Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 10:00 PM BST

PDB ID	:	5U73
Title	:	Crystal structure of human Niemann-Pick C1 protein
Authors	:	Li, X.; Wang, J.; Blobel, G.
Deposited on	:	2016-12-11
Resolution	:	3.35 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 following versions of software and data (see references ⓘ) were used in the production of this report:

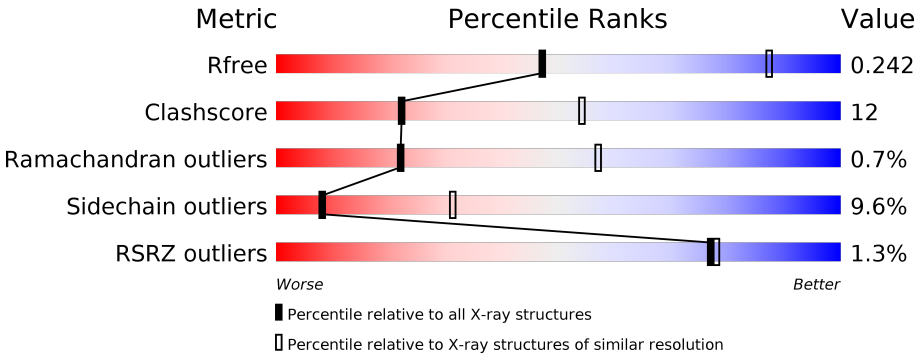
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.35 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}	130704	1060 (3.38-3.30)
Clashscore	141614	1111 (3.38-3.30)
Ramachandran outliers	138981	1090 (3.38-3.30)
Sidechain outliers	138945	1089 (3.38-3.30)
RSRZ outliers	127900	1028 (3.38-3.30)

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% 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	1278	% 47% 21% • 30%
2	B	2	50% 50%
3	C	3	100%
3	D	3	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MAN	D	3	-	-	-	X
4	NAG	A	1302	-	-	-	X
4	NAG	A	1314	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7262 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 Niemann-Pick C1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	898	Total	C	N	O	S	0	0	0
			7044	4581	1136	1281	46			

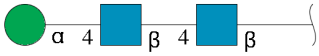
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	642	ILE	MET	conflict	UNP O15118

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

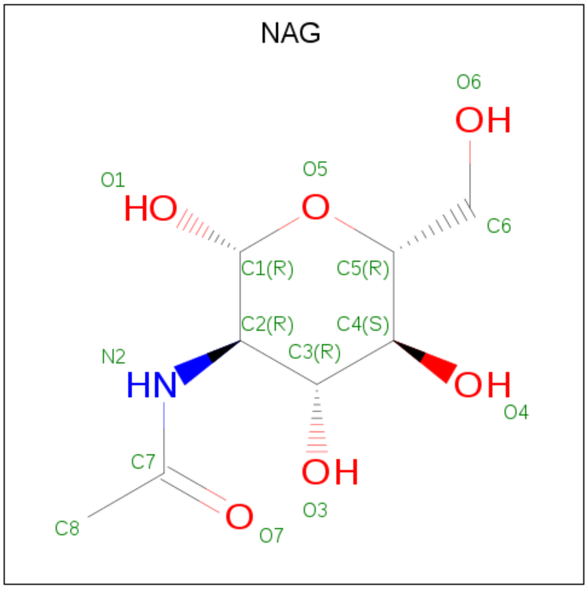
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called 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
3	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



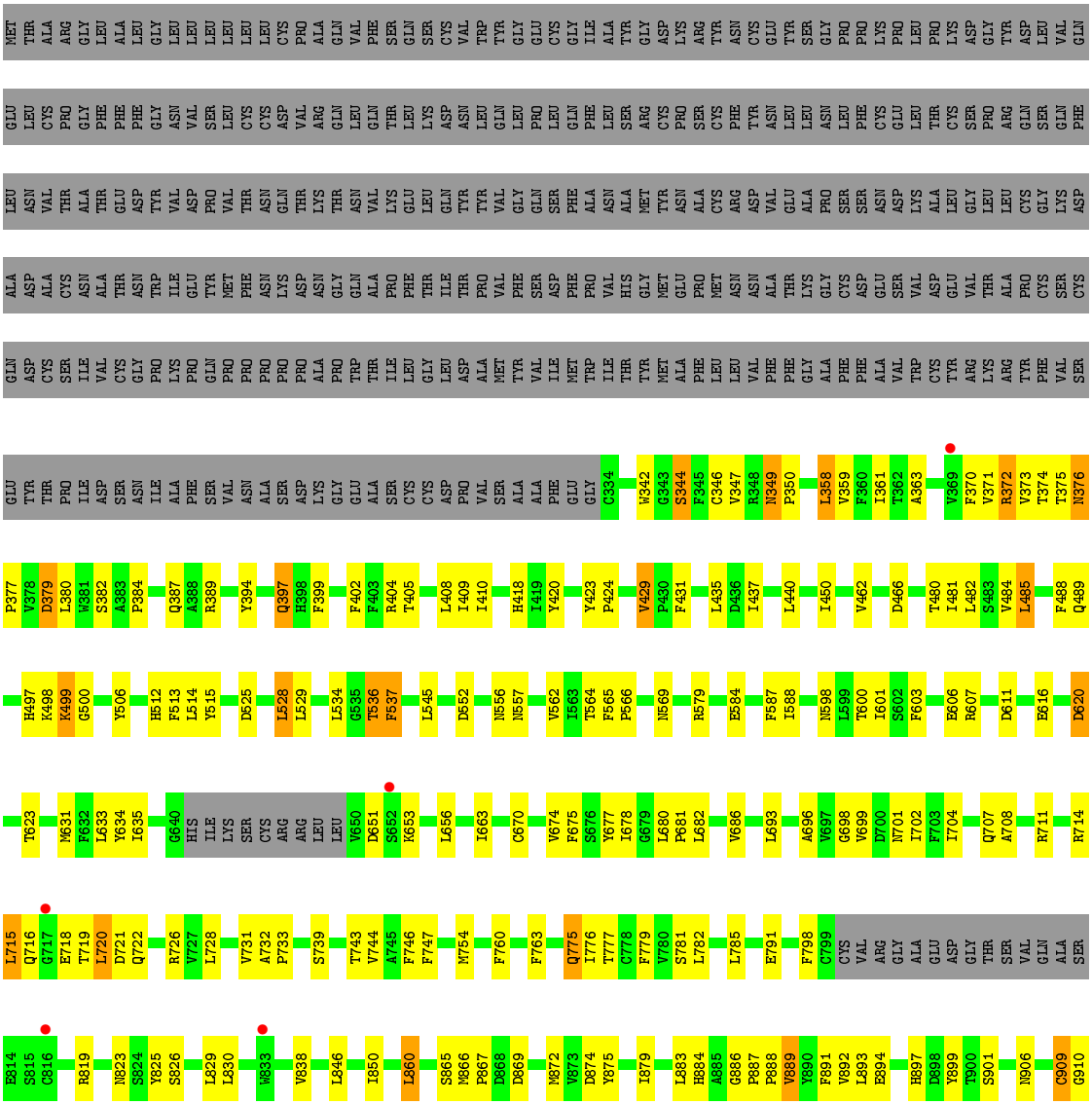
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0

