# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 02:20 PM BST

| | | |
|---|---|---|
| PDB ID | : | 1IVD |
| Title | : | STRUCTURES OF AROMATIC INHIBITORS OF INFLUENZA VIRUS NEURAMINIDASE |
| Authors | : | Jedrzejas, M.J.; Luo, M. |
| Deposited on | : | 1994-12-12 |
| Resolution | : | 1.90 Å(reported) |

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

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

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

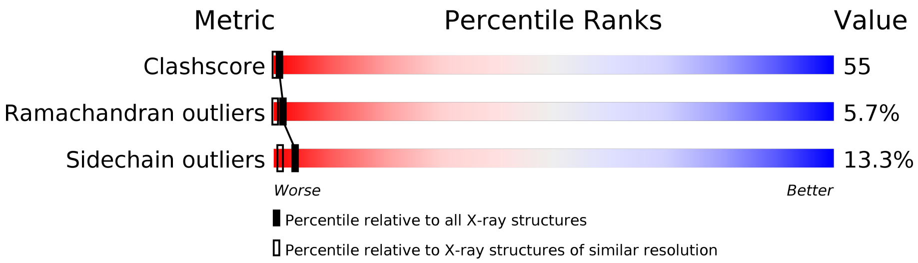
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.13.1 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.13.1 |

# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

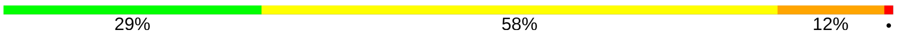
The reported resolution of this entry is 1.90 Å.

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) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| Clashscore | 141614 | 6847 (1.90-1.90) |
| Ramachandran outliers | 138981 | 6760 (1.90-1.90) |
| Sidechain outliers | 138945 | 6760 (1.90-1.90) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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%

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 388 |  |
| 1 | B | 388 |  |
| 2 | C | 2 |  |
| 2 | F | 2 |  |
| 2 | G | 2 |  |
| 2 | J | 2 |  |
| 3 | D | 4 |  |
| 4 | E | 6 |  |
| 4 | I | 6 |  |

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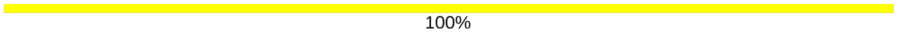
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 5 | H | 4 |  |

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 |
|---|---|---|---|---|---|---|---|
| 4 | NAG | E | 1 | - | X | X | - |
| 4 | MAN | E | 6 | - | - | X | - |
| 4 | NAG | I | 1 | - | X | - | - |
| 5 | FUC | H | 4 | X | - | - | - |

# 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8595 atoms, of which 2036 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

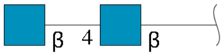
- Molecule 1 is a protein called INFLUENZA A SUBTYPE N2 NEURAMINIDASE.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | S | | | |
| 1 | A | 388 | 3745 | 1866 | 723 | 545 | 588 | 23 | 0 | 0 | 0 |
| 1 | B | 388 | 3745 | 1866 | 723 | 545 | 588 | 23 | 0 | 0 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

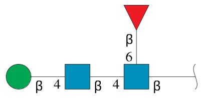
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 339 | ASP | ASN | conflict | UNP P06820 |
| B | 339 | ASP | ASN | conflict | UNP P06820 |

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



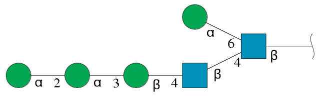
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | | | |
| 2 | C | 2 | 55 | 16 | 27 | 2 | 10 | 0 | 0 | 0 |
| 2 | F | 2 | 55 | 16 | 27 | 2 | 10 | 0 | 0 | 0 |
| 2 | G | 2 | 55 | 16 | 27 | 2 | 10 | 0 | 0 | 0 |
| 2 | J | 2 | 55 | 16 | 27 | 2 | 10 | 0 | 0 | 0 |

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



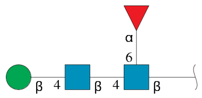
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | | | |
| 3 | D | 4 | 96 | 28 | 47 | 2 | 19 | 0 | 0 | 0 |

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | | | |
| 4 | E | 6 | 139 | 40 | 67 | 2 | 30 | 0 | 0 | 0 |
| 4 | I | 6 | 139 | 40 | 67 | 2 | 30 | 0 | 0 | 0 |

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

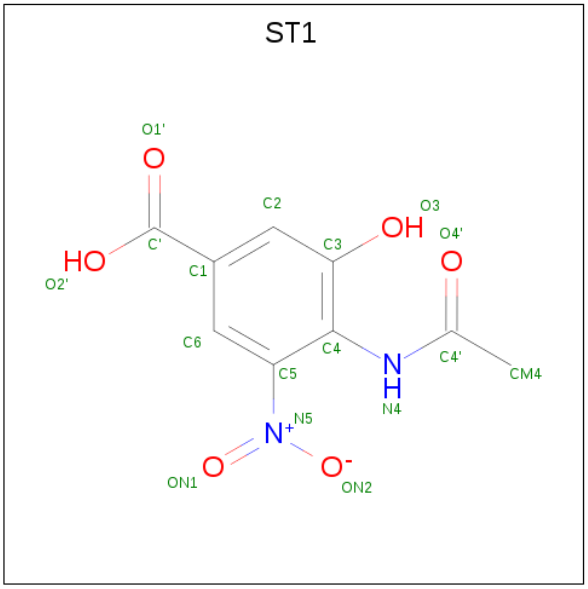


| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | | | |
| 5 | H | 4 | 96 | 28 | 47 | 2 | 19 | 0 | 0 | 0 |

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Ca | | |
| 6 | B | 1 | 1 | 1 | 0 | 0 |
| 6 | A | 1 | 1 | 1 | 0 | 0 |

- Molecule 7 is 4-(ACETYLAMINO)-3-HYDROXY-5-NITROBENZOIC ACID (three-letter code: ST1) (formula: $C_9H_8N_2O_6$).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | H | N | O | | |
| 7 | A | 1 | 19 | 9 | 2 | 2 | 6 | 0 | 0 |
| 7 | B | 1 | 19 | 9 | 2 | 2 | 6 | 0 | 0 |

- Molecule 8 is water.

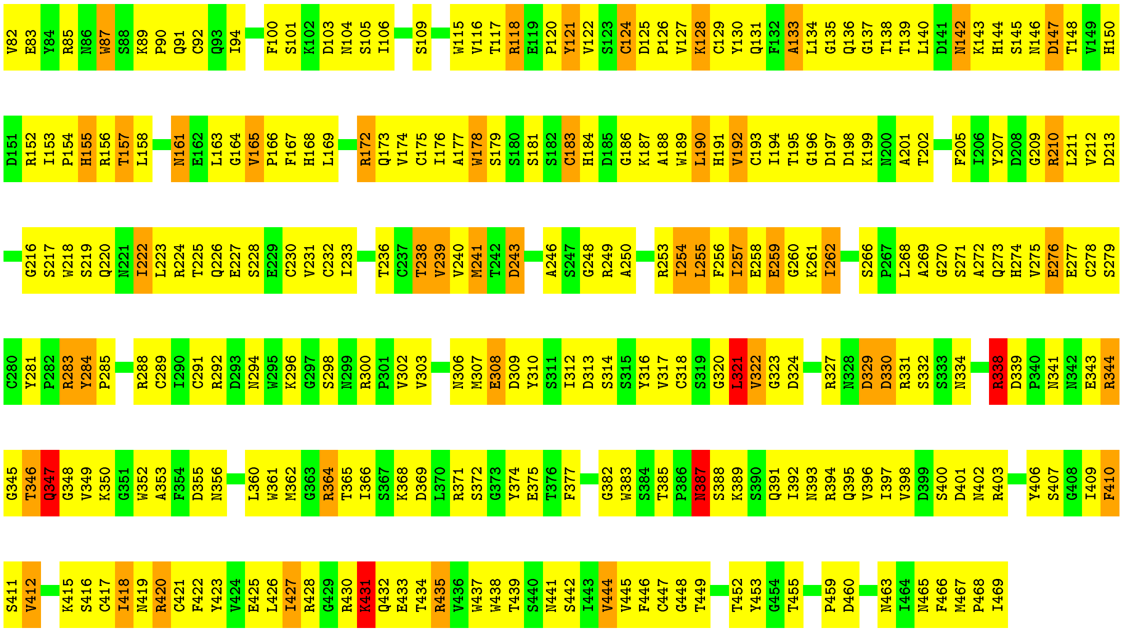
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| 8 | A | 121 | Total<br>363 | H<br>242 | O<br>121 | 1 | 0 |
| 8 | B | 4 | Total<br>12 | H<br>8 | O<br>4 | 0 | 0 |

# 3 Residue-property plots ⓘ

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. 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. 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.

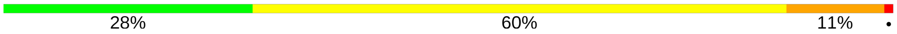
- Molecule 1: INFLUENZA A SUBTYPE N2 NEURAMINIDASE

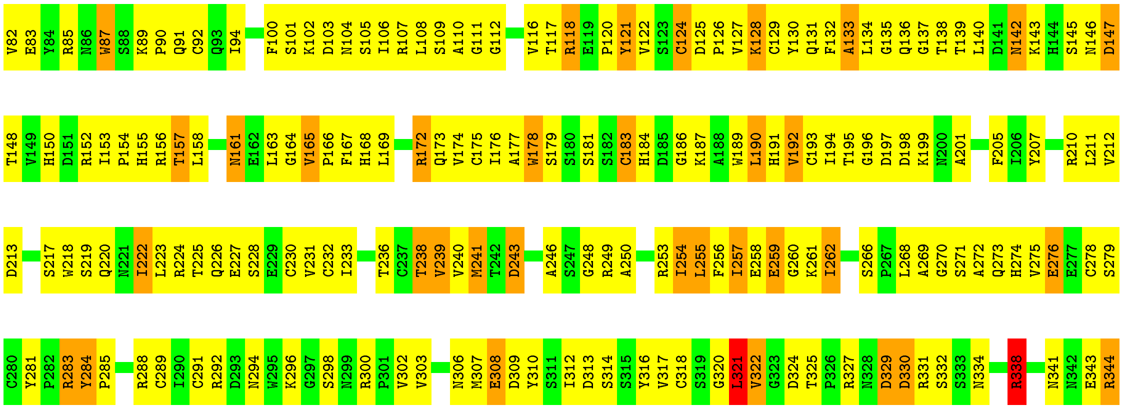
Chain A:

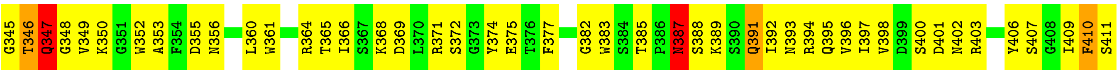


- Molecule 1: INFLUENZA A SUBTYPE N2 NEURAMINIDASE

Chain B:







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

Chain C:

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

Chain F:

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

Chain G:

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

Chain J:

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

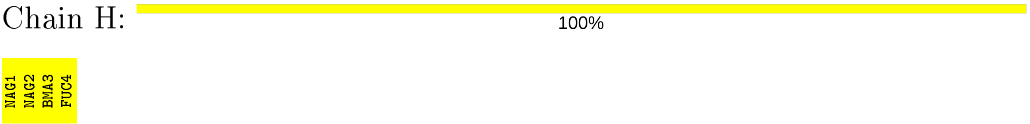
Chain E:

- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



# 4 Data and refinement statistics ⓘ

| Property | Value | Source |
|---|---|---|
| Space group | C 2 2 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 120.42Å 139.83Å 140.07Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 5.00 – 1.90<br>25.93 – 1.76 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | (Not available) (5.00-1.90)<br>28.4 (25.93-1.76) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.71 (at 1.76Å) | Xtriage |
| Refinement program | X-PLOR | Depositor |
| R, $R_{free}$ | 0.225 , (Not available)<br>0.287 , (Not available) | Depositor<br>DCC |
| $R_{free}$ test set | No test flags present. | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 4.1 | Xtriage |
| Anisotropy | 3.656 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.36 , 65.6 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.42$, $< L^2 > = 0.24$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.72 | EDS |
| Total number of atoms | 8595 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 7.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 5 Model quality ⓘ

## 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, ST1, CA, FUC, FUL, MAN

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 | 0.64 | 0/3092 | 0.94 | 4/4194 (0.1%) |
| 1 | B | 0.64 | 0/3092 | 0.94 | 4/4194 (0.1%) |
| All | All | 0.64 | 0/6184 | 0.94 | 8/8388 (0.1%) |

There are no bond length outliers.

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 1 | A | 243 | ASP | N-CA-C | -5.70 | 95.60 | 111.00 |
| 1 | B | 243 | ASP | N-CA-C | -5.70 | 95.60 | 111.00 |
| 1 | A | 338 | ARG | NE-CZ-NH1 | 5.12 | 122.86 | 120.30 |
| 1 | B | 338 | ARG | NE-CZ-NH1 | 5.12 | 122.86 | 120.30 |
| 1 | A | 444 | VAL | N-CA-C | -5.06 | 97.35 | 111.00 |
| 1 | B | 444 | VAL | N-CA-C | -5.06 | 97.35 | 111.00 |
| 1 | A | 321 | LEU | CA-CB-CG | -5.01 | 103.77 | 115.30 |
| 1 | B | 321 | LEU | CA-CB-CG | -5.01 | 103.77 | 115.30 |

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 | 3022 | 723 | 2850 | 335 | 5 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | B | 3022 | 723 | 2850 | 352 | 4 |
| 2 | C | 28 | 27 | 25 | 6 | 0 |
| 2 | F | 28 | 27 | 25 | 6 | 0 |
| 2 | G | 28 | 27 | 25 | 5 | 0 |
| 2 | J | 28 | 27 | 25 | 5 | 0 |
| 3 | D | 49 | 47 | 42 | 2 | 5 |
| 4 | E | 72 | 67 | 60 | 26 | 6 |
| 4 | I | 72 | 67 | 60 | 3 | 4 |
| 5 | H | 49 | 47 | 42 | 0 | 0 |
| 6 | A | 1 | 0 | 0 | 0 | 0 |
| 6 | B | 1 | 0 | 0 | 0 | 0 |
| 7 | A | 17 | 2 | 7 | 1 | 0 |
| 7 | B | 17 | 2 | 7 | 1 | 0 |
| 8 | A | 121 | 242 | 0 | 27 | 2 |
| 8 | B | 4 | 8 | 0 | 5 | 0 |
| All | All | 6559 | 2036 | 6018 | 678 | 13 |

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 55.

