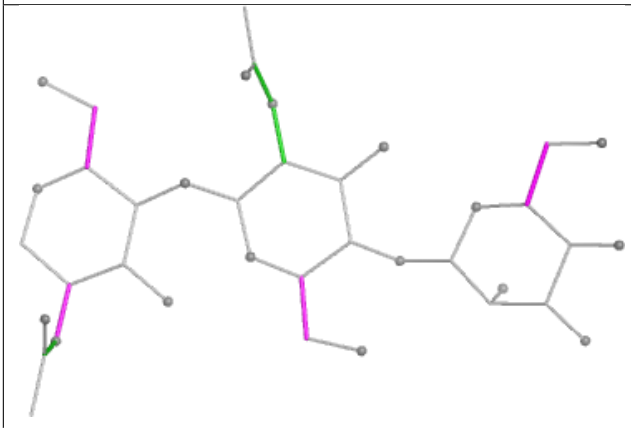
## Oligosaccharide Chain N



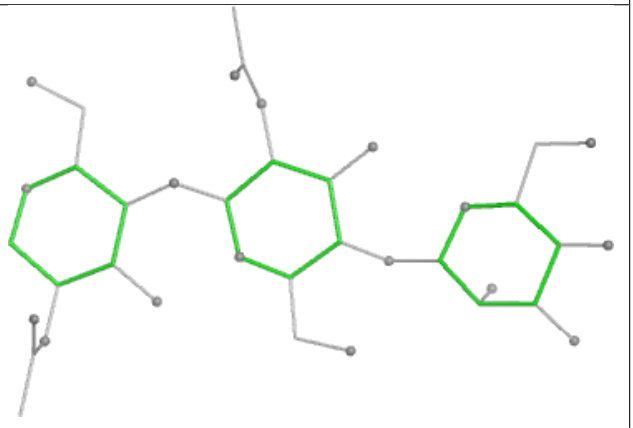
Bond lengths



Bond angles

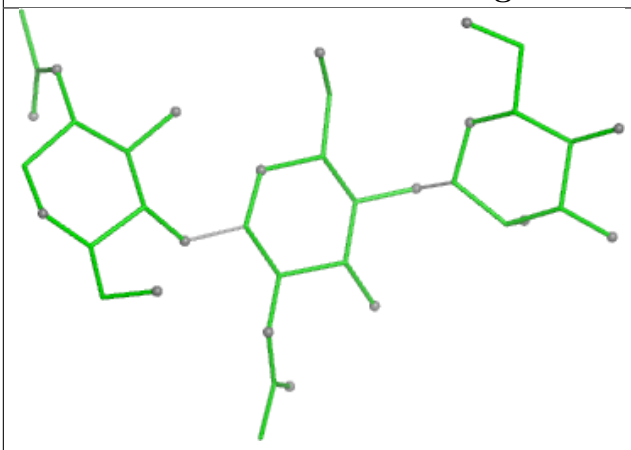


Torsions

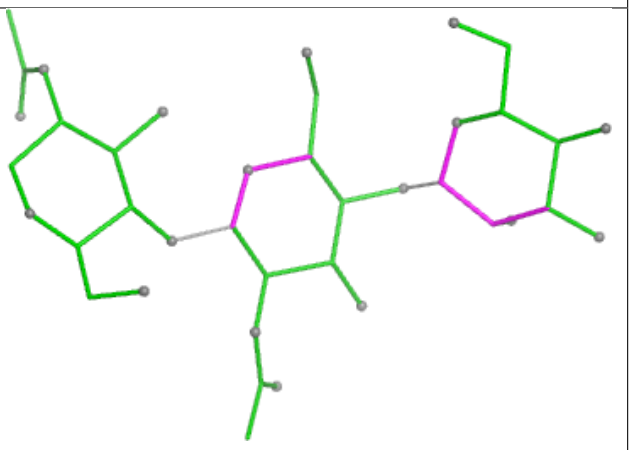


Rings

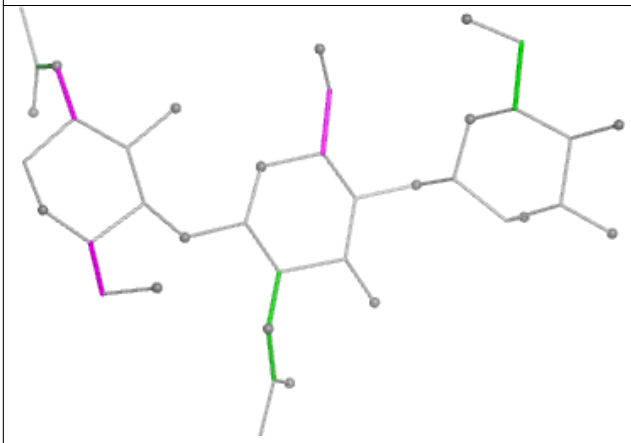
**Oligosaccharide Chain O**



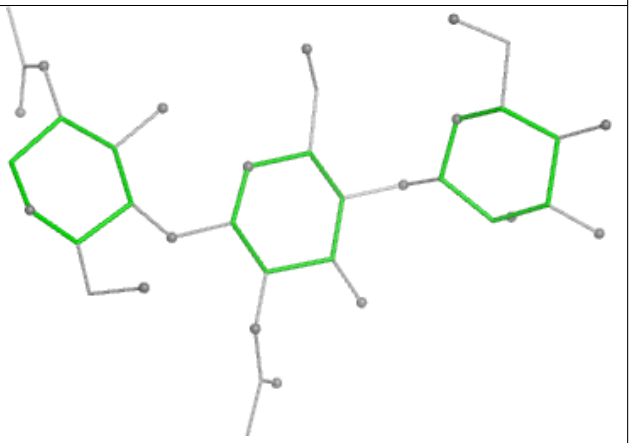
**Bond lengths**



**Bond angles**

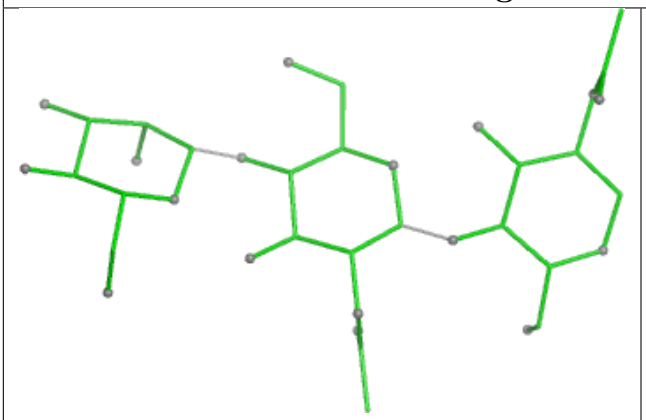


**Torsions**

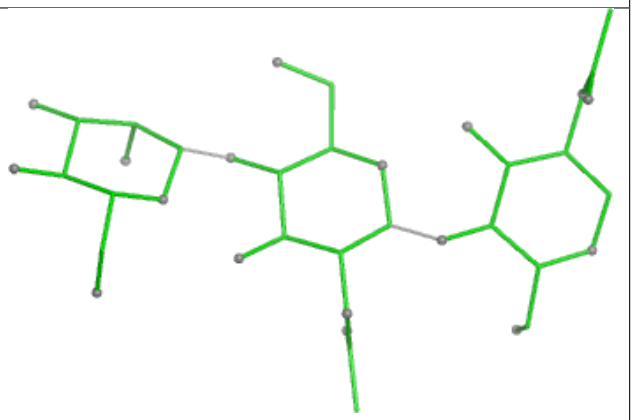


**Rings**

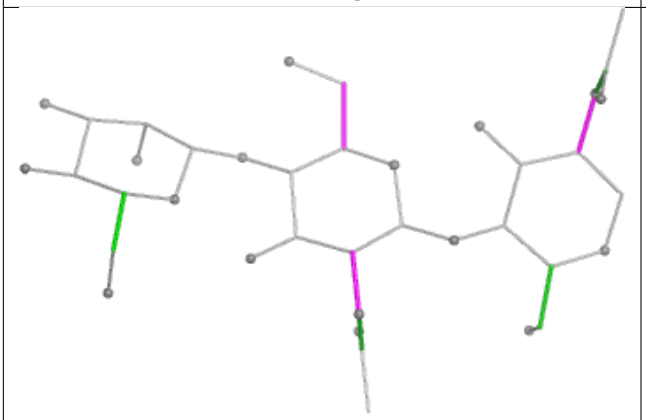
**Oligosaccharide Chain P**



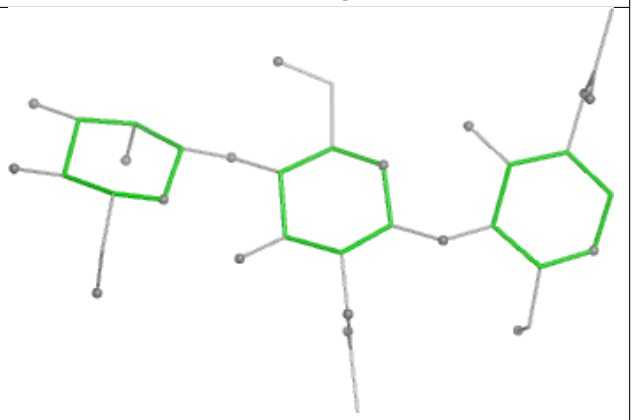
**Bond lengths**



**Bond angles**

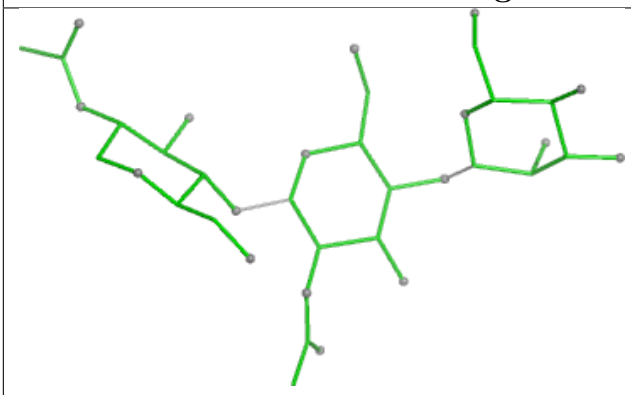


**Torsions**

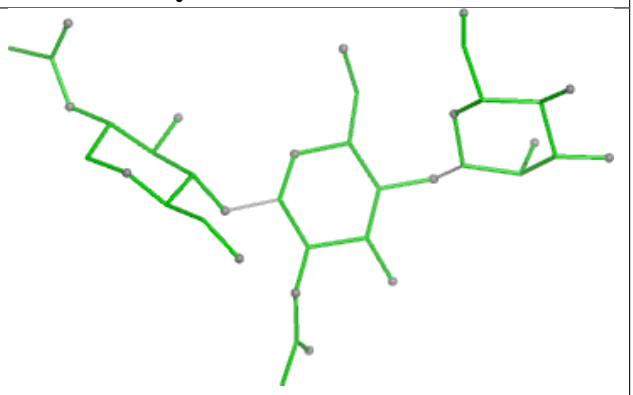


**Rings**

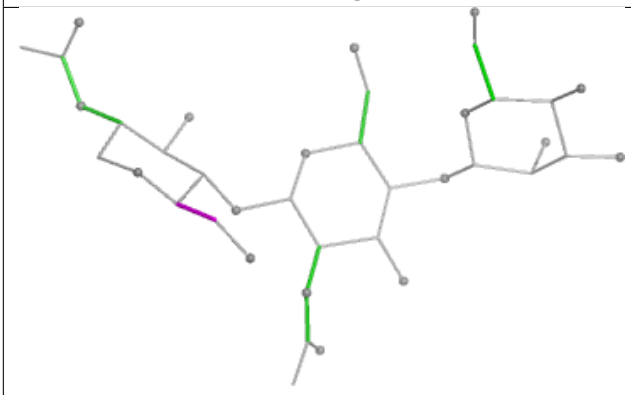
**Oligosaccharide Chain Q**



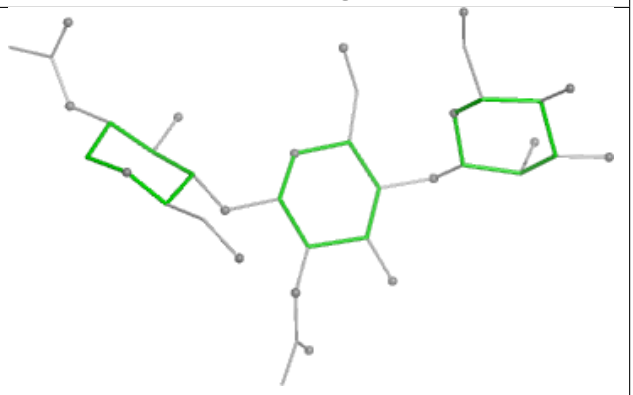
**Bond lengths**



**Bond angles**

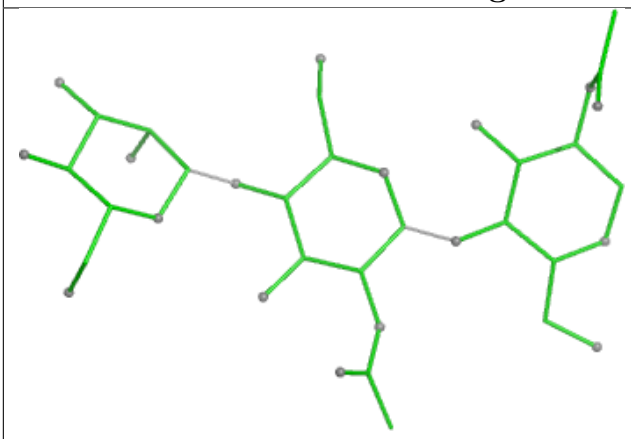


**Torsions**

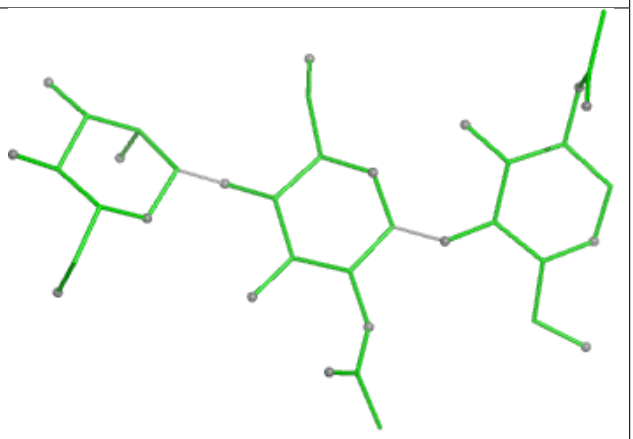


**Rings**

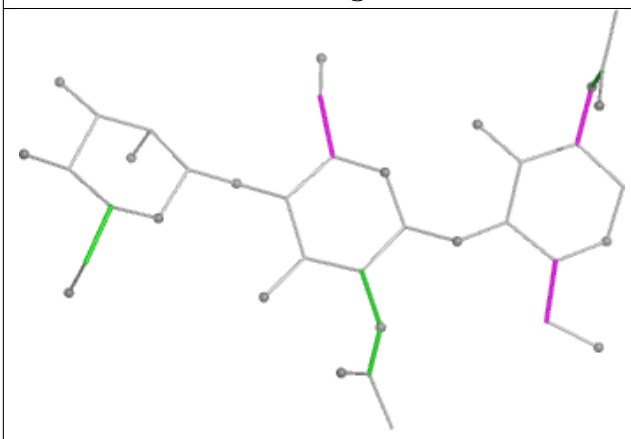
**Oligosaccharide Chain W**



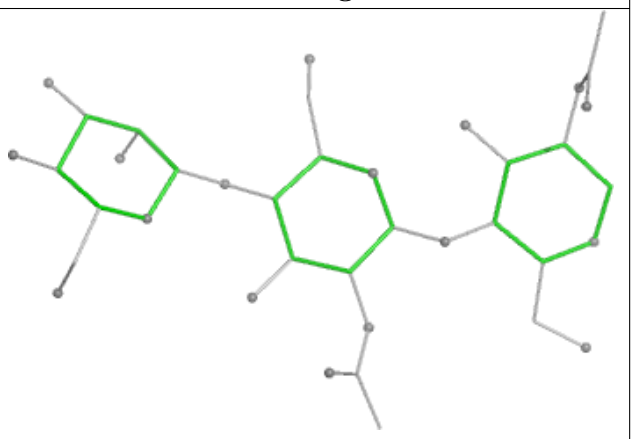
**Bond lengths**



**Bond angles**

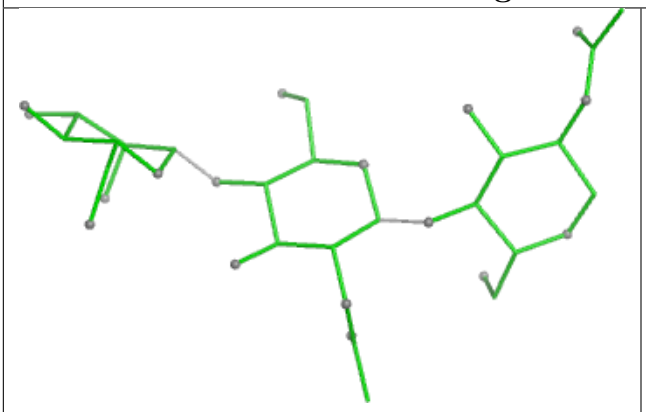


**Torsions**

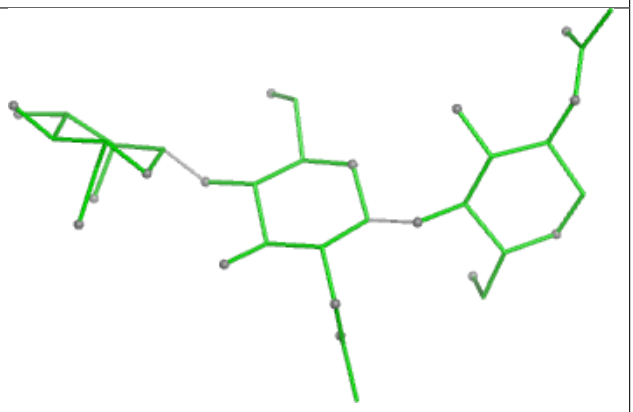


**Rings**

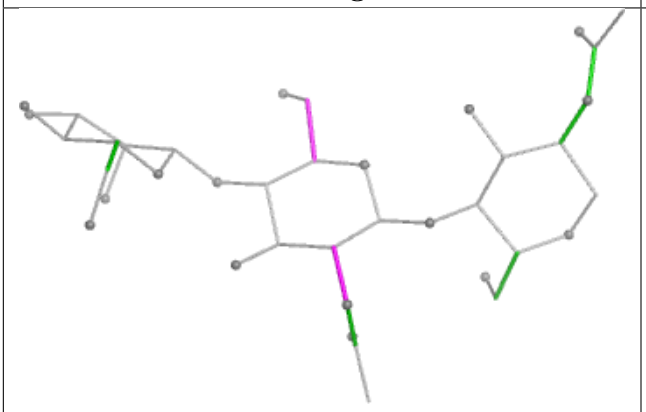
**Oligosaccharide Chain X**



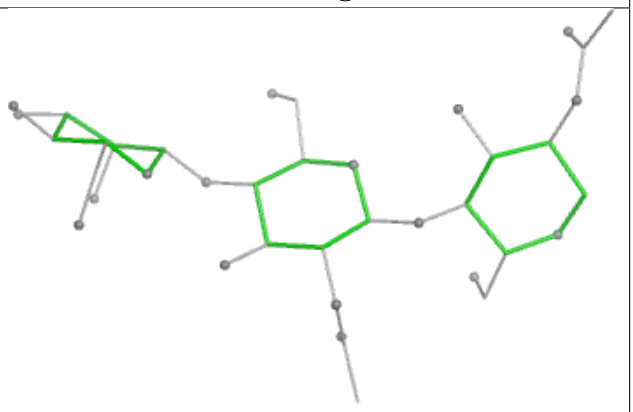
**Bond lengths**



**Bond angles**

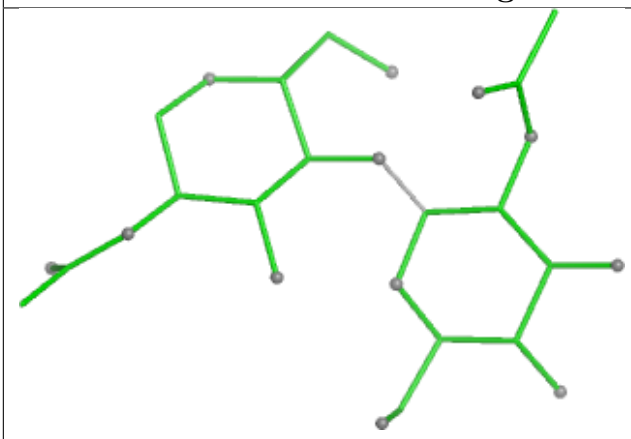


**Torsions**

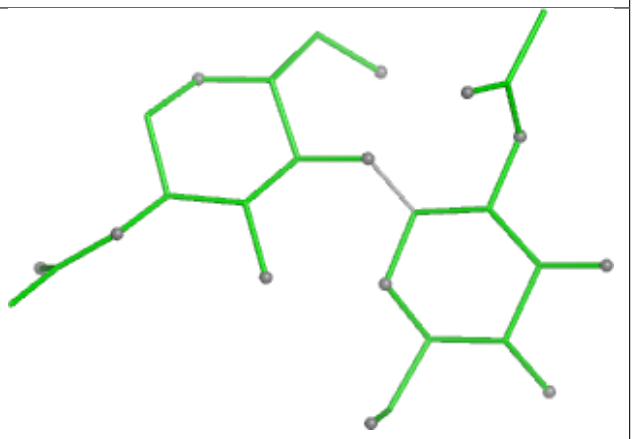