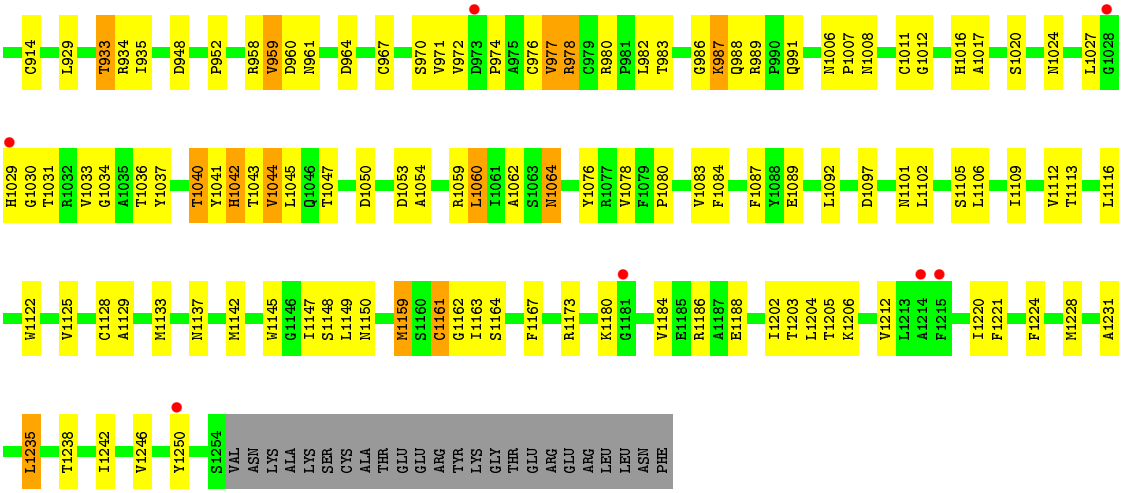
3 Residue-property plots (i)

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

- Molecule 1: Niemann-Pick C1 protein

Chain A:





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

Chain B:

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

Chain C:

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

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	181.94Å 223.07Å 63.21Å 90.00° 105.31° 90.00°	Depositor
Resolution (Å)	41.15 – 3.35 41.15 – 3.35	Depositor EDS
% Data completeness (in resolution range)	51.5 (41.15-3.35) 51.5 (41.15-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.45 (at 3.32Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.233 , 0.258 0.230 , 0.242	Depositor DCC
R_{free} test set	873 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	24.8	Xtriage
Anisotropy	0.617	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 31.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	7262	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: NAG, 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	0.26	0/7221	0.44	0/9827

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	536	THR	Peptide

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	7044	0	6960	168	0
2	B	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	39	0	34	0	0
3	D	39	0	34	3	0
4	A	112	0	103	1	0
All	All	7262	0	7156	169	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 12.