All (678) 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:B:455:THR:CG2 | 4:E:1:NAG:H61 | 1.57 | 1.35 |
| 1:B:107:ARG:CZ | 8:B:497:HOH:O | 1.78 | 1.31 |
| 8:A:515:HOH:O | 1:B:100:PHE:CZ | 1.83 | 1.31 |
| 1:B:455:THR:CG2 | 4:E:1:NAG:C6 | 2.15 | 1.24 |
| 1:B:205:PHE:HD2 | 1:B:257:ILE:HD12 | 1.08 | 1.17 |
| 1:B:455:THR:HG21 | 4:E:1:NAG:C6 | 1.75 | 1.15 |
| 1:A:205:PHE:HD2 | 1:A:257:ILE:HD12 | 1.08 | 1.12 |
| 1:B:455:THR:HG22 | 4:E:1:NAG:H61 | 1.26 | 1.09 |
| 1:A:169:LEU:HD11 | 1:B:112:GLY:HA3 | 1.31 | 1.07 |
| 1:A:115:TRP:CZ2 | 1:B:108:LEU:HD11 | 1.90 | 1.05 |
| 1:A:205:PHE:CD2 | 1:A:257:ILE:HD12 | 1.95 | 1.01 |
| 1:A:142:ASN:ND2 | 1:B:110:ALA:HB3 | 1.74 | 1.01 |
| 1:B:205:PHE:CD2 | 1:B:257:ILE:HD12 | 1.95 | 1.00 |
| 1:A:177:ALA:HB2 | 1:A:193:CYS:HB3 | 1.42 | 0.99 |
| 1:B:177:ALA:HB2 | 1:B:193:CYS:HB3 | 1.42 | 0.99 |
| 1:A:136:GLN:HG3 | 1:A:148:THR:HG23 | 1.46 | 0.96 |
| 1:A:409:ILE:HD11 | 1:A:420:ARG:HB3 | 1.47 | 0.95 |
| 1:B:409:ILE:HD11 | 1:B:420:ARG:HB3 | 1.47 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:A:518:HOH:O | 1:B:412:VAL:HG23 | 1.66 | 0.94 |
| 1:A:142:ASN:HD21 | 1:B:110:ALA:HB3 | 1.28 | 0.94 |
| 1:B:136:GLN:HG3 | 1:B:148:THR:HG23 | 1.46 | 0.94 |
| 1:A:281:TYR:HB3 | 8:A:525:HOH:O | 1.66 | 0.93 |
| 1:B:455:THR:HB | 4:E:1:NAG:O5 | 1.69 | 0.92 |
| 1:A:106:ILE:HG12 | 8:A:557:HOH:O | 1.69 | 0.91 |
| 1:B:396:VAL:CG1 | 4:E:6:MAN:O2 | 2.18 | 0.90 |
| 1:A:202:THR:HB | 1:B:454:GLY:H | 1.35 | 0.90 |
| 1:A:136:GLN:O | 1:A:138:THR:HG22 | 1.72 | 0.90 |
| 1:B:136:GLN:O | 1:B:138:THR:HG22 | 1.72 | 0.89 |
| 1:B:455:THR:CB | 4:E:1:NAG:H61 | 2.03 | 0.88 |
| 1:B:257:ILE:HD11 | 1:B:260:GLY:HA2 | 1.55 | 0.87 |
| 1:A:257:ILE:HD11 | 1:A:260:GLY:HA2 | 1.55 | 0.86 |
| 1:B:272:ALA:HA | 1:B:316:TYR:CE1 | 2.11 | 0.86 |
| 1:A:272:ALA:HA | 1:A:316:TYR:CE1 | 2.11 | 0.86 |
| 1:A:195:THR:HG21 | 1:B:458:TRP:HE1 | 1.43 | 0.83 |
| 1:A:169:LEU:CD1 | 1:B:112:GLY:HA3 | 2.09 | 0.83 |
| 1:B:396:VAL:HG11 | 4:E:6:MAN:O2 | 1.79 | 0.82 |
| 1:B:455:THR:HG21 | 4:E:1:NAG:H5 | 1.60 | 0.80 |
| 1:B:240:VAL:HG12 | 1:B:254:ILE:HG23 | 1.63 | 0.80 |
| 1:A:240:VAL:HG12 | 1:A:254:ILE:HG23 | 1.63 | 0.79 |
| 1:B:249:ARG:HG3 | 1:B:250:ALA:H | 1.47 | 0.79 |
| 1:B:331:ARG:HA | 1:B:331:ARG:NH1 | 1.99 | 0.78 |
| 1:A:331:ARG:HH11 | 1:A:331:ARG:HA | 1.48 | 0.78 |
| 1:B:331:ARG:HA | 1:B:331:ARG:HH11 | 1.48 | 0.77 |
| 1:B:455:THR:HG21 | 4:E:1:NAG:C5 | 2.13 | 0.77 |
| 1:A:249:ARG:HG3 | 1:A:250:ALA:H | 1.47 | 0.77 |
| 1:A:331:ARG:HA | 1:A:331:ARG:NH1 | 1.99 | 0.77 |
| 1:A:138:THR:HA | 1:B:108:LEU:HD23 | 1.64 | 0.77 |
| 1:A:101:SER:HA | 8:A:500:HOH:O | 1.84 | 0.76 |
| 1:A:272:ALA:HA | 1:A:316:TYR:HE1 | 1.48 | 0.76 |
| 1:B:452:THR:HG22 | 1:B:453:TYR:H | 1.51 | 0.76 |
| 1:A:318:CYS:HB3 | 1:A:385:THR:O | 1.86 | 0.76 |
| 1:A:452:THR:HG22 | 1:A:453:TYR:H | 1.51 | 0.76 |
| 1:A:296:LYS:O | 1:A:345:GLY:HA3 | 1.86 | 0.76 |
| 1:B:318:CYS:HB3 | 1:B:385:THR:O | 1.86 | 0.75 |
| 1:B:272:ALA:HA | 1:B:316:TYR:HE1 | 1.48 | 0.74 |
| 1:B:455:THR:HG22 | 4:E:1:NAG:C6 | 2.00 | 0.74 |
| 1:A:115:TRP:HZ2 | 1:B:108:LEU:HD11 | 1.51 | 0.73 |
| 1:B:438:TRP:HD1 | 1:B:469:ILE:HG13 | 1.53 | 0.73 |
| 1:A:158:LEU:O | 1:A:174:VAL:HG12 | 1.88 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:296:LYS:O | 1:B:345:GLY:HA3 | 1.86 | 0.73 |
| 1:B:271:SER:HB3 | 1:B:338:ARG:O | 1.89 | 0.73 |
| 1:B:158:LEU:O | 1:B:174:VAL:HG12 | 1.88 | 0.73 |
| 1:A:283:ARG:HE | 1:A:288:ARG:HE | 1.36 | 0.72 |
| 1:A:438:TRP:HD1 | 1:A:469:ILE:HG13 | 1.53 | 0.72 |
| 1:B:283:ARG:HE | 1:B:288:ARG:HE | 1.36 | 0.72 |
| 1:A:271:SER:HB3 | 1:A:338:ARG:O | 1.89 | 0.72 |
| 1:B:455:THR:CB | 4:E:1:NAG:C5 | 2.68 | 0.71 |
| 1:B:338:ARG:HB2 | 1:B:338:ARG:HH11 | 1.55 | 0.71 |
| 1:B:257:ILE:HD11 | 1:B:260:GLY:CA | 2.19 | 0.71 |
| 1:A:257:ILE:HD11 | 1:A:260:GLY:CA | 2.19 | 0.71 |
| 1:A:268:LEU:HD12 | 1:A:312:ILE:HG21 | 1.73 | 0.71 |
| 1:A:183:CYS:HB2 | 1:A:232:CYS:SG | 2.31 | 0.70 |
| 1:B:183:CYS:HB2 | 1:B:232:CYS:SG | 2.31 | 0.70 |
| 1:B:438:TRP:CD1 | 1:B:469:ILE:HG13 | 2.26 | 0.70 |
| 1:A:338:ARG:HB2 | 1:A:338:ARG:HH11 | 1.55 | 0.70 |
| 1:A:438:TRP:CD1 | 1:A:469:ILE:HG13 | 2.26 | 0.70 |
| 1:B:157:THR:HG22 | 1:B:176:ILE:HA | 1.73 | 0.70 |
| 1:A:125:ASP:HB3 | 1:A:184:HIS:ND1 | 2.06 | 0.70 |
| 1:A:394:ARG:HG3 | 1:A:395:GLN:N | 2.06 | 0.70 |
| 1:B:125:ASP:HB3 | 1:B:184:HIS:ND1 | 2.06 | 0.70 |
| 8:A:501:HOH:O | 1:B:108:LEU:HD22 | 1.91 | 0.70 |
| 1:A:430:ARG:HD3 | 1:A:437:TRP:HA | 1.72 | 0.70 |
| 1:B:394:ARG:HG3 | 1:B:395:GLN:N | 2.06 | 0.70 |
| 1:B:268:LEU:HD12 | 1:B:312:ILE:HG21 | 1.73 | 0.70 |
| 1:A:289:CYS:HB2 | 1:A:303:VAL:HB | 1.74 | 0.69 |
| 1:A:374:TYR:HB3 | 1:A:398:VAL:HG23 | 1.74 | 0.69 |
| 1:B:321:LEU:O | 1:B:322:VAL:HB | 1.93 | 0.69 |
| 1:B:430:ARG:HG3 | 1:B:431:LYS:H | 1.57 | 0.69 |
| 1:B:430:ARG:HD3 | 1:B:437:TRP:HA | 1.72 | 0.69 |
| 1:A:157:THR:HG22 | 1:A:176:ILE:HA | 1.73 | 0.69 |
| 1:B:87:TRP:HD1 | 1:B:233:ILE:HG12 | 1.58 | 0.69 |
| 1:B:217:SER:HA | 1:B:223:LEU:HD22 | 1.75 | 0.69 |
| 1:A:430:ARG:HG3 | 1:A:431:LYS:H | 1.57 | 0.69 |
| 1:A:155:HIS:HB3 | 1:B:104:ASN:ND2 | 2.06 | 0.69 |
| 1:A:87:TRP:HD1 | 1:A:233:ILE:HG12 | 1.58 | 0.68 |
| 1:B:289:CYS:HB2 | 1:B:303:VAL:HB | 1.74 | 0.68 |
| 1:B:455:THR:HB | 4:E:1:NAG:C5 | 2.22 | 0.68 |
| 1:B:419:ASN:HB3 | 8:B:517:HOH:O | 1.92 | 0.68 |
| 1:B:455:THR:OG1 | 4:E:1:NAG:C1 | 2.41 | 0.68 |
| 1:A:134:LEU:HB2 | 1:A:156:ARG:NH2 | 2.08 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:134:LEU:HB2 | 1:B:156:ARG:NH2 | 2.08 | 0.68 |
| 1:A:321:LEU:O | 1:A:322:VAL:HB | 1.93 | 0.68 |
| 1:A:216:GLY:H | 1:B:452:THR:HB | 1.59 | 0.68 |
| 1:A:103:ASP:HB3 | 8:A:502:HOH:O | 1.94 | 0.68 |
| 1:A:116:VAL:HG11 | 1:A:148:THR:HG21 | 1.76 | 0.68 |
| 1:B:116:VAL:HG11 | 1:B:148:THR:HG21 | 1.76 | 0.67 |
| 1:B:374:TYR:HB3 | 1:B:398:VAL:HG23 | 1.74 | 0.67 |
| 1:A:321:LEU:HD13 | 1:A:377:PHE:CE1 | 2.30 | 0.67 |
| 1:B:396:VAL:O | 1:B:396:VAL:HG13 | 1.95 | 0.67 |
| 1:A:116:VAL:CG1 | 1:A:148:THR:HG21 | 2.24 | 0.67 |
| 1:A:396:VAL:O | 1:A:396:VAL:HG13 | 1.95 | 0.67 |
| 1:A:217:SER:HA | 1:A:223:LEU:HD22 | 1.75 | 0.67 |
| 1:B:238:THR:OG1 | 1:B:307:MET:SD | 2.52 | 0.67 |
| 1:B:455:THR:CB | 4:E:1:NAG:O5 | 2.41 | 0.67 |
| 1:A:238:THR:OG1 | 1:A:307:MET:SD | 2.52 | 0.67 |
| 1:B:116:VAL:CG1 | 1:B:148:THR:HG21 | 2.24 | 0.66 |
| 1:A:144:HIS:CD2 | 1:B:466:PHE:HD2 | 2.13 | 0.66 |
| 1:A:249:ARG:HG3 | 1:A:250:ALA:N | 2.11 | 0.66 |
| 1:B:300:ARG:O | 1:B:317:VAL:HG23 | 1.95 | 0.66 |
| 1:B:321:LEU:HD13 | 1:B:377:PHE:CE1 | 2.30 | 0.66 |
| 1:A:300:ARG:O | 1:A:317:VAL:HG23 | 1.95 | 0.66 |
| 1:B:455:THR:HG21 | 4:E:1:NAG:O6 | 1.93 | 0.66 |
| 1:B:226:GLN:HE21 | 1:B:240:VAL:H | 1.44 | 0.66 |
| 1:B:455:THR:HB | 4:E:1:NAG:H61 | 1.77 | 0.65 |
| 1:A:412:VAL:HG11 | 1:A:421:CYS:SG | 2.36 | 0.65 |
| 1:B:412:VAL:HG11 | 1:B:421:CYS:SG | 2.36 | 0.65 |
| 1:B:249:ARG:HG3 | 1:B:250:ALA:N | 2.11 | 0.65 |
| 1:B:312:ILE:HG22 | 1:B:313:ASP:H | 1.62 | 0.65 |
| 1:A:419:ASN:HD21 | 1:A:448:GLY:HA3 | 1.61 | 0.65 |
| 1:B:419:ASN:HD21 | 1:B:448:GLY:HA3 | 1.61 | 0.65 |
| 1:A:312:ILE:HG22 | 1:A:313:ASP:H | 1.62 | 0.64 |
| 1:A:134:LEU:HD11 | 8:A:521:HOH:O | 1.98 | 0.64 |
| 1:B:228:SER:HB2 | 1:B:350:LYS:NZ | 2.13 | 0.64 |
| 1:A:366:ILE:HG21 | 1:A:400:SER:HB3 | 1.80 | 0.64 |
| 1:B:366:ILE:HG21 | 1:B:400:SER:HB3 | 1.80 | 0.64 |
| 1:A:228:SER:HB2 | 1:A:350:LYS:NZ | 2.13 | 0.63 |
| 1:A:226:GLN:HE21 | 1:A:240:VAL:H | 1.44 | 0.63 |
| 1:B:219:SER:O | 1:B:220:GLN:HB2 | 1.99 | 0.63 |
| 1:B:334:ASN:HA | 1:B:387:ASN:HD21 | 1.63 | 0.63 |
| 1:A:115:TRP:CZ2 | 1:B:108:LEU:CD1 | 2.76 | 0.63 |
| 1:A:101:SER:HB2 | 1:A:445:VAL:HG22 | 1.80 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:212:VAL:HB | 1:A:260:GLY:O | 1.98 | 0.63 |
| 1:B:212:VAL:HB | 1:B:260:GLY:O | 1.98 | 0.63 |
| 1:A:430:ARG:HD2 | 1:A:434:THR:HA | 1.81 | 0.63 |
| 1:B:101:SER:HB2 | 1:B:445:VAL:HG22 | 1.80 | 0.63 |
| 1:B:320:GLY:H | 1:B:388:SER:H | 1.47 | 0.63 |
| 1:A:146:ASN:OD1 | 1:A:437:TRP:HB3 | 1.99 | 0.63 |
| 1:A:177:ALA:CB | 1:A:193:CYS:HB3 | 2.24 | 0.63 |
| 1:B:452:THR:HG22 | 1:B:453:TYR:N | 2.14 | 0.63 |
| 1:B:372:SER:HA | 1:B:403:ARG:HA | 1.81 | 0.63 |
| 1:B:455:THR:CG2 | 4:E:1:NAG:C5 | 2.74 | 0.63 |
| 1:A:372:SER:HA | 1:A:403:ARG:HA | 1.81 | 0.63 |
| 1:B:430:ARG:HD2 | 1:B:434:THR:HA | 1.81 | 0.63 |
| 1:B:146:ASN:OD1 | 1:B:437:TRP:HB3 | 1.99 | 0.62 |
| 1:A:320:GLY:N | 1:A:388:SER:H | 1.97 | 0.62 |
| 1:A:409:ILE:HD12 | 1:A:421:CYS:O | 1.99 | 0.62 |
| 1:A:412:VAL:CG1 | 1:A:421:CYS:SG | 2.87 | 0.62 |
| 1:A:190:LEU:HD11 | 1:A:257:ILE:HD13 | 1.82 | 0.62 |
| 1:A:317:VAL:HB | 8:A:543:HOH:O | 1.98 | 0.62 |
| 1:B:412:VAL:CG1 | 1:B:421:CYS:SG | 2.87 | 0.62 |
| 1:B:320:GLY:N | 1:B:388:SER:H | 1.97 | 0.62 |
| 1:B:455:THR:CB | 4:E:1:NAG:C6 | 2.71 | 0.62 |
| 1:A:117:THR:HG21 | 1:A:167:PHE:HD2 | 1.65 | 0.62 |
| 1:A:334:ASN:HA | 1:A:387:ASN:HD21 | 1.63 | 0.62 |
| 1:B:85:ARG:HH12 | 1:B:125:ASP:HA | 1.65 | 0.62 |
| 1:B:409:ILE:HD12 | 1:B:421:CYS:O | 1.99 | 0.62 |
| 1:A:85:ARG:HH12 | 1:A:125:ASP:HA | 1.65 | 0.62 |
| 1:A:219:SER:O | 1:A:220:GLN:HB2 | 1.99 | 0.62 |
| 1:B:117:THR:HG21 | 1:B:167:PHE:HD2 | 1.65 | 0.62 |
| 1:A:118:ARG:HA | 1:A:441:ASN:OD1 | 1.99 | 0.61 |
| 1:B:196:GLY:HA3 | 1:B:201:ALA:HA | 1.82 | 0.61 |
| 1:B:118:ARG:HA | 1:B:441:ASN:OD1 | 1.99 | 0.61 |
| 1:A:320:GLY:H | 1:A:388:SER:H | 1.47 | 0.61 |
| 1:A:146:ASN:O | 1:A:147:ASP:HB2 | 2.01 | 0.61 |
| 1:A:452:THR:HG22 | 1:A:453:TYR:N | 2.14 | 0.61 |
| 1:B:107:ARG:NH2 | 8:B:497:HOH:O | 2.04 | 0.61 |
| 1:B:275:VAL:HG13 | 1:B:278:CYS:SG | 2.41 | 0.61 |
| 1:A:283:ARG:CZ | 1:A:288:ARG:HH21 | 2.14 | 0.61 |
| 1:A:196:GLY:HA3 | 1:A:201:ALA:HA | 1.82 | 0.61 |
| 1:B:283:ARG:CZ | 1:B:288:ARG:HH21 | 2.14 | 0.61 |
| 1:B:302:VAL:HG21 | 1:B:383:TRP:CZ3 | 2.36 | 0.61 |
| 1:A:302:VAL:HG21 | 1:A:383:TRP:CZ3 | 2.36 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:146:ASN:O | 1:B:147:ASP:HB2 | 2.01 | 0.60 |
| 1:A:463:ASN:HB3 | 1:A:466:PHE:CG | 2.36 | 0.60 |
| 1:B:190:LEU:HD11 | 1:B:257:ILE:HD13 | 1.82 | 0.60 |
| 1:B:246:ALA:O | 1:B:274:HIS:NE2 | 2.34 | 0.60 |
| 1:A:275:VAL:HG13 | 1:A:278:CYS:SG | 2.41 | 0.60 |
| 1:B:329:ASP:HA | 1:B:368:LYS:HD3 | 1.84 | 0.60 |
| 1:A:138:THR:HA | 1:B:108:LEU:CD2 | 2.32 | 0.60 |
| 1:A:246:ALA:O | 1:A:274:HIS:NE2 | 2.34 | 0.59 |
| 1:B:463:ASN:HB3 | 1:B:466:PHE:CG | 2.36 | 0.59 |
| 1:A:312:ILE:HG22 | 1:A:313:ASP:N | 2.17 | 0.59 |
| 1:A:172:ARG:HB3 | 1:B:165:VAL:HG12 | 1.83 | 0.59 |
| 1:A:329:ASP:HA | 1:A:368:LYS:HD3 | 1.84 | 0.59 |
| 1:B:257:ILE:O | 1:B:257:ILE:HG12 | 2.03 | 0.59 |
| 1:B:402:ASN:ND2 | 1:B:459:PRO:HB3 | 2.18 | 0.59 |
| 1:A:402:ASN:ND2 | 1:A:459:PRO:HB3 | 2.18 | 0.58 |
| 1:B:352:TRP:HD1 | 1:B:407:SER:HG | 1.50 | 0.58 |
| 1:B:312:ILE:HG22 | 1:B:313:ASP:N | 2.17 | 0.58 |
| 1:A:291:CYS:O | 1:A:300:ARG:HD3 | 2.03 | 0.58 |
| 1:B:291:CYS:O | 1:B:300:ARG:HD3 | 2.03 | 0.58 |
| 1:B:116:VAL:O | 1:B:135:GLY:HA2 | 2.02 | 0.58 |
| 1:B:396:VAL:HG12 | 4:E:6:MAN:O2 | 2.01 | 0.58 |
| 1:A:116:VAL:O | 1:A:135:GLY:HA2 | 2.02 | 0.58 |
| 1:A:258:GLU:O | 1:A:259:GLU:HB2 | 2.03 | 0.58 |
| 1:A:139:THR:O | 1:A:142:ASN:HB2 | 2.04 | 0.58 |
| 1:B:139:THR:O | 1:B:142:ASN:HB2 | 2.04 | 0.58 |
| 1:B:258:GLU:O | 1:B:259:GLU:HB2 | 2.03 | 0.58 |
| 1:B:327:ARG:HH11 | 1:B:327:ARG:HG2 | 1.68 | 0.58 |
| 2:C:1:NAG:C3 | 2:C:2:NAG:O5 | 2.51 | 0.58 |
| 1:B:177:ALA:CB | 1:B:193:CYS:HB3 | 2.24 | 0.58 |
| 1:A:431:LYS:H | 1:A:434:THR:HG22 | 1.69 | 0.57 |
| 1:B:455:THR:CG2 | 4:E:1:NAG:O6 | 2.50 | 0.57 |
| 1:A:218:TRP:HH2 | 1:A:241:MET:HB2 | 1.69 | 0.57 |
| 1:B:218:TRP:HH2 | 1:B:241:MET:HB2 | 1.69 | 0.57 |
| 1:B:131:GLN:NE2 | 1:B:164:GLY:H | 2.02 | 0.57 |
| 1:B:283:ARG:NE | 1:B:288:ARG:HH21 | 2.03 | 0.57 |
| 1:B:431:LYS:H | 1:B:434:THR:HG22 | 1.69 | 0.57 |
| 1:A:131:GLN:NE2 | 1:A:164:GLY:H | 2.02 | 0.57 |
| 1:B:91:GLN:HG3 | 1:B:420:ARG:NH1 | 2.20 | 0.57 |
| 1:A:327:ARG:HG2 | 1:A:327:ARG:HH11 | 1.68 | 0.57 |
| 1:A:283:ARG:NE | 1:A:288:ARG:HH21 | 2.03 | 0.57 |
| 1:A:257:ILE:HG12 | 1:A:257:ILE:O | 2.03 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:142:ASN:ND2 | 1:B:110:ALA:CB | 2.60 | 0.56 |
| 1:A:341:ASN:OD1 | 1:A:343:GLU:HG3 | 2.05 | 0.56 |
| 1:A:91:GLN:HG3 | 1:A:420:ARG:NH1 | 2.20 | 0.56 |
| 1:B:430:ARG:HG3 | 1:B:431:LYS:N | 2.21 | 0.56 |
| 1:A:155:HIS:HE2 | 1:B:461:GLY:HA3 | 1.70 | 0.56 |
| 1:B:324:ASP:O | 1:B:327:ARG:HD3 | 2.05 | 0.56 |
| 1:A:430:ARG:HG3 | 1:A:431:LYS:N | 2.21 | 0.56 |
| 1:B:341:ASN:OD1 | 1:B:343:GLU:HG3 | 2.05 | 0.56 |
| 2:G:1:NAG:C3 | 2:G:2:NAG:O5 | 2.51 | 0.56 |
| 1:A:279:SER:HB3 | 1:A:409:ILE:HG22 | 1.87 | 0.56 |
| 1:B:455:THR:HB | 4:E:1:NAG:C6 | 2.34 | 0.56 |
| 1:B:279:SER:HB3 | 1:B:409:ILE:HG22 | 1.87 | 0.56 |
| 1:B:136:GLN:HA | 1:B:136:GLN:OE1 | 2.06 | 0.55 |
| 1:A:410:PHE:CD1 | 1:A:410:PHE:C | 2.80 | 0.55 |
| 1:B:147:ASP:O | 1:B:150:HIS:HD2 | 1.90 | 0.55 |
| 1:A:197:ASP:O | 1:A:201:ALA:HB2 | 2.07 | 0.55 |
| 1:A:324:ASP:O | 1:A:327:ARG:HD3 | 2.05 | 0.55 |
| 2:G:1:NAG:N2 | 2:J:2:NAG:H82 | 2.22 | 0.55 |
| 1:A:150:HIS:HB3 | 8:A:585:HOH:O | 2.05 | 0.55 |
| 1:B:338:ARG:CB | 1:B:338:ARG:HH11 | 2.20 | 0.55 |
| 1:A:276:GLU:O | 1:A:292:ARG:HB3 | 2.07 | 0.55 |
| 1:B:276:GLU:O | 1:B:292:ARG:HB3 | 2.07 | 0.55 |
| 1:B:318:CYS:HB3 | 1:B:385:THR:C | 2.28 | 0.55 |
| 1:B:197:ASP:O | 1:B:201:ALA:HB2 | 2.07 | 0.54 |
| 1:B:288:ARG:NH1 | 1:B:383:TRP:CZ2 | 2.75 | 0.54 |
| 1:B:395:GLN:HA | 8:B:511:HOH:O | 2.06 | 0.54 |
| 1:A:136:GLN:HA | 1:A:136:GLN:OE1 | 2.06 | 0.54 |
| 1:A:155:HIS:HB3 | 1:B:104:ASN:HD21 | 1.70 | 0.54 |
| 1:B:410:PHE:C | 1:B:410:PHE:CD1 | 2.80 | 0.54 |
| 1:A:168:HIS:CD2 | 1:A:168:HIS:H | 2.25 | 0.54 |
| 1:A:318:CYS:HB3 | 1:A:385:THR:C | 2.28 | 0.54 |
| 1:B:228:SER:HB2 | 1:B:350:LYS:CE | 2.38 | 0.54 |
| 1:A:228:SER:HB2 | 1:A:350:LYS:CE | 2.38 | 0.54 |
| 1:A:147:ASP:O | 1:A:150:HIS:HD2 | 1.90 | 0.54 |
| 1:A:228:SER:HB2 | 1:A:350:LYS:HE2 | 1.90 | 0.54 |
| 1:B:346:THR:O | 1:B:347:GLN:O | 2.26 | 0.54 |
| 1:A:143:LYS:NZ | 1:B:466:PHE:HA | 2.23 | 0.53 |
| 1:A:213:ASP:OD2 | 1:A:262:ILE:HG13 | 2.08 | 0.53 |
| 1:B:168:HIS:CD2 | 1:B:168:HIS:H | 2.25 | 0.53 |
| 2:C:1:NAG:N2 | 2:F:2:NAG:H82 | 2.22 | 0.53 |
| 1:A:288:ARG:NH1 | 1:A:383:TRP:CZ2 | 2.75 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:411:SER:HB3 | 1:A:418:ILE:HD11 | 1.90 | 0.53 |
| 1:A:199:LYS:HA | 1:A:220:GLN:O | 2.09 | 0.53 |
| 1:B:199:LYS:HA | 1:B:220:GLN:O | 2.09 | 0.53 |
| 1:B:213:ASP:OD2 | 1:B:262:ILE:HG13 | 2.08 | 0.53 |
| 1:B:468:PRO:O | 1:B:469:ILE:HB | 2.08 | 0.53 |
| 1:A:468:PRO:O | 1:A:469:ILE:HB | 2.08 | 0.53 |
| 1:A:198:ASP:HB3 | 1:A:222:ILE:HG12 | 1.91 | 0.53 |
| 1:B:87:TRP:CD1 | 1:B:233:ILE:HG12 | 2.43 | 0.53 |
| 1:A:152:ARG:HD3 | 8:A:578:HOH:O | 2.07 | 0.53 |
| 1:A:177:ALA:HB2 | 1:A:193:CYS:CB | 2.28 | 0.53 |
| 1:A:338:ARG:CB | 1:A:338:ARG:HH11 | 2.20 | 0.53 |
| 1:A:409:ILE:HG13 | 1:A:410:PHE:N | 2.23 | 0.53 |
| 1:B:409:ILE:HG13 | 1:B:410:PHE:N | 2.23 | 0.53 |
| 1:A:463:ASN:OD1 | 1:A:465:ASN:HB2 | 2.09 | 0.53 |
| 1:B:411:SER:HB3 | 1:B:418:ILE:HD11 | 1.90 | 0.53 |
| 1:B:463:ASN:OD1 | 1:B:465:ASN:HB2 | 2.09 | 0.53 |
| 1:A:176:ILE:O | 1:A:177:ALA:HB2 | 2.09 | 0.52 |
| 1:A:346:THR:O | 1:A:347:GLN:O | 2.26 | 0.52 |
| 1:A:212:VAL:HG12 | 1:A:261:LYS:HE2 | 1.91 | 0.52 |
| 1:B:106:ILE:O | 1:B:109:SER:HB2 | 2.10 | 0.52 |
| 1:A:155:HIS:NE2 | 1:B:461:GLY:HA3 | 2.24 | 0.52 |
| 1:A:82:VAL:O | 1:A:187:LYS:HE2 | 2.10 | 0.52 |
| 1:B:228:SER:HB2 | 1:B:350:LYS:HE2 | 1.90 | 0.52 |
| 1:B:107:ARG:NH1 | 8:B:497:HOH:O | 2.15 | 0.52 |
| 1:A:106:ILE:O | 1:A:109:SER:HB2 | 2.10 | 0.52 |
| 1:A:421:CYS:HA | 1:A:447:CYS:HA | 1.92 | 0.52 |
| 1:A:281:TYR:OH | 1:A:288:ARG:HD2 | 2.10 | 0.52 |
| 1:A:402:ASN:HD22 | 1:A:459:PRO:HB3 | 1.75 | 0.52 |
| 1:A:209:GLY:O | 1:B:100:PHE:HZ | 1.93 | 0.51 |
| 1:A:329:ASP:OD1 | 1:A:330:ASP:N | 2.43 | 0.51 |
| 1:B:177:ALA:HB2 | 1:B:193:CYS:CB | 2.28 | 0.51 |
| 1:B:329:ASP:OD1 | 1:B:330:ASP:N | 2.43 | 0.51 |
| 4:I:2:NAG:H5 | 4:I:3:BMA:O2 | 2.10 | 0.51 |
| 1:B:134:LEU:HB2 | 1:B:156:ARG:HH21 | 1.75 | 0.51 |
| 1:B:281:TYR:OH | 1:B:288:ARG:HD2 | 2.10 | 0.51 |
| 1:B:128:LYS:HB3 | 1:B:130:TYR:CZ | 2.45 | 0.51 |
| 1:B:388:SER:C | 1:B:389:LYS:HG2 | 2.30 | 0.51 |
| 1:B:82:VAL:O | 1:B:187:LYS:HE2 | 2.10 | 0.51 |
| 1:B:402:ASN:HD22 | 1:B:459:PRO:HB3 | 1.75 | 0.51 |
| 1:A:388:SER:C | 1:A:389:LYS:HG2 | 2.30 | 0.51 |
| 1:B:198:ASP:HB3 | 1:B:222:ILE:HG12 | 1.91 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:E:2:NAG:H5 | 4:E:3:BMA:O2 | 2.10 | 0.51 |
| 1:B:212:VAL:HG12 | 1:B:261:LYS:HE2 | 1.91 | 0.51 |
| 1:A:128:LYS:HB3 | 1:A:130:TYR:CZ | 2.45 | 0.51 |
| 1:A:134:LEU:HB2 | 1:A:156:ARG:HH21 | 1.75 | 0.51 |
| 1:B:120:PRO:HG2 | 1:B:423:TYR:CE2 | 2.46 | 0.51 |
| 1:A:87:TRP:CD1 | 1:A:233:ILE:HG12 | 2.43 | 0.51 |
| 1:A:129:CYS:O | 1:A:163:LEU:N | 2.45 | 0.50 |
| 1:A:320:GLY:CA | 1:A:387:ASN:HD22 | 2.24 | 0.50 |
| 8:A:515:HOH:O | 1:B:100:PHE:CE2 | 2.36 | 0.50 |
| 1:B:176:ILE:O | 1:B:177:ALA:HB2 | 2.09 | 0.50 |
| 1:B:421:CYS:HA | 1:B:447:CYS:HA | 1.92 | 0.50 |
| 1:A:120:PRO:HG2 | 1:A:423:TYR:CE2 | 2.46 | 0.50 |
| 1:A:142:ASN:OD1 | 1:B:111:GLY:HA3 | 2.12 | 0.50 |
| 1:B:172:ARG:HG3 | 1:B:172:ARG:HH11 | 1.77 | 0.50 |
| 1:A:101:SER:HB2 | 1:A:445:VAL:CG2 | 2.41 | 0.50 |
| 8:A:515:HOH:O | 1:B:100:PHE:HZ | 1.50 | 0.50 |
| 1:B:352:TRP:NE1 | 1:B:374:TYR:OH | 2.45 | 0.50 |
| 1:B:101:SER:HB2 | 1:B:445:VAL:CG2 | 2.41 | 0.50 |
| 1:A:176:ILE:HD11 | 1:B:102:LYS:HB2 | 1.93 | 0.50 |
| 1:B:117:THR:HG21 | 1:B:167:PHE:CD2 | 2.46 | 0.50 |
| 1:B:320:GLY:CA | 1:B:387:ASN:HD22 | 2.24 | 0.50 |
| 1:B:227:GLU:O | 1:B:350:LYS:HE2 | 2.12 | 0.50 |
| 1:A:199:LYS:O | 1:A:220:GLN:HA | 2.12 | 0.50 |
| 2:J:1:NAG:O6 | 2:J:2:NAG:N2 | 2.45 | 0.50 |
| 1:A:403:ARG:HG2 | 8:A:550:HOH:O | 2.12 | 0.50 |
| 1:B:199:LYS:O | 1:B:220:GLN:HA | 2.12 | 0.50 |
| 1:B:270:GLY:HA3 | 1:B:314:SER:OG | 2.12 | 0.50 |
| 1:A:125:ASP:HB2 | 1:A:126:PRO:CD | 2.42 | 0.49 |
| 1:B:348:GLY:O | 1:B:371:ARG:NH2 | 2.44 | 0.49 |
| 1:B:423:TYR:HB2 | 1:B:445:VAL:HG12 | 1.94 | 0.49 |
| 1:B:419:ASN:ND2 | 1:B:448:GLY:HA3 | 2.26 | 0.49 |
| 1:B:125:ASP:HB2 | 1:B:126:PRO:CD | 2.42 | 0.49 |
| 1:B:302:VAL:HG21 | 1:B:383:TRP:CH2 | 2.47 | 0.49 |
| 1:A:227:GLU:O | 1:A:350:LYS:HE2 | 2.12 | 0.49 |
| 1:A:344:ARG:NH2 | 1:A:368:LYS:O | 2.46 | 0.49 |
| 1:B:134:LEU:CB | 1:B:156:ARG:HH21 | 2.26 | 0.49 |
| 1:B:419:ASN:ND2 | 1:B:420:ARG:N | 2.61 | 0.49 |
| 1:A:172:ARG:HH11 | 1:A:172:ARG:HG3 | 1.77 | 0.49 |
| 1:A:419:ASN:ND2 | 1:A:420:ARG:N | 2.61 | 0.49 |
| 1:B:344:ARG:NH2 | 1:B:368:LYS:O | 2.46 | 0.49 |
| 1:A:202:THR:HB | 1:B:454:GLY:N | 2.16 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:212:VAL:HB | 1:A:260:GLY:C | 2.33 | 0.49 |
| 1:A:270:GLY:HA3 | 1:A:314:SER:OG | 2.12 | 0.49 |
| 1:A:302:VAL:HG21 | 1:A:383:TRP:CH2 | 2.47 | 0.49 |
| 1:A:423:TYR:HB2 | 1:A:445:VAL:HG12 | 1.94 | 0.49 |
| 1:A:419:ASN:ND2 | 1:A:448:GLY:HA3 | 2.26 | 0.49 |
| 1:A:348:GLY:O | 1:A:371:ARG:NH2 | 2.44 | 0.49 |
| 1:A:406:TYR:HD2 | 8:A:488:HOH:O | 1.95 | 0.49 |
| 1:B:320:GLY:HA3 | 1:B:387:ASN:HD22 | 1.78 | 0.49 |
| 1:B:425:GLU:HB2 | 1:B:441:ASN:HD22 | 1.78 | 0.49 |
| 1:A:320:GLY:HA3 | 1:A:387:ASN:HD22 | 1.78 | 0.49 |
| 2:F:1:NAG:O6 | 2:F:2:NAG:N2 | 2.45 | 0.49 |
| 1:A:172:ARG:CB | 1:B:165:VAL:HG12 | 2.42 | 0.49 |
| 1:A:403:ARG:NH1 | 1:A:433:GLU:HG3 | 2.28 | 0.49 |
| 1:B:212:VAL:HB | 1:B:260:GLY:C | 2.33 | 0.49 |
| 1:B:419:ASN:ND2 | 1:B:420:ARG:O | 2.45 | 0.49 |
| 1:A:419:ASN:ND2 | 1:A:420:ARG:O | 2.45 | 0.49 |
| 1:A:425:GLU:HB2 | 1:A:441:ASN:HD22 | 1.78 | 0.48 |
| 1:B:327:ARG:HG2 | 1:B:327:ARG:NH1 | 2.28 | 0.48 |
| 1:B:422:PHE:CE1 | 1:B:446:PHE:HB2 | 2.47 | 0.48 |
| 1:A:140:LEU:HD23 | 1:A:468:PRO:HG2 | 1.95 | 0.48 |
| 1:A:327:ARG:NH1 | 1:A:327:ARG:HG2 | 2.28 | 0.48 |
| 1:A:124:CYS:HB3 | 1:A:129:CYS:HA | 1.96 | 0.48 |
| 1:A:179:SER:HB3 | 1:A:194:ILE:HB | 1.95 | 0.48 |
| 1:A:422:PHE:CE1 | 1:A:446:PHE:HB2 | 2.47 | 0.48 |
| 1:A:426:LEU:HD21 | 1:A:444:VAL:HG23 | 1.95 | 0.48 |
| 1:B:281:TYR:CZ | 1:B:288:ARG:HD2 | 2.49 | 0.48 |
| 1:B:85:ARG:NH1 | 1:B:184:HIS:HB3 | 2.29 | 0.48 |
| 1:A:430:ARG:O | 1:A:431:LYS:HB2 | 2.14 | 0.48 |
| 8:A:501:HOH:O | 1:B:108:LEU:HD13 | 2.14 | 0.48 |
| 1:B:129:CYS:SG | 1:B:410:PHE:HZ | 2.37 | 0.48 |
| 1:A:128:LYS:HB3 | 1:A:130:TYR:CE1 | 2.49 | 0.48 |
| 1:A:134:LEU:CB | 1:A:156:ARG:HH21 | 2.26 | 0.48 |
| 1:A:124:CYS:CB | 1:A:129:CYS:HA | 2.43 | 0.48 |
| 1:A:441:ASN:C | 8:A:557:HOH:O | 2.51 | 0.48 |
| 1:B:192:VAL:HG11 | 1:B:239:VAL:HG21 | 1.96 | 0.48 |
| 1:A:138:THR:OG1 | 1:A:139:THR:N | 2.44 | 0.48 |
| 1:A:144:HIS:HE1 | 1:B:462:ALA:HB1 | 1.77 | 0.48 |
| 1:A:352:TRP:NE1 | 1:A:374:TYR:OH | 2.45 | 0.48 |
| 1:B:124:CYS:CB | 1:B:129:CYS:HA | 2.43 | 0.48 |
| 1:B:139:THR:HG22 | 1:B:140:LEU:N | 2.28 | 0.48 |
| 1:B:128:LYS:HB3 | 1:B:130:TYR:CE1 | 2.49 | 0.47 |