**Rings**

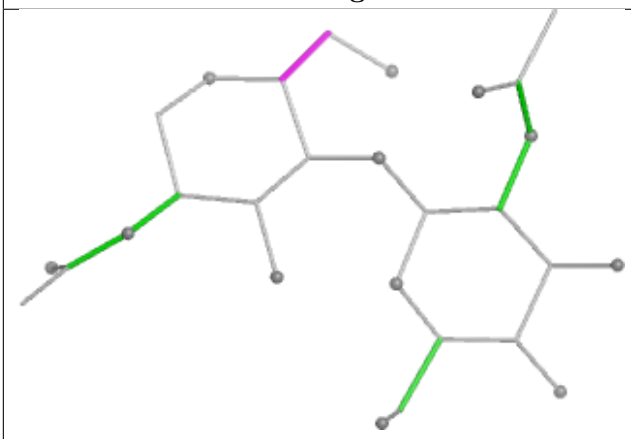
**Oligosaccharide Chain L**



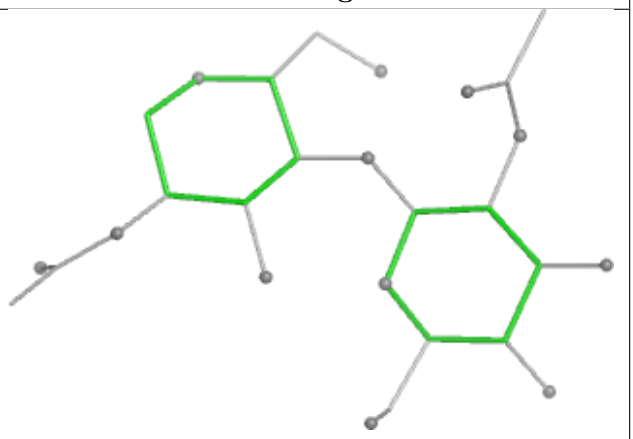
**Bond lengths**



**Bond angles**

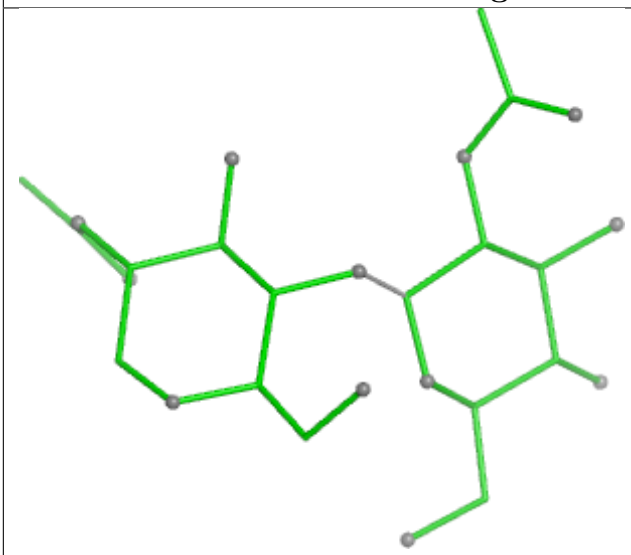


**Torsions**

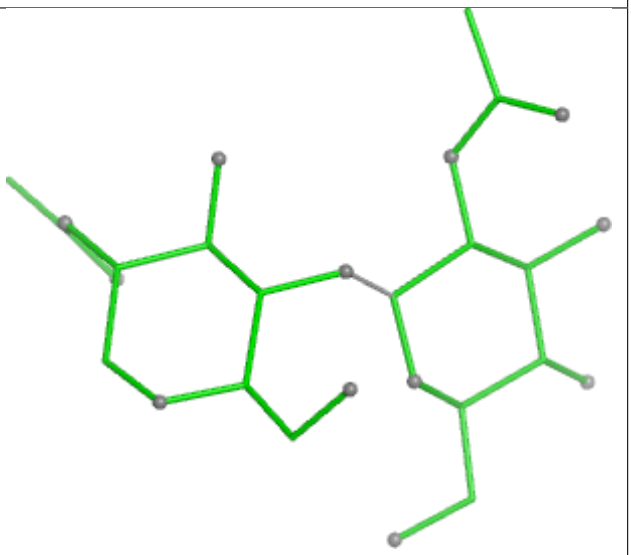


**Rings**

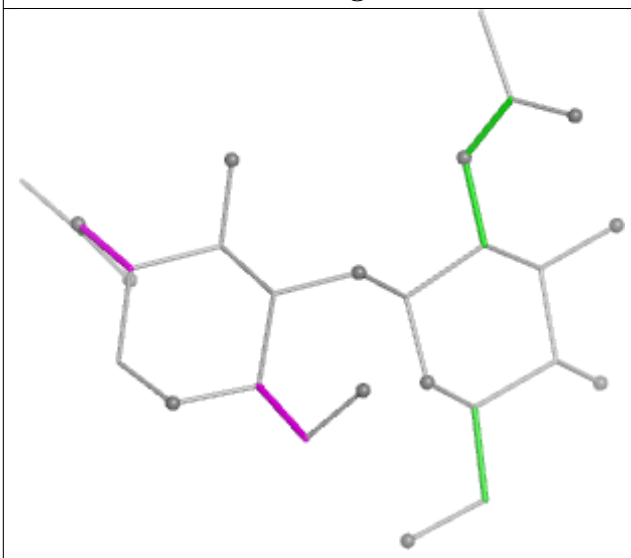
**Oligosaccharide Chain M**



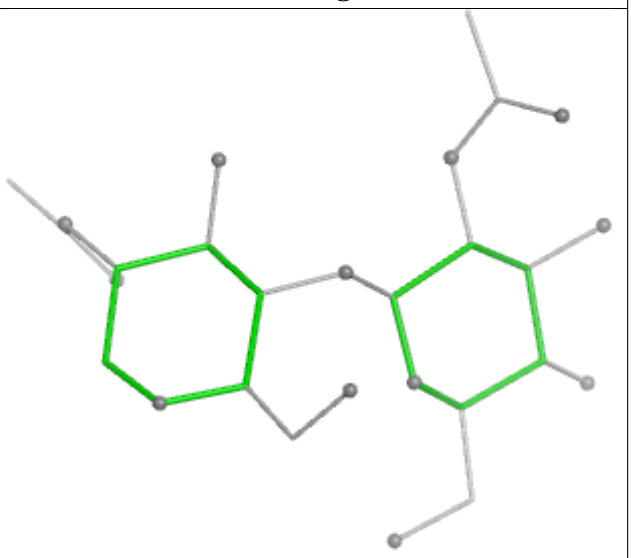
**Bond lengths**



**Bond angles**

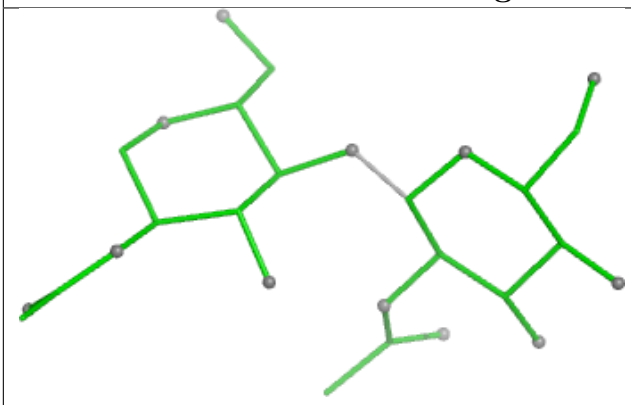


**Torsions**

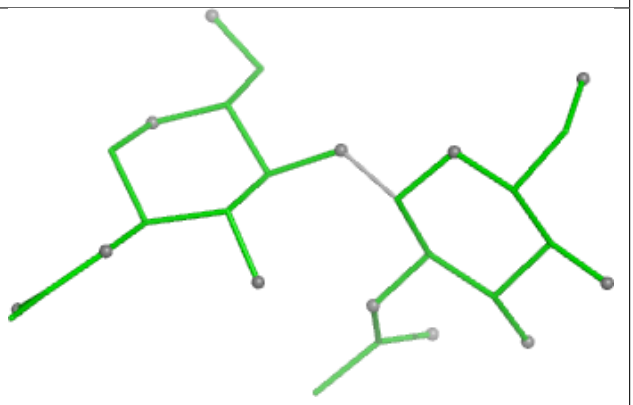


**Rings**

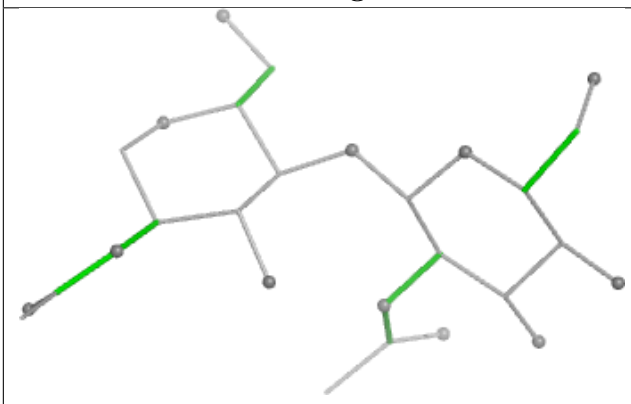
**Oligosaccharide Chain R**



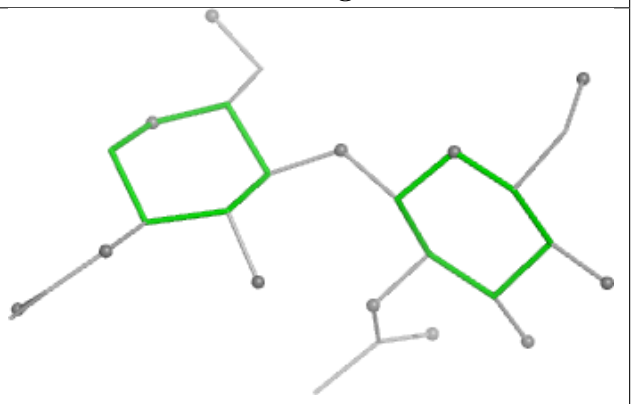
**Bond lengths**



**Bond angles**

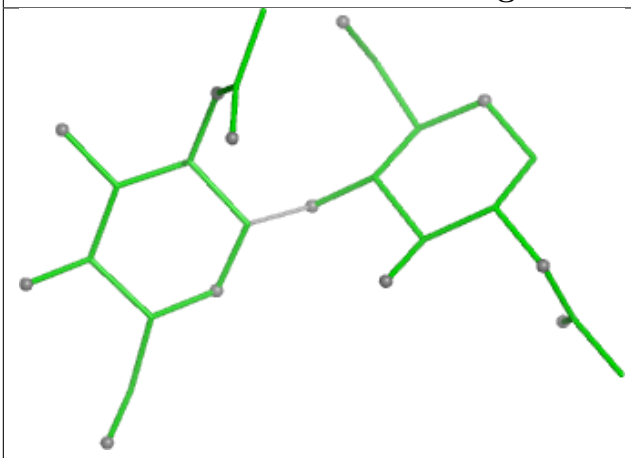


**Torsions**

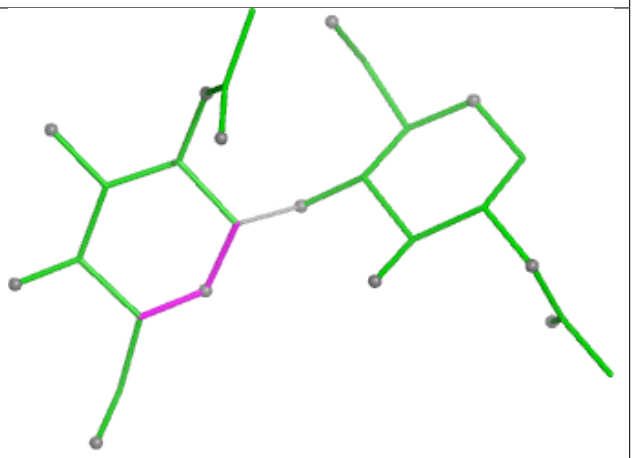


**Rings**

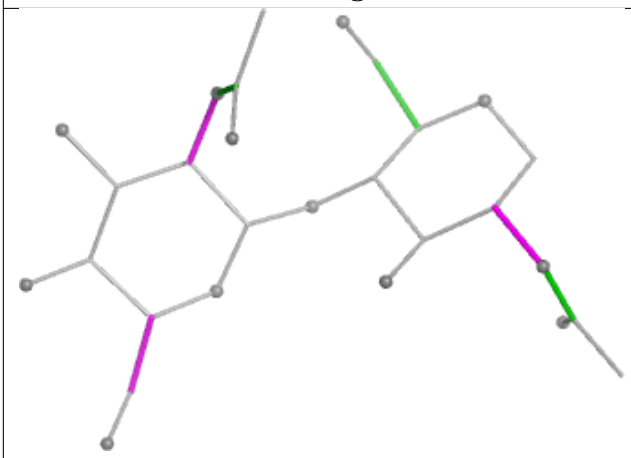
**Oligosaccharide Chain S**



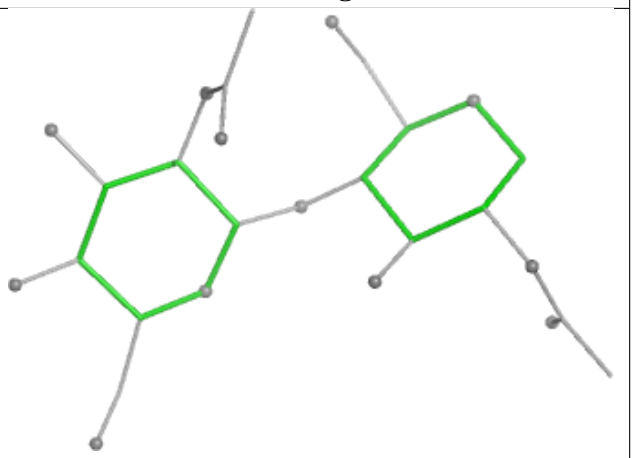
**Bond lengths**



**Bond angles**

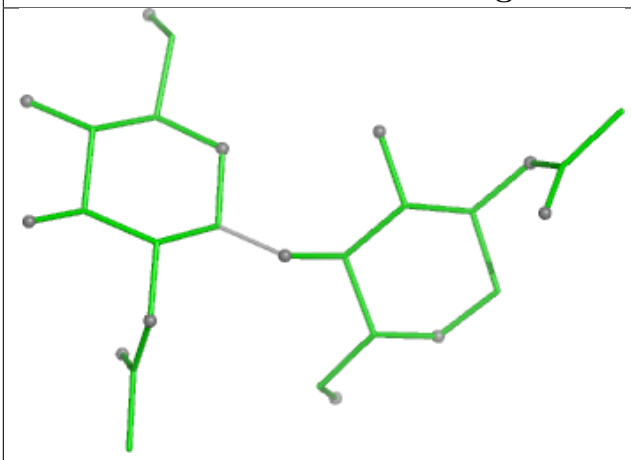


**Torsions**

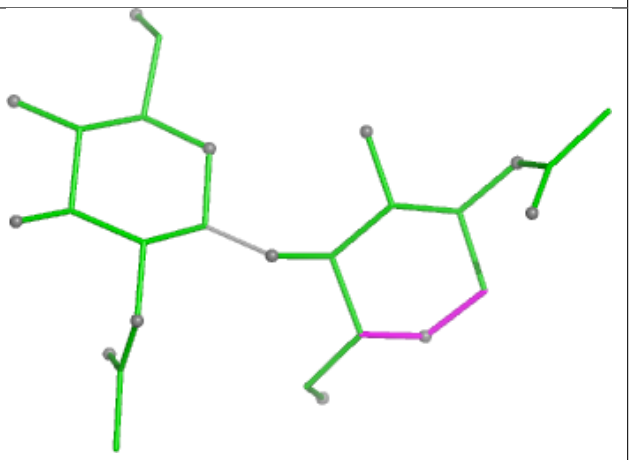


**Rings**

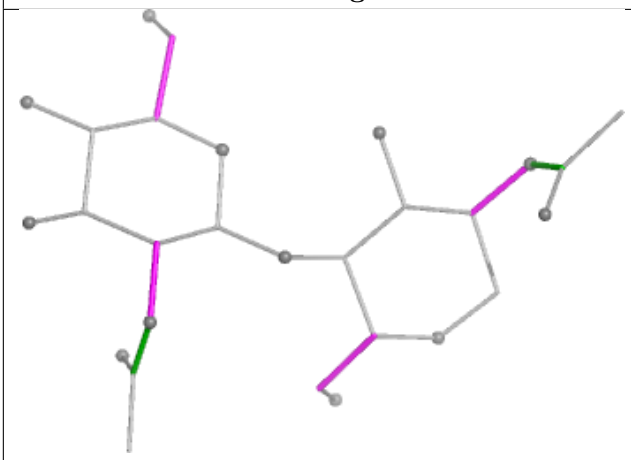
**Oligosaccharide Chain T**



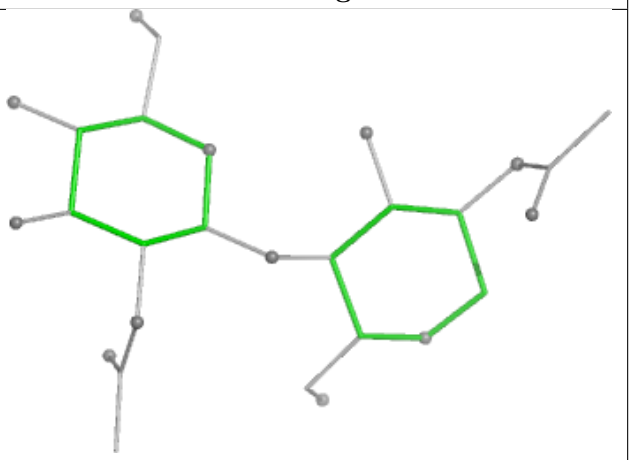
**Bond lengths**



**Bond angles**

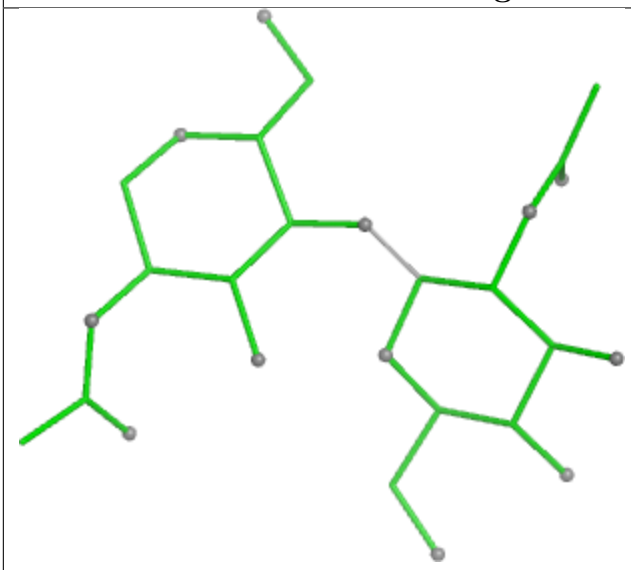


**Torsions**

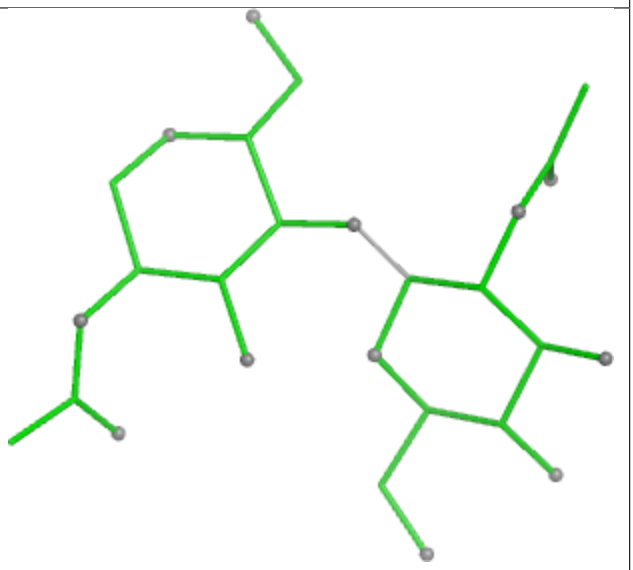


**Rings**

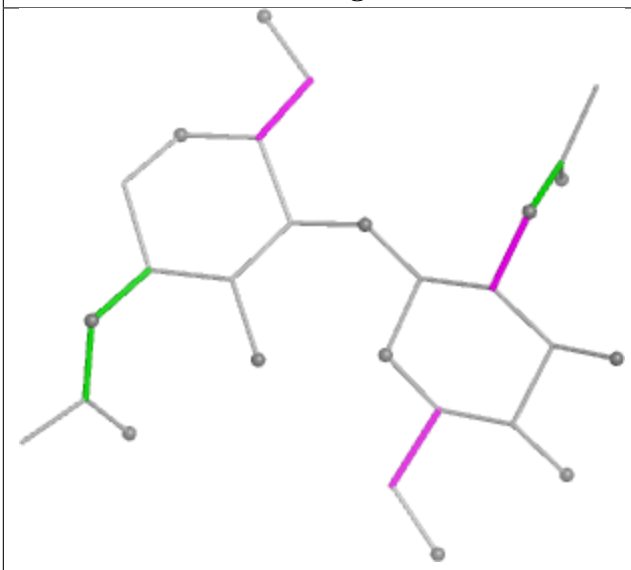
**Oligosaccharide Chain U**



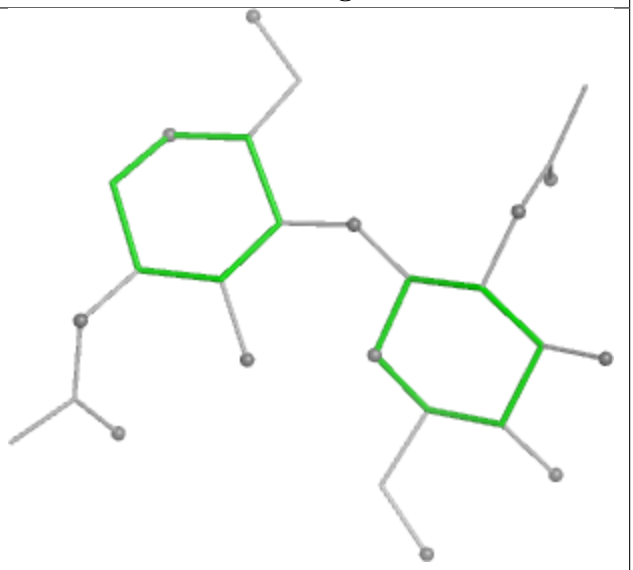
**Bond lengths**



**Bond angles**

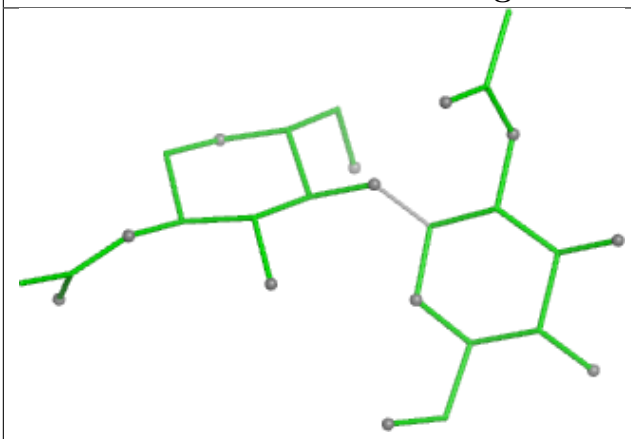


**Torsions**

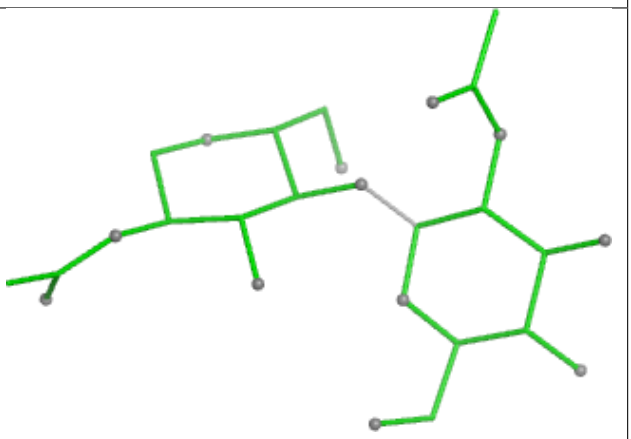


