



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:00 AM UTC

PDB ID : 7S0I / pdb_00007s0i
Title : CRYSTAL STRUCTURE OF N1 NEURAMINIDASE FROM A/Michigan/4
5/2015(H1N1)
Authors : Zhu, X.; Wilson, I.A.
Deposited on : 2021-08-30
Resolution : 2.89 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.

The types of validation reports are described at

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

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

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

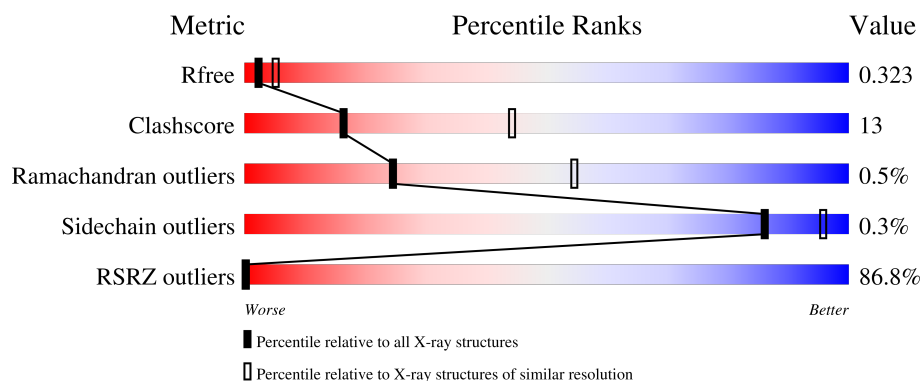
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 of 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	393	85% 72% 25% ..
2	B	4	25% 25% 50%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3064 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	387	2993	1881	513	577	22	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

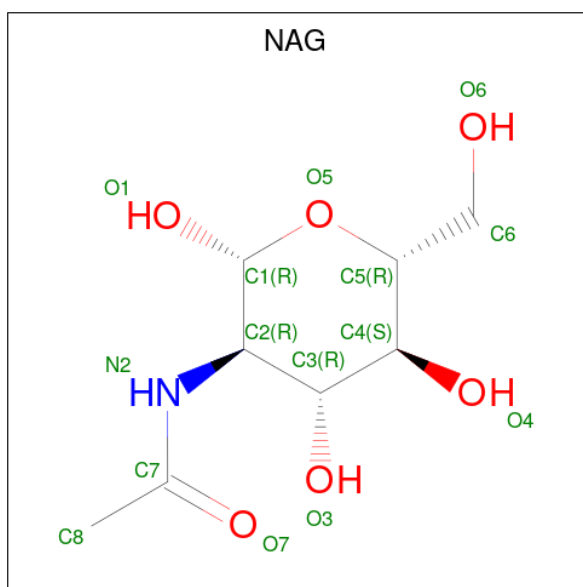
Chain	Residue	Modelled	Actual	Comment	Reference
A	77	GLY	-	expression tag	UNP A0A0X9QTS2
A	78	SER	-	expression tag	UNP A0A0X9QTS2
A	79	PRO	-	expression tag	UNP A0A0X9QTS2
A	80	SER	-	expression tag	UNP A0A0X9QTS2
A	81	ARG	-	expression tag	UNP A0A0X9QTS2

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-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	N	O			
2	B	4	50	28	2	20	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Ca	0	0
			3	3		

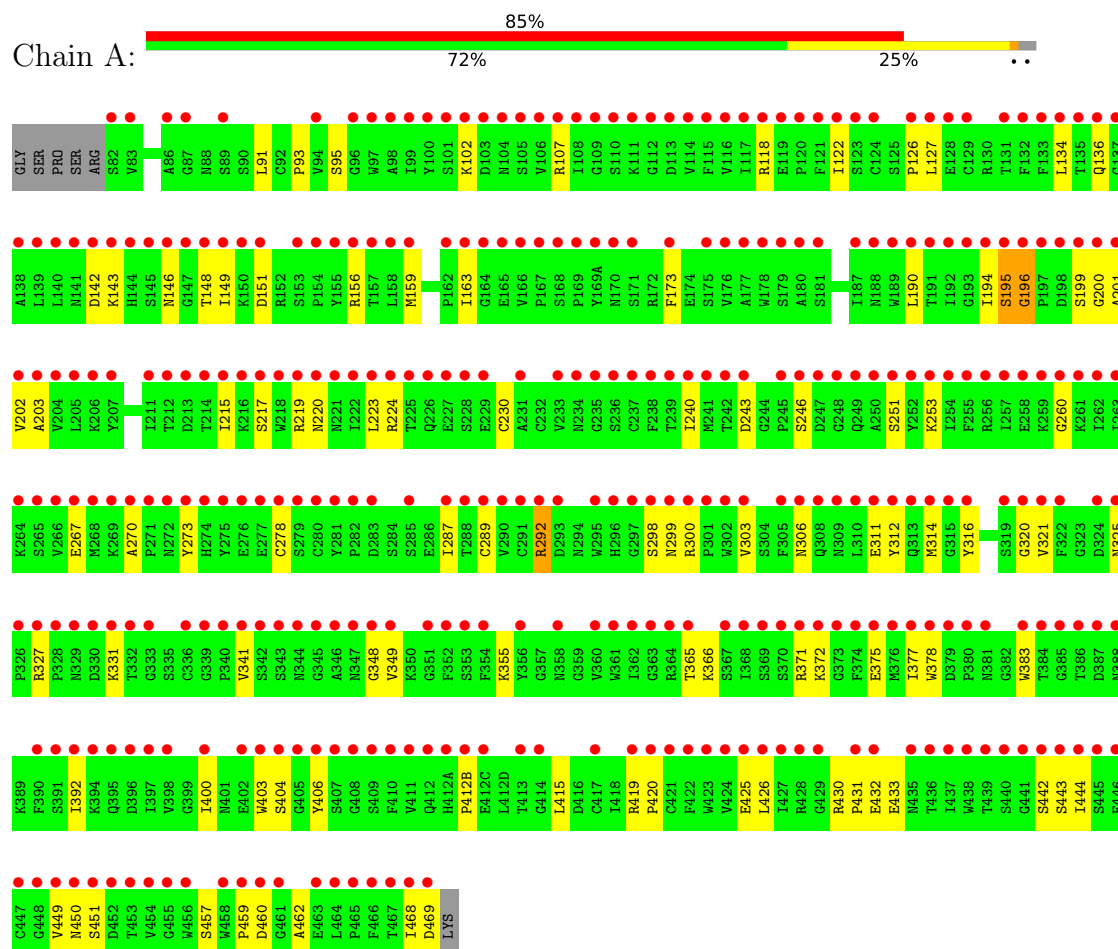
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	O	0	0
			4	4		