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| **Atom-1** | **Atom-2** | **Interatomic distance (Å)** | **Clash overlap (Å)** |
|---|---|---|---|
| 1:B:165:VAL:HG23 | 1:B:166:PRO:O | 2.14 | 0.47 |
| 1:B:410:PHE:O | 1:B:421:CYS:N | 2.43 | 0.47 |
| 1:B:430:ARG:O | 1:B:431:LYS:HB2 | 2.14 | 0.47 |
| 2:G:1:NAG:H3 | 2:G:2:NAG:O5 | 2.14 | 0.47 |
| 1:A:85:ARG:NH1 | 1:A:184:HIS:HB3 | 2.29 | 0.47 |
| 1:A:239:VAL:HG13 | 1:A:239:VAL:O | 2.13 | 0.47 |
| 1:B:239:VAL:HG13 | 1:B:239:VAL:O | 2.13 | 0.47 |
| 1:B:140:LEU:HD23 | 1:B:468:PRO:HG2 | 1.95 | 0.47 |
| 1:B:129:CYS:O | 1:B:163:LEU:N | 2.45 | 0.47 |
| 1:B:407:SER:HB2 | 1:B:423:TYR:O | 2.13 | 0.47 |
| 1:A:100:PHE:HB3 | 1:A:445:VAL:HG23 | 1.97 | 0.47 |
| 1:B:179:SER:HB3 | 1:B:194:ILE:HB | 1.95 | 0.47 |
| 1:A:165:VAL:HG23 | 1:A:166:PRO:O | 2.14 | 0.47 |
| 1:A:189:TRP:O | 1:A:207:TYR:HA | 2.14 | 0.47 |
| 1:A:407:SER:HB2 | 1:A:423:TYR:O | 2.13 | 0.47 |
| 1:A:431:LYS:NZ | 1:A:431:LYS:HA | 2.29 | 0.47 |
| 1:B:125:ASP:HB3 | 1:B:184:HIS:CE1 | 2.49 | 0.47 |
| 1:B:153:ILE:HG13 | 1:B:153:ILE:O | 2.14 | 0.47 |
| 1:B:431:LYS:NZ | 1:B:431:LYS:HA | 2.29 | 0.47 |
| 2:C:1:NAG:H3 | 2:C:2:NAG:O5 | 2.14 | 0.47 |
| 1:A:281:TYR:CZ | 1:A:288:ARG:HD2 | 2.49 | 0.47 |
| 1:B:249:ARG:CG | 1:B:250:ALA:N | 2.78 | 0.47 |
| 1:B:426:LEU:HD21 | 1:B:444:VAL:HG23 | 1.95 | 0.47 |
| 1:A:177:ALA:HA | 1:A:195:THR:OG1 | 2.15 | 0.47 |
| 1:A:268:LEU:HG | 1:A:269:ALA:N | 2.30 | 0.47 |
| 1:A:129:CYS:SG | 1:A:410:PHE:HZ | 2.37 | 0.47 |
| 1:A:410:PHE:O | 1:A:421:CYS:N | 2.43 | 0.47 |
| 1:B:268:LEU:HG | 1:B:269:ALA:N | 2.30 | 0.47 |
| 1:B:403:ARG:NH1 | 1:B:433:GLU:HG3 | 2.28 | 0.47 |
| 1:A:139:THR:HG22 | 1:A:140:LEU:N | 2.28 | 0.47 |
| 1:A:255:LEU:HD23 | 1:A:255:LEU:N | 2.30 | 0.47 |
| 1:A:320:GLY:H | 1:A:388:SER:N | 2.11 | 0.47 |
| 1:A:115:TRP:CH2 | 1:B:108:LEU:HD11 | 2.47 | 0.47 |
| 1:A:188:ALA:HB1 | 8:A:510:HOH:O | 2.14 | 0.47 |
| 1:A:120:PRO:HG3 | 1:A:425:GLU:HB3 | 1.96 | 0.47 |
| 1:B:120:PRO:HG3 | 1:B:425:GLU:HB3 | 1.96 | 0.47 |
| 1:B:426:LEU:HD11 | 1:B:444:VAL:CG2 | 2.45 | 0.47 |
| 1:A:153:ILE:HG13 | 1:A:153:ILE:O | 2.14 | 0.47 |
| 1:A:218:TRP:CG | 1:A:253:ARG:NH2 | 2.83 | 0.47 |
| 1:B:138:THR:OG1 | 1:B:139:THR:N | 2.44 | 0.47 |
| 1:A:117:THR:HG21 | 1:A:167:PHE:CD2 | 2.46 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:306:ASN:OD1 | 1:A:308:GLU:HB2 | 2.15 | 0.47 |
| 1:B:218:TRP:CG | 1:B:253:ARG:NH2 | 2.83 | 0.47 |
| 1:A:152:ARG:O | 1:A:153:ILE:HG23 | 2.15 | 0.46 |
| 1:A:211:LEU:HD23 | 1:A:211:LEU:O | 2.15 | 0.46 |
| 1:A:352:TRP:HD1 | 1:A:407:SER:HG | 1.61 | 0.46 |
| 1:A:236:THR:HG23 | 1:A:258:GLU:HG2 | 1.98 | 0.46 |
| 1:A:284:TYR:OH | 2:F:1:NAG:H3 | 2.15 | 0.46 |
| 1:B:211:LEU:HD23 | 1:B:211:LEU:O | 2.15 | 0.46 |
| 1:A:179:SER:OG | 1:A:225:THR:HG22 | 2.15 | 0.46 |
| 1:A:283:ARG:NE | 1:A:288:ARG:HE | 2.11 | 0.46 |
| 1:B:100:PHE:HB3 | 1:B:445:VAL:HG23 | 1.97 | 0.46 |
| 1:B:124:CYS:HB3 | 1:B:129:CYS:HA | 1.96 | 0.46 |
| 1:B:152:ARG:O | 1:B:153:ILE:HG23 | 2.15 | 0.46 |
| 1:B:189:TRP:O | 1:B:207:TYR:HA | 2.14 | 0.46 |
| 1:B:457:SER:HB3 | 4:E:6:MAN:O3 | 2.15 | 0.46 |
| 1:B:177:ALA:HA | 1:B:195:THR:OG1 | 2.15 | 0.46 |
| 1:B:283:ARG:NE | 1:B:288:ARG:HE | 2.11 | 0.46 |
| 1:A:248:GLY:O | 1:A:274:HIS:CE1 | 2.69 | 0.46 |
| 1:A:426:LEU:HD11 | 1:A:444:VAL:CG2 | 2.45 | 0.46 |
| 1:B:248:GLY:O | 1:B:274:HIS:CE1 | 2.69 | 0.46 |
| 1:B:306:ASN:OD1 | 1:B:308:GLU:HB2 | 2.15 | 0.46 |
| 1:A:125:ASP:HB3 | 1:A:184:HIS:CE1 | 2.49 | 0.46 |
| 1:A:352:TRP:HE1 | 1:A:374:TYR:HH | 1.63 | 0.46 |
| 1:A:106:ILE:HG13 | 1:A:428:ARG:HG3 | 1.98 | 0.46 |
| 1:A:91:GLN:HG2 | 1:A:92:CYS:N | 2.31 | 0.46 |
| 1:B:255:LEU:HD23 | 1:B:255:LEU:N | 2.30 | 0.46 |
| 1:A:198:ASP:HB3 | 1:A:222:ILE:CG1 | 2.46 | 0.46 |
| 1:B:120:PRO:CG | 1:B:425:GLU:HB3 | 2.46 | 0.46 |
| 1:B:284:TYR:OH | 2:J:1:NAG:H3 | 2.15 | 0.46 |
| 1:B:410:PHE:CD1 | 1:B:411:SER:O | 2.69 | 0.46 |
| 1:B:426:LEU:HD13 | 1:B:460:ASP:N | 2.31 | 0.46 |
| 1:A:183:CYS:CB | 1:A:232:CYS:SG | 3.00 | 0.46 |
| 1:A:249:ARG:HA | 8:A:526:HOH:O | 2.15 | 0.46 |
| 1:A:410:PHE:HD1 | 1:A:410:PHE:C | 2.19 | 0.46 |
| 1:A:120:PRO:CG | 1:A:425:GLU:HB3 | 2.46 | 0.46 |
| 1:B:133:ALA:HB3 | 1:B:167:PHE:HE2 | 1.80 | 0.46 |
| 1:A:284:TYR:CE2 | 1:A:285:PRO:HG3 | 2.51 | 0.46 |
| 1:B:143:LYS:HE3 | 1:B:143:LYS:HB2 | 1.79 | 0.46 |
| 1:B:432:GLN:O | 1:B:434:THR:HG23 | 2.16 | 0.46 |
| 1:B:91:GLN:HG2 | 1:B:92:CYS:N | 2.31 | 0.46 |
| 1:A:321:LEU:O | 1:A:322:VAL:CB | 2.64 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:284:TYR:CE2 | 1:B:285:PRO:HG3 | 2.51 | 0.45 |
| 1:A:192:VAL:HG11 | 1:A:239:VAL:HG21 | 1.96 | 0.45 |
| 1:A:426:LEU:HD13 | 1:A:460:ASP:N | 2.31 | 0.45 |
| 1:A:432:GLN:O | 1:A:434:THR:HG23 | 2.16 | 0.45 |
| 1:B:183:CYS:CB | 1:B:232:CYS:SG | 3.00 | 0.45 |
| 1:A:392:ILE:HG12 | 1:A:393:ASN:N | 2.32 | 0.45 |
| 1:A:115:TRP:CH2 | 1:B:108:LEU:HD21 | 2.52 | 0.45 |
| 1:B:179:SER:OG | 1:B:225:THR:HG22 | 2.15 | 0.45 |
| 1:B:392:ILE:HG12 | 1:B:393:ASN:N | 2.32 | 0.45 |
| 1:B:106:ILE:HG13 | 1:B:428:ARG:HG3 | 1.98 | 0.45 |
| 1:B:288:ARG:HH11 | 1:B:288:ARG:HG3 | 1.82 | 0.45 |
| 1:A:133:ALA:HB3 | 1:A:167:PHE:HE2 | 1.80 | 0.45 |
| 1:B:198:ASP:HB3 | 1:B:222:ILE:CG1 | 2.46 | 0.45 |
| 2:C:2:NAG:C6 | 2:C:2:NAG:H2 | 2.46 | 0.45 |
| 2:G:2:NAG:C6 | 2:G:2:NAG:H2 | 2.46 | 0.45 |
| 1:A:144:HIS:CD2 | 1:B:466:PHE:CD2 | 3.00 | 0.45 |
| 1:A:387:ASN:HD22 | 1:A:387:ASN:HA | 1.61 | 0.45 |
| 1:A:410:PHE:CD1 | 1:A:411:SER:O | 2.69 | 0.45 |
| 1:A:87:TRP:CZ3 | 1:A:418:ILE:HD13 | 2.52 | 0.45 |
| 1:B:181:SER:HB3 | 1:B:192:VAL:HG13 | 1.98 | 0.45 |
| 1:B:236:THR:HG23 | 1:B:258:GLU:HG2 | 1.98 | 0.45 |
| 1:B:410:PHE:C | 1:B:410:PHE:HD1 | 2.19 | 0.45 |
| 1:B:87:TRP:CZ3 | 1:B:418:ILE:HD13 | 2.52 | 0.45 |
| 1:B:321:LEU:O | 1:B:322:VAL:CB | 2.64 | 0.45 |
| 1:A:210:ARG:NH2 | 8:A:518:HOH:O | 2.49 | 0.45 |
| 1:A:298:SER:O | 1:A:322:VAL:HG13 | 2.17 | 0.45 |
| 1:B:120:PRO:O | 1:B:121:TYR:HB3 | 2.17 | 0.45 |
| 1:B:211:LEU:HD23 | 1:B:211:LEU:C | 2.37 | 0.45 |
| 1:B:298:SER:O | 1:B:322:VAL:HG13 | 2.17 | 0.45 |
| 1:A:178:TRP:CE2 | 1:A:195:THR:HA | 2.53 | 0.44 |
| 1:A:278:CYS:HB3 | 1:A:289:CYS:HB3 | 1.99 | 0.44 |
| 1:A:442:SER:HB2 | 1:A:460:ASP:OD1 | 2.17 | 0.44 |
| 1:A:140:LEU:CD2 | 1:A:468:PRO:HG2 | 2.47 | 0.44 |
| 1:B:306:ASN:OD1 | 1:B:308:GLU:CB | 2.65 | 0.44 |
| 1:B:320:GLY:H | 1:B:388:SER:N | 2.11 | 0.44 |
| 1:A:190:LEU:CD1 | 1:A:257:ILE:HD13 | 2.46 | 0.44 |
| 1:B:139:THR:HB | 1:B:142:ASN:OD1 | 2.17 | 0.44 |
| 1:B:184:HIS:HD2 | 1:B:186:GLY:H | 1.64 | 0.44 |
| 1:B:442:SER:HB2 | 1:B:460:ASP:OD1 | 2.17 | 0.44 |
| 2:G:1:NAG:HN2 | 2:J:2:NAG:H82 | 1.82 | 0.44 |
| 1:A:139:THR:HB | 1:A:142:ASN:OD1 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:184:HIS:HD2 | 1:A:186:GLY:H | 1.64 | 0.44 |
| 1:A:211:LEU:HD23 | 1:A:211:LEU:C | 2.37 | 0.44 |
| 1:A:240:VAL:HG21 | 1:A:278:CYS:SG | 2.57 | 0.44 |
| 1:A:396:VAL:O | 1:A:398:VAL:N | 2.51 | 0.44 |
| 1:B:181:SER:HB3 | 1:B:192:VAL:CG1 | 2.48 | 0.44 |
| 1:B:195:THR:HG22 | 1:B:196:GLY:N | 2.33 | 0.44 |
| 1:A:181:SER:HB3 | 1:A:192:VAL:HG13 | 1.98 | 0.44 |
| 1:A:90:PRO:O | 1:A:417:CYS:HA | 2.18 | 0.44 |
| 1:B:90:PRO:O | 1:B:417:CYS:HA | 2.18 | 0.44 |
| 1:A:181:SER:HB3 | 1:A:192:VAL:CG1 | 2.48 | 0.44 |
| 1:A:288:ARG:HH11 | 1:A:288:ARG:HG3 | 1.82 | 0.44 |
| 1:A:415:LYS:O | 1:A:415:LYS:HG2 | 2.18 | 0.44 |
| 1:B:278:CYS:HB3 | 1:B:289:CYS:HB3 | 1.99 | 0.44 |
| 1:A:195:THR:HG22 | 1:A:196:GLY:N | 2.33 | 0.44 |
| 1:A:306:ASN:OD1 | 1:A:308:GLU:CB | 2.65 | 0.44 |
| 1:B:178:TRP:CE2 | 1:B:195:THR:HA | 2.53 | 0.44 |
| 1:B:240:VAL:HG21 | 1:B:278:CYS:SG | 2.57 | 0.44 |
| 1:B:415:LYS:HG2 | 1:B:415:LYS:O | 2.18 | 0.44 |
| 1:B:199:LYS:HG2 | 1:B:220:GLN:O | 2.18 | 0.44 |
| 1:B:218:TRP:NE1 | 1:B:243:ASP:HB3 | 2.33 | 0.44 |
| 1:A:249:ARG:CG | 1:A:250:ALA:N | 2.78 | 0.43 |
| 1:B:131:GLN:HE21 | 1:B:164:GLY:H | 1.66 | 0.43 |
| 1:A:143:LYS:HZ3 | 1:B:466:PHE:HA | 1.82 | 0.43 |
| 1:B:140:LEU:CD2 | 1:B:468:PRO:HG2 | 2.47 | 0.43 |
| 1:B:190:LEU:CG | 1:B:257:ILE:HD13 | 2.48 | 0.43 |
| 1:B:406:TYR:H | 1:B:425:GLU:HG2 | 1.83 | 0.43 |
| 1:A:406:TYR:H | 1:A:425:GLU:HG2 | 1.83 | 0.43 |
| 1:B:106:ILE:HG23 | 1:B:467:MET:CE | 2.48 | 0.43 |
| 1:A:120:PRO:O | 1:A:121:TYR:HB3 | 2.17 | 0.43 |
| 1:A:106:ILE:HG23 | 1:A:467:MET:CE | 2.48 | 0.43 |
| 1:B:169:LEU:HA | 1:B:169:LEU:HD23 | 1.79 | 0.43 |
| 2:C:1:NAG:HN2 | 2:F:2:NAG:H82 | 1.82 | 0.43 |
| 1:B:153:ILE:HG12 | 1:B:156:ARG:HG3 | 2.01 | 0.43 |
| 1:B:183:CYS:N | 1:B:230:CYS:SG | 2.91 | 0.43 |
| 1:A:183:CYS:N | 1:A:230:CYS:SG | 2.91 | 0.43 |
| 1:B:153:ILE:CG1 | 1:B:156:ARG:HG3 | 2.49 | 0.43 |
| 1:B:396:VAL:O | 1:B:398:VAL:N | 2.51 | 0.43 |
| 3:D:2:NAG:O6 | 3:D:3:BMA:O2 | 2.33 | 0.43 |
| 1:A:105:SER:HB2 | 1:A:442:SER:HA | 2.00 | 0.43 |
| 1:A:153:ILE:HG12 | 1:A:156:ARG:HG3 | 2.01 | 0.43 |
| 1:A:190:LEU:CG | 1:A:257:ILE:HD13 | 2.48 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:324:ASP:H | 1:A:327:ARG:HD3 | 1.84 | 0.43 |
| 1:A:350:LYS:HG2 | 1:A:407:SER:O | 2.18 | 0.43 |
| 1:A:365:THR:HG21 | 1:A:371:ARG:HA | 2.01 | 0.43 |
| 1:B:127:VAL:HG23 | 1:B:128:LYS:N | 2.34 | 0.43 |
| 1:B:324:ASP:H | 1:B:327:ARG:HD3 | 1.84 | 0.43 |
| 1:B:350:LYS:HG2 | 1:B:407:SER:O | 2.18 | 0.43 |
| 1:A:153:ILE:CG1 | 1:A:156:ARG:HG3 | 2.49 | 0.43 |
| 1:A:131:GLN:HE21 | 1:A:164:GLY:H | 1.66 | 0.43 |
| 1:A:161:ASN:HD22 | 1:A:161:ASN:HA | 1.62 | 0.43 |
| 1:A:218:TRP:NE1 | 1:A:243:ASP:HB3 | 2.33 | 0.43 |
| 1:A:366:ILE:HG21 | 1:A:400:SER:CB | 2.49 | 0.43 |
| 1:B:300:ARG:HH22 | 1:B:349:VAL:HG13 | 1.84 | 0.43 |
| 1:B:309:ASP:O | 1:B:310:TYR:HB2 | 2.19 | 0.43 |
| 1:B:463:ASN:O | 1:B:467:MET:HG2 | 2.19 | 0.43 |
| 1:B:109:SER:HB3 | 1:B:140:LEU:HD13 | 2.00 | 0.42 |
| 1:B:153:ILE:HB | 1:B:154:PRO:HD2 | 2.00 | 0.42 |
| 1:A:161:ASN:HB3 | 1:A:165:VAL:HG22 | 2.01 | 0.42 |
| 1:B:325:THR:HG1 | 1:B:365:THR:HG1 | 1.66 | 0.42 |
| 1:B:327:ARG:NH1 | 1:B:368:LYS:HA | 2.34 | 0.42 |
| 1:A:292:ARG:CZ | 1:A:294:ASN:HD21 | 2.32 | 0.42 |
| 1:A:332:SER:O | 1:A:334:ASN:OD1 | 2.37 | 0.42 |
| 1:A:327:ARG:NH1 | 1:A:368:LYS:HA | 2.34 | 0.42 |
| 1:A:442:SER:N | 8:A:557:HOH:O | 2.53 | 0.42 |
| 1:B:292:ARG:CZ | 1:B:294:ASN:HD21 | 2.32 | 0.42 |
| 1:B:365:THR:HG21 | 1:B:371:ARG:HA | 2.01 | 0.42 |
| 1:A:144:HIS:CE1 | 1:B:463:ASN:H | 2.37 | 0.42 |
| 1:A:153:ILE:HB | 1:A:154:PRO:HD2 | 2.00 | 0.42 |
| 1:A:199:LYS:HG2 | 1:A:220:GLN:O | 2.18 | 0.42 |
| 1:A:463:ASN:O | 1:A:467:MET:HG2 | 2.19 | 0.42 |
| 1:A:409:ILE:HG12 | 8:A:525:HOH:O | 2.19 | 0.42 |
| 1:B:128:LYS:HE2 | 1:B:128:LYS:HB2 | 1.82 | 0.42 |
| 1:B:427:ILE:HD11 | 1:B:439:THR:HG23 | 2.02 | 0.42 |
| 1:A:109:SER:HB3 | 1:A:140:LEU:HD13 | 2.00 | 0.42 |
| 1:A:302:VAL:HG21 | 1:A:383:TRP:HZ3 | 1.84 | 0.42 |
| 1:B:103:ASP:O | 1:B:104:ASN:HB2 | 2.20 | 0.42 |
| 1:B:161:ASN:HB3 | 1:B:165:VAL:HG22 | 2.01 | 0.42 |
| 1:B:332:SER:O | 1:B:334:ASN:OD1 | 2.37 | 0.42 |
| 1:A:103:ASP:O | 1:A:104:ASN:HB2 | 2.20 | 0.42 |
| 1:B:105:SER:HB2 | 1:B:442:SER:HA | 2.00 | 0.42 |
| 4:I:1:NAG:O4 | 4:I:2:NAG:O6 | 2.33 | 0.42 |
| 1:A:309:ASP:O | 1:A:310:TYR:HB2 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:F:1:NAG:H5 | 2:F:2:NAG:HN2 | 1.85 | 0.42 |
| 1:A:127:VAL:HG23 | 1:A:128:LYS:N | 2.34 | 0.42 |
| 1:A:323:GLY:HA3 | 8:A:534:HOH:O | 2.19 | 0.42 |
| 1:A:402:ASN:ND2 | 1:A:459:PRO:CB | 2.83 | 0.42 |
| 1:A:467:MET:HE3 | 1:A:468:PRO:HD2 | 2.02 | 0.42 |
| 1:B:157:THR:OG1 | 1:B:173:GLN:HG2 | 2.20 | 0.42 |
| 1:A:427:ILE:HD11 | 1:A:439:THR:HG23 | 2.02 | 0.42 |
| 1:A:431:LYS:HZ2 | 1:A:431:LYS:HA | 1.85 | 0.42 |
| 1:A:455:THR:HG23 | 8:A:555:HOH:O | 2.20 | 0.42 |
| 1:B:419:ASN:HD21 | 1:B:448:GLY:CA | 2.32 | 0.42 |
| 4:E:2:NAG:O4 | 4:E:6:MAN:C6 | 2.68 | 0.42 |
| 1:A:375:GLU:HA | 1:A:395:GLN:O | 2.20 | 0.41 |
| 1:B:402:ASN:ND2 | 1:B:459:PRO:CB | 2.83 | 0.41 |
| 1:A:157:THR:OG1 | 1:A:173:GLN:HG2 | 2.20 | 0.41 |
| 1:B:161:ASN:HD22 | 1:B:161:ASN:HA | 1.62 | 0.41 |
| 1:B:302:VAL:HG21 | 1:B:383:TRP:HZ3 | 1.84 | 0.41 |
| 1:B:353:ALA:HB1 | 1:B:360:LEU:HD11 | 2.02 | 0.41 |
| 4:I:2:NAG:O4 | 4:I:6:MAN:C6 | 2.68 | 0.41 |
| 2:J:1:NAG:H5 | 2:J:2:NAG:HN2 | 1.85 | 0.41 |
| 1:A:158:LEU:HB3 | 1:A:175:CYS:SG | 2.60 | 0.41 |
| 1:A:256:PHE:CD2 | 1:A:310:TYR:CD1 | 3.08 | 0.41 |
| 1:A:118:ARG:CA | 1:A:441:ASN:OD1 | 2.67 | 0.41 |
| 1:A:94:ILE:HD11 | 1:A:361:TRP:CD2 | 2.55 | 0.41 |
| 1:B:134:LEU:CB | 1:B:156:ARG:NH2 | 2.80 | 0.41 |
| 1:B:190:LEU:CD1 | 1:B:257:ILE:HD13 | 2.46 | 0.41 |
| 1:A:136:GLN:O | 1:A:138:THR:N | 2.54 | 0.41 |
| 1:A:266:SER:OG | 1:A:310:TYR:HB3 | 2.21 | 0.41 |
| 1:A:425:GLU:HB2 | 1:A:441:ASN:ND2 | 2.35 | 0.41 |
| 1:A:300:ARG:HH22 | 1:A:349:VAL:HG13 | 1.84 | 0.41 |
| 1:A:409:ILE:CG1 | 8:A:525:HOH:O | 2.68 | 0.41 |
| 1:A:463:ASN:HB3 | 1:A:466:PHE:CD2 | 2.56 | 0.41 |
| 1:A:435:ARG:HH21 | 1:A:465:ASN:HA | 1.86 | 0.41 |
| 1:B:125:ASP:O | 1:B:127:VAL:N | 2.54 | 0.41 |
| 1:B:136:GLN:O | 1:B:138:THR:N | 2.54 | 0.41 |
| 1:B:158:LEU:HB3 | 1:B:175:CYS:SG | 2.60 | 0.41 |
| 1:B:94:ILE:HD11 | 1:B:361:TRP:CD2 | 2.55 | 0.41 |
| 1:B:266:SER:OG | 1:B:310:TYR:HB3 | 2.21 | 0.41 |
| 1:B:366:ILE:HG21 | 1:B:400:SER:CB | 2.49 | 0.41 |
| 1:B:375:GLU:HA | 1:B:395:GLN:O | 2.20 | 0.41 |
| 1:A:327:ARG:C | 1:A:344:ARG:HE | 2.24 | 0.41 |
| 1:A:432:GLN:O | 1:A:434:THR:N | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:228:SER:HB2 | 1:B:350:LYS:HZ3 | 1.85 | 0.41 |
| 1:A:125:ASP:O | 1:A:127:VAL:N | 2.54 | 0.41 |
| 1:A:147:ASP:O | 1:A:150:HIS:CD2 | 2.73 | 0.41 |
| 7:A:471:ST1:O3 | 7:A:471:ST1:HM43 | 2.21 | 0.41 |
| 1:B:425:GLU:HB2 | 1:B:441:ASN:ND2 | 2.35 | 0.41 |
| 1:A:181:SER:OG | 1:A:230:CYS:HB3 | 2.21 | 0.41 |
| 1:A:191:HIS:O | 1:A:193:CYS:SG | 2.79 | 0.41 |
| 1:A:218:TRP:CH2 | 1:A:241:MET:HB2 | 2.51 | 0.41 |
| 1:A:283:ARG:HD3 | 1:A:283:ARG:O | 2.20 | 0.41 |
| 1:B:256:PHE:CD2 | 1:B:310:TYR:CD1 | 3.08 | 0.41 |
| 1:B:387:ASN:HA | 1:B:387:ASN:HD22 | 1.61 | 0.41 |
| 1:B:391:GLN:HE22 | 1:B:394:ARG:HB2 | 1.86 | 0.41 |
| 1:B:463:ASN:HB3 | 1:B:466:PHE:CD2 | 2.56 | 0.41 |
| 1:B:132:PHE:CD1 | 1:B:132:PHE:N | 2.89 | 0.41 |
| 1:B:191:HIS:O | 1:B:193:CYS:SG | 2.79 | 0.41 |
| 1:B:283:ARG:O | 1:B:283:ARG:HD3 | 2.20 | 0.41 |
| 1:B:414:GLY:N | 1:B:417:CYS:O | 2.54 | 0.41 |
| 1:A:216:GLY:N | 1:B:452:THR:HB | 2.31 | 0.41 |
| 7:B:471:ST1:HM43 | 7:B:471:ST1:O3 | 2.21 | 0.41 |
| 1:A:127:VAL:HG23 | 1:A:128:LYS:H | 1.86 | 0.40 |
| 1:A:338:ARG:NH1 | 1:A:339:ASP:OD1 | 2.55 | 0.40 |
| 1:A:362:MET:CE | 1:A:364:ARG:HG2 | 2.51 | 0.40 |
| 1:B:120:PRO:HG2 | 1:B:423:TYR:HE2 | 1.86 | 0.40 |
| 1:B:327:ARG:C | 1:B:344:ARG:HE | 2.24 | 0.40 |
| 2:C:1:NAG:O3 | 2:F:2:NAG:C8 | 2.69 | 0.40 |
| 1:A:277:GLU:N | 8:A:522:HOH:O | 2.53 | 0.40 |
| 1:A:353:ALA:HB1 | 1:A:360:LEU:HD11 | 2.02 | 0.40 |
| 1:B:320:GLY:N | 1:B:388:SER:N | 2.68 | 0.40 |
| 1:B:432:GLN:O | 1:B:434:THR:N | 2.54 | 0.40 |
| 4:E:2:NAG:O4 | 4:E:6:MAN:H61 | 2.22 | 0.40 |
| 1:A:128:LYS:HE2 | 1:A:128:LYS:HB2 | 1.82 | 0.40 |
| 1:A:136:GLN:OE1 | 1:A:156:ARG:CG | 2.69 | 0.40 |
| 1:A:144:HIS:HE1 | 1:B:462:ALA:CB | 2.34 | 0.40 |
| 1:A:317:VAL:HG21 | 8:A:535:HOH:O | 2.21 | 0.40 |
| 1:A:142:ASN:HD21 | 1:B:110:ALA:CB | 2.14 | 0.40 |
| 1:A:284:TYR:CG | 1:A:285:PRO:HA | 2.57 | 0.40 |
| 1:B:256:PHE:N | 1:B:256:PHE:CD1 | 2.90 | 0.40 |
| 1:B:368:LYS:NZ | 1:B:369:ASP:OD2 | 2.54 | 0.40 |
| 1:B:91:GLN:OE1 | 1:B:420:ARG:NH1 | 2.51 | 0.40 |
| 1:A:368:LYS:NZ | 1:A:369:ASP:OD2 | 2.54 | 0.40 |
| 1:B:136:GLN:OE1 | 1:B:156:ARG:CG | 2.69 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:256:PHE:CD2 | 1:B:310:TYR:CE1 | 3.10 | 0.40 |
| 1:B:349:VAL:HG22 | 1:B:350:LYS:N | 2.37 | 0.40 |
| 1:B:467:MET:HE3 | 1:B:468:PRO:HD2 | 2.02 | 0.40 |
| 3:D:2:NAG:H3 | 3:D:3:BMA:O5 | 2.22 | 0.40 |