**Rings**

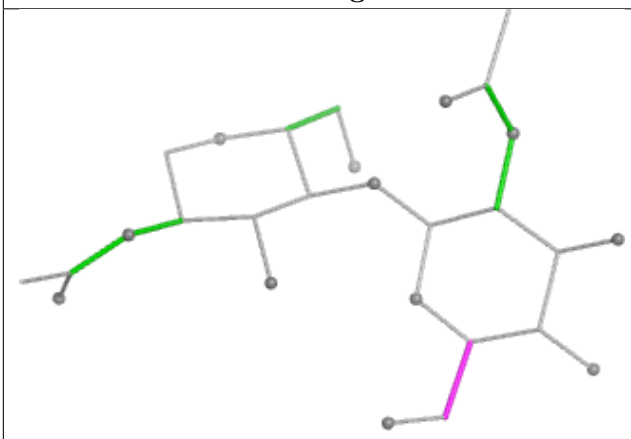
**Oligosaccharide Chain V**



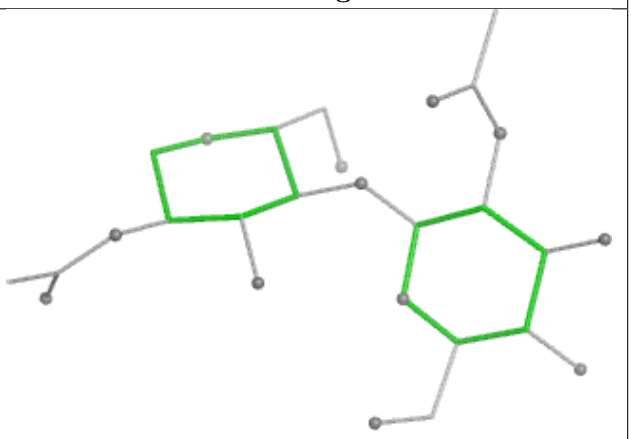
**Bond lengths**



**Bond angles**

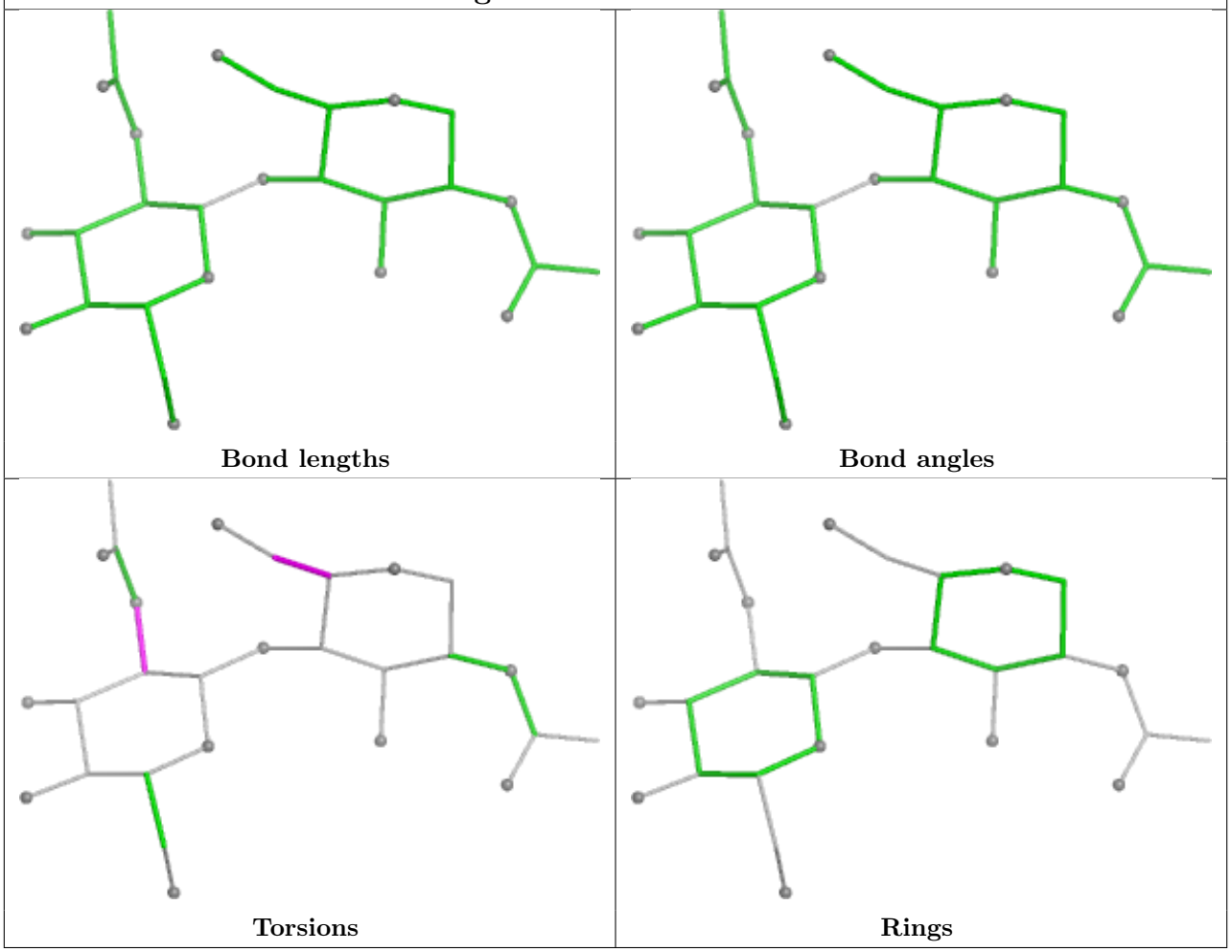


**Torsions**



**Rings**

**Oligosaccharide Chain Y**




## 5.6 Ligand geometry (i)

Of 55 ligands modelled in this entry, 27 are monoatomic - leaving 28 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 9 | NAG | A | 4504 | 1 | 14,14,15 | 0.20 | 0 | 17,19,21 | 0.47 | 0 |
| 9 | NAG | B | 4507 | 1 | 14,14,15 | 0.23 | 0 | 17,19,21 | 0.40 | 0 |
| 9 | NAG | B | 4505 | - | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.42 | 0 |
| 10 | NGA | B | 4510 | 1 | 14,14,15 | 0.56 | 0 | 17,19,21 | 0.70 | 0 |
| 9 | NAG | A | 4501 | 1 | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.46 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 10 | NGA | A | 4512 | 1 | 14,14,15 | 0.58 | 0 | 17,19,21 | 0.78 | 0 |
| 10 | NGA | B | 4512 | 1 | 14,14,15 | 0.61 | 0 | 17,19,21 | 0.67 | 0 |
| 9 | NAG | A | 4508 | 1 | 14,14,15 | 0.19 | 0 | 17,19,21 | 0.42 | 0 |
| 9 | NAG | B | 4504 | 1 | 14,14,15 | 0.23 | 0 | 17,19,21 | 0.42 | 0 |
| 9 | NAG | A | 4502 | 1 | 14,14,15 | 0.26 | 0 | 17,19,21 | 0.45 | 0 |
| 9 | NAG | A | 4507 | 1 | 14,14,15 | 0.19 | 0 | 17,19,21 | 0.40 | 0 |
| 9 | NAG | A | 4503 | 1 | 14,14,15 | 0.28 | 0 | 17,19,21 | 0.52 | 0 |
| 10 | NGA | A | 4513 | - | 14,14,15 | 0.60 | 0 | 17,19,21 | 0.60 | 0 |
| 9 | NAG | B | 4508 | 1 | 14,14,15 | 0.23 | 0 | 17,19,21 | 0.53 | 0 |