All (169) 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:1231:ALA:O	1:A:1235:LEU:HB2	1.74	0.86
1:A:404:ARG:NH1	1:A:584:GLU:OE2	2.11	0.82
1:A:906:ASN:OD1	1:A:989:ARG:NH1	2.16	0.78
1:A:914:CYS:SG	1:A:989:ARG:NH2	2.56	0.77
1:A:635:ILE:HD11	1:A:1204:LEU:HD13	1.66	0.76
1:A:1011:CYS:SG	1:A:1012:GLY:N	2.59	0.71
1:A:711:ARG:HB3	1:A:819:ARG:HH12	1.54	0.71
1:A:1097:ASP:O	1:A:1101:ASN:ND2	2.24	0.71
1:A:552:ASP:OD2	3:D:3:MAN:H61	1.92	0.70
1:A:702:ILE:HG13	1:A:775:GLN:HE21	1.57	0.69
1:A:556:ASN:ND2	1:A:557:ASN:OD1	2.25	0.69
1:A:552:ASP:CG	3:D:2:NAG:H62	2.13	0.69
1:A:404:ARG:HG2	1:A:569:ASN:HB2	1.75	0.68
1:A:718:GLU:OE2	1:A:726:ARG:NH1	2.26	0.68
1:A:346:CYS:HB3	1:A:781:SER:HB3	1.76	0.68
1:A:489:GLN:NE2	1:A:534:LEU:O	2.27	0.67
1:A:350:PRO:HG3	1:A:785:LEU:HD21	1.77	0.66
1:A:1062:ALA:HB2	1:A:1080:PRO:HD3	1.77	0.66
1:A:958:ARG:HG3	1:A:967:CYS:HB2	1.76	0.65
1:A:1164:SER:HA	1:A:1167:PHE:HD2	1.61	0.65
1:A:394:TYR:O	1:A:397:GLN:HG3	1.98	0.63
1:A:404:ARG:HD3	1:A:584:GLU:OE2	1.99	0.63
1:A:909:CYS:SG	1:A:910:GLY:N	2.71	0.62
1:A:901:SER:HA	1:A:991:GLN:HG3	1.81	0.62
1:A:344:SER:HB2	1:A:721:ASP:HB3	1.82	0.62
1:A:893:LEU:HD13	1:A:1078:VAL:HG22	1.82	0.61
1:A:1167:PHE:HE1	1:A:1202:ILE:HG12	1.65	0.61
1:A:537:PHE:HE1	1:A:1017:ALA:HB1	1.63	0.61
1:A:359:VAL:O	1:A:363:ALA:HB2	2.02	0.59
1:A:616:GLU:HB2	1:A:867:PRO:HD3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1016:HIS:HA	1:A:1020:SER:HB3	1.83	0.59
1:A:1047:THR:OG1	1:A:1050:ASP:OD1	2.21	0.59
1:A:711:ARG:CB	1:A:819:ARG:HH12	2.15	0.59
1:A:887:PRO:O	1:A:1042:HIS:HB2	2.03	0.59
1:A:429:VAL:HG11	1:A:514:LEU:HD21	1.86	0.57
1:A:537:PHE:CE1	1:A:1017:ALA:HB1	2.38	0.57
1:A:1180:LYS:HB2	1:A:1186:ARG:HG3	1.86	0.57
1:A:711:ARG:HB3	1:A:819:ARG:NH1	2.18	0.57
1:A:1125:VAL:O	1:A:1129:ALA:HB2	2.05	0.56
1:A:375:THR:HB	1:A:681:PRO:HB3	1.88	0.56
1:A:1133:MET:O	1:A:1137:ASN:ND2	2.35	0.56
1:A:481:ILE:HD12	1:A:565:PHE:CE2	2.42	0.55
1:A:702:ILE:HG13	1:A:775:GLN:NE2	2.20	0.55
1:A:958:ARG:HB2	1:A:976:CYS:HB3	1.89	0.55
1:A:866:MET:HG2	1:A:872:MET:HB3	1.88	0.54
1:A:1142:MET:HG2	1:A:1147:ILE:HD11	1.89	0.54
1:A:960:ASP:OD1	1:A:961:ASN:N	2.39	0.54
1:A:933:THR:O	1:A:933:THR:OG1	2.24	0.54
1:A:1212:VAL:HG13	1:A:1221:PHE:HE2	1.72	0.54
1:A:382:SER:OG	1:A:389:ARG:NH1	2.40	0.54
1:A:826:SER:O	1:A:830:LEU:HB2	2.06	0.54
1:A:746:PHE:CZ	1:A:1162:GLY:HA3	2.43	0.54
1:A:1161:CYS:SG	1:A:1162:GLY:N	2.81	0.54
1:A:513:PHE:HD1	1:A:514:LEU:HD12	1.73	0.54
1:A:952:PRO:HG2	1:A:987:LYS:HA	1.89	0.53
1:A:1125:VAL:O	1:A:1129:ALA:CB	2.56	0.53