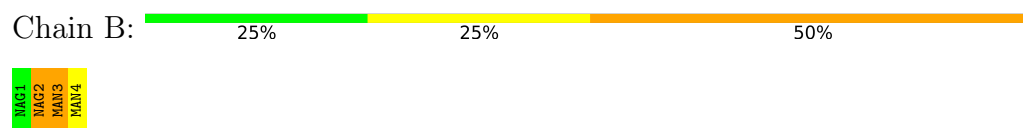
3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Neuraminidase



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	92.13Å 92.13Å 104.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.07 – 2.89 46.07 – 2.89	Depositor EDS
% Data completeness (in resolution range)	91.0 (46.07-2.89) 91.2 (46.07-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.35	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.292 , 0.321 0.292 , 0.323	Depositor DCC
R_{free} test set	459 reflections (4.32%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	1.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 12.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	3064	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.46	1/3075 (0.0%)	0.88	4/4175 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	292	ARG	C-O	-6.48	1.16	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	GLY	N-CA-C	-6.20	99.70	112.34
1	A	194	ILE	CA-C-N	6.09	132.33	122.53
1	A	194	ILE	C-N-CA	6.09	132.33	122.53
1	A	195	SER	N-CA-C	-5.64	100.91	108.86

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2993	0	2831	76	0
2	B	50	0	43	1	0
3	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	3	0	0	0	0
5	A	4	0	0	0	0
All	All	3064	0	2887	77	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (77) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:GLN:HE21	1:A:148:THR:HG22	1.13	1.14
1:A:403:TRP:O	1:A:426:LEU:HD12	1.49	1.11
1:A:136:GLN:NE2	1:A:148:THR:HG22	1.70	1.07
1:A:136:GLN:HE21	1:A:148:THR:CG2	1.81	0.93
1:A:136:GLN:NE2	1:A:148:THR:CG2	2.32	0.91
1:A:136:GLN:NE2	1:A:148:THR:CB	2.36	0.89
1:A:136:GLN:HE22	1:A:148:THR:HA	1.39	0.88
1:A:404:SER:HA	1:A:426:LEU:HD13	1.58	0.83
1:A:136:GLN:HE22	1:A:148:THR:CA	1.91	0.82
1:A:432:GLU:HG2	1:A:433:GLU:HG3	1.61	0.80
1:A:449:VAL:HG22	1:A:451:SER:H	1.47	0.80
1:A:136:GLN:NE2	1:A:148:THR:HB	2.04	0.73
1:A:403:TRP:O	1:A:426:LEU:CD1	2.34	0.72
1:A:136:GLN:HE22	1:A:148:THR:CB	2.04	0.69
1:A:196:GLY:HA3	1:A:201:ALA:HA	1.75	0.68
1:A:195:SER:O	1:A:202:VAL:N	2.25	0.68
1:A:406:TYR:HB2	1:A:425:GLU:OE2	1.96	0.66
1:A:300:ARG:HH22	1:A:349:VAL:HG23	1.61	0.65
1:A:219:ARG:NH2	1:A:251:SER:HB2	2.11	0.65
1:A:240:ILE:HG21	1:A:278:CYS:SG	2.37	0.64
1:A:298:SER:H	1:A:341:VAL:HG13	1.68	0.59
1:A:270:ALA:HB2	1:A:314:MET:HE1	1.85	0.59
1:A:136:GLN:HG2	1:A:156:ARG:HE	1.69	0.58
1:A:196:GLY:CA	1:A:201:ALA:HA	2.34	0.57
1:A:375:GLU:OE1	1:A:377:ILE:HD11	2.04	0.57
1:A:102:LYS:HG3	1:A:444:ILE:HG22	1.86	0.57
1:A:349:VAL:HG12	1:A:371:ARG:NH1	2.19	0.57
1:A:201:ALA:HB3	1:A:223:LEU:HB3	1.87	0.56
1:A:299:ASN:OD1	1:A:341:VAL:HG12	2.04	0.56
1:A:190:LEU:HD13	1:A:260:GLY:HA2	1.86	0.56
1:A:366:LYS:HG2	1:A:375:GLU:OE2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:LEU:HD22	1:A:420:PRO:HG3	1.88	0.56
1:A:142:ASP:OD1	1:A:143:LYS:N	2.38	0.56
1:A:219:ARG:HB2	1:A:243:ASP:CG	2.31	0.56
1:A:126:PRO:HB2	1:A:127:LEU:HD22	1.89	0.54
1:A:107:ARG:HD2	1:A:460:ASP:O	2.08	0.54
1:A:325:ASN:OD1	1:A:371:ARG:HG3	2.07	0.53
1:A:366:LYS:HB3	1:A:400:ILE:HD12	1.90	0.53
1:A:199:SER:O	1:A:220:ASN:ND2	2.39	0.53
1:A:196:GLY:C	1:A:201:ALA:HA	2.34	0.53
1:A:457:SER:O	1:A:459:PRO:HD3	2.09	0.52
1:A:93:PRO:O	1:A:450:ASN:ND2	2.38	0.52
1:A:468:ILE:O	1:A:469:ASP:HB2	2.09	0.52
1:A:159:MET:HG2	1:A:173:PHE:HA	1.93	0.51
1:A:203:ALA:HB3	1:A:215:ILE:HG22	1.92	0.51
1:A:412(B):PRO:HB3	1:A:415:LEU:O	2.11	0.50
1:A:430:ARG:HB3	1:A:431:PRO:HA	1.94	0.50
1:A:442:SER:OG	1:A:443:SER:N	2.44	0.50
1:A:118:ARG:NE	1:A:425:GLU:OE1	2.41	0.49
1:A:270:ALA:HB1	1:A:273:TYR:HB2	1.94	0.49
1:A:224:ARG:NH2	1:A:246:SER:OG	2.45	0.48
1:A:143:LYS:O	1:A:146:ASN:HB2	2.12	0.48
1:A:289:CYS:HB2	1:A:303:VAL:HG13	1.95	0.48
1:A:95:SER:OG	1:A:450:ASN:HA	2.15	0.47
1:A:287:ILE:HD12	1:A:287:ILE:N	2.30	0.47
1:A:201:ALA:N	1:A:217:SER:OG	2.49	0.46
1:A:253:LYS:HG2	1:A:267:GLU:HA	1.96	0.46
1:A:378:TRP:HB3	1:A:392:ILE:HB	1.97	0.46
1:A:134:LEU:O	1:A:156:ARG:NH2	2.49	0.46
1:A:306:ASN:ND2	1:A:311:GLU:HB2	2.32	0.44
1:A:327:ARG:HH12	1:A:365:THR:HB	1.82	0.44
1:A:404:SER:HA	1:A:426:LEU:CD1	2.40	0.44
1:A:149:ILE:HD11	1:A:431:PRO:HG3	2.00	0.43
1:A:292:ARG:HH21	1:A:348:GLY:N	2.16	0.43
2:B:2:NAG:H4	2:B:3:MAN:H5	2.01	0.43
1:A:320:GLY:HA3	1:A:331:LYS:O	2.19	0.42
1:A:355:LYS:HE2	1:A:383:TRP:CD1	2.53	0.42
1:A:107:ARG:HG2	1:A:462:ALA:HB2	2.01	0.41
1:A:372:LYS:HB3	1:A:400:ILE:O	2.19	0.41
1:A:127:LEU:HD13	1:A:127:LEU:HA	1.85	0.41
1:A:419:ARG:HA	1:A:420:PRO:HD3	1.89	0.41
1:A:151:ASP:O	1:A:156:ARG:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:TYR:HD1	1:A:312:TYR:H	1.66	0.41
1:A:312:TYR:CD1	1:A:312:TYR:N	2.89	0.41
1:A:122:ILE:HD13	1:A:163:ILE:HD11	2.02	0.41
1:A:273:TYR:CD1	1:A:316:TYR:HE1	2.38	0.41
1:A:289:CYS:HB2	1:A:303:VAL:CG1	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	385/393 (98%)	370 (96%)	13 (3%)	2 (0%)	24 54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	GLY
1	A	321	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	334/339 (98%)	333 (100%)	1 (0%)	86 96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	230	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	GLN
1	A	296	HIS
1	A	344	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 ⓘ