All (13) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:463:ASN:HD22 | 4:E:5:MAN:H62[3_654] | 1.02 | 0.58 |
| 3:D:4:FUL:H1 | 4:E:4:MAN:O3[3_654] | 1.02 | 0.58 |
| 3:D:4:FUL:H3 | 4:E:4:MAN:HO3[3_654] | 1.04 | 0.56 |
| 3:D:4:FUL:C1 | 4:E:4:MAN:O3[3_654] | 1.85 | 0.35 |
| 1:A:455:THR:OG1 | 4:I:1:NAG:H1[4_555] | 1.42 | 0.18 |
| 1:A:455:THR:CG2 | 4:I:1:NAG:H61[4_555] | 1.43 | 0.17 |
| 1:B:270:GLY:CA | 8:A:489:HOH:O[7_544] | 2.10 | 0.10 |
| 1:A:164:GLY:O | 1:B:173:GLN:H[4_555] | 1.54 | 0.06 |
| 1:A:455:THR:CG2 | 4:I:1:NAG:C6[4_555] | 2.15 | 0.05 |
| 3:D:4:FUL:H3 | 4:E:4:MAN:O2[3_654] | 1.56 | 0.04 |
| 3:D:4:FUL:H5 | 4:E:4:MAN:O5[3_654] | 1.58 | 0.02 |
| 1:B:270:GLY:C | 8:A:489:HOH:O[7_544] | 2.18 | 0.02 |
| 1:A:396:VAL:CG1 | 4:I:6:MAN:O2[4_555] | 2.18 | 0.02 |

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | A | 386/388 (100%) | 294 (76%) | 70 (18%) | 22 (6%) | 1 0 |
| 1 | B | 386/388 (100%) | 294 (76%) | 70 (18%) | 22 (6%) | 1 0 |
| All | All | 772/776 (100%) | 588 (76%) | 140 (18%) | 44 (6%) | 1 0 |

All (44) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 145 | SER |
| 1 | A | 284 | TYR |
| 1 | A | 329 | ASP |
| 1 | A | 346 | THR |
| 1 | A | 347 | GLN |
| 1 | A | 397 | ILE |
| 1 | A | 412 | VAL |
| 1 | B | 145 | SER |
| 1 | B | 284 | TYR |
| 1 | B | 329 | ASP |
| 1 | B | 346 | THR |
| 1 | B | 347 | GLN |
| 1 | B | 397 | ILE |
| 1 | B | 412 | VAL |
| 1 | A | 87 | TRP |
| 1 | A | 118 | ARG |
| 1 | A | 259 | GLU |
| 1 | A | 322 | VAL |
| 1 | A | 416 | SER |
| 1 | B | 87 | TRP |
| 1 | B | 118 | ARG |
| 1 | B | 259 | GLU |
| 1 | B | 322 | VAL |
| 1 | B | 416 | SER |
| 1 | A | 133 | ALA |
| 1 | A | 137 | GLY |
| 1 | A | 147 | ASP |
| 1 | A | 431 | LYS |
| 1 | B | 133 | ALA |
| 1 | B | 137 | GLY |
| 1 | B | 147 | ASP |
| 1 | B | 431 | LYS |
| 1 | A | 356 | ASN |
| 1 | B | 356 | ASN |
| 1 | A | 121 | TYR |
| 1 | A | 222 | ILE |
| 1 | B | 121 | TYR |
| 1 | B | 222 | ILE |
| 1 | A | 239 | VAL |
| 1 | A | 387 | ASN |
| 1 | B | 239 | VAL |
| 1 | B | 387 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 382 | GLY |
| 1 | B | 382 | GLY |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | A | 338/338 (100%) | 293 (87%) | 45 (13%) | 4 | 1 |
| 1 | B | 338/338 (100%) | 293 (87%) | 45 (13%) | 4 | 1 |
| All | All | 676/676 (100%) | 586 (87%) | 90 (13%) | 4 | 1 |

All (90) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 83 | GLU |
| 1 | A | 89 | LYS |
| 1 | A | 122 | VAL |
| 1 | A | 124 | CYS |
| 1 | A | 128 | LYS |
| 1 | A | 142 | ASN |
| 1 | A | 155 | HIS |
| 1 | A | 157 | THR |
| 1 | A | 161 | ASN |
| 1 | A | 165 | VAL |
| 1 | A | 172 | ARG |
| 1 | A | 178 | TRP |
| 1 | A | 183 | CYS |
| 1 | A | 190 | LEU |
| 1 | A | 192 | VAL |
| 1 | A | 210 | ARG |
| 1 | A | 224 | ARG |
| 1 | A | 231 | VAL |
| 1 | A | 238 | THR |
| 1 | A | 241 | MET |
| 1 | A | 254 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 255 | LEU |
| 1 | A | 257 | ILE |
| 1 | A | 262 | ILE |
| 1 | A | 273 | GLN |
| 1 | A | 276 | GLU |
| 1 | A | 283 | ARG |
| 1 | A | 308 | GLU |
| 1 | A | 321 | LEU |
| 1 | A | 330 | ASP |
| 1 | A | 338 | ARG |
| 1 | A | 344 | ARG |
| 1 | A | 347 | GLN |
| 1 | A | 355 | ASP |
| 1 | A | 364 | ARG |
| 1 | A | 387 | ASN |
| 1 | A | 391 | GLN |
| 1 | A | 401 | ASP |
| 1 | A | 410 | PHE |
| 1 | A | 418 | ILE |
| 1 | A | 420 | ARG |
| 1 | A | 427 | ILE |
| 1 | A | 431 | LYS |
| 1 | A | 435 | ARG |
| 1 | A | 449 | THR |
| 1 | B | 83 | GLU |
| 1 | B | 89 | LYS |
| 1 | B | 122 | VAL |
| 1 | B | 124 | CYS |
| 1 | B | 128 | LYS |
| 1 | B | 142 | ASN |
| 1 | B | 155 | HIS |
| 1 | B | 157 | THR |
| 1 | B | 161 | ASN |
| 1 | B | 165 | VAL |
| 1 | B | 172 | ARG |
| 1 | B | 178 | TRP |
| 1 | B | 183 | CYS |
| 1 | B | 190 | LEU |
| 1 | B | 192 | VAL |
| 1 | B | 210 | ARG |
| 1 | B | 224 | ARG |
| 1 | B | 231 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 238 | THR |
| 1 | B | 241 | MET |
| 1 | B | 254 | ILE |
| 1 | B | 255 | LEU |
| 1 | B | 257 | ILE |
| 1 | B | 262 | ILE |
| 1 | B | 273 | GLN |
| 1 | B | 276 | GLU |
| 1 | B | 283 | ARG |
| 1 | B | 308 | GLU |
| 1 | B | 321 | LEU |
| 1 | B | 330 | ASP |
| 1 | B | 338 | ARG |
| 1 | B | 344 | ARG |
| 1 | B | 347 | GLN |
| 1 | B | 355 | ASP |
| 1 | B | 364 | ARG |
| 1 | B | 387 | ASN |
| 1 | B | 391 | GLN |
| 1 | B | 401 | ASP |
| 1 | B | 410 | PHE |
| 1 | B | 418 | ILE |
| 1 | B | 420 | ARG |
| 1 | B | 427 | ILE |
| 1 | B | 431 | LYS |
| 1 | B | 435 | ARG |
| 1 | B | 449 | THR |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 104 | ASN |
| 1 | A | 131 | GLN |
| 1 | A | 144 | HIS |
| 1 | A | 150 | HIS |
| 1 | A | 161 | ASN |
| 1 | A | 173 | GLN |
| 1 | A | 220 | GLN |
| 1 | A | 221 | ASN |
| 1 | A | 226 | GLN |
| 1 | A | 334 | ASN |
| 1 | A | 387 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 393 | ASN |
| 1 | A | 402 | ASN |
| 1 | A | 419 | ASN |
| 1 | B | 104 | ASN |
| 1 | B | 131 | GLN |
| 1 | B | 150 | HIS |
| 1 | B | 161 | ASN |
| 1 | B | 168 | HIS |
| 1 | B | 173 | GLN |
| 1 | B | 220 | GLN |
| 1 | B | 226 | GLN |
| 1 | B | 334 | ASN |
| 1 | B | 387 | ASN |
| 1 | B | 393 | ASN |
| 1 | B | 402 | ASN |
| 1 | B | 419 | ASN |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