| 10 | NGA | A | 4514 | - | 14,14,15 | 0.59 | 0 | 17,19,21 | 0.71 | 0 |
| 10 | NGA | B | 4513 | - | 14,14,15 | 0.54 | 0 | 17,19,21 | 0.61 | 0 |
| 10 | NGA | B | 4511 | 1 | 14,14,15 | 0.56 | 0 | 17,19,21 | 0.64 | 0 |
| 9 | NAG | B | 4502 | 1 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.39 | 0 |
| 9 | NAG | A | 4506 | 1 | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.48 | 0 |
| 9 | NAG | A | 4528 | - | 14,14,15 | 0.50 | 0 | 17,19,21 | 0.38 | 0 |
| 10 | NGA | A | 4511 | 1 | 14,14,15 | 0.61 | 0 | 17,19,21 | 0.80 | 0 |
| 9 | NAG | B | 4501 | 1 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.45 | 0 |
| 9 | NAG | A | 4509 | - | 14,14,15 | 0.20 | 0 | 17,19,21 | 0.42 | 0 |
| 10 | NGA | B | 4509 | - | 14,14,15 | 0.63 | 0 | 17,19,21 | 0.79 | 0 |
| 9 | NAG | A | 4505 | - | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.49 | 0 |
| 9 | NAG | A | 4510 | - | 14,14,15 | 0.33 | 0 | 17,19,21 | 0.96 | 1 (5%) |
| 9 | NAG | B | 4503 | - | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.40 | 0 |
| 9 | NAG | B | 4506 | 1 | 14,14,15 | 0.16 | 0 | 17,19,21 | 0.44 | 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 |
|---|---|---|---|---|---|---|---|
| 9 | NAG | A | 4504 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 9 | NAG | B | 4507 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 9 | NAG | B | 4505 | - | - | 2/6/23/26 | 0/1/1/1 |
| 10 | NGA | B | 4510 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 9 | NAG | A | 4501 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 10 | NGA | A | 4512 | 1 | - | 4/6/23/26 | 0/1/1/1 |