4 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	B	1	1,2	14,14,15	0.26	0	17,19,21	0.65	0
2	NAG	B	2	2	14,14,15	0.67	1 (7%)	17,19,21	0.64	0
2	MAN	B	3	2	11,11,12	0.91	1 (9%)	15,15,17	0.79	1 (6%)
2	MAN	B	4	2	11,11,12	1.00	1 (9%)	15,15,17	0.78	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	MAN	B	3	2	-	0/2/19/22	0/1/1/1
2	MAN	B	4	2	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	O5-C1	-2.42	1.39	1.43
2	B	4	MAN	O5-C1	-2.20	1.40	1.43
2	B	3	MAN	C4-C3	2.04	1.57	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	MAN	O2-C2-C3	-2.11	105.79	110.15

There are no chirality outliers.

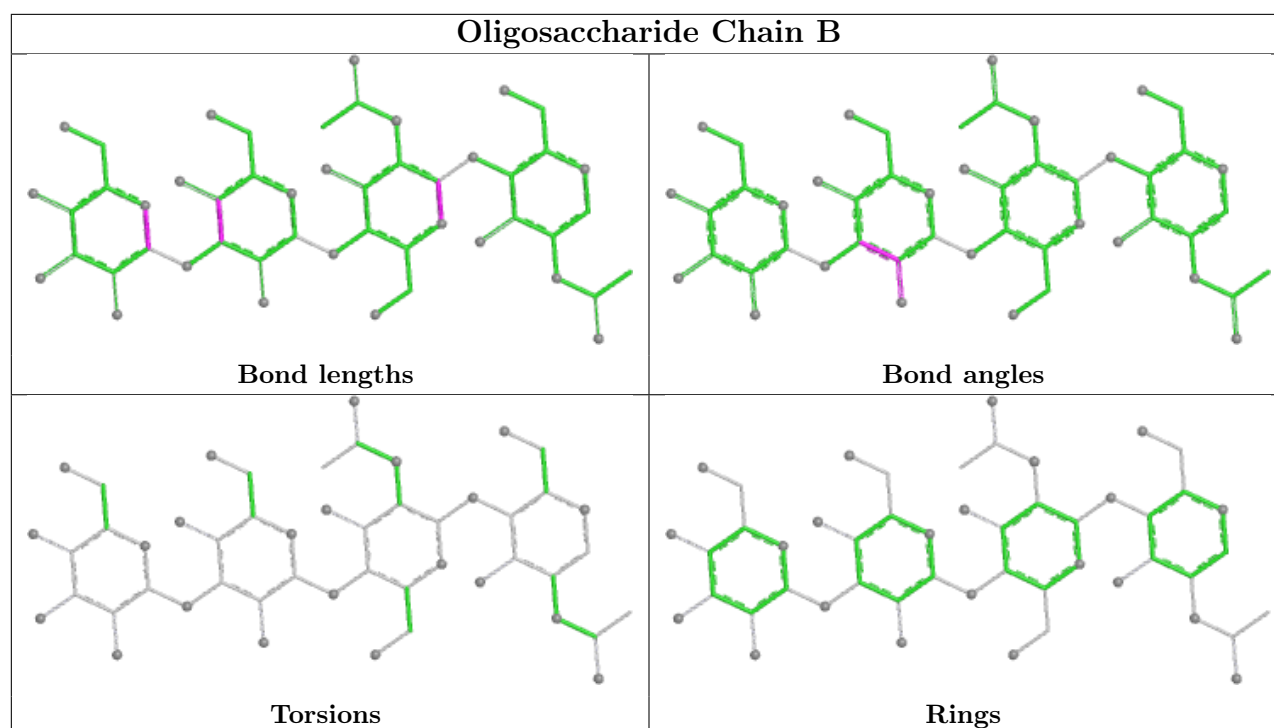
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	1	0
2	B	3	MAN	1	0