28 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 | $\#\|Z\| > 2$ |
| 2 | NAG | C | 1 | 1,2 | 14,14,15 | 1.75 | 3 (21%) | 17,19,21 | 2.38 | 8 (47%) |
| 2 | NAG | C | 2 | 2 | 14,14,15 | 2.02 | 4 (28%) | 17,19,21 | 2.72 | 5 (29%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | #\|Z\| > 2 | Counts | RMSZ | #\|Z\| > 2 |
| 3 | NAG | D | 1 | 1,3 | 14,14,15 | 1.93 | 3 (21%) | 17,19,21 | 2.54 | 6 (35%) |
| 3 | NAG | D | 2 | 3 | 14,14,15 | 1.82 | 1 (7%) | 17,19,21 | 3.11 | 7 (41%) |
| 3 | BMA | D | 3 | 3 | 11,11,12 | 2.22 | 5 (45%) | 15,15,17 | 2.29 | 3 (20%) |
| 3 | FUL | D | 4 | 3 | 10,10,11 | 2.59 | 4 (40%) | 14,14,16 | 2.80 | 7 (50%) |
| 4 | NAG | E | 1 | 1,4 | 14,14,15 | 4.71 | 9 (64%) | 17,19,21 | 4.09 | 10 (58%) |
| 4 | NAG | E | 2 | 4 | 14,14,15 | 1.93 | 5 (35%) | 17,19,21 | 2.28 | 8 (47%) |
| 4 | BMA | E | 3 | 4 | 11,11,12 | 2.50 | 2 (18%) | 15,15,17 | 2.96 | 5 (33%) |
| 4 | MAN | E | 4 | 4 | 11,11,12 | 2.88 | 5 (45%) | 15,15,17 | 1.98 | 3 (20%) |
| 4 | MAN | E | 5 | 4 | 11,11,12 | 2.48 | 5 (45%) | 15,15,17 | 2.80 | 4 (26%) |
| 4 | MAN | E | 6 | 4 | 11,11,12 | 3.28 | 5 (45%) | 15,15,17 | 2.73 | 8 (53%) |
| 2 | NAG | F | 1 | 1,2 | 14,14,15 | 2.15 | 5 (35%) | 17,19,21 | 2.80 | 7 (41%) |
| 2 | NAG | F | 2 | 2 | 14,14,15 | 1.51 | 4 (28%) | 17,19,21 | 3.56 | 10 (58%) |
| 2 | NAG | G | 1 | 1,2 | 14,14,15 | 1.75 | 3 (21%) | 17,19,21 | 2.38 | 8 (47%) |
| 2 | NAG | G | 2 | 2 | 14,14,15 | 2.02 | 4 (28%) | 17,19,21 | 2.72 | 5 (29%) |
| 5 | NAG | H | 1 | 1,5 | 14,14,15 | 1.93 | 3 (21%) | 17,19,21 | 2.54 | 6 (35%) |
| 5 | NAG | H | 2 | 5 | 14,14,15 | 1.82 | 1 (7%) | 17,19,21 | 3.11 | 7 (41%) |
| 5 | BMA | H | 3 | 5 | 11,11,12 | 2.22 | 5 (45%) | 15,15,17 | 2.29 | 3 (20%) |
| 5 | FUC | H | 4 | 5 | 10,10,11 | 2.59 | 4 (40%) | 14,14,16 | 2.80 | 7 (50%) |
| 4 | NAG | I | 1 | 1,4 | 14,14,15 | 4.71 | 9 (64%) | 17,19,21 | 4.09 | 10 (58%) |
| 4 | NAG | I | 2 | 4 | 14,14,15 | 1.93 | 5 (35%) | 17,19,21 | 2.28 | 8 (47%) |
| 4 | BMA | I | 3 | 4 | 11,11,12 | 2.50 | 2 (18%) | 15,15,17 | 2.96 | 5 (33%) |
| 4 | MAN | I | 4 | 4 | 11,11,12 | 2.88 | 5 (45%) | 15,15,17 | 1.98 | 3 (20%) |
| 4 | MAN | I | 5 | 4 | 11,11,12 | 2.48 | 5 (45%) | 15,15,17 | 2.80 | 4 (26%) |
| 4 | MAN | I | 6 | 4 | 11,11,12 | 3.28 | 5 (45%) | 15,15,17 | 2.73 | 8 (53%) |
| 2 | NAG | J | 1 | 1,2 | 14,14,15 | 2.15 | 5 (35%) | 17,19,21 | 2.80 | 7 (41%) |
| 2 | NAG | J | 2 | 2 | 14,14,15 | 1.51 | 4 (28%) | 17,19,21 | 3.56 | 10 (58%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 2 | NAG | C | 1 | 1,2 | - | 2/6/23/26 | 0/1/1/1 |
| 2 | NAG | C | 2 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | D | 1 | 1,3 | - | 4/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 3 | NAG | D | 2 | 3 | - | 1/6/23/26 | 0/1/1/1 |
| 3 | BMA | D | 3 | 3 | - | 0/2/19/22 | 1/1/1/1 |
| 3 | FUL | D | 4 | 3 | - | - | 0/1/1/1 |
| 4 | NAG | E | 1 | 1,4 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | E | 2 | 4 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | BMA | E | 3 | 4 | - | 0/2/19/22 | 0/1/1/1 |
| 4 | MAN | E | 4 | 4 | - | 1/2/19/22 | 0/1/1/1 |
| 4 | MAN | E | 5 | 4 | - | 1/2/19/22 | 0/1/1/1 |
| 4 | MAN | E | 6 | 4 | - | 0/2/19/22 | 1/1/1/1 |
| 2 | NAG | F | 1 | 1,2 | - | 2/6/23/26 | 0/1/1/1 |
| 2 | NAG | F | 2 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 2 | NAG | G | 1 | 1,2 | - | 2/6/23/26 | 0/1/1/1 |
| 2 | NAG | G | 2 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 5 | NAG | H | 1 | 1,5 | - | 4/6/23/26 | 0/1/1/1 |
| 5 | NAG | H | 2 | 5 | - | 1/6/23/26 | 0/1/1/1 |
| 5 | BMA | H | 3 | 5 | - | 0/2/19/22 | 1/1/1/1 |
| 5 | FUC | H | 4 | 5 | 1/1/5/5 | - | 0/1/1/1 |
| 4 | NAG | I | 1 | 1,4 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | I | 2 | 4 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | BMA | I | 3 | 4 | - | 0/2/19/22 | 0/1/1/1 |
| 4 | MAN | I | 4 | 4 | - | 1/2/19/22 | 0/1/1/1 |
| 4 | MAN | I | 5 | 4 | - | 1/2/19/22 | 0/1/1/1 |
| 4 | MAN | I | 6 | 4 | - | 0/2/19/22 | 1/1/1/1 |
| 2 | NAG | J | 1 | 1,2 | - | 2/6/23/26 | 0/1/1/1 |
| 2 | NAG | J | 2 | 2 | - | 2/6/23/26 | 0/1/1/1 |

All (120) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | E | 1 | NAG | C1-C2 | 8.71 | 1.65 | 1.52 |
| 4 | I | 1 | NAG | C1-C2 | 8.71 | 1.65 | 1.52 |
| 4 | E | 6 | MAN | C4-C5 | 7.76 | 1.69 | 1.53 |
| 4 | I | 6 | MAN | C4-C5 | 7.76 | 1.69 | 1.53 |
| 4 | E | 1 | NAG | O5-C1 | 7.63 | 1.55 | 1.43 |
| 4 | I | 1 | NAG | O5-C1 | 7.63 | 1.55 | 1.43 |
| 4 | I | 3 | BMA | C1-C2 | 6.77 | 1.67 | 1.52 |
| 4 | E | 3 | BMA | C1-C2 | 6.77 | 1.67 | 1.52 |
| 4 | E | 1 | NAG | C4-C5 | 6.47 | 1.66 | 1.53 |
| 4 | I | 1 | NAG | C4-C5 | 6.47 | 1.66 | 1.53 |
| 4 | I | 4 | MAN | C2-C3 | 6.32 | 1.61 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | E | 4 | MAN | C2-C3 | 6.32 | 1.61 | 1.52 |
| 4 | E | 1 | NAG | C3-C2 | 5.95 | 1.65 | 1.52 |
| 4 | I | 1 | NAG | C3-C2 | 5.95 | 1.65 | 1.52 |
| 3 | D | 2 | NAG | C4-C3 | 5.66 | 1.66 | 1.52 |
| 5 | H | 2 | NAG | C4-C3 | 5.66 | 1.66 | 1.52 |
| 4 | E | 6 | MAN | O5-C5 | 5.61 | 1.54 | 1.43 |
| 4 | I | 6 | MAN | O5-C5 | 5.61 | 1.54 | 1.43 |
| 3 | D | 1 | NAG | C1-C2 | 5.32 | 1.60 | 1.52 |
| 5 | H | 1 | NAG | C1-C2 | 5.32 | 1.60 | 1.52 |
| 4 | E | 1 | NAG | O5-C5 | 4.98 | 1.53 | 1.43 |
| 4 | I | 1 | NAG | O5-C5 | 4.98 | 1.53 | 1.43 |
| 2 | F | 1 | NAG | O5-C1 | 4.93 | 1.51 | 1.43 |
| 2 | J | 1 | NAG | O5-C1 | 4.93 | 1.51 | 1.43 |
| 2 | G | 2 | NAG | C4-C3 | 4.93 | 1.64 | 1.52 |
| 2 | C | 2 | NAG | C4-C3 | 4.93 | 1.64 | 1.52 |
| 4 | E | 1 | NAG | C4-C3 | 4.93 | 1.64 | 1.52 |
| 4 | I | 1 | NAG | C4-C3 | 4.93 | 1.64 | 1.52 |
| 5 | H | 4 | FUC | C4-C5 | 4.74 | 1.63 | 1.52 |
| 3 | D | 4 | FUL | C4-C5 | 4.74 | 1.63 | 1.52 |
| 4 | E | 5 | MAN | C4-C5 | 4.53 | 1.62 | 1.53 |
| 4 | I | 5 | MAN | C4-C5 | 4.53 | 1.62 | 1.53 |
| 4 | E | 1 | NAG | C6-C5 | 4.47 | 1.66 | 1.51 |
| 4 | I | 1 | NAG | C6-C5 | 4.47 | 1.66 | 1.51 |
| 2 | C | 1 | NAG | O5-C5 | 4.36 | 1.52 | 1.43 |
| 2 | G | 1 | NAG | O5-C5 | 4.36 | 1.52 | 1.43 |
| 4 | I | 4 | MAN | O5-C5 | 4.33 | 1.52 | 1.43 |
| 4 | E | 4 | MAN | O5-C5 | 4.33 | 1.52 | 1.43 |
| 5 | H | 4 | FUC | C4-C3 | 4.25 | 1.63 | 1.52 |
| 3 | D | 4 | FUL | C4-C3 | 4.25 | 1.63 | 1.52 |
| 4 | I | 3 | BMA | C4-C5 | 4.21 | 1.61 | 1.53 |
| 4 | E | 3 | BMA | C4-C5 | 4.21 | 1.61 | 1.53 |
| 4 | E | 1 | NAG | C2-N2 | 4.17 | 1.53 | 1.46 |
| 4 | I | 1 | NAG | C2-N2 | 4.17 | 1.53 | 1.46 |
| 4 | E | 5 | MAN | O5-C5 | 4.06 | 1.51 | 1.43 |
| 4 | I | 5 | MAN | O5-C5 | 4.06 | 1.51 | 1.43 |
| 4 | I | 2 | NAG | C6-C5 | 4.01 | 1.65 | 1.51 |
| 4 | E | 2 | NAG | C6-C5 | 4.01 | 1.65 | 1.51 |
| 4 | E | 5 | MAN | O5-C1 | 3.91 | 1.50 | 1.43 |
| 4 | I | 5 | MAN | O5-C1 | 3.91 | 1.50 | 1.43 |
| 5 | H | 4 | FUC | O2-C2 | -3.59 | 1.35 | 1.43 |
| 3 | D | 4 | FUL | O2-C2 | -3.59 | 1.35 | 1.43 |
| 2 | J | 2 | NAG | C3-C2 | 3.53 | 1.60 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | F | 2 | NAG | C3-C2 | 3.53 | 1.60 | 1.52 |
| 5 | H | 3 | BMA | C1-C2 | 3.50 | 1.60 | 1.52 |
| 3 | D | 3 | BMA | C1-C2 | 3.50 | 1.60 | 1.52 |
| 5 | H | 3 | BMA | C4-C3 | 3.39 | 1.61 | 1.52 |
| 3 | D | 3 | BMA | C4-C3 | 3.39 | 1.61 | 1.52 |
| 2 | C | 1 | NAG | C4-C3 | 3.36 | 1.60 | 1.52 |
| 2 | G | 1 | NAG | C4-C3 | 3.36 | 1.60 | 1.52 |
| 4 | I | 4 | MAN | C1-C2 | 3.35 | 1.59 | 1.52 |
| 4 | E | 4 | MAN | C1-C2 | 3.35 | 1.59 | 1.52 |
| 4 | I | 4 | MAN | O4-C4 | -3.30 | 1.35 | 1.43 |
| 4 | E | 4 | MAN | O4-C4 | -3.30 | 1.35 | 1.43 |
| 2 | G | 2 | NAG | C4-C5 | 3.19 | 1.59 | 1.53 |
| 2 | C | 2 | NAG | C4-C5 | 3.19 | 1.59 | 1.53 |
| 2 | F | 1 | NAG | O4-C4 | 3.16 | 1.50 | 1.43 |
| 2 | J | 1 | NAG | O4-C4 | 3.16 | 1.50 | 1.43 |
| 5 | H | 3 | BMA | C2-C3 | 3.09 | 1.57 | 1.52 |
| 3 | D | 3 | BMA | C2-C3 | 3.09 | 1.57 | 1.52 |
| 4 | I | 2 | NAG | C4-C5 | 2.86 | 1.59 | 1.53 |
| 4 | E | 2 | NAG | C4-C5 | 2.86 | 1.59 | 1.53 |
| 2 | F | 1 | NAG | C2-N2 | 2.84 | 1.51 | 1.46 |
| 2 | J | 1 | NAG | C2-N2 | 2.84 | 1.51 | 1.46 |
| 4 | E | 6 | MAN | O4-C4 | 2.83 | 1.49 | 1.43 |
| 4 | I | 6 | MAN | O4-C4 | 2.83 | 1.49 | 1.43 |
| 4 | E | 6 | MAN | C1-C2 | 2.80 | 1.58 | 1.52 |
| 4 | I | 6 | MAN | C1-C2 | 2.80 | 1.58 | 1.52 |
| 5 | H | 4 | FUC | C6-C5 | 2.79 | 1.58 | 1.51 |
| 3 | D | 4 | FUL | C6-C5 | 2.79 | 1.58 | 1.51 |
| 5 | H | 3 | BMA | C4-C5 | 2.73 | 1.58 | 1.53 |
| 3 | D | 3 | BMA | C4-C5 | 2.73 | 1.58 | 1.53 |
| 2 | F | 1 | NAG | O5-C5 | 2.72 | 1.49 | 1.43 |
| 2 | J | 1 | NAG | O5-C5 | 2.72 | 1.49 | 1.43 |
| 2 | F | 1 | NAG | C1-C2 | 2.70 | 1.56 | 1.52 |
| 2 | J | 1 | NAG | C1-C2 | 2.70 | 1.56 | 1.52 |
| 5 | H | 3 | BMA | O5-C1 | 2.64 | 1.47 | 1.43 |
| 3 | D | 3 | BMA | O5-C1 | 2.64 | 1.47 | 1.43 |
| 2 | J | 2 | NAG | C4-C5 | 2.55 | 1.58 | 1.53 |
| 2 | F | 2 | NAG | C4-C5 | 2.55 | 1.58 | 1.53 |
| 4 | I | 2 | NAG | O5-C1 | -2.55 | 1.39 | 1.43 |
| 4 | E | 2 | NAG | O5-C1 | -2.55 | 1.39 | 1.43 |
| 4 | E | 1 | NAG | O6-C6 | 2.53 | 1.53 | 1.42 |
| 4 | I | 1 | NAG | O6-C6 | 2.53 | 1.53 | 1.42 |
| 2 | G | 2 | NAG | O4-C4 | 2.53 | 1.48 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | C | 2 | NAG | O4-C4 | 2.53 | 1.48 | 1.43 |
| 2 | G | 2 | NAG | C8-C7 | 2.45 | 1.55 | 1.50 |
| 2 | C | 2 | NAG | C8-C7 | 2.45 | 1.55 | 1.50 |
| 3 | D | 1 | NAG | O5-C5 | 2.45 | 1.48 | 1.43 |
| 5 | H | 1 | NAG | O5-C5 | 2.45 | 1.48 | 1.43 |
| 2 | J | 2 | NAG | C4-C3 | 2.27 | 1.58 | 1.52 |
| 2 | F | 2 | NAG | C4-C3 | 2.27 | 1.58 | 1.52 |
| 4 | E | 6 | MAN | O2-C2 | -2.23 | 1.38 | 1.43 |
| 4 | I | 6 | MAN | O2-C2 | -2.23 | 1.38 | 1.43 |
| 3 | D | 1 | NAG | C4-C5 | 2.20 | 1.57 | 1.53 |
| 5 | H | 1 | NAG | C4-C5 | 2.20 | 1.57 | 1.53 |
| 4 | I | 4 | MAN | O5-C1 | 2.15 | 1.47 | 1.43 |
| 4 | E | 4 | MAN | O5-C1 | 2.15 | 1.47 | 1.43 |
| 4 | I | 2 | NAG | C4-C3 | 2.13 | 1.57 | 1.52 |
| 4 | E | 2 | NAG | C4-C3 | 2.13 | 1.57 | 1.52 |
| 4 | I | 2 | NAG | C3-C2 | 2.09 | 1.57 | 1.52 |
| 4 | E | 2 | NAG | C3-C2 | 2.09 | 1.57 | 1.52 |
| 4 | E | 5 | MAN | C6-C5 | 2.08 | 1.58 | 1.51 |
| 4 | I | 5 | MAN | C6-C5 | 2.08 | 1.58 | 1.51 |
| 2 | C | 1 | NAG | C1-C2 | 2.07 | 1.55 | 1.52 |
| 2 | G | 1 | NAG | C1-C2 | 2.07 | 1.55 | 1.52 |
| 2 | J | 2 | NAG | O5-C5 | 2.06 | 1.47 | 1.43 |
| 2 | F | 2 | NAG | O5-C5 | 2.06 | 1.47 | 1.43 |
| 4 | E | 5 | MAN | C1-C2 | 2.01 | 1.56 | 1.52 |
| 4 | I | 5 | MAN | C1-C2 | 2.01 | 1.56 | 1.52 |