1:A:698:GLY:O	1:A:775:GLN:NE2	2.42	0.53
1:A:1164:SER:HA	1:A:1167:PHE:CD2	2.42	0.52
1:A:372:ARG:O	1:A:372:ARG:HG2	2.09	0.52
1:A:499:LYS:HG3	1:A:528:LEU:HD23	1.92	0.52
1:A:715:LEU:H	1:A:718:GLU:HG3	1.74	0.52
1:A:1024:ASN:HB2	1:A:1034:GLY:O	2.10	0.51
1:A:1060:LEU:O	1:A:1064:ASN:HB2	2.11	0.51
1:A:358:LEU:HD12	1:A:361:ILE:HD12	1.93	0.51
1:A:376:ASN:H	1:A:377:PRO:HD3	1.75	0.51
1:A:897:HIS:HB3	1:A:899:TYR:CE2	2.45	0.50
1:A:418:HIS:O	1:A:431:PHE:HB2	2.12	0.50
1:A:1045:LEU:HD21	1:A:1054:ALA:HB2	1.94	0.50
1:A:402:PHE:CE1	1:A:888:PRO:HG2	2.47	0.49
1:A:952:PRO:HG3	1:A:980:ARG:HB2	1.93	0.49
1:A:1106:LEU:HD22	1:A:1128:CYS:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:LEU:HB2	1:A:564:THR:HB	1.95	0.49
1:A:488:PHE:HE1	1:A:512:HIS:HD1	1.61	0.49
1:A:384:PRO:HA	1:A:389:ARG:HG2	1.95	0.48
1:A:399:PHE:O	1:A:399:PHE:CG	2.66	0.48
1:A:588:ILE:HG23	1:A:603:PHE:HE2	1.78	0.48
1:A:1224:PHE:O	1:A:1228:MET:HB2	2.13	0.48
1:A:714:ARG:NH2	1:A:791:GLU:OE2	2.41	0.48
1:A:933:THR:O	1:A:935:ILE:N	2.46	0.48
1:A:744:VAL:HG11	1:A:1112:VAL:HG21	1.94	0.48
1:A:866:MET:HG3	1:A:867:PRO:HD2	1.96	0.48
1:A:376:ASN:N	1:A:377:PRO:CD	2.77	0.48
1:A:1220:ILE:H	1:A:1220:ILE:HD12	1.79	0.48
1:A:1238:THR:O	1:A:1242:ILE:HB	2.14	0.48
1:A:865:SER:HA	1:A:1220:ILE:HD11	1.94	0.47
1:A:375:THR:HG23	1:A:380:LEU:HD11	1.96	0.47
1:A:1040:THR:OG1	1:A:1041:TYR:N	2.47	0.47
1:A:825:TYR:HE2	1:A:829:LEU:HD22	1.79	0.47
1:A:875:TYR:O	1:A:879:ILE:HG23	2.14	0.47
1:A:409:ILE:HG12	1:A:562:VAL:HG22	1.96	0.47
1:A:686:VAL:HG22	1:A:760:PHE:HA	1.97	0.47
1:A:674:VAL:O	1:A:678:ILE:HG13	2.14	0.47
1:A:420:TYR:HB3	1:A:429:VAL:HG23	1.96	0.47
1:A:634:TYR:HH	1:A:1203:THR:HG1	1.62	0.47
1:A:846:LEU:HD22	1:A:1133:MET:HG2	1.95	0.47
3:D:1:NAG:O3	3:D:2:NAG:O6	2.33	0.47
1:A:423:TYR:HA	1:A:424:PRO:HA	1.72	0.47
1:A:1029:HIS:N	1:A:1030:GLY:HA2	2.28	0.46
1:A:739:SER:O	1:A:743:THR:HG23	2.16	0.46
1:A:670:CYS:O	1:A:674:VAL:HG12	2.14	0.46
1:A:971:VAL:HG22	1:A:972:VAL:H	1.79	0.46
1:A:361:ILE:HA	1:A:670:CYS:SG	2.56	0.46
1:A:983:THR:O	1:A:986:GLY:N	2.48	0.46
1:A:342:TRP:HE1	1:A:777:THR:HA	1.81	0.46
1:A:846:LEU:O	1:A:850:ILE:HG13	2.16	0.45
1:A:894:GLU:HB2	1:A:1076:TYR:HB2	1.97	0.45
1:A:371:VAL:HG13	1:A:373:VAL:HG13	1.99	0.45
1:A:450:ILE:HD13	1:A:587:PHE:HE1	1.82	0.45
1:A:663:ILE:HD11	1:A:782:LEU:HD12	1.98	0.45
1:A:513:PHE:CD1	1:A:514:LEU:HD12	2.52	0.44
1:A:678:ILE:H	1:A:678:ILE:HG13	1.62	0.44
1:A:1044:VAL:HG23	1:A:1045:LEU:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:GLN:HB3	1:A:1089:GLU:OE2	2.18	0.44