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



5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	$\# Z > 2$
3	NAG	A	501	1	14,14,15	0.63	0	17,19,21	0.94	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	501	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

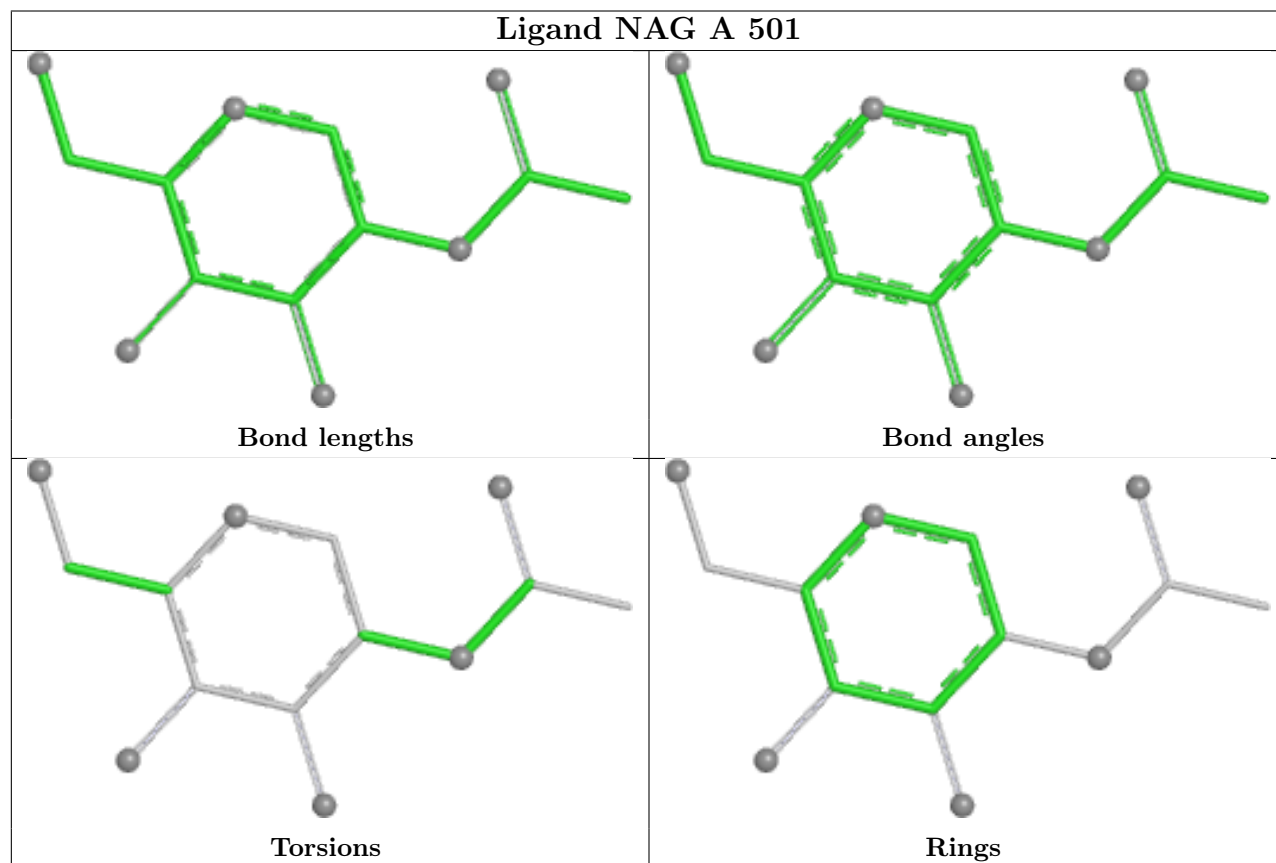
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	387/393 (98%)	3.41	336 (86%) 0 0	23, 34, 45, 77	0