All (182) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 4 | E | 5 | MAN | C1-O5-C5 | 8.47 | 123.66 | 112.19 |
| 4 | I | 5 | MAN | C1-O5-C5 | 8.47 | 123.66 | 112.19 |
| 2 | G | 2 | NAG | C1-O5-C5 | 7.81 | 122.77 | 112.19 |
| 2 | C | 2 | NAG | C1-O5-C5 | 7.81 | 122.77 | 112.19 |
| 4 | E | 1 | NAG | O7-C7-C8 | -7.80 | 107.56 | 122.06 |
| 4 | I | 1 | NAG | O7-C7-C8 | -7.80 | 107.56 | 122.06 |
| 3 | D | 1 | NAG | C1-C2-N2 | 7.78 | 123.78 | 110.49 |
| 5 | H | 1 | NAG | C1-C2-N2 | 7.78 | 123.78 | 110.49 |
| 4 | E | 1 | NAG | C8-C7-N2 | 7.61 | 128.98 | 116.10 |
| 4 | I | 1 | NAG | C8-C7-N2 | 7.61 | 128.98 | 116.10 |
| 4 | E | 1 | NAG | O5-C1-C2 | 6.95 | 122.26 | 111.29 |
| 4 | I | 1 | NAG | O5-C1-C2 | 6.95 | 122.26 | 111.29 |
| 2 | F | 1 | NAG | C1-O5-C5 | 6.79 | 121.40 | 112.19 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 2 | J | 1 | NAG | C1-O5-C5 | 6.79 | 121.40 | 112.19 |
| 2 | J | 2 | NAG | C2-N2-C7 | -6.46 | 113.70 | 122.90 |
| 2 | F | 2 | NAG | C2-N2-C7 | -6.46 | 113.70 | 122.90 |
| 4 | I | 3 | BMA | O2-C2-C1 | 6.28 | 121.99 | 109.15 |
| 4 | E | 3 | BMA | O2-C2-C1 | 6.28 | 121.99 | 109.15 |
| 4 | I | 3 | BMA | O5-C1-C2 | 6.03 | 120.08 | 110.77 |
| 4 | E | 3 | BMA | O5-C1-C2 | 6.03 | 120.08 | 110.77 |
| 4 | E | 6 | MAN | C3-C4-C5 | -5.90 | 99.72 | 110.24 |
| 4 | I | 6 | MAN | C3-C4-C5 | -5.90 | 99.72 | 110.24 |
| 3 | D | 2 | NAG | C4-C3-C2 | -5.88 | 102.41 | 111.02 |
| 5 | H | 2 | NAG | C4-C3-C2 | -5.88 | 102.41 | 111.02 |
| 2 | J | 2 | NAG | C4-C3-C2 | -5.87 | 102.41 | 111.02 |
| 2 | F | 2 | NAG | C4-C3-C2 | -5.87 | 102.41 | 111.02 |
| 4 | E | 1 | NAG | C6-C5-C4 | 5.70 | 126.35 | 113.00 |
| 4 | I | 1 | NAG | C6-C5-C4 | 5.70 | 126.35 | 113.00 |
| 3 | D | 2 | NAG | O4-C4-C3 | 5.70 | 123.52 | 110.35 |
| 5 | H | 2 | NAG | O4-C4-C3 | 5.70 | 123.52 | 110.35 |
| 2 | J | 2 | NAG | O3-C3-C2 | 5.56 | 120.97 | 109.47 |
| 2 | F | 2 | NAG | O3-C3-C2 | 5.56 | 120.97 | 109.47 |
| 2 | F | 1 | NAG | O5-C1-C2 | 5.44 | 119.88 | 111.29 |
| 2 | J | 1 | NAG | O5-C1-C2 | 5.44 | 119.88 | 111.29 |
| 4 | I | 2 | NAG | O5-C5-C6 | 5.33 | 115.56 | 107.20 |
| 4 | E | 2 | NAG | O5-C5-C6 | 5.33 | 115.56 | 107.20 |
| 4 | I | 3 | BMA | C1-O5-C5 | 5.23 | 119.28 | 112.19 |
| 4 | E | 3 | BMA | C1-O5-C5 | 5.23 | 119.28 | 112.19 |
| 5 | H | 3 | BMA | O2-C2-C1 | 5.21 | 119.82 | 109.15 |
| 3 | D | 3 | BMA | O2-C2-C1 | 5.21 | 119.82 | 109.15 |
| 3 | D | 2 | NAG | O3-C3-C2 | -5.19 | 98.73 | 109.47 |
| 5 | H | 2 | NAG | O3-C3-C2 | -5.19 | 98.73 | 109.47 |
| 5 | H | 3 | BMA | C1-O5-C5 | 5.16 | 119.19 | 112.19 |
| 3 | D | 3 | BMA | C1-O5-C5 | 5.16 | 119.19 | 112.19 |
| 2 | J | 2 | NAG | C3-C4-C5 | -5.10 | 101.15 | 110.24 |
| 2 | F | 2 | NAG | C3-C4-C5 | -5.10 | 101.15 | 110.24 |
| 4 | E | 1 | NAG | O5-C5-C4 | -4.93 | 98.83 | 110.83 |
| 4 | I | 1 | NAG | O5-C5-C4 | -4.93 | 98.83 | 110.83 |
| 4 | E | 6 | MAN | O4-C4-C5 | 4.87 | 121.39 | 109.30 |
| 4 | I | 6 | MAN | O4-C4-C5 | 4.87 | 121.39 | 109.30 |
| 2 | C | 1 | NAG | C4-C3-C2 | -4.84 | 103.92 | 111.02 |
| 2 | G | 1 | NAG | C4-C3-C2 | -4.84 | 103.92 | 111.02 |
| 5 | H | 4 | FUC | O5-C1-C2 | -4.82 | 103.34 | 110.77 |
| 3 | D | 4 | FUL | O5-C1-C2 | -4.82 | 103.34 | 110.77 |
| 2 | J | 2 | NAG | C6-C5-C4 | 4.81 | 124.28 | 113.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 2 | F | 2 | NAG | C6-C5-C4 | 4.81 | 124.28 | 113.00 |
| 4 | E | 5 | MAN | C1-C2-C3 | 4.75 | 115.51 | 109.67 |
| 4 | I | 5 | MAN | C1-C2-C3 | 4.75 | 115.51 | 109.67 |
| 2 | G | 2 | NAG | C6-C5-C4 | 4.48 | 123.49 | 113.00 |
| 2 | C | 2 | NAG | C6-C5-C4 | 4.48 | 123.49 | 113.00 |
| 4 | I | 4 | MAN | O4-C4-C3 | -4.38 | 100.22 | 110.35 |
| 4 | E | 4 | MAN | O4-C4-C3 | -4.38 | 100.22 | 110.35 |
| 3 | D | 2 | NAG | O3-C3-C4 | 4.27 | 120.22 | 110.35 |
| 5 | H | 2 | NAG | O3-C3-C4 | 4.27 | 120.22 | 110.35 |
| 3 | D | 2 | NAG | C2-N2-C7 | -4.22 | 116.90 | 122.90 |
| 5 | H | 2 | NAG | C2-N2-C7 | -4.22 | 116.90 | 122.90 |
| 5 | H | 4 | FUC | C2-C3-C4 | -4.21 | 103.60 | 110.89 |
| 3 | D | 4 | FUL | C2-C3-C4 | -4.21 | 103.60 | 110.89 |
| 3 | D | 2 | NAG | C3-C4-C5 | -4.02 | 103.07 | 110.24 |
| 5 | H | 2 | NAG | C3-C4-C5 | -4.02 | 103.07 | 110.24 |
| 2 | J | 2 | NAG | C1-C2-N2 | 4.00 | 117.33 | 110.49 |
| 2 | F | 2 | NAG | C1-C2-N2 | 4.00 | 117.33 | 110.49 |
| 4 | E | 6 | MAN | C1-C2-C3 | 3.93 | 114.49 | 109.67 |
| 4 | I | 6 | MAN | C1-C2-C3 | 3.93 | 114.49 | 109.67 |
| 4 | E | 1 | NAG | C4-C3-C2 | 3.87 | 116.69 | 111.02 |
| 4 | I | 1 | NAG | C4-C3-C2 | 3.87 | 116.69 | 111.02 |
| 5 | H | 4 | FUC | O3-C3-C4 | 3.84 | 119.22 | 110.35 |
| 3 | D | 4 | FUL | O3-C3-C4 | 3.84 | 119.22 | 110.35 |
| 2 | C | 1 | NAG | O4-C4-C3 | 3.79 | 119.11 | 110.35 |
| 2 | G | 1 | NAG | O4-C4-C3 | 3.79 | 119.11 | 110.35 |
| 2 | G | 2 | NAG | O5-C1-C2 | -3.76 | 105.35 | 111.29 |
| 2 | C | 2 | NAG | O5-C1-C2 | -3.76 | 105.35 | 111.29 |
| 2 | G | 2 | NAG | C1-C2-N2 | 3.74 | 116.87 | 110.49 |
| 2 | C | 2 | NAG | C1-C2-N2 | 3.74 | 116.87 | 110.49 |
| 4 | E | 1 | NAG | O5-C5-C6 | 3.67 | 112.95 | 107.20 |
| 4 | I | 1 | NAG | O5-C5-C6 | 3.67 | 112.95 | 107.20 |
| 5 | H | 4 | FUC | C1-C2-C3 | -3.63 | 105.20 | 109.67 |
| 3 | D | 4 | FUL | C1-C2-C3 | -3.63 | 105.20 | 109.67 |
| 2 | C | 1 | NAG | C1-O5-C5 | 3.59 | 117.06 | 112.19 |
| 2 | G | 1 | NAG | C1-O5-C5 | 3.59 | 117.06 | 112.19 |
| 5 | H | 4 | FUC | C3-C4-C5 | 3.59 | 115.36 | 109.77 |
| 3 | D | 4 | FUL | C3-C4-C5 | 3.59 | 115.36 | 109.77 |
| 4 | I | 4 | MAN | C3-C4-C5 | 3.58 | 116.62 | 110.24 |
| 4 | E | 4 | MAN | C3-C4-C5 | 3.58 | 116.62 | 110.24 |
| 4 | I | 2 | NAG | C4-C3-C2 | -3.51 | 105.88 | 111.02 |
| 4 | E | 2 | NAG | C4-C3-C2 | -3.51 | 105.88 | 111.02 |
| 4 | E | 6 | MAN | O2-C2-C3 | -3.44 | 103.24 | 110.14 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 4 | I | 6 | MAN | O2-C2-C3 | -3.44 | 103.24 | 110.14 |
| 2 | J | 2 | NAG | O4-C4-C5 | 3.40 | 117.73 | 109.30 |
| 2 | F | 2 | NAG | O4-C4-C5 | 3.40 | 117.73 | 109.30 |
| 2 | F | 1 | NAG | O3-C3-C2 | 3.38 | 116.46 | 109.47 |
| 2 | J | 1 | NAG | O3-C3-C2 | 3.38 | 116.46 | 109.47 |
| 4 | E | 1 | NAG | O3-C3-C4 | -3.33 | 102.65 | 110.35 |
| 4 | I | 1 | NAG | O3-C3-C4 | -3.33 | 102.65 | 110.35 |
| 2 | F | 1 | NAG | C8-C7-N2 | 3.28 | 121.65 | 116.10 |
| 2 | J | 1 | NAG | C8-C7-N2 | 3.28 | 121.65 | 116.10 |
| 5 | H | 4 | FUC | O3-C3-C2 | -3.12 | 104.02 | 109.99 |
| 3 | D | 4 | FUL | O3-C3-C2 | -3.12 | 104.02 | 109.99 |
| 2 | C | 1 | NAG | C2-N2-C7 | 3.12 | 127.34 | 122.90 |
| 2 | G | 1 | NAG | C2-N2-C7 | 3.12 | 127.34 | 122.90 |
| 3 | D | 1 | NAG | C2-N2-C7 | 3.10 | 127.31 | 122.90 |
| 5 | H | 1 | NAG | C2-N2-C7 | 3.10 | 127.31 | 122.90 |
| 2 | F | 1 | NAG | O7-C7-C8 | -3.07 | 116.35 | 122.06 |
| 2 | J | 1 | NAG | O7-C7-C8 | -3.07 | 116.35 | 122.06 |
| 3 | D | 1 | NAG | C3-C4-C5 | 3.06 | 115.69 | 110.24 |
| 5 | H | 1 | NAG | C3-C4-C5 | 3.06 | 115.69 | 110.24 |
| 4 | I | 2 | NAG | C1-O5-C5 | 3.05 | 116.33 | 112.19 |
| 4 | E | 2 | NAG | C1-O5-C5 | 3.05 | 116.33 | 112.19 |
| 2 | C | 1 | NAG | C8-C7-N2 | -3.05 | 110.94 | 116.10 |
| 2 | G | 1 | NAG | C8-C7-N2 | -3.05 | 110.94 | 116.10 |
| 5 | H | 3 | BMA | C1-C2-C3 | -3.01 | 105.97 | 109.67 |
| 3 | D | 3 | BMA | C1-C2-C3 | -3.01 | 105.97 | 109.67 |
| 2 | J | 2 | NAG | O5-C1-C2 | -2.94 | 106.64 | 111.29 |
| 2 | F | 2 | NAG | O5-C1-C2 | -2.94 | 106.64 | 111.29 |
| 4 | I | 2 | NAG | C2-N2-C7 | -2.93 | 118.73 | 122.90 |
| 4 | E | 2 | NAG | C2-N2-C7 | -2.93 | 118.73 | 122.90 |
| 4 | I | 2 | NAG | O5-C5-C4 | -2.92 | 103.73 | 110.83 |
| 4 | E | 2 | NAG | O5-C5-C4 | -2.92 | 103.73 | 110.83 |
| 2 | F | 1 | NAG | O4-C4-C3 | -2.90 | 103.64 | 110.35 |
| 2 | J | 1 | NAG | O4-C4-C3 | -2.90 | 103.64 | 110.35 |
| 3 | D | 1 | NAG | O3-C3-C2 | 2.89 | 115.45 | 109.47 |
| 5 | H | 1 | NAG | O3-C3-C2 | 2.89 | 115.45 | 109.47 |
| 2 | F | 1 | NAG | C1-C2-N2 | -2.87 | 105.58 | 110.49 |
| 2 | J | 1 | NAG | C1-C2-N2 | -2.87 | 105.58 | 110.49 |
| 4 | E | 1 | NAG | O4-C4-C5 | 2.80 | 116.25 | 109.30 |
| 4 | I | 1 | NAG | O4-C4-C5 | 2.80 | 116.25 | 109.30 |
| 4 | E | 5 | MAN | O2-C2-C3 | -2.74 | 104.66 | 110.14 |
| 4 | I | 5 | MAN | O2-C2-C3 | -2.74 | 104.66 | 110.14 |
| 4 | E | 5 | MAN | O2-C2-C1 | -2.69 | 103.65 | 109.15 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|---|---|---|---|---|---|---|---|
| 4 | I | 5 | MAN | O2-C2-C1 | -2.69 | 103.65 | 109.15 |
| 2 | C | 1 | NAG | O3-C3-C4 | 2.57 | 116.28 | 110.35 |
| 2 | G | 1 | NAG | O3-C3-C4 | 2.57 | 116.28 | 110.35 |
| 2 | C | 1 | NAG | C3-C4-C5 | -2.55 | 105.69 | 110.24 |
| 2 | G | 1 | NAG | C3-C4-C5 | -2.55 | 105.69 | 110.24 |
| 4 | I | 2 | NAG | C1-C2-N2 | 2.55 | 114.84 | 110.49 |
| 4 | E | 2 | NAG | C1-C2-N2 | 2.55 | 114.84 | 110.49 |
| 4 | I | 4 | MAN | O3-C3-C2 | 2.51 | 114.81 | 109.99 |
| 4 | E | 4 | MAN | O3-C3-C2 | 2.51 | 114.81 | 109.99 |
| 3 | D | 1 | NAG | O5-C1-C2 | -2.50 | 107.34 | 111.29 |
| 5 | H | 1 | NAG | O5-C1-C2 | -2.50 | 107.34 | 111.29 |
| 4 | E | 6 | MAN | O3-C3-C2 | 2.49 | 114.76 | 109.99 |
| 4 | I | 6 | MAN | O3-C3-C2 | 2.49 | 114.76 | 109.99 |
| 4 | E | 6 | MAN | C6-C5-C4 | 2.44 | 118.72 | 113.00 |
| 4 | I | 6 | MAN | C6-C5-C4 | 2.44 | 118.72 | 113.00 |
| 4 | E | 1 | NAG | O6-C6-C5 | 2.40 | 119.53 | 111.29 |
| 4 | I | 1 | NAG | O6-C6-C5 | 2.40 | 119.53 | 111.29 |
| 4 | I | 3 | BMA | O2-C2-C3 | -2.40 | 105.34 | 110.14 |
| 4 | E | 3 | BMA | O2-C2-C3 | -2.40 | 105.34 | 110.14 |
| 5 | H | 4 | FUC | C6-C5-C4 | 2.40 | 117.50 | 113.07 |
| 3 | D | 4 | FUL | C6-C5-C4 | 2.40 | 117.50 | 113.07 |
| 2 | C | 1 | NAG | O3-C3-C2 | 2.36 | 114.34 | 109.47 |
| 2 | G | 1 | NAG | O3-C3-C2 | 2.36 | 114.34 | 109.47 |
| 2 | J | 2 | NAG | C8-C7-N2 | 2.32 | 120.03 | 116.10 |
| 2 | F | 2 | NAG | C8-C7-N2 | 2.32 | 120.03 | 116.10 |
| 4 | E | 6 | MAN | O2-C2-C1 | 2.28 | 113.81 | 109.15 |
| 4 | I | 6 | MAN | O2-C2-C1 | 2.28 | 113.81 | 109.15 |
| 2 | J | 2 | NAG | O7-C7-C8 | -2.27 | 117.84 | 122.06 |
| 2 | F | 2 | NAG | O7-C7-C8 | -2.27 | 117.84 | 122.06 |
| 4 | I | 3 | BMA | C3-C4-C5 | -2.20 | 106.32 | 110.24 |
| 4 | E | 3 | BMA | C3-C4-C5 | -2.20 | 106.32 | 110.24 |
| 4 | I | 2 | NAG | O3-C3-C2 | 2.18 | 113.98 | 109.47 |
| 4 | E | 2 | NAG | O3-C3-C2 | 2.18 | 113.98 | 109.47 |
| 4 | I | 2 | NAG | O6-C6-C5 | 2.14 | 118.63 | 111.29 |
| 4 | E | 2 | NAG | O6-C6-C5 | 2.14 | 118.63 | 111.29 |
| 3 | D | 1 | NAG | O4-C4-C3 | -2.07 | 105.56 | 110.35 |
| 5 | H | 1 | NAG | O4-C4-C3 | -2.07 | 105.56 | 110.35 |
| 4 | E | 6 | MAN | O6-C6-C5 | -2.04 | 104.31 | 111.29 |
| 4 | I | 6 | MAN | O6-C6-C5 | -2.04 | 104.31 | 111.29 |
| 2 | G | 2 | NAG | O5-C5-C4 | -2.03 | 105.88 | 110.83 |
| 2 | C | 2 | NAG | O5-C5-C4 | -2.03 | 105.88 | 110.83 |
| 3 | D | 2 | NAG | O5-C1-C2 | -2.01 | 108.12 | 111.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | H | 2 | NAG | O5-C1-C2 | -2.01 | 108.12 | 111.29 |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 5 | H | 4 | FUC | C1 |

All (42) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 3 | D | 1 | NAG | C3-C2-N2-C7 |
| 5 | H | 1 | NAG | C3-C2-N2-C7 |
| 3 | D | 1 | NAG | O5-C5-C6-O6 |
| 5 | H | 1 | NAG | O5-C5-C6-O6 |
| 2 | G | 2 | NAG | O5-C5-C6-O6 |
| 4 | I | 2 | NAG | O5-C5-C6-O6 |
| 4 | E | 2 | NAG | O5-C5-C6-O6 |
| 2 | C | 2 | NAG | O5-C5-C6-O6 |
| 4 | I | 2 | NAG | C4-C5-C6-O6 |
| 4 | E | 2 | NAG | C4-C5-C6-O6 |
| 2 | G | 2 | NAG | C4-C5-C6-O6 |
| 2 | C | 2 | NAG | C4-C5-C6-O6 |
| 3 | D | 1 | NAG | C4-C5-C6-O6 |
| 5 | H | 1 | NAG | C4-C5-C6-O6 |
| 4 | E | 1 | NAG | O5-C5-C6-O6 |
| 4 | I | 1 | NAG | O5-C5-C6-O6 |
| 4 | E | 1 | NAG | C1-C2-N2-C7 |
| 4 | I | 1 | NAG | C1-C2-N2-C7 |
| 2 | J | 2 | NAG | C1-C2-N2-C7 |
| 2 | F | 2 | NAG | C1-C2-N2-C7 |
| 2 | F | 1 | NAG | O5-C5-C6-O6 |
| 2 | J | 1 | NAG | O5-C5-C6-O6 |
| 3 | D | 2 | NAG | O5-C5-C6-O6 |
| 5 | H | 2 | NAG | O5-C5-C6-O6 |
| 4 | I | 4 | MAN | O5-C5-C6-O6 |
| 4 | E | 4 | MAN | O5-C5-C6-O6 |
| 2 | C | 1 | NAG | C1-C2-N2-C7 |
| 2 | G | 1 | NAG | C1-C2-N2-C7 |
| 3 | D | 1 | NAG | C1-C2-N2-C7 |
| 5 | H | 1 | NAG | C1-C2-N2-C7 |
| 4 | E | 5 | MAN | C4-C5-C6-O6 |
| 4 | I | 5 | MAN | C4-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | C | 1 | NAG | C3-C2-N2-C7 |
| 2 | G | 1 | NAG | C3-C2-N2-C7 |
| 4 | E | 1 | NAG | C4-C5-C6-O6 |
| 4 | I | 1 | NAG | C4-C5-C6-O6 |
| 4 | E | 1 | NAG | C3-C2-N2-C7 |
| 2 | J | 2 | NAG | C3-C2-N2-C7 |
| 2 | F | 1 | NAG | C3-C2-N2-C7 |
| 2 | J | 1 | NAG | C3-C2-N2-C7 |
| 4 | I | 1 | NAG | C3-C2-N2-C7 |
| 2 | F | 2 | NAG | C3-C2-N2-C7 |

All (4) ring outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 4 | E | 6 | MAN | C1-C2-C3-C4-C5-O5 |
| 4 | I | 6 | MAN | C1-C2-C3-C4-C5-O5 |
| 5 | H | 3 | BMA | C1-C2-C3-C4-C5-O5 |
| 3 | D | 3 | BMA | C1-C2-C3-C4-C5-O5 |

21 monomers are involved in 58 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 4 | E | 1 | NAG | 19 | 0 |
| 2 | J | 2 | NAG | 4 | 0 |
| 2 | C | 1 | NAG | 5 | 0 |
| 2 | F | 1 | NAG | 3 | 0 |
| 3 | D | 3 | BMA | 2 | 0 |
| 2 | G | 2 | NAG | 3 | 0 |
| 4 | E | 5 | MAN | 0 | 1 |
| 2 | J | 1 | NAG | 3 | 0 |
| 4 | I | 3 | BMA | 1 | 0 |
| 4 | E | 6 | MAN | 6 | 0 |
| 4 | I | 2 | NAG | 3 | 0 |
| 3 | D | 2 | NAG | 2 | 0 |
| 4 | E | 4 | MAN | 0 | 5 |
| 4 | I | 1 | NAG | 1 | 3 |
| 2 | F | 2 | NAG | 5 | 0 |
| 4 | I | 6 | MAN | 1 | 1 |
| 4 | E | 2 | NAG | 3 | 0 |
| 4 | E | 3 | BMA | 1 | 0 |
| 2 | C | 2 | NAG | 3 | 0 |
| 2 | G | 1 | NAG | 4 | 0 |

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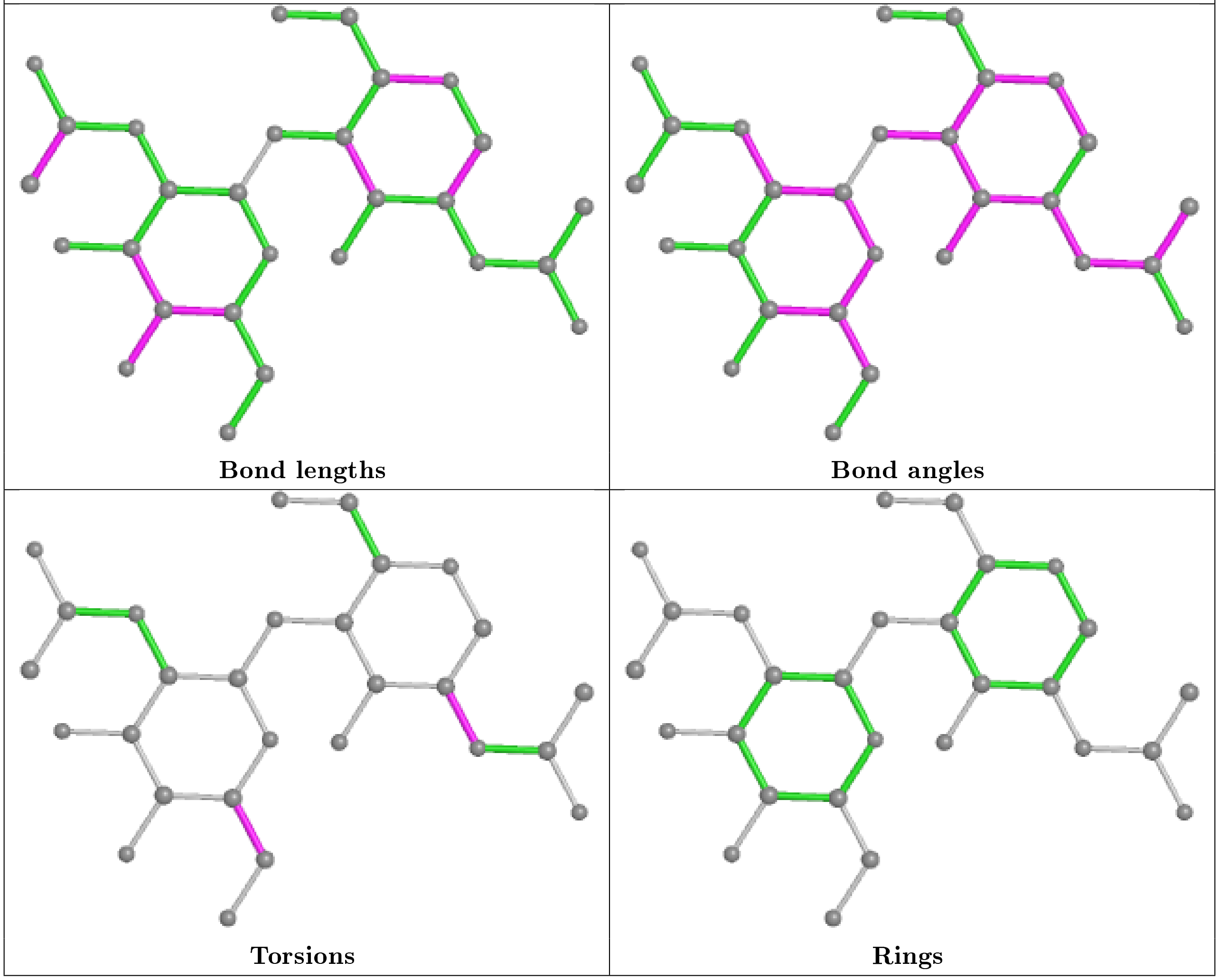
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 3 | D | 4 | FUL | 0 | 5 |