| 10 | NGA | B | 4512 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 9 | NAG | A | 4508 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 9 | NAG | B | 4504 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 9 | NAG | A | 4502 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 9 | NAG | A | 4507 | 1 | - | 1/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 9 | NAG | A | 4503 | 1 | - | 1/6/23/26 | 0/1/1/1 |
| 10 | NGA | A | 4513 | - | - | 0/6/23/26 | 0/1/1/1 |
| 9 | NAG | B | 4508 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 10 | NGA | A | 4514 | - | - | 0/6/23/26 | 0/1/1/1 |
| 10 | NGA | B | 4513 | - | - | 3/6/23/26 | 0/1/1/1 |
| 10 | NGA | B | 4511 | 1 | 1/1/5/7 | 3/6/23/26 | 0/1/1/1 |
| 9 | NAG | B | 4502 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 9 | NAG | A | 4506 | 1 | - | 1/6/23/26 | 0/1/1/1 |
| 9 | NAG | A | 4528 | - | - | 2/6/23/26 | 0/1/1/1 |
| 10 | NGA | A | 4511 | 1 | - | 4/6/23/26 | 0/1/1/1 |
| 9 | NAG | B | 4501 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 9 | NAG | A | 4509 | - | - | 0/6/23/26 | 0/1/1/1 |
| 10 | NGA | B | 4509 | - | - | 3/6/23/26 | 0/1/1/1 |
| 9 | NAG | A | 4505 | - | - | 2/6/23/26 | 0/1/1/1 |
| 9 | NAG | A | 4510 | - | - | 5/6/23/26 | 0/1/1/1 |
| 9 | NAG | B | 4503 | - | - | 2/6/23/26 | 0/1/1/1 |
| 9 | NAG | B | 4506 | 1 | - | 0/6/23/26 | 0/1/1/1 |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | A | 4510 | NAG | C2-N2-C7 | 3.12 | 127.35 | 122.90 |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 10 | B | 4511 | NGA | C1 |