All (336) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	112	GLY	10.9
1	A	254	ILE	8.6
1	A	310	LEU	7.7
1	A	312	TYR	7.4
1	A	269	LYS	7.4
1	A	344	ASN	7.3
1	A	87	GLY	6.7
1	A	138	ALA	6.7
1	A	456	TRP	6.6
1	A	99	ILE	6.5
1	A	180	ALA	6.2
1	A	215	ILE	6.2
1	A	192	ILE	6.0
1	A	242	THR	6.0
1	A	268	MET	5.9
1	A	154	PRO	5.8
1	A	427	ILE	5.8
1	A	328	PRO	5.7
1	A	272	ASN	5.7
1	A	193	GLY	5.7
1	A	211	ILE	5.7
1	A	406	TYR	5.6
1	A	196	GLY	5.6
1	A	202	VAL	5.6
1	A	145	SER	5.6
1	A	97	TRP	5.5
1	A	390	PHE	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	410	PHE	5.4
1	A	301	PRO	5.4
1	A	195	SER	5.4
1	A	122	ILE	5.4
1	A	441	GLY	5.3
1	A	168	SER	5.3
1	A	131	THR	5.3
1	A	275	TYR	5.2
1	A	225	THR	5.1
1	A	181	SER	5.1
1	A	365	THR	5.0
1	A	388	ASN	5.0
1	A	381	ASN	5.0
1	A	445	SER	4.9
1	A	405	GLY	4.9
1	A	240	ILE	4.9
1	A	368	ILE	4.9
1	A	291	CYS	4.9
1	A	349	VAL	4.9
1	A	351	GLY	4.9
1	A	175	SER	4.9
1	A	223	LEU	4.9
1	A	452	ASP	4.9
1	A	409	SER	4.8
1	A	413	THR	4.8
1	A	287	ILE	4.8
1	A	290	VAL	4.8
1	A	397	ILE	4.7
1	A	455	GLY	4.7
1	A	135	THR	4.7
1	A	454	VAL	4.7
1	A	448	GLY	4.7
1	A	163	ILE	4.7
1	A	336	CYS	4.7
1	A	412	GLN	4.7
1	A	262	ILE	4.7
1	A	142	ASP	4.6
1	A	321	VAL	4.6
1	A	265	SER	4.6
1	A	197	PRO	4.5
1	A	346	ALA	4.5
1	A	383	TRP	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	256	ARG	4.5
1	A	203	ALA	4.5
1	A	121	PHE	4.5
1	A	148	THR	4.4
1	A	177	ALA	4.4
1	A	110	SER	4.4
1	A	257	ILE	4.4
1	A	247	ASP	4.4
1	A	453	THR	4.4
1	A	176	VAL	4.4
1	A	179	SER	4.4
1	A	432	GLU	4.3
1	A	464	LEU	4.3
1	A	140	LEU	4.3
1	A	205	LEU	4.3
1	A	241	MET	4.3
1	A	426	LEU	4.3
1	A	82	SER	4.2
1	A	101	SER	4.2
1	A	153	SER	4.2
1	A	266	VAL	4.2
1	A	261	LYS	4.2
1	A	282	PRO	4.2
1	A	157	THR	4.2
1	A	264	LYS	4.2
1	A	199	SER	4.2
1	A	106	VAL	4.1
1	A	169	PRO	4.1
1	A	378	TRP	4.1
1	A	322	PHE	4.1
1	A	144	HIS	4.1
1	A	126	PRO	4.0
1	A	222	ILE	4.0
1	A	281	TYR	4.0
1	A	371	ARG	4.0
1	A	273	TYR	4.0
1	A	278	CYS	4.0
1	A	414	GLY	4.0
1	A	352	PHE	4.0
1	A	250	ALA	3.9
1	A	331	LYS	3.9
1	A	360	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	171	SER	3.9
1	A	108	ILE	3.9
1	A	194	ILE	3.9
1	A	164	GLY	3.9
1	A	348	GLY	3.9
1	A	111	LYS	3.9
1	A	104	ASN	3.9
1	A	218	TRP	3.9
1	A	347	ASN	3.9
1	A	255	PHE	3.9
1	A	435	ASN	3.9
1	A	320	GLY	3.8
1	A	341	VAL	3.8
1	A	271	PRO	3.8
1	A	231	ALA	3.8
1	A	419	ARG	3.8
1	A	369	SER	3.8
1	A	189	TRP	3.8
1	A	325	ASN	3.8
1	A	408	GLY	3.8
1	A	354	PHE	3.8
1	A	165	GLU	3.7
1	A	412(C)	GLU	3.7
1	A	118	ARG	3.7
1	A	253	LYS	3.7
1	A	404	SER	3.7
1	A	226	GLN	3.7
1	A	314	MET	3.7
1	A	191	THR	3.7
1	A	386	THR	3.7
1	A	298	SER	3.7
1	A	391	SER	3.7
1	A	248	GLY	3.6
1	A	279	SER	3.6
1	A	367	SER	3.6
1	A	420	PRO	3.6
1	A	98	ALA	3.6
1	A	293	ASP	3.6
1	A	308	GLN	3.6
1	A	343	SER	3.5
1	A	139	LEU	3.5
1	A	364	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	100	TYR	3.5
1	A	380	PRO	3.5
1	A	115	PHE	3.5
1	A	238	PHE	3.5
1	A	411	VAL	3.5
1	A	251	SER	3.5
1	A	438	TRP	3.5
1	A	460	ASP	3.5
1	A	429	GLY	3.5
1	A	440	SER	3.5
1	A	327	ARG	3.5
1	A	394	LYS	3.4
1	A	123	SER	3.4
1	A	217	SER	3.4
1	A	423	TRP	3.4
1	A	306	ASN	3.4
1	A	200	GLY	3.4
1	A	216	LYS	3.4
1	A	204	VAL	3.4
1	A	449	VAL	3.4
1	A	267	GLU	3.4
1	A	342	SER	3.4
1	A	295	TRP	3.4
1	A	207	TYR	3.4
1	A	96	GLY	3.4
1	A	303	VAL	3.4
1	A	229	GLU	3.4
1	A	214	THR	3.4
1	A	170	ASN	3.4
1	A	235	GLY	3.4
1	A	276	GLU	3.4
1	A	162	PRO	3.4
1	A	167	PRO	3.4
1	A	442	SER	3.4
1	A	425	GLU	3.3
1	A	412(B)	PRO	3.3
1	A	421	CYS	3.3
1	A	274	HIS	3.3
1	A	127	LEU	3.3
1	A	143	LYS	3.3
1	A	345	GLY	3.3
1	A	134	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	311	GLU	3.2
1	A	151	ASP	3.2
1	A	243	ASP	3.2
1	A	353	SER	3.2
1	A	362	ILE	3.2
1	A	309	ASN	3.2
1	A	447	CYS	3.2
1	A	296	HIS	3.2
1	A	169(A)	TYR	3.1
1	A	407	SER	3.1
1	A	233	VAL	3.1
1	A	128	GLU	3.1
1	A	150	LYS	3.1
1	A	379	ASP	3.1
1	A	374	PHE	3.1
1	A	384	THR	3.1
1	A	155	TYR	3.1
1	A	329	ASN	3.1
1	A	249	GLN	3.1
1	A	120	PRO	3.1
1	A	305	PHE	3.1
1	A	86	ALA	3.0
1	A	213	ASP	3.0
1	A	221	ASN	3.0
1	A	443	SER	3.0
1	A	313	GLN	3.0
1	A	263	ILE	3.0
1	A	156	ARG	3.0
1	A	289	CYS	3.0
1	A	227	GLU	3.0
1	A	105	SER	3.0
1	A	137	GLY	3.0
1	A	141	ASN	3.0
1	A	188	ASN	3.0
1	A	239	THR	3.0
1	A	302	TRP	2.9
1	A	252	TYR	2.9
1	A	395	GLN	2.9
1	A	245	PRO	2.9
1	A	124	CYS	2.9
1	A	132	PHE	2.9
1	A	446	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	463	GLU	2.9
1	A	220	ASN	2.9
1	A	228	SER	2.9
1	A	236	SER	2.9
1	A	372	LYS	2.9
1	A	158	LEU	2.9
1	A	461	GLY	2.9
1	A	201	ALA	2.9
1	A	260	GLY	2.9
1	A	173	PHE	2.9
1	A	319	SER	2.9
1	A	468	ILE	2.9
1	A	361	TRP	2.8
1	A	396	ASP	2.8
1	A	469	ASP	2.8
1	A	116	VAL	2.8
1	A	270	ALA	2.8
1	A	103	ASP	2.8
1	A	198	ASP	2.8
1	A	363	GLY	2.8
1	A	237	CYS	2.8
1	A	277	GLU	2.8
1	A	224	ARG	2.8
1	A	392	ILE	2.8
1	A	206	LYS	2.8
1	A	451	SER	2.8
1	A	403	TRP	2.7
1	A	102	LYS	2.7
1	A	330	ASP	2.7
1	A	280	CYS	2.7
1	A	444	ILE	2.7
1	A	422	PHE	2.7
1	A	159	MET	2.7
1	A	234	ASN	2.7
1	A	107	ARG	2.7
1	A	424	VAL	2.7
1	A	340	PRO	2.7
1	A	387	ASP	2.7
1	A	117	ILE	2.6
1	A	300	ARG	2.6
1	A	119	GLU	2.6
1	A	398	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	89	SER	2.6
1	A	437	ILE	2.6
1	A	133	PHE	2.6
1	A	458	TRP	2.6
1	A	316	TYR	2.6
1	A	146	ASN	2.6
1	A	315	GLY	2.6
1	A	339	GLY	2.6
1	A	385	GLY	2.6
1	A	94	VAL	2.6
1	A	129	CYS	2.6
1	A	136	GLN	2.6
1	A	258	GLU	2.6
1	A	297	GLY	2.5
1	A	114	VAL	2.5
1	A	375	GLU	2.5
1	A	324	ASP	2.5
1	A	285	SER	2.5
1	A	436	THR	2.5
1	A	246	SER	2.5
1	A	376	MET	2.5
1	A	356	TYR	2.5
1	A	212	THR	2.5
1	A	283	ASP	2.4
1	A	147	GLY	2.4
1	A	149	ILE	2.4
1	A	417	CYS	2.4
1	A	467	THR	2.4
1	A	377	ILE	2.4
1	A	259	LYS	2.4
1	A	190	LEU	2.4
1	A	459	PRO	2.4
1	A	450	ASN	2.3
1	A	466	PHE	2.3
1	A	439	THR	2.3
1	A	400	ILE	2.3
1	A	109	GLY	2.3
1	A	412(A)	HIS	2.3
1	A	292	ARG	2.3
1	A	326	PRO	2.3
1	A	83	VAL	2.3
1	A	333	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	402	GLU	2.2
1	A	370	SER	2.2
1	A	113	ASP	2.2
1	A	428	ARG	2.2
1	A	373	GLY	2.2
1	A	358	ASN	2.2
1	A	219	ARG	2.2
1	A	288	THR	2.1
1	A	431	PRO	2.1
1	A	332	THR	2.1
1	A	178	TRP	2.1
1	A	187	ILE	2.1
1	A	465	PRO	2.1
1	A	299	ASN	2.0
1	A	166	VAL	2.0