1:A:653:LYS:N	1:A:653:LYS:HD2	2.32	0.44
1:A:431:PHE:HA	1:A:556:ASN:O	2.18	0.44
1:A:500:GLY:HA2	1:A:506:TYR:CE2	2.53	0.44
1:A:1084:PHE:HA	1:A:1087:PHE:HD2	1.82	0.44
1:A:680:LEU:HD12	1:A:681:PRO:HD2	1.99	0.44
1:A:1109:ILE:O	1:A:1113:THR:OG1	2.15	0.44
1:A:370:PHE:CD2	1:A:371:VAL:HG23	2.52	0.44
1:A:631:MET:O	1:A:635:ILE:HG12	2.18	0.44
1:A:699:VAL:HG11	1:A:1204:LEU:HD21	1.99	0.44
1:A:732:ALA:N	1:A:733:PRO:HD2	2.32	0.44
1:A:977:VAL:HG12	1:A:978:ARG:H	1.82	0.44
1:A:1204:LEU:HG	1:A:1205:THR:N	2.32	0.44
1:A:779:PHE:HA	1:A:782:LEU:HB2	2.00	0.43
1:A:515:TYR:CE2	1:A:525:ASP:HA	2.54	0.43
1:A:462:VAL:HG21	1:A:579:ARG:HG3	2.00	0.43
1:A:899:TYR:HH	1:A:1036:THR:HG1	1.66	0.43
1:A:733:PRO:HB2	1:A:1173:ARG:CZ	2.49	0.43
1:A:620:ASP:HA	1:A:623:THR:HG23	2.01	0.43
1:A:986:GLY:O	1:A:988:GLN:N	2.45	0.43
1:A:410:ILE:HG13	1:A:601:ILE:HG22	2.00	0.43
1:A:359:VAL:O	1:A:363:ALA:CB	2.66	0.43
1:A:377:PRO:HB2	1:A:379:ASP:OD2	2.19	0.43
1:A:497:HIS:HB3	1:A:528:LEU:HD21	2.00	0.43
1:A:370:PHE:CE2	1:A:371:VAL:HG23	2.53	0.43
1:A:959:VAL:HG22	1:A:964:ASP:HA	2.01	0.42
1:A:484:VAL:HG13	1:A:485:LEU:HD13	2.01	0.42
1:A:480:THR:O	1:A:566:PRO:HD2	2.19	0.42
1:A:838:VAL:HG21	1:A:1246:VAL:HG21	2.00	0.42
1:A:892:VAL:O	1:A:1078:VAL:HA	2.19	0.42
1:A:860:LEU:HA	1:A:860:LEU:HD13	1.88	0.42
1:A:1006:ASN:HB3	1:A:1007:PRO:HD2	2.01	0.42
1:A:347:VAL:HG11	1:A:720:LEU:HB3	2.02	0.41
1:A:720:LEU:HD22	1:A:720:LEU:HA	1.90	0.41
1:A:704:ILE:O	1:A:708:ALA:HB2	2.20	0.41
1:A:437:ILE:HA	1:A:440:LEU:HD12	2.03	0.41
1:A:974:PRO:O	4:A:1314:NAG:H82	2.20	0.41
1:A:349:ASN:ND2	1:A:349:ASN:O	2.50	0.41
1:A:1059:ARG:O	1:A:1062:ALA:HB3	2.20	0.41
1:A:719:THR:HG23	1:A:722:GLN:H	1.86	0.41
1:A:781:SER:O	1:A:785:LEU:HD23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:VAL:HG21	1:A:883:LEU:HD13	2.03	0.41
1:A:1102:LEU:O	1:A:1105:SER:HB2	2.21	0.41
1:A:686:VAL:HG11	1:A:763:PHE:CD1	2.55	0.41
1:A:701:ASN:HB2	1:A:775:GLN:NE2	2.35	0.41
1:A:707:GLN:HB3	1:A:711:ARG:HH21	1.86	0.41
1:A:760:PHE:CZ	1:A:1159:MET:HB2	2.56	0.40
1:A:891:PHE:O	1:A:1037:TYR:HA	2.21	0.40
1:A:889:VAL:HG23	1:A:1040:THR:HG23	2.04	0.40
1:A:693:LEU:HB2	1:A:1159:MET:HE2	2.03	0.40
1:A:1184:VAL:O	1:A:1188:GLU:HG3	2.21	0.40
1:A:350:PRO:HB3	1:A:781:SER:HB2	2.03	0.40
1:A:886:GLY:N	1:A:1043:THR:O	2.54	0.40
1:A:978:ARG:HG2	1:A:978:ARG:H	1.70	0.40
1:A:696:ALA:O	1:A:699:VAL:HG12	2.22	0.40
1:A:1148:SER:HB2	1:A:1150:ASN:ND2	2.36	0.40
1:A:431:PHE:HD2	1:A:435:LEU:HB3	1.85	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	892/1278 (70%)	788 (88%)	98 (11%)	6 (1%)	22 57