All (49) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 9 | A | 4528 | NAG | C3-C2-N2-C7 |
| 10 | A | 4511 | NGA | C1-C2-N2-C7 |
| 10 | A | 4511 | NGA | C8-C7-N2-C2 |
| 10 | A | 4511 | NGA | O7-C7-N2-C2 |
| 10 | A | 4512 | NGA | C1-C2-N2-C7 |
| 10 | A | 4512 | NGA | C8-C7-N2-C2 |
| 10 | A | 4512 | NGA | O7-C7-N2-C2 |

*Continued on next page...*

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 10 | B | 4509 | NGA | C3-C2-N2-C7 |
| 10 | B | 4509 | NGA | C8-C7-N2-C2 |
| 10 | B | 4509 | NGA | O7-C7-N2-C2 |
| 10 | B | 4512 | NGA | C8-C7-N2-C2 |
| 10 | B | 4512 | NGA | O7-C7-N2-C2 |
| 10 | B | 4513 | NGA | C3-C2-N2-C7 |
| 10 | B | 4513 | NGA | C8-C7-N2-C2 |
| 10 | B | 4513 | NGA | O7-C7-N2-C2 |
| 10 | B | 4510 | NGA | C8-C7-N2-C2 |
| 9 | A | 4501 | NAG | O5-C5-C6-O6 |
| 9 | A | 4502 | NAG | O5-C5-C6-O6 |
| 10 | B | 4511 | NGA | C8-C7-N2-C2 |
| 10 | B | 4511 | NGA | O7-C7-N2-C2 |
| 9 | A | 4504 | NAG | O5-C5-C6-O6 |
| 9 | B | 4503 | NAG | O5-C5-C6-O6 |
| 9 | B | 4501 | NAG | O5-C5-C6-O6 |
| 10 | B | 4510 | NGA | O7-C7-N2-C2 |
| 9 | B | 4503 | NAG | C4-C5-C6-O6 |
| 9 | A | 4504 | NAG | C4-C5-C6-O6 |
| 9 | B | 4502 | NAG | O5-C5-C6-O6 |
| 9 | A | 4502 | NAG | C4-C5-C6-O6 |
| 9 | B | 4501 | NAG | C4-C5-C6-O6 |
| 9 | A | 4510 | NAG | C8-C7-N2-C2 |
| 9 | A | 4510 | NAG | O7-C7-N2-C2 |
| 9 | A | 4501 | NAG | C4-C5-C6-O6 |
| 9 | A | 4510 | NAG | O5-C5-C6-O6 |
| 9 | B | 4505 | NAG | O5-C5-C6-O6 |
| 9 | B | 4505 | NAG | C4-C5-C6-O6 |
| 10 | B | 4511 | NGA | O5-C5-C6-O6 |
| 10 | A | 4512 | NGA | O5-C5-C6-O6 |
| 9 | A | 4510 | NAG | C4-C5-C6-O6 |
| 9 | A | 4507 | NAG | O5-C5-C6-O6 |
| 10 | A | 4511 | NGA | O5-C5-C6-O6 |
| 9 | A | 4528 | NAG | O5-C5-C6-O6 |
| 9 | B | 4508 | NAG | O5-C5-C6-O6 |
| 9 | A | 4505 | NAG | O5-C5-C6-O6 |
| 9 | A | 4503 | NAG | C3-C2-N2-C7 |
| 9 | A | 4505 | NAG | C3-C2-N2-C7 |
| 9 | A | 4506 | NAG | C3-C2-N2-C7 |
| 9 | B | 4508 | NAG | C3-C2-N2-C7 |
| 9 | B | 4502 | NAG | C4-C5-C6-O6 |
| 9 | A | 4510 | NAG | C3-C2-N2-C7 |

There are no ring outliers.

7 monomers are involved in 13 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 10 | B | 4510 | NGA | 1 | 0 |
| 10 | A | 4512 | NGA | 1 | 0 |
| 10 | A | 4514 | NGA | 3 | 0 |
| 10 | B | 4513 | NGA | 1 | 0 |
| 9 | A | 4528 | NAG | 3 | 0 |
| 10 | B | 4509 | NGA | 1 | 0 |
| 9 | A | 4510 | NAG | 3 | 0 |

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

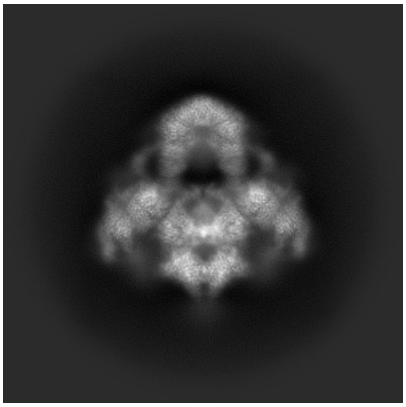
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-52617. These allow visual inspection of the internal detail of the map and identification of artifacts.

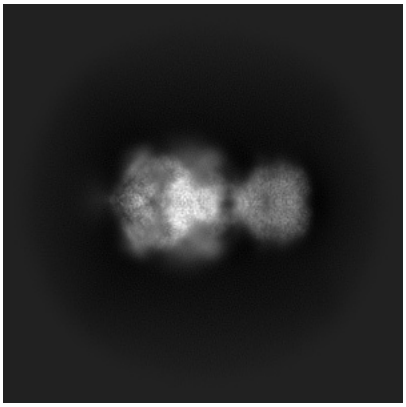
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

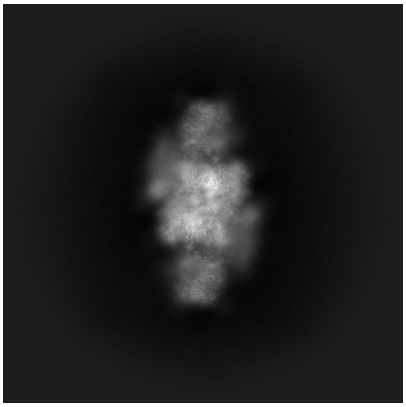
### 6.1.1 Primary map



X



Y

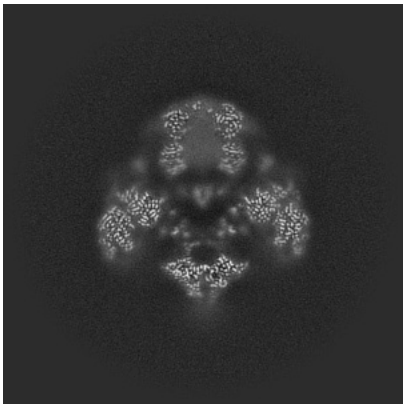


Z

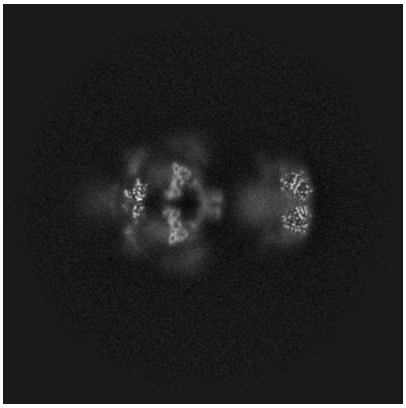
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

### 6.2.1 Primary map



X Index: 280



Y Index: 280

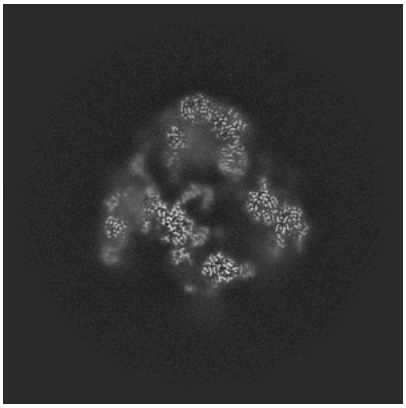


Z Index: 280

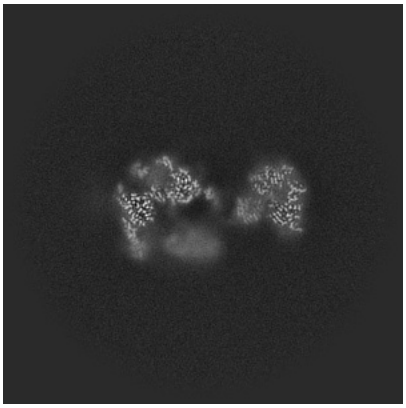
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

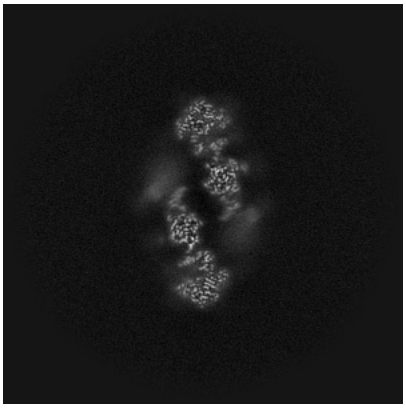
### 6.3.1 Primary map



X Index: 266



Y Index: 306

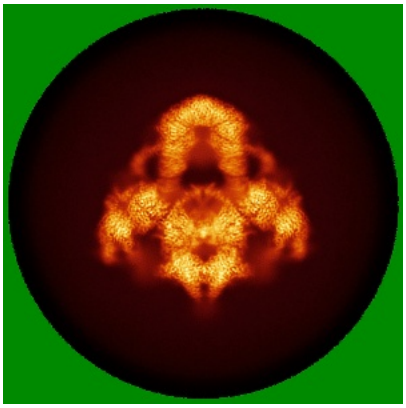


Z Index: 254

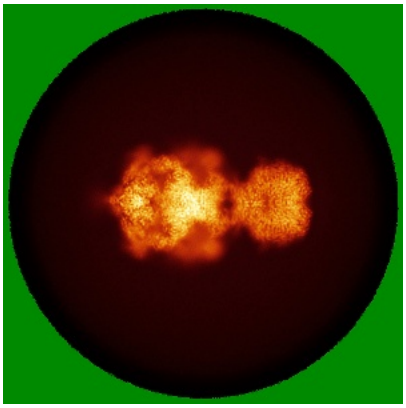
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) (i)