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

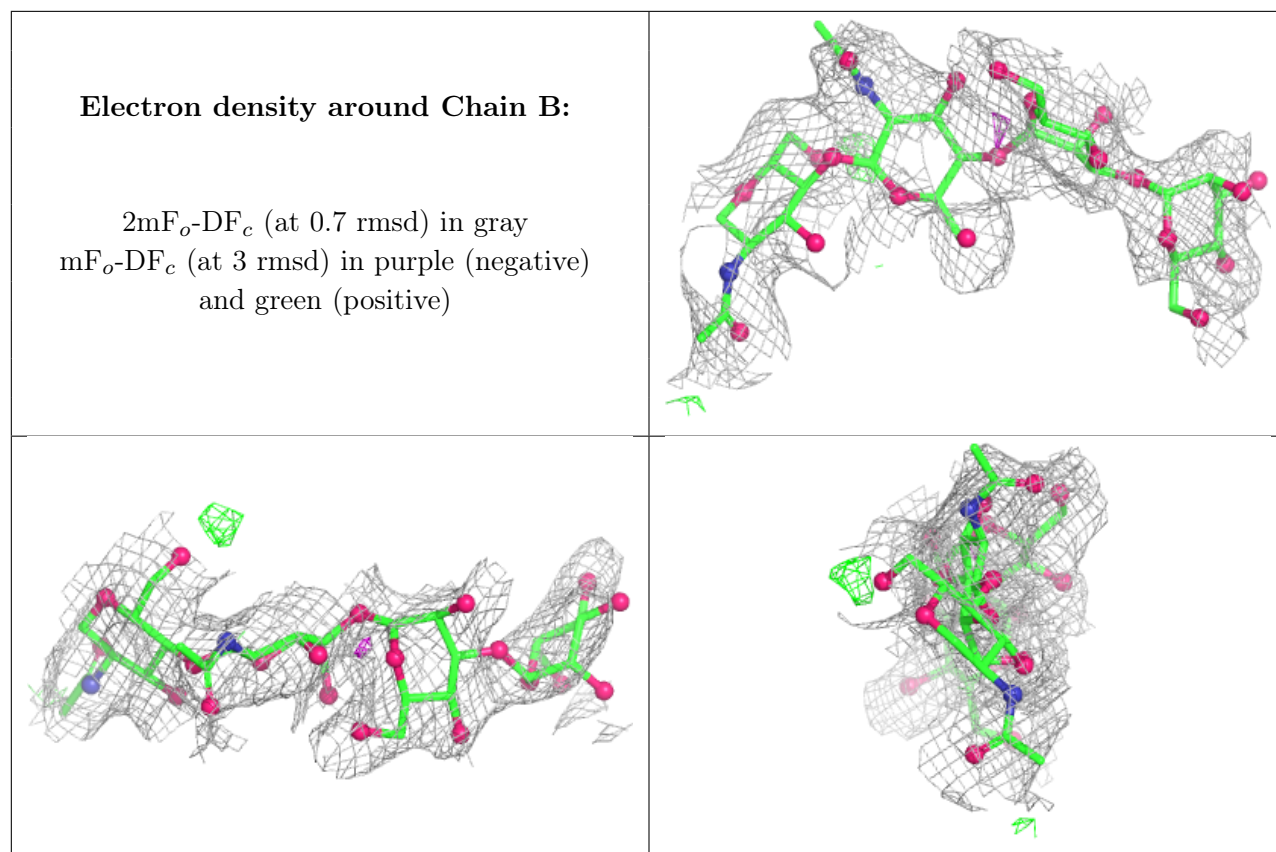
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MAN	B	3	11/12	0.51	0.25	53,62,68,68	0
2	MAN	B	4	11/12	0.54	0.39	54,66,74,77	0
2	NAG	B	2	14/15	0.55	0.21	54,59,62,63	0
2	NAG	B	1	14/15	0.58	0.20	37,44,49,51	0