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	934	ARG
1	A	529	LEU
1	A	536	THR
1	A	537	PHE
1	A	987	LYS

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Mol	Chain	Res	Type
1	A	376	ASN

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	782/1109 (70%)	707 (90%)	75 (10%)	8 31

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

Mol	Chain	Res	Type
1	A	344	SER
1	A	349	ASN
1	A	358	LEU
1	A	372	ARG
1	A	374	THR
1	A	379	ASP
1	A	397	GLN
1	A	405	THR
1	A	408	LEU
1	A	429	VAL
1	A	466	ASP
1	A	485	LEU
1	A	498	LYS
1	A	499	LYS
1	A	528	LEU
1	A	545	LEU
1	A	598	ASN
1	A	600	THR
1	A	606	GLU
1	A	607	ARG
1	A	611	ASP
1	A	620	ASP
1	A	633	LEU
1	A	651	ASP
1	A	656	LEU

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Mol	Chain	Res	Type
1	A	675	PHE
1	A	677	TYR
1	A	682	LEU
1	A	715	LEU
1	A	716	GLN
1	A	720	LEU
1	A	728	LEU
1	A	731	VAL
1	A	747	PHE
1	A	754	MET
1	A	775	GLN
1	A	776	ILE
1	A	798	PHE
1	A	823	ASN
1	A	860	LEU
1	A	869	ASP
1	A	874	ASP
1	A	884	HIS
1	A	889	VAL
1	A	909	CYS
1	A	929	LEU
1	A	933	THR
1	A	948	ASP
1	A	959	VAL
1	A	970	SER
1	A	977	VAL
1	A	978	ARG
1	A	982	LEU
1	A	1008	ASN
1	A	1027	LEU
1	A	1031	THR
1	A	1033	VAL
1	A	1040	THR
1	A	1042	HIS
1	A	1044	VAL
1	A	1053	ASP
1	A	1060	LEU
1	A	1064	ASN
1	A	1083	VAL
1	A	1092	LEU
1	A	1116	LEU
1	A	1122	TRP