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 C**



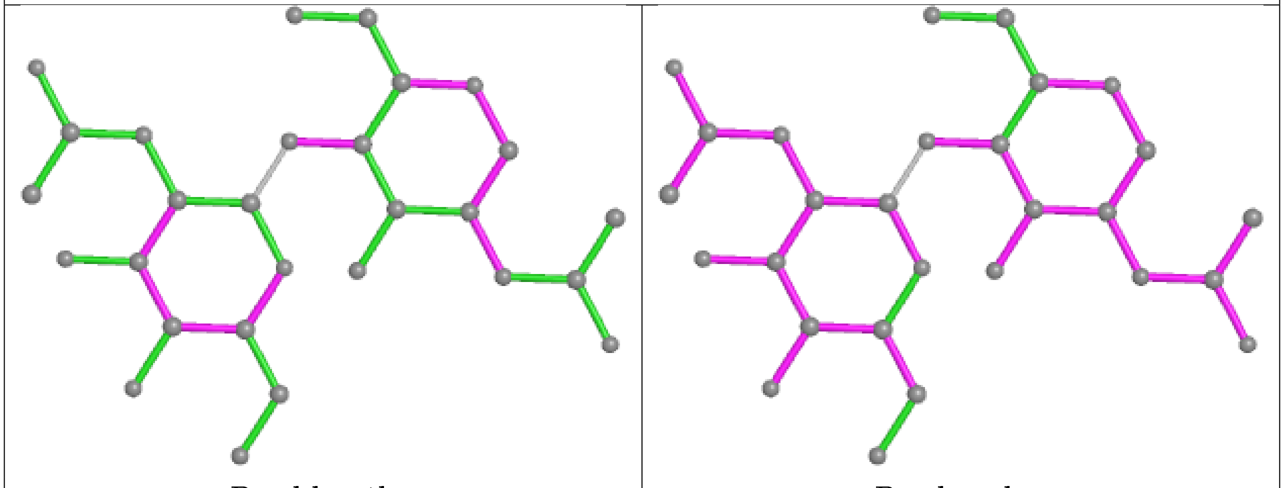
**Bond lengths**

**Bond angles**

**Torsions**

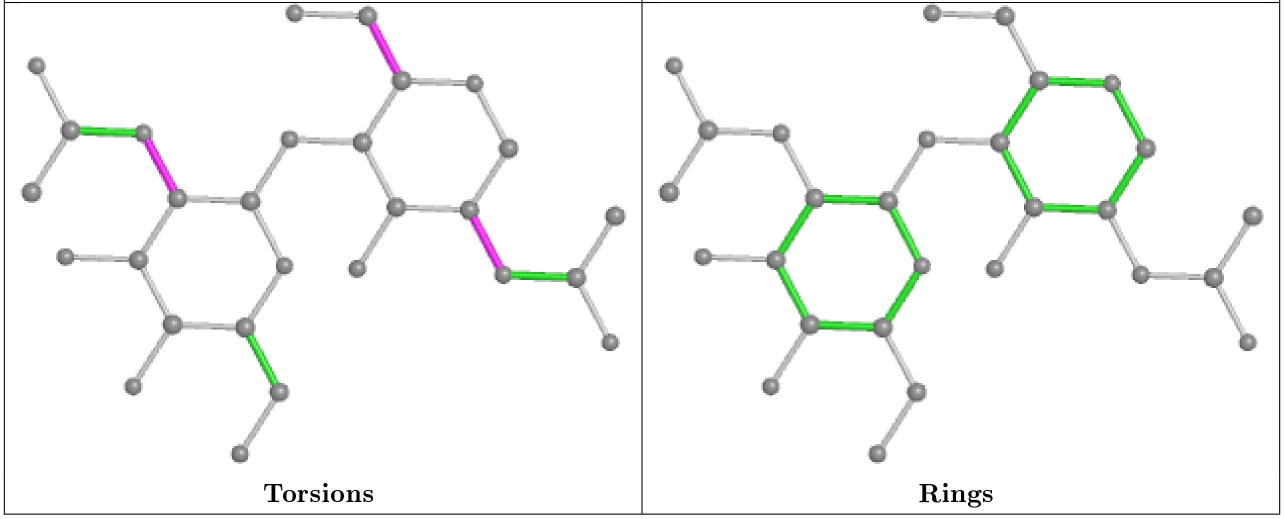
**Rings**

**Oligosaccharide Chain F**



Bond lengths

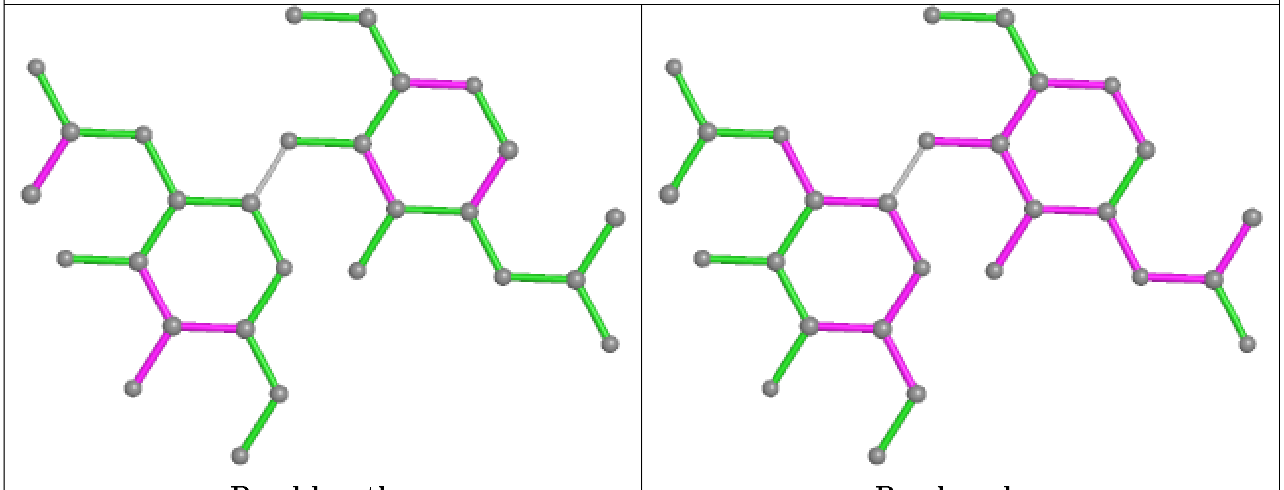
Bond angles



Torsions

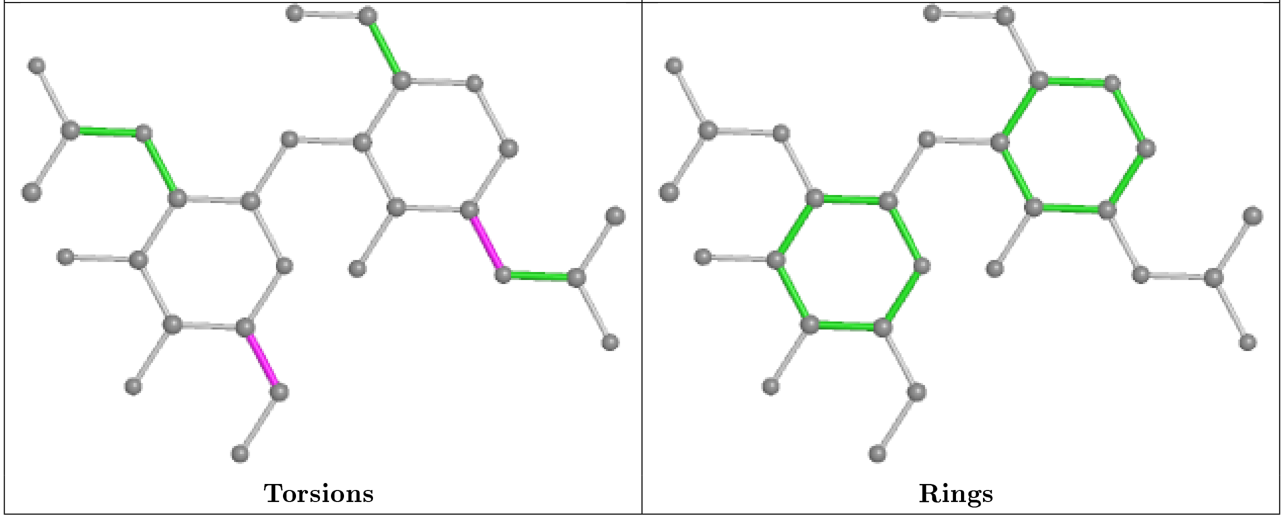
Rings

## Oligosaccharide Chain G



Bond lengths

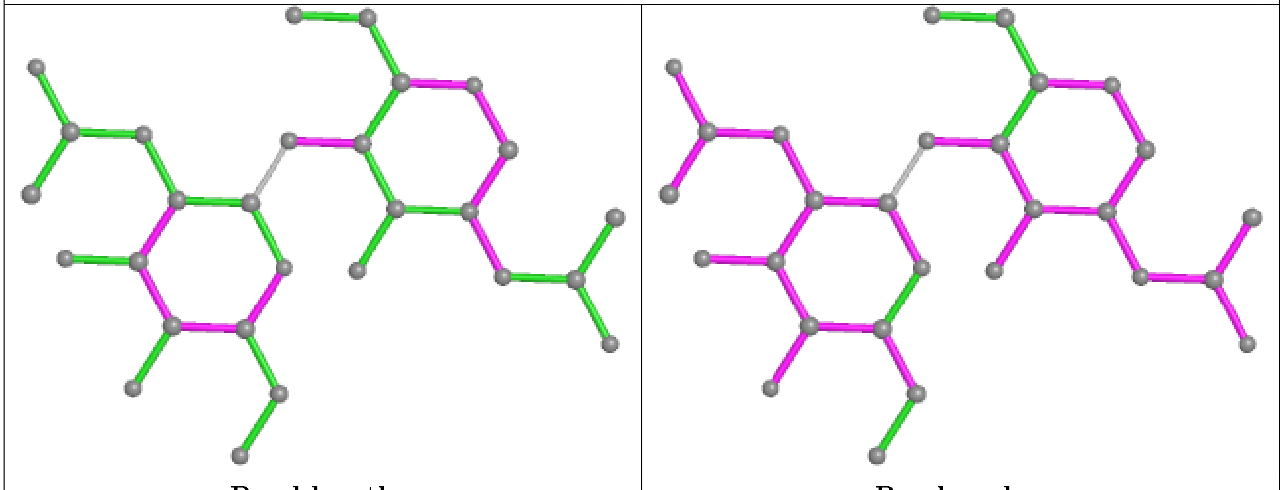
Bond angles



Torsions

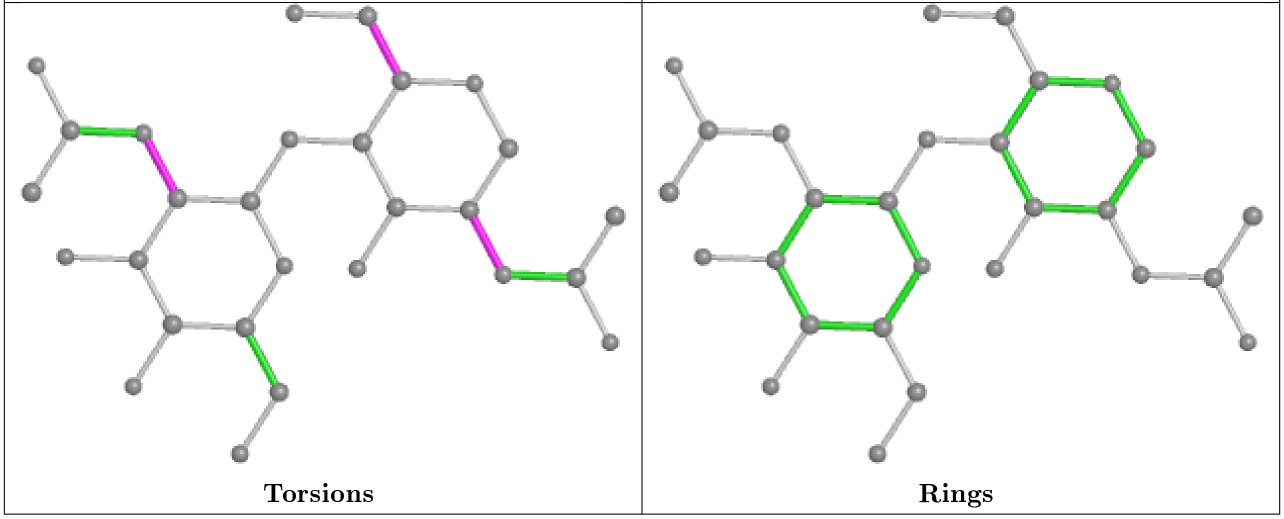
Rings

**Oligosaccharide Chain J**



Bond lengths

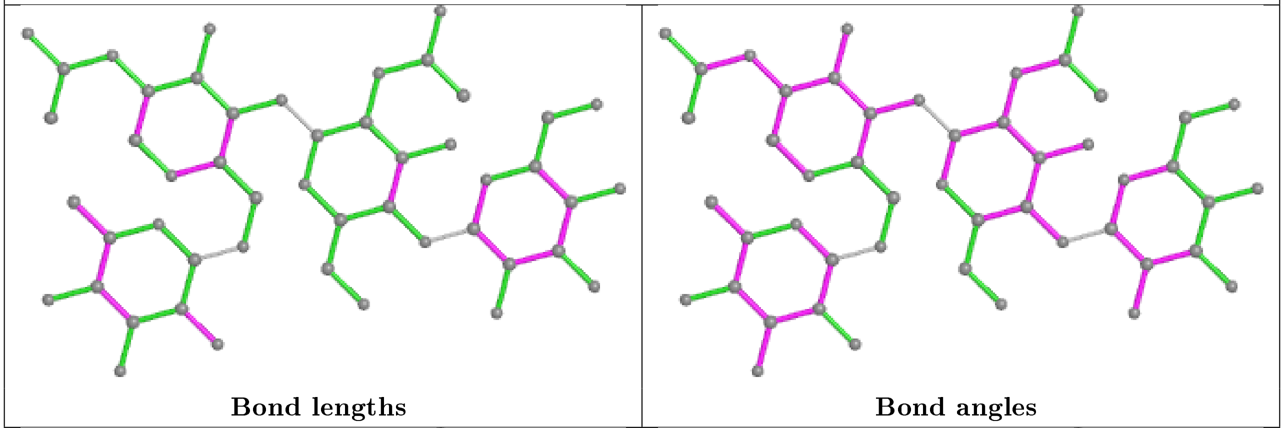
Bond angles



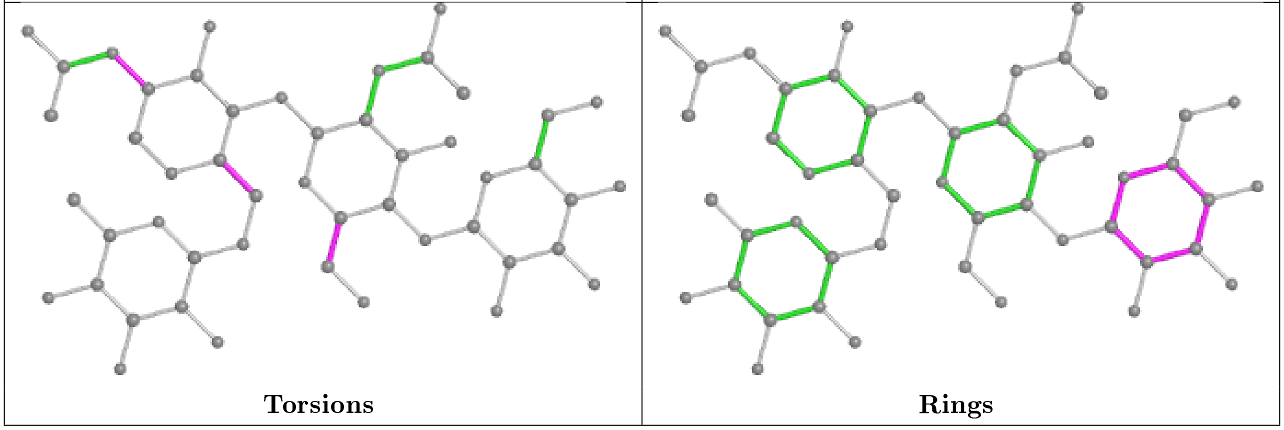
Torsions

Rings

**Oligosaccharide Chain D**

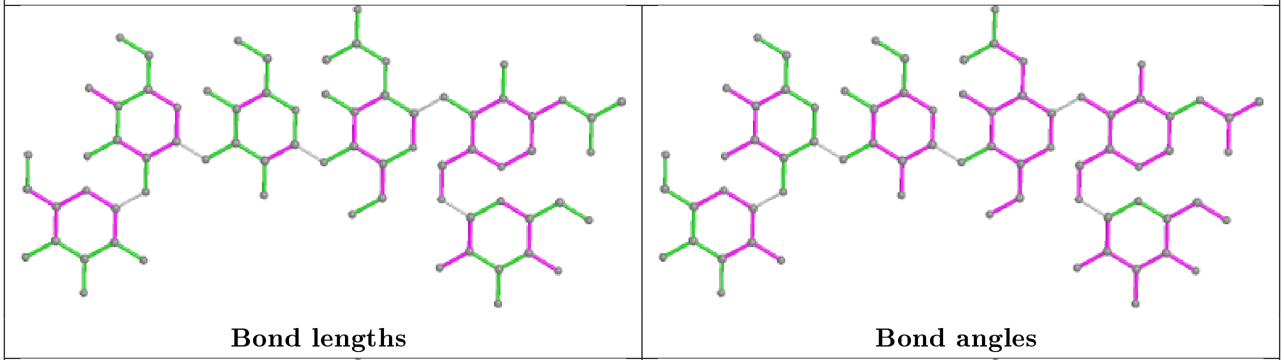


**Bond lengths** **Bond angles**

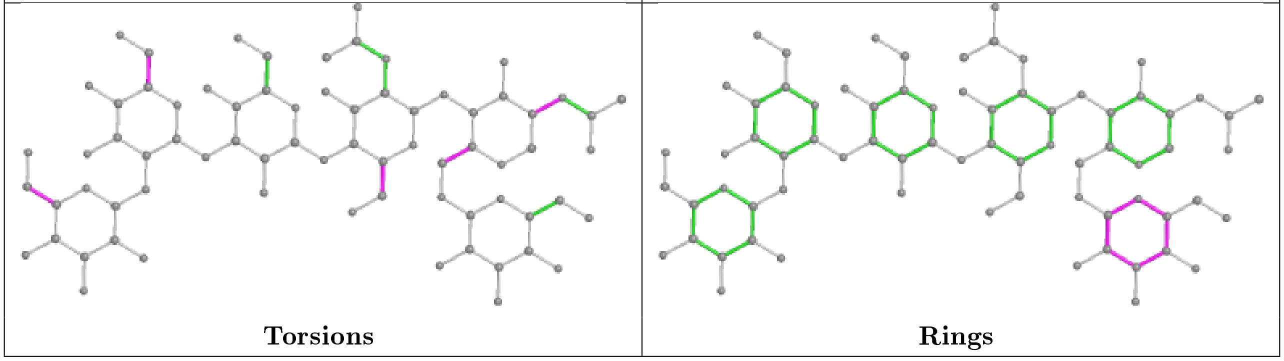


**Torsions** **Rings**

**Oligosaccharide Chain E**



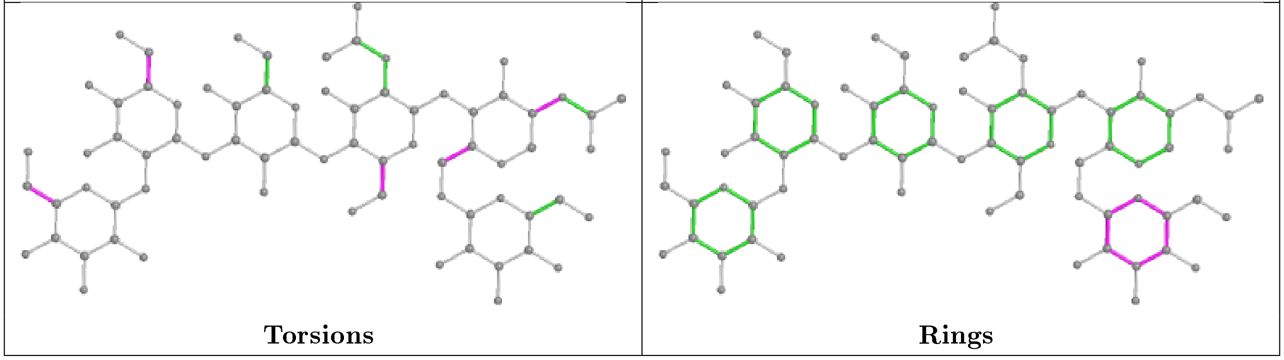
**Bond lengths** **Bond angles**



**Torsions** **Rings**

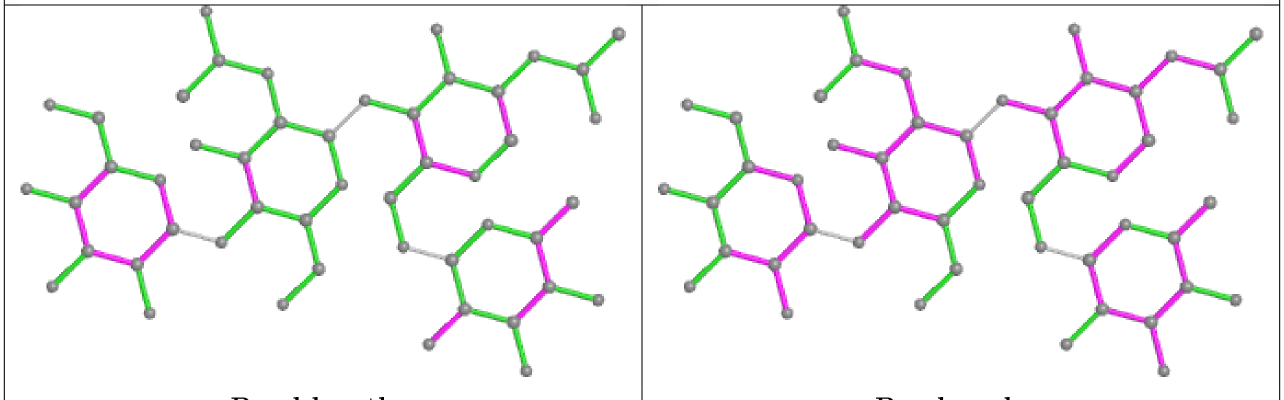
**Oligosaccharide Chain I**

**Bond lengths** **Bond angles**

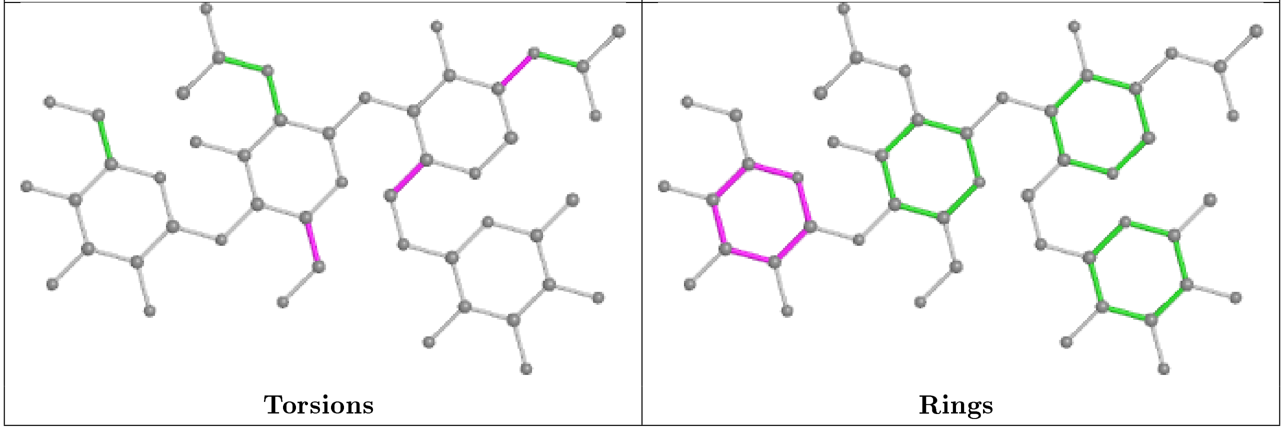


**Torsions** **Rings**

**Oligosaccharide Chain H**



**Bond lengths** **Bond angles**



**Torsions** **Rings**

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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 | $\#\|Z\| > 2$ |
| 7 | ST1 | A | 471 | - | 14,17,17 | 2.50 | 3 (21%) | 16,24,24 | 2.46 | 4 (25%) |
| 7 | ST1 | B | 471 | - | 14,17,17 | 2.50 | 3 (21%) | 16,24,24 | 2.46 | 4 (25%) |

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 | ST1 | A | 471 | - | - | 4/6/12/12 | 0/1/1/1 |
| 7 | ST1 | B | 471 | - | - | 4/6/12/12 | 0/1/1/1 |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | B | 471 | ST1 | C1-C' | -6.84 | 1.40 | 1.47 |
| 7 | A | 471 | ST1 | C1-C' | -6.84 | 1.40 | 1.47 |
| 7 | B | 471 | ST1 | C5-N5 | -5.28 | 1.36 | 1.45 |
| 7 | A | 471 | ST1 | C5-N5 | -5.28 | 1.36 | 1.45 |
| 7 | B | 471 | ST1 | C4-N4 | -2.04 | 1.39 | 1.43 |
| 7 | A | 471 | ST1 | C4-N4 | -2.04 | 1.39 | 1.43 |

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | B | 471 | ST1 | C4-N4-C4' | -7.25 | 110.54 | 122.79 |
| 7 | A | 471 | ST1 | C4-N4-C4' | -7.25 | 110.54 | 122.79 |
| 7 | B | 471 | ST1 | ON1-N5-C5 | -4.49 | 111.35 | 119.03 |
| 7 | A | 471 | ST1 | ON1-N5-C5 | -4.49 | 111.35 | 119.03 |
| 7 | B | 471 | ST1 | CM4-C4'-N4 | 3.12 | 119.56 | 114.98 |

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*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | A | 471 | ST1 | CM4-C4'-N4 | 3.12 | 119.56 | 114.98 |
| 7 | B | 471 | ST1 | C5-C4-N4 | -2.32 | 119.07 | 123.20 |
| 7 | A | 471 | ST1 | C5-C4-N4 | -2.32 | 119.07 | 123.20 |

There are no chirality outliers.