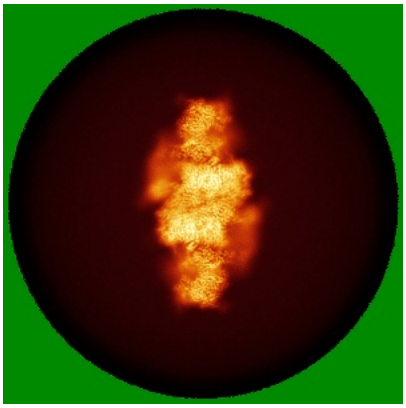
### 6.4.1 Primary map



X



Y

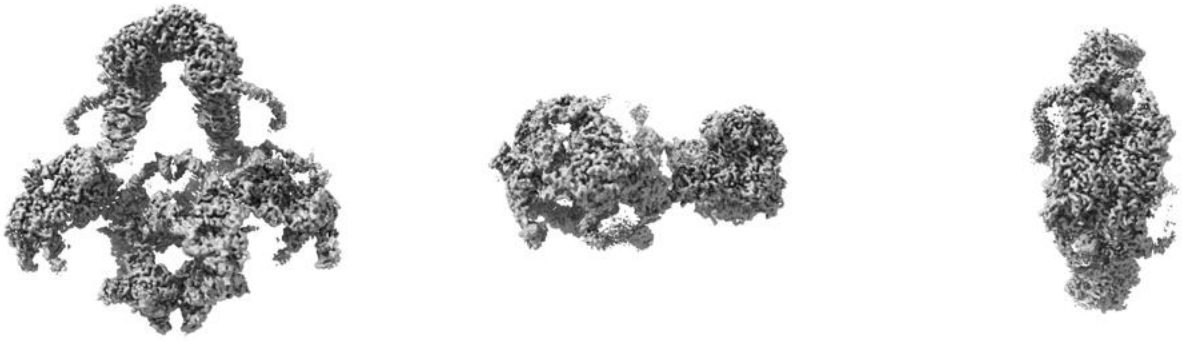


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.318. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

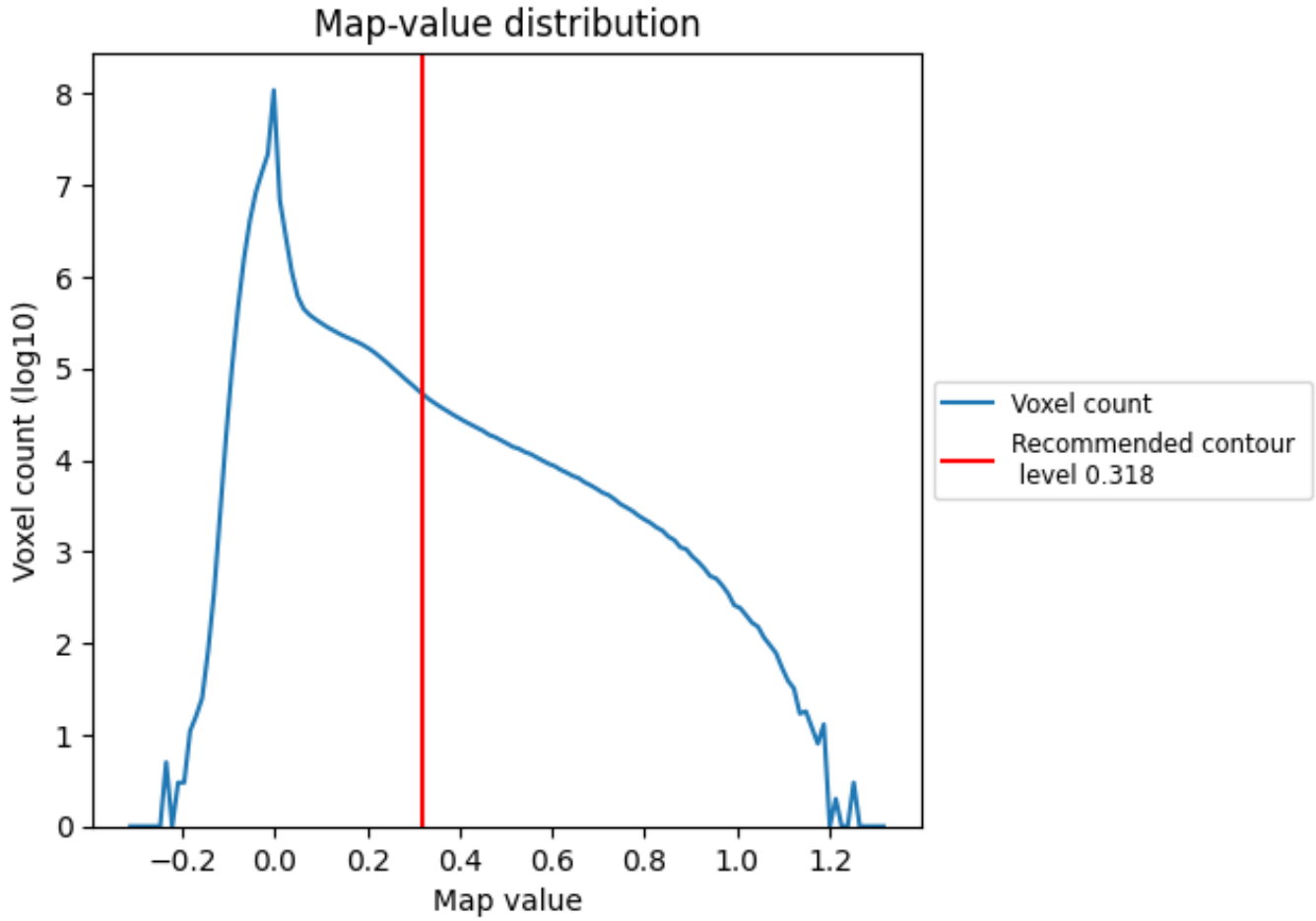
## 6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

# 7 Map analysis

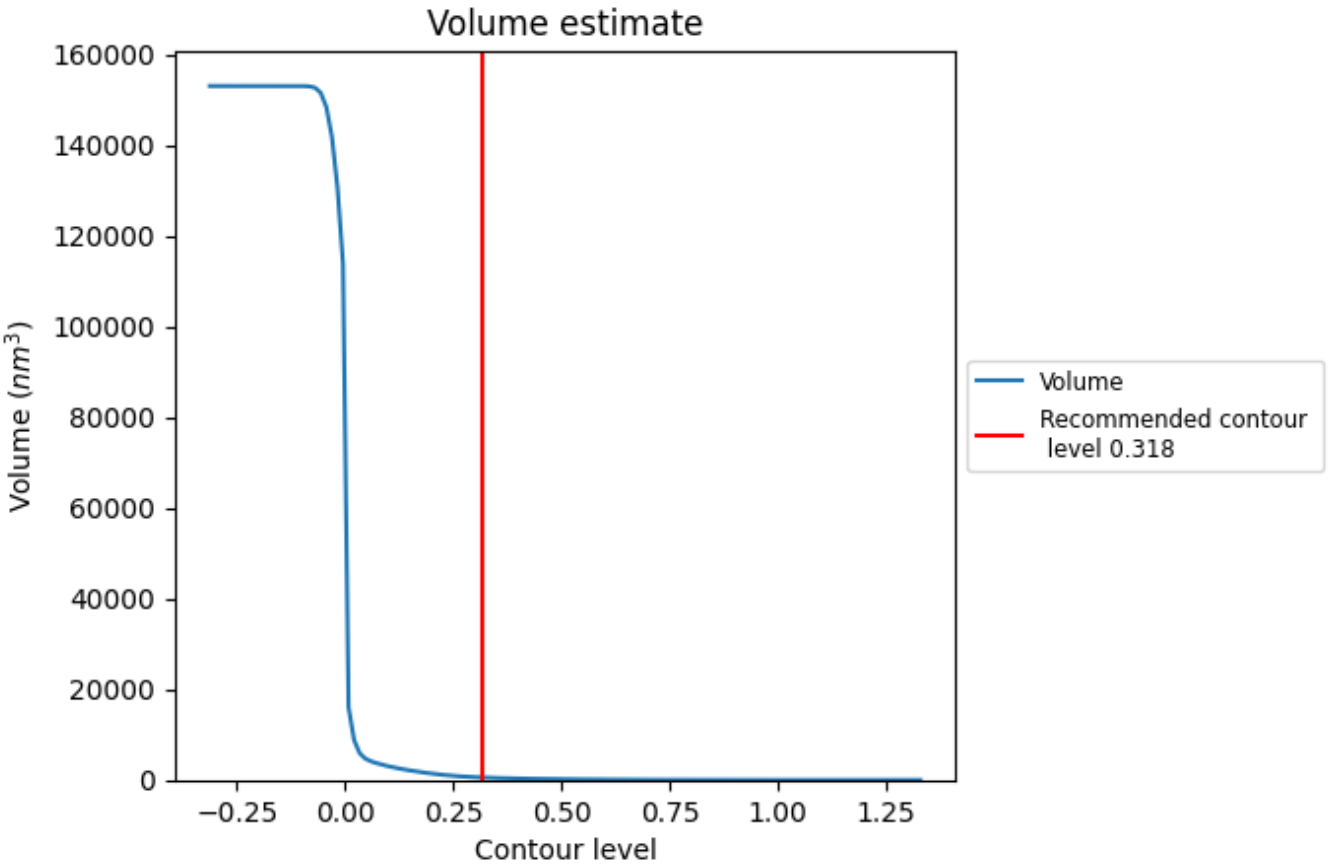
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

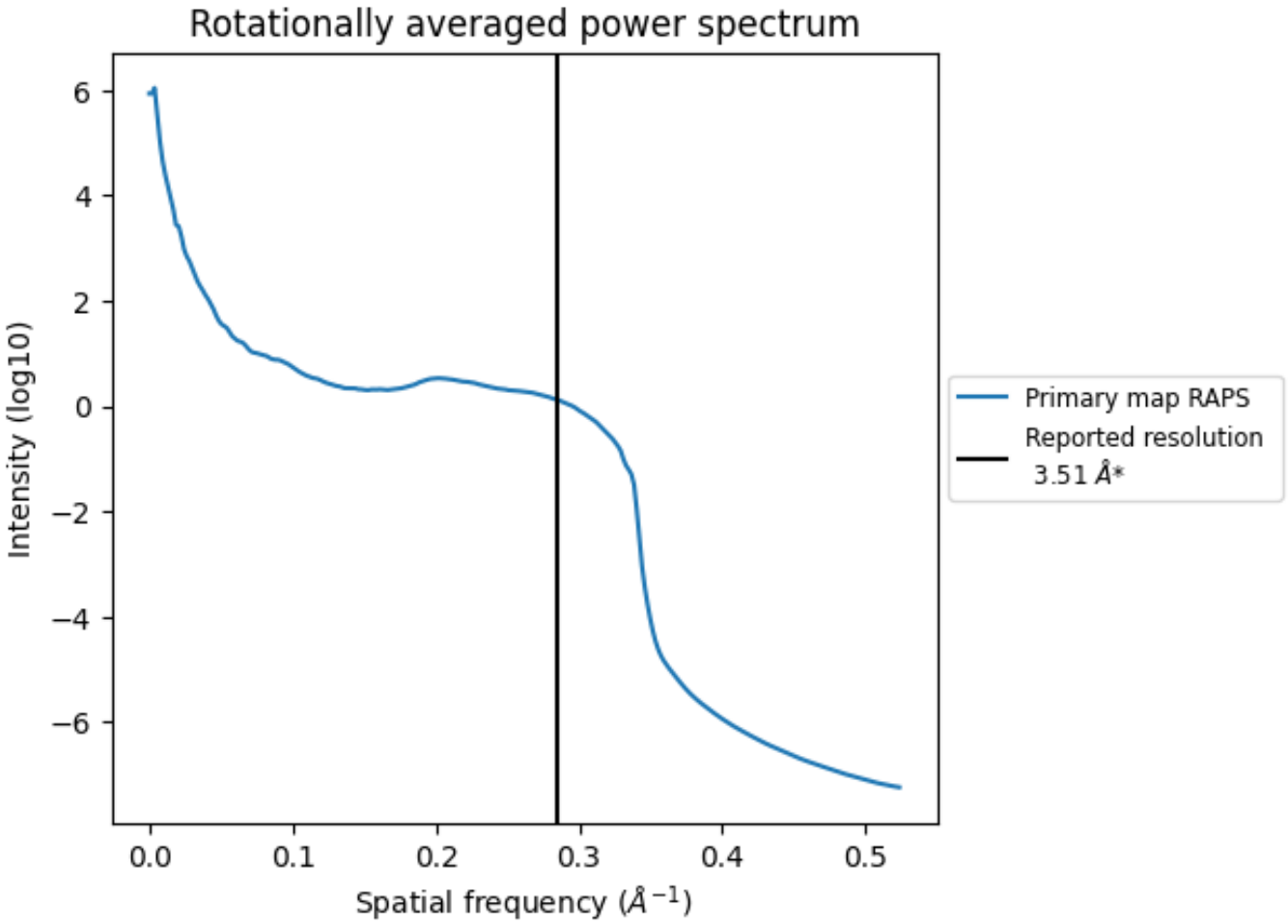
## 7.2 Volume estimate




The volume at the recommended contour level is 543 $nm^3$; this corresponds to an approximate mass of 491 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