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Mol	Chain	Res	Type
1	A	1145	TRP
1	A	1149	LEU
1	A	1159	MET
1	A	1161	CYS
1	A	1163	ILE
1	A	1206	LYS
1	A	1235	LEU
1	A	1250	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	447	GLN
1	A	490	ASN
1	A	578	GLN
1	A	775	GLN

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

8 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	0.90	2 (14%)	17,19,21	0.85	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	B	2	2	14,14,15	0.32	0	17,19,21	0.58	0
3	NAG	C	1	1,3	14,14,15	0.85	2 (14%)	17,19,21	0.72	1 (5%)
3	NAG	C	2	3	14,14,15	1.21	2 (14%)	17,19,21	1.27	1 (5%)
3	MAN	C	3	3	11,11,12	1.72	3 (27%)	15,15,17	1.76	5 (33%)
3	NAG	D	1	1,3	14,14,15	0.94	2 (14%)	17,19,21	0.81	0
3	NAG	D	2	3	14,14,15	1.11	2 (14%)	17,19,21	1.47	2 (11%)
3	MAN	D	3	3	11,11,12	1.66	2 (18%)	15,15,17	1.98	5 (33%)

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	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
3	NAG	C	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	MAN	C	3	3	-	1/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	1/6/23/26	0/1/1/1
3	MAN	D	3	3	-	0/2/19/22	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	MAN	C1-C2	4.21	1.61	1.52
3	D	3	MAN	O5-C5	3.55	1.50	1.43
3	D	3	MAN	C4-C5	3.34	1.60	1.53
3	C	2	NAG	C1-C2	3.34	1.57	1.52
3	D	2	NAG	O5-C1	3.22	1.48	1.43
3	C	2	NAG	O5-C1	2.90	1.48	1.43
2	B	1	NAG	C1-C2	2.62	1.56	1.52
3	D	1	NAG	O5-C1	2.54	1.47	1.43
3	C	3	MAN	O5-C5	2.54	1.48	1.43
3	D	2	NAG	C1-C2	2.46	1.56	1.52
3	D	1	NAG	C1-C2	2.30	1.55	1.52
3	C	1	NAG	C1-C2	2.30	1.55	1.52
3	C	3	MAN	C4-C5	2.21	1.57	1.53
3	C	1	NAG	O5-C1	2.04	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	O5-C1	2.02	1.46	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	2	NAG	O4-C4-C5	-4.98	96.93	109.30
3	C	2	NAG	O4-C4-C5	-4.87	97.21	109.30
3	D	3	MAN	C1-C2-C3	-4.71	103.88	109.67
3	C	3	MAN	O2-C2-C1	3.80	116.93	109.15
3	D	3	MAN	C1-O5-C5	3.15	116.46	112.19
2	B	1	NAG	C1-O5-C5	3.12	116.41	112.19
3	C	3	MAN	C1-C2-C3	-3.06	105.90	109.67
3	D	2	NAG	C1-O5-C5	2.82	116.01	112.19
3	C	3	MAN	O2-C2-C3	-2.77	104.59	110.14
3	D	3	MAN	C3-C4-C5	2.58	114.83	110.24
3	C	3	MAN	C1-O5-C5	2.57	115.68	112.19
3	D	3	MAN	O5-C1-C2	-2.38	107.10	110.77
3	C	3	MAN	O5-C1-C2	-2.26	107.29	110.77
3	C	1	NAG	C1-O5-C5	2.15	115.10	112.19
3	D	3	MAN	O5-C5-C4	2.13	116.01	110.83

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	3	MAN	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6

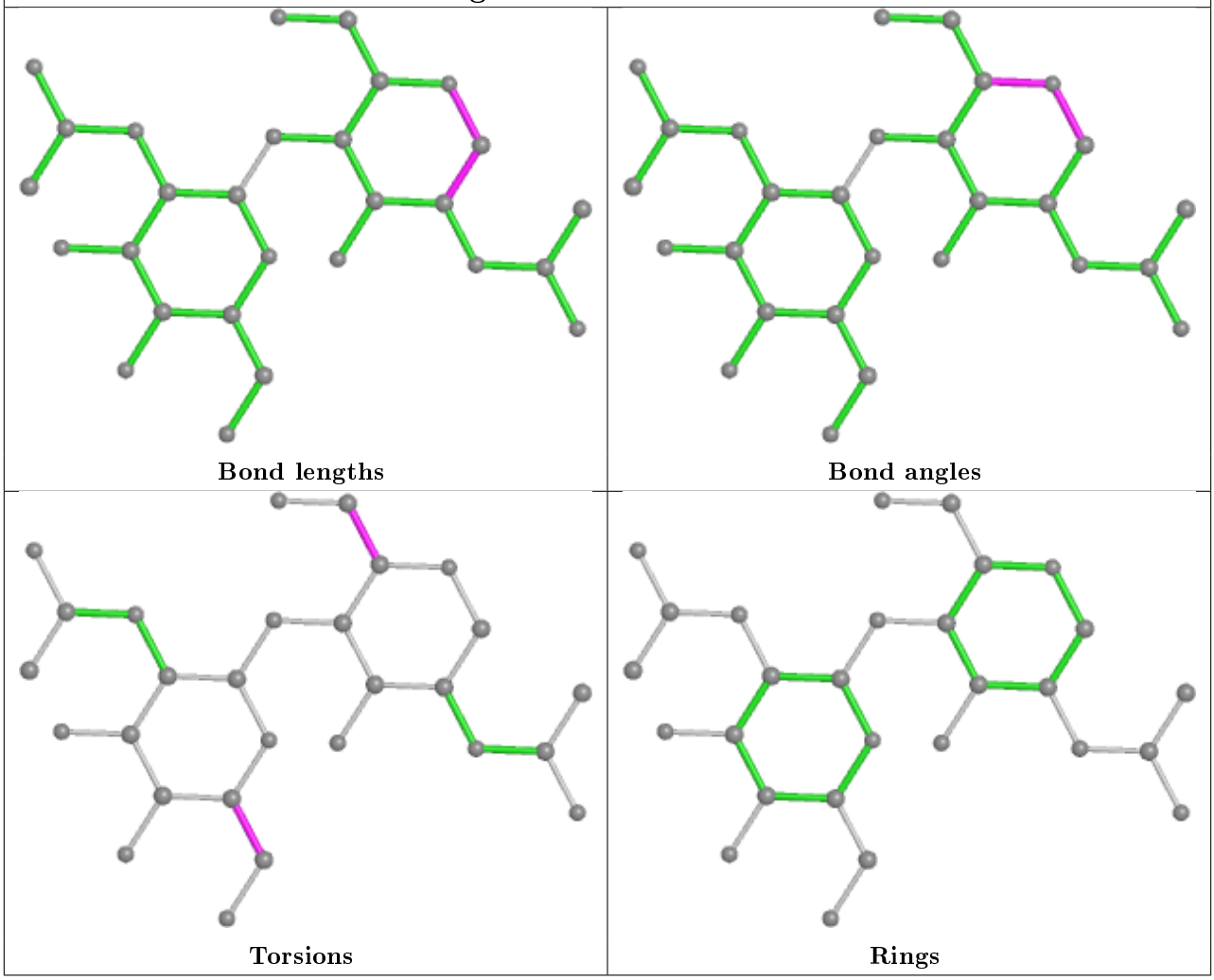
There are no ring outliers.