All (8) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 7 | B | 471 | ST1 | O4'-C4'-N4-C4 |
| 7 | B | 471 | ST1 | CM4-C4'-N4-C4 |
| 7 | A | 471 | ST1 | O4'-C4'-N4-C4 |
| 7 | A | 471 | ST1 | CM4-C4'-N4-C4 |
| 7 | B | 471 | ST1 | C6-C5-N5-ON1 |
| 7 | A | 471 | ST1 | C6-C5-N5-ON1 |
| 7 | B | 471 | ST1 | C4-C5-N5-ON1 |
| 7 | A | 471 | ST1 | C4-C5-N5-ON1 |

There are no ring outliers.

2 monomers are involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 7 | A | 471 | ST1 | 1 | 0 |
| 7 | B | 471 | ST1 | 1 | 0 |

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

# 6 Fit of model and data ⓘ

## 6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

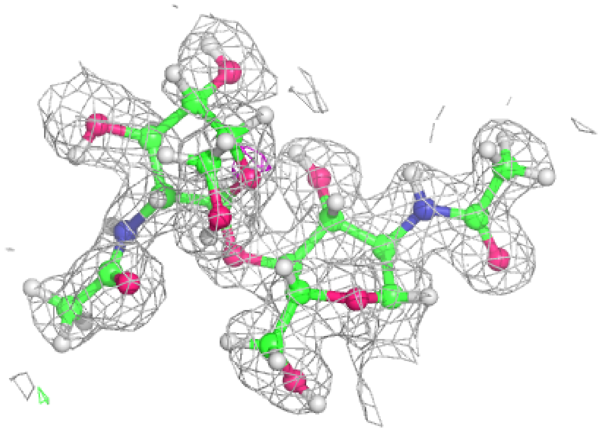
## 6.3 Carbohydrates ⓘ

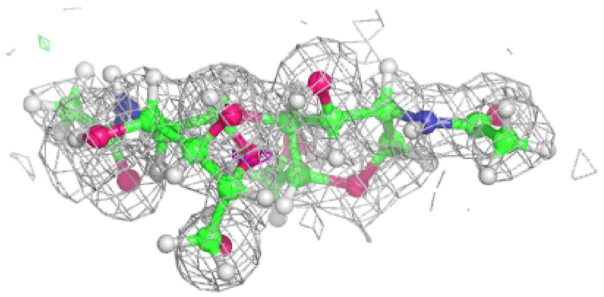
Unable to reproduce the depositors R factor - this section is therefore empty.

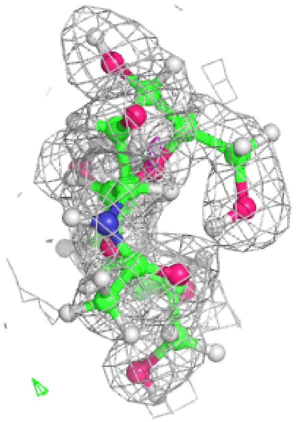
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain C:**

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

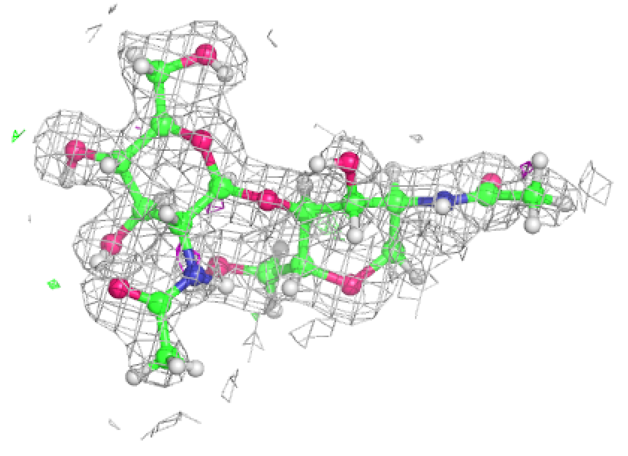


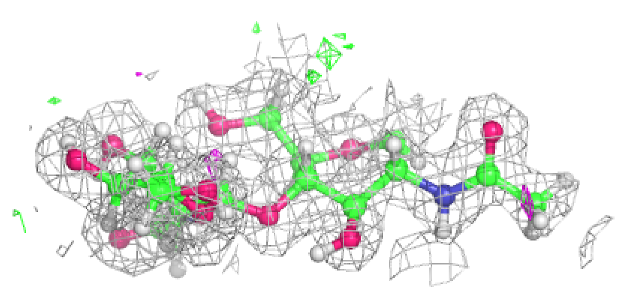


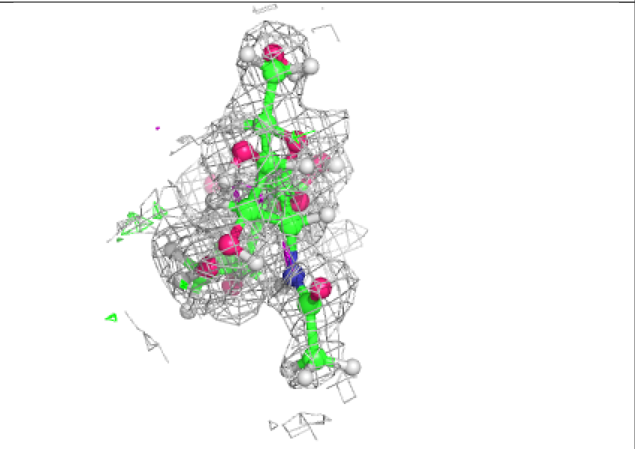


**Electron density around Chain F:**

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

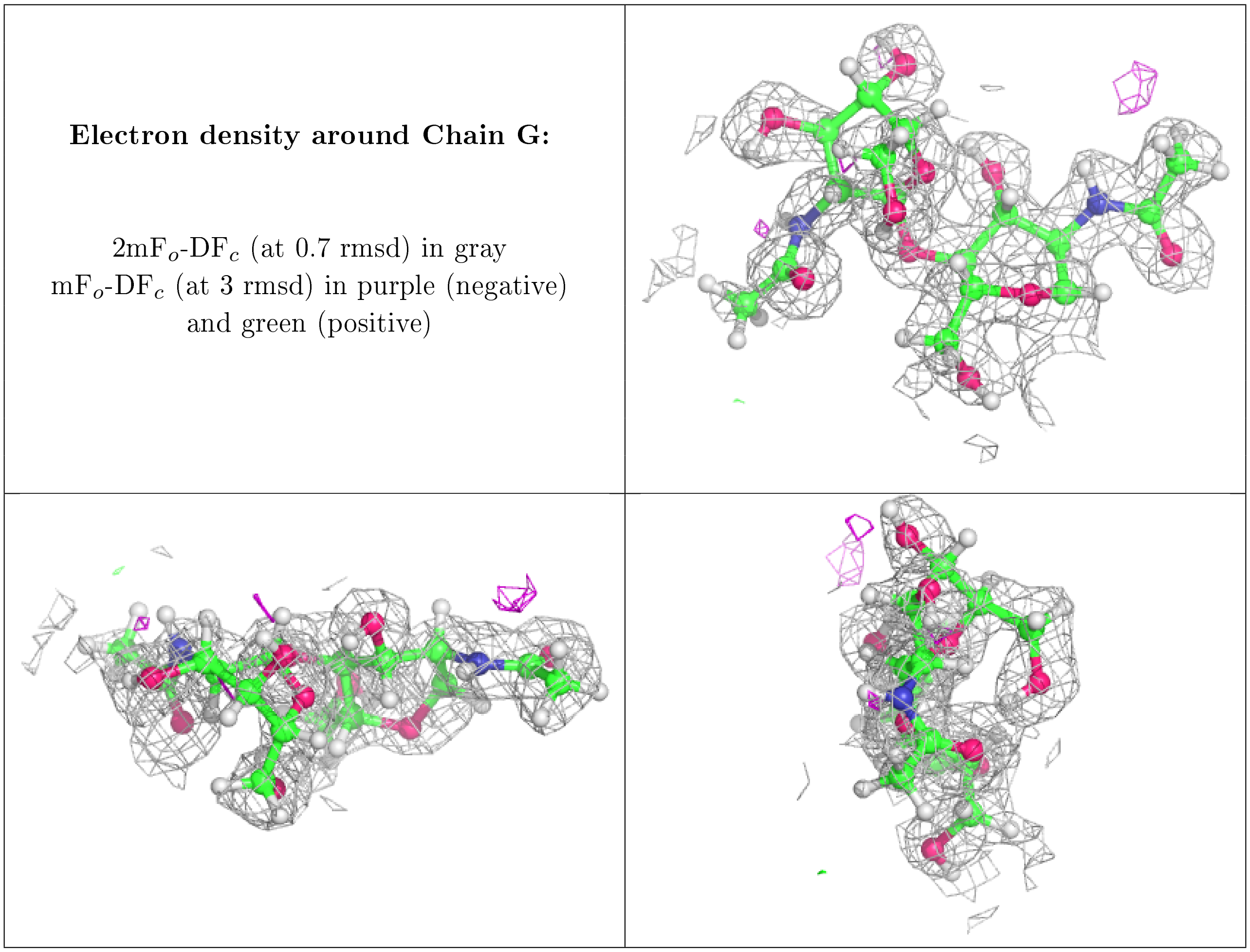






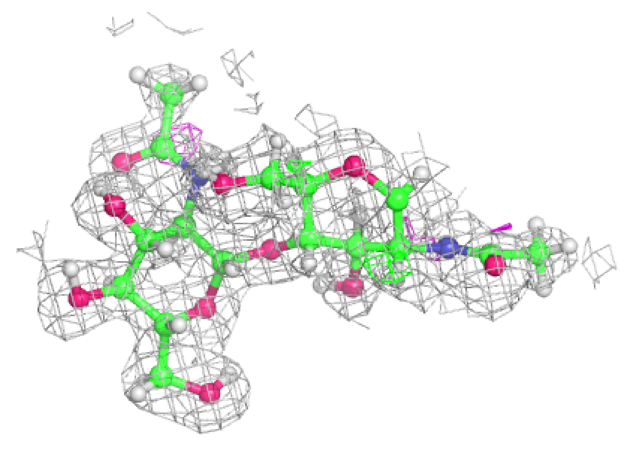
**Electron density around Chain G:**

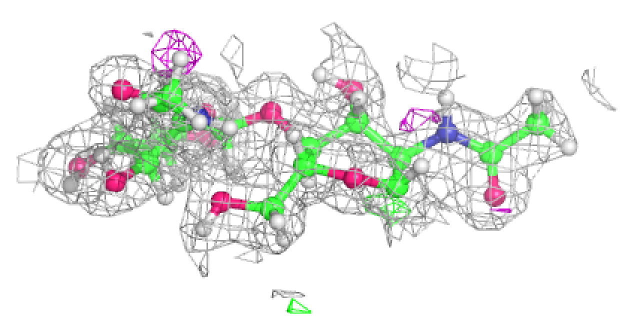
$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

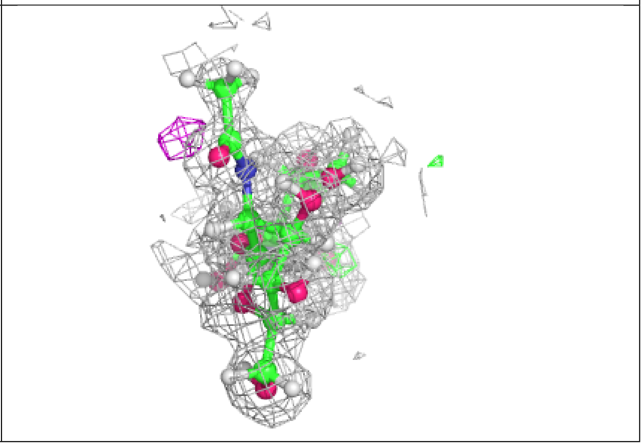


**Electron density around Chain J:**

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

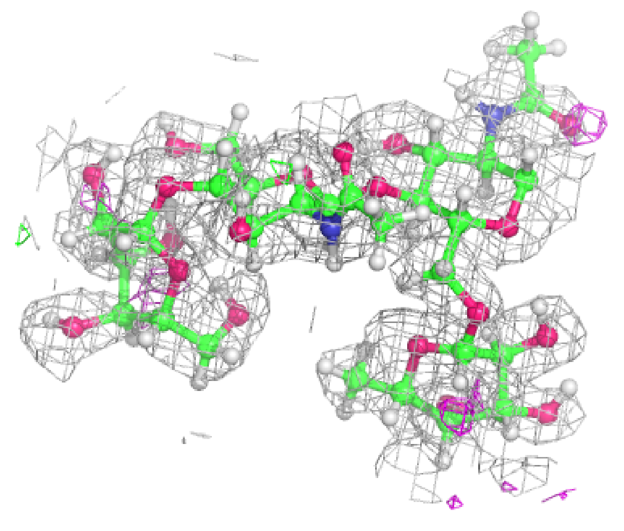


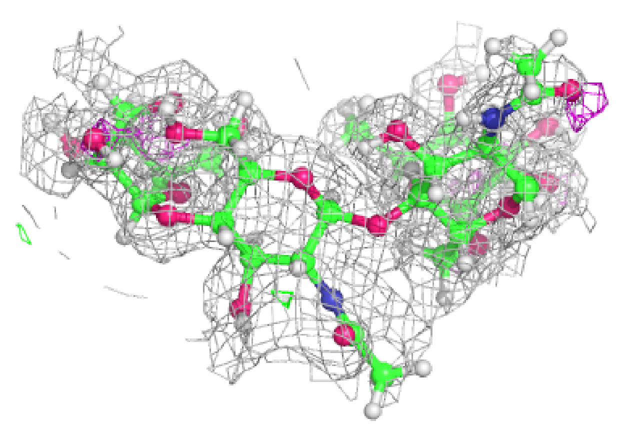


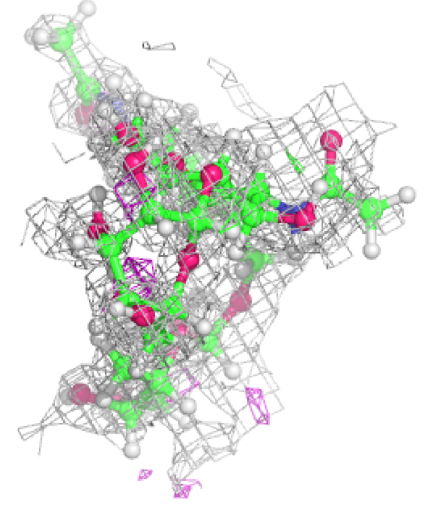


**Electron density around Chain D:**

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

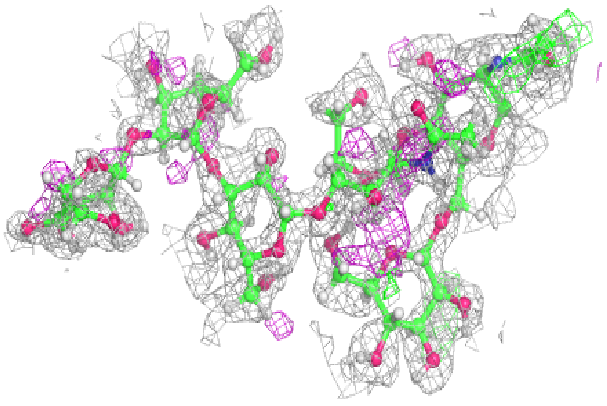


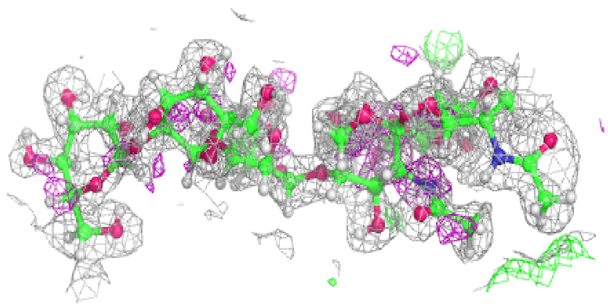


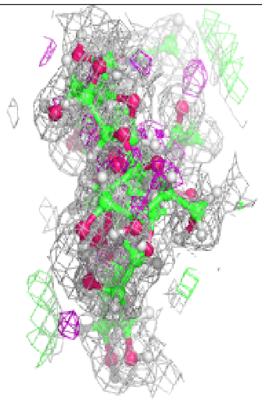


**Electron density around Chain E:**

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

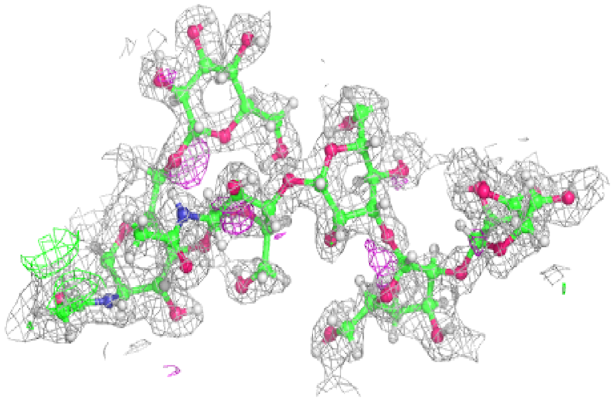


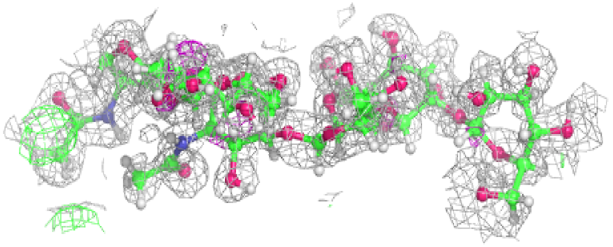


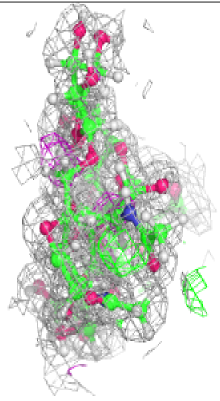


**Electron density around Chain I:**

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

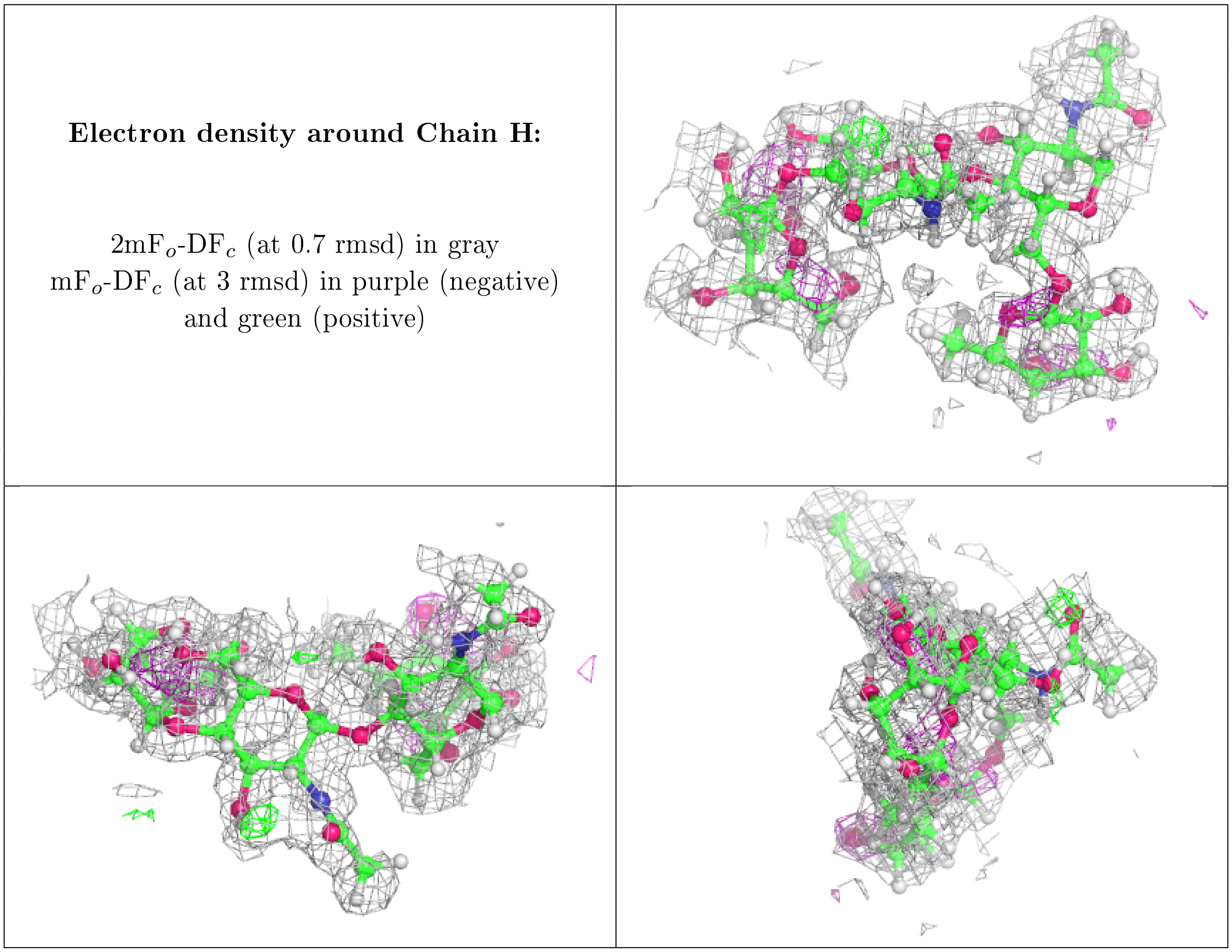






**Electron density around Chain H:**

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



## 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.