## 7.3 Rotationally averaged power spectrum (i)




*Reported resolution corresponds to spatial frequency of 0.285 Å$^{-1}$

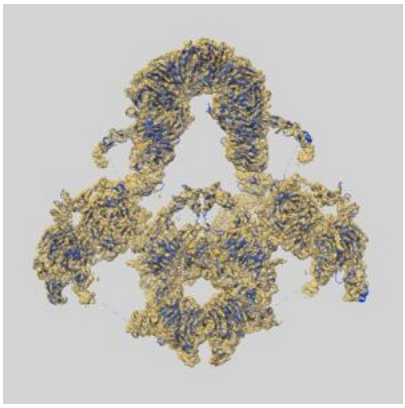
# 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

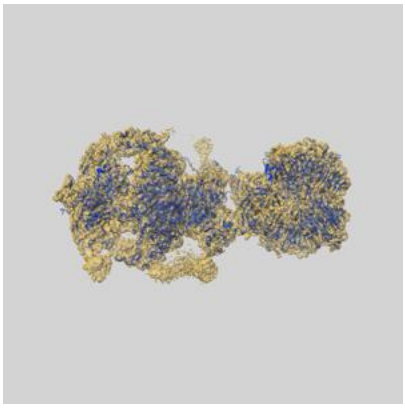
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-52617 and PDB model 9I3V. Per-residue inclusion information can be found in section 3 on page 12.

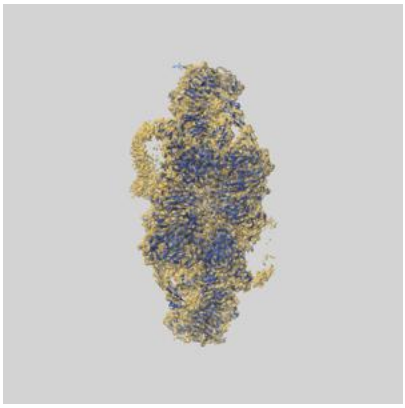
## 9.1 Map-model overlay



X



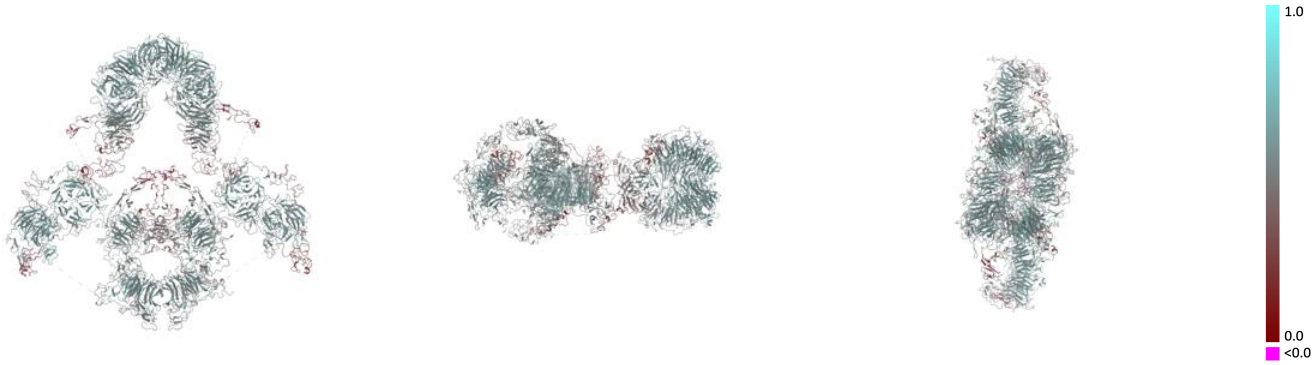
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.318 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

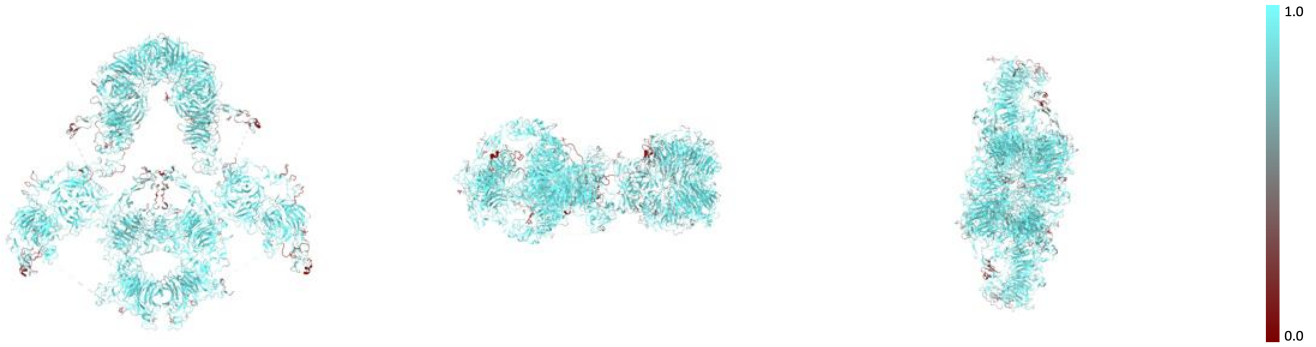
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

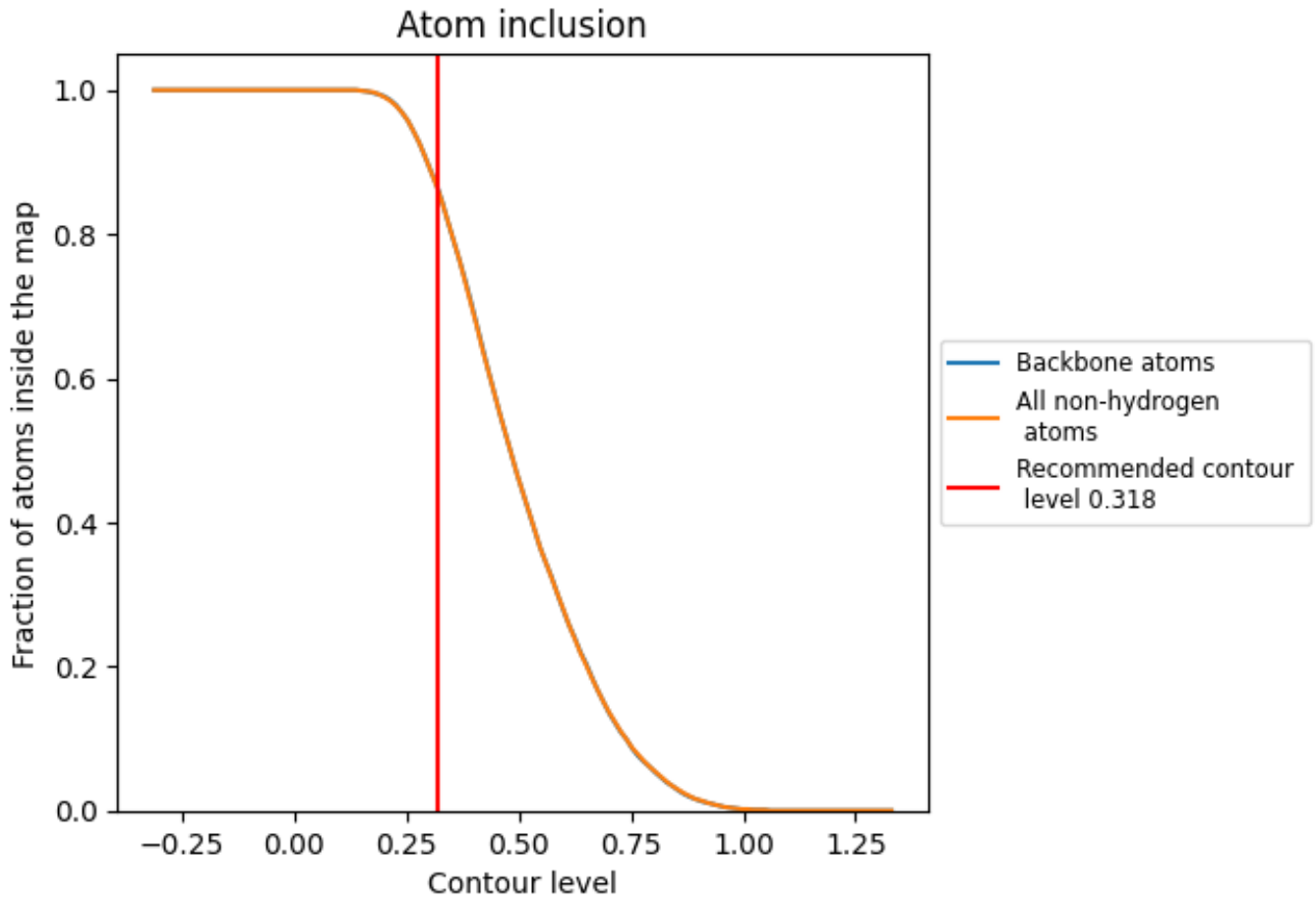
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.318).

## 9.4 Atom inclusion (i)




At the recommended contour level, 87% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.318) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.8650 | 0.5090 |
| A | 0.8690 | 0.5080 |
| B | 0.8780 | 0.5090 |
| C | 0.9710 | 0.5480 |
| D | 0.9600 | 0.5350 |
| E | 1.0000 | 0.5550 |
| F | 1.0000 | 0.5580 |
| G | 0.6310 | 0.5050 |
| H | 0.6670 | 0.5440 |
| I | 0.9250 | 0.5340 |
| J | 1.0000 | 0.5120 |
| K | 0.1540 | 0.3550 |
| L | 0.7500 | 0.4740 |
| M | 0.2140 | 0.3770 |
| N | 0.7180 | 0.5700 |
| O | 0.8720 | 0.4550 |
| P | 0.6410 | 0.4730 |
| Q | 0.5130 | 0.4350 |
| R | 0.6790 | 0.4350 |
| S | 0.1790 | 0.2990 |
| T | 0.8570 | 0.4080 |
| U | 0.8930 | 0.5090 |
| V | 0.8570 | 0.5050 |
| W | 0.7950 | 0.5580 |
| X | 0.5900 | 0.4790 |
| Y | 0.7500 | 0.5180 |