3 monomers are involved in 3 short contacts:

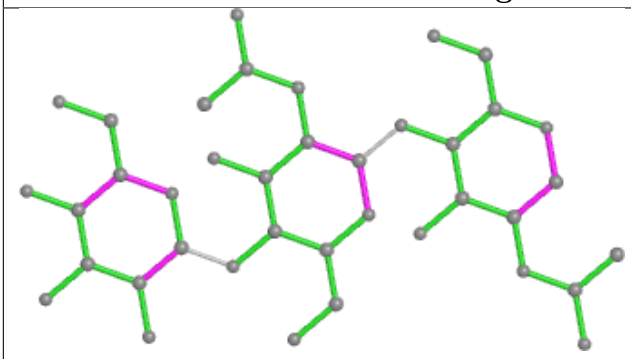
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3	MAN	1	0
3	D	1	NAG	1	0
3	D	2	NAG	2	0

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

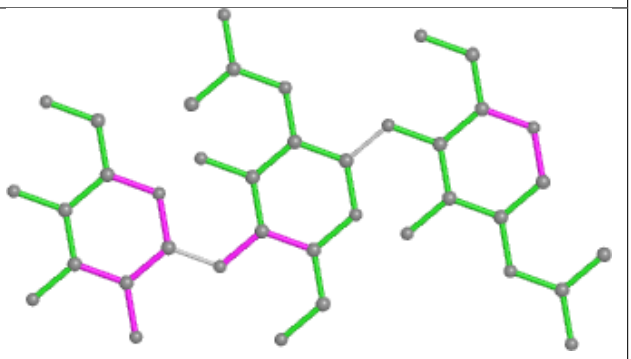
Oligosaccharide Chain B



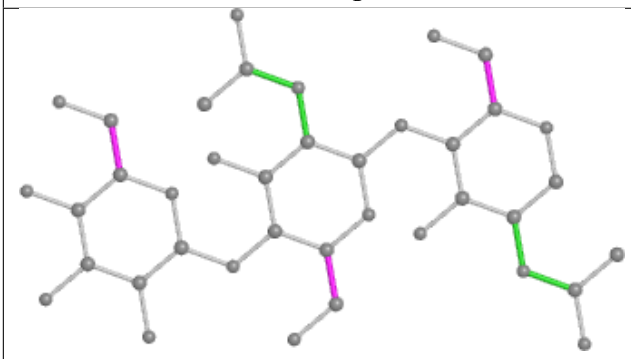
Oligosaccharide Chain C



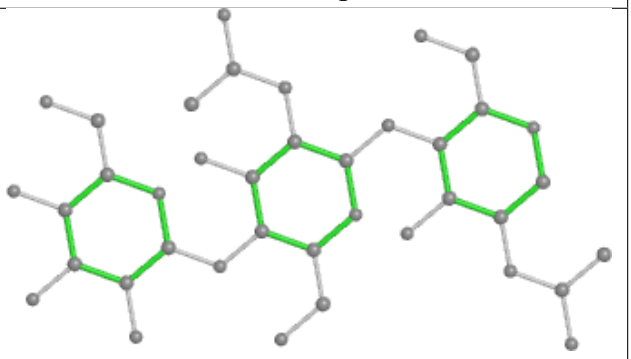
Bond lengths



Bond angles

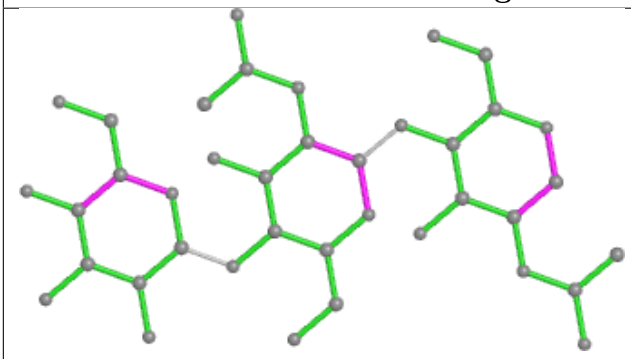


Torsions

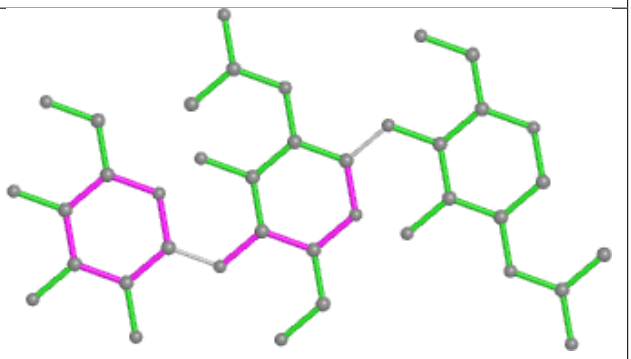


Rings

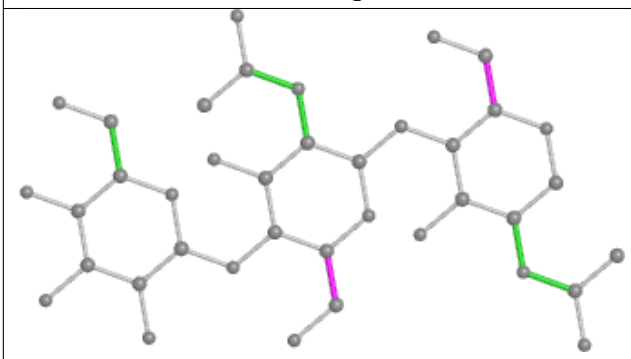
Oligosaccharide Chain D



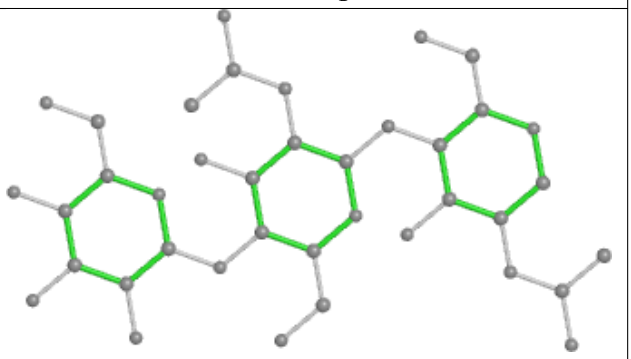
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	1301	1	14,14,15	0.24	0	17,19,21	0.39	0
4	NAG	A	1315	1	14,14,15	0.75	1 (7%)	17,19,21	1.13	1 (5%)
4	NAG	A	1309	1	14,14,15	0.23	0	17,19,21	0.33	0
4	NAG	A	1314	1	14,14,15	0.37	0	17,19,21	0.39	0
4	NAG	A	1310	1	14,14,15	0.49	0	17,19,21	0.76	1 (5%)
4	NAG	A	1316	1	14,14,15	1.03	1 (7%)	17,19,21	0.86	1 (5%)
4	NAG	A	1302	1	14,14,15	0.25	0	17,19,21	0.46	0
4	NAG	A	1305	1	14,14,15	0.24	0	17,19,21	0.54	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
4	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1315	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1314	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1316	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1316	NAG	O5-C1	-3.47	1.38	1.43
4	A	1315	NAG	C1-C2	2.60	1.56	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1315	NAG	C1-O5-C5	4.10	117.75	112.19
4	A	1310	NAG	C1-O5-C5	2.65	115.78	112.19
4	A	1316	NAG	C3-C4-C5	2.26	114.27	110.24

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1315	NAG	O5-C5-C6-O6
4	A	1305	NAG	O5-C5-C6-O6
4	A	1309	NAG	O5-C5-C6-O6
4	A	1302	NAG	O5-C5-C6-O6
4	A	1305	NAG	C4-C5-C6-O6
4	A	1309	NAG	C4-C5-C6-O6
4	A	1314	NAG	O5-C5-C6-O6
4	A	1316	NAG	C4-C5-C6-O6
4	A	1315	NAG	C4-C5-C6-O6
4	A	1302	NAG	C4-C5-C6-O6
4	A	1316	NAG	O5-C5-C6-O6
4	A	1315	NAG	C1-C2-N2-C7
4	A	1314	NAG	C4-C5-C6-O6
4	A	1314	NAG	C1-C2-N2-C7
4	A	1315	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1314	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	898/1278 (70%)	-0.43	12 (1%) 77 78	8, 47, 93, 144	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1029	HIS	3.6
1	A	816	CYS	3.4
1	A	1215	PHE	3.0
1	A	1214	ALA	2.9
1	A	717	GLY	2.7
1	A	973	ASP	2.6
1	A	1250	TYR	2.4
1	A	833	TRP	2.2
1	A	1028	GLY	2.1
1	A	652	SER	2.1
1	A	1181	GLY	2.1
1	A	369	VAL	2.0

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

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

6.3 Carbohydrates