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.



6.4 Ligands [i](#)

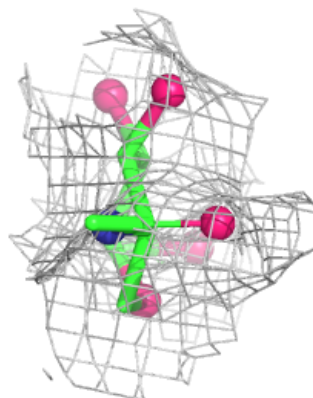
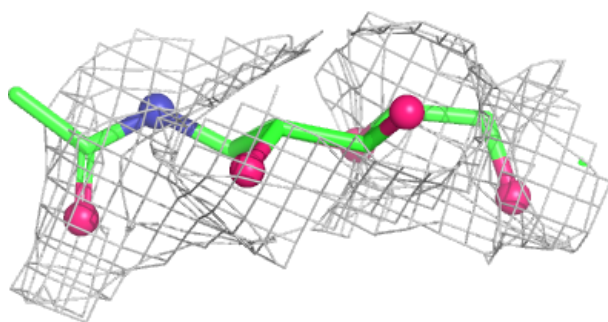
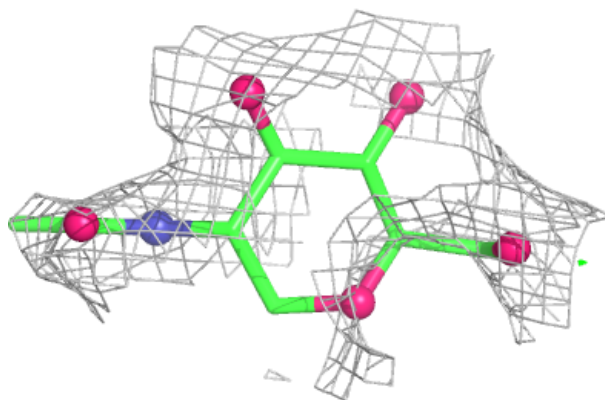
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	A	501	14/15	0.58	0.19	54,64,67,67	0
4	CA	A	503	1/1	0.59	0.22	31,31,31,31	0
4	CA	A	504	1/1	0.89	0.51	41,41,41,41	1
4	CA	A	502	1/1	0.93	0.12	24,24,24,24	0

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

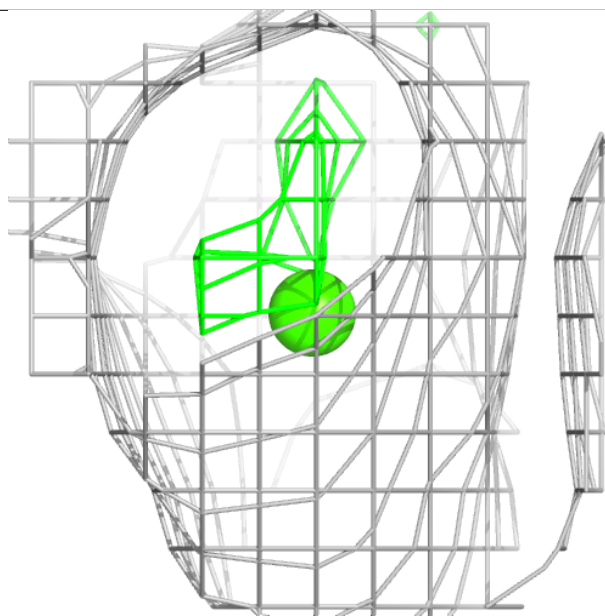
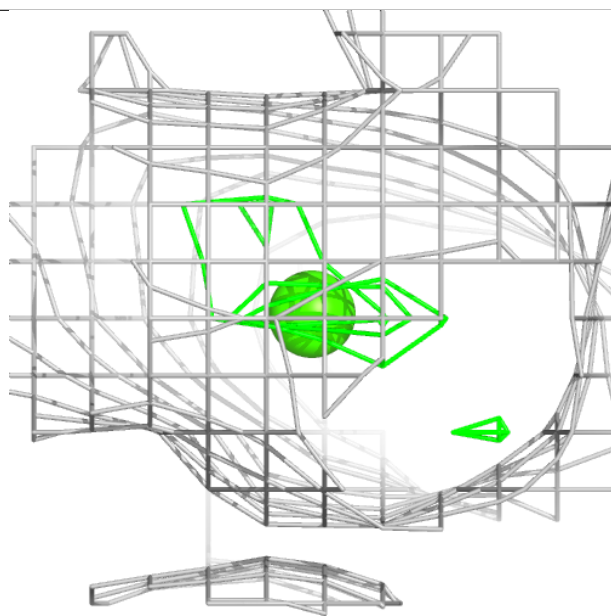
Electron density around NAG A 501:

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



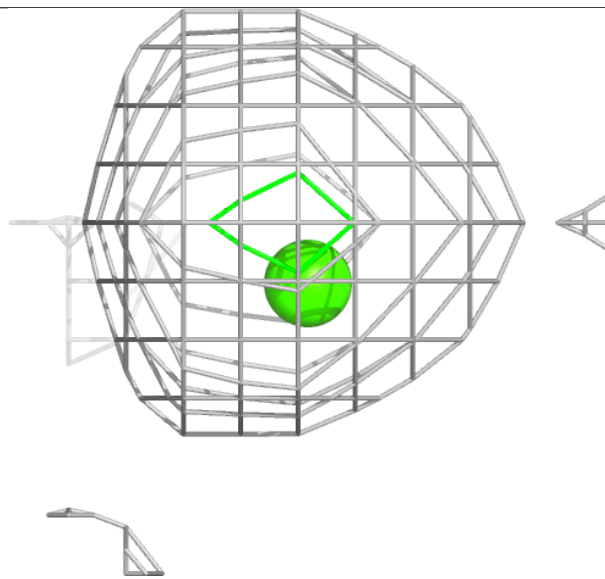
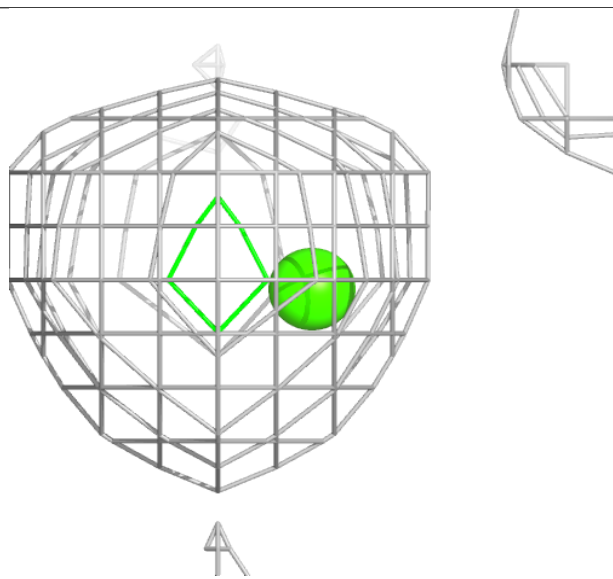
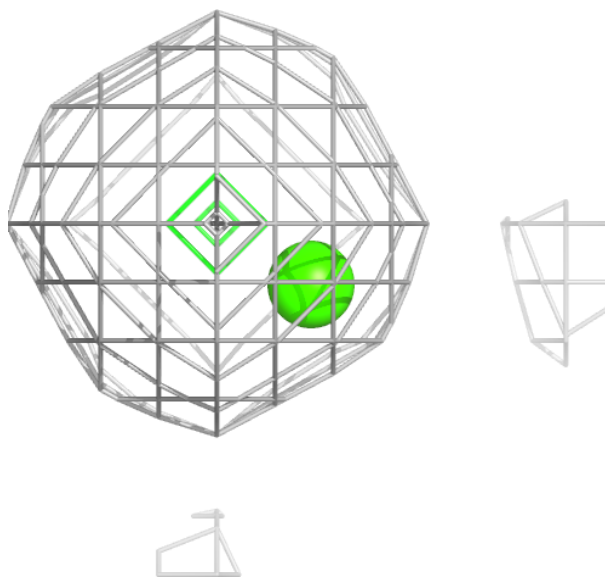
Electron density around CA A 503:

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



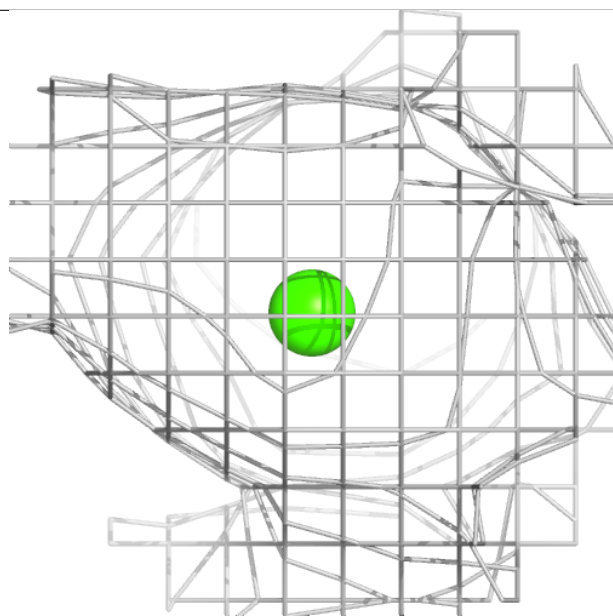
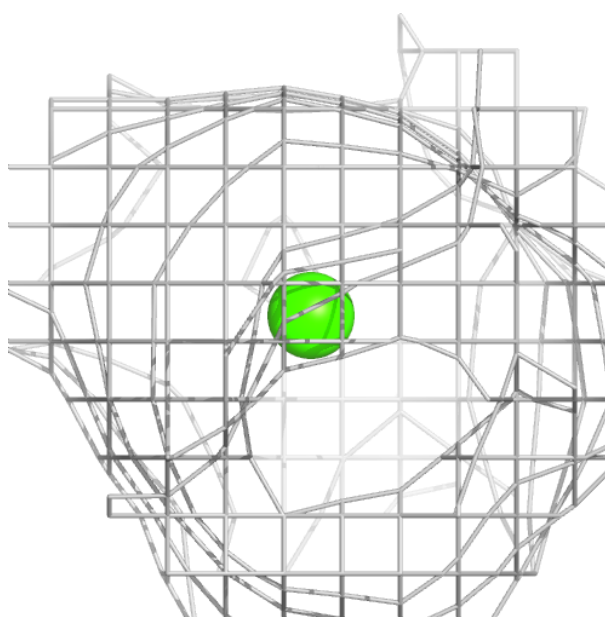
Electron density around CA A 504:

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



Electron density around CA A 502:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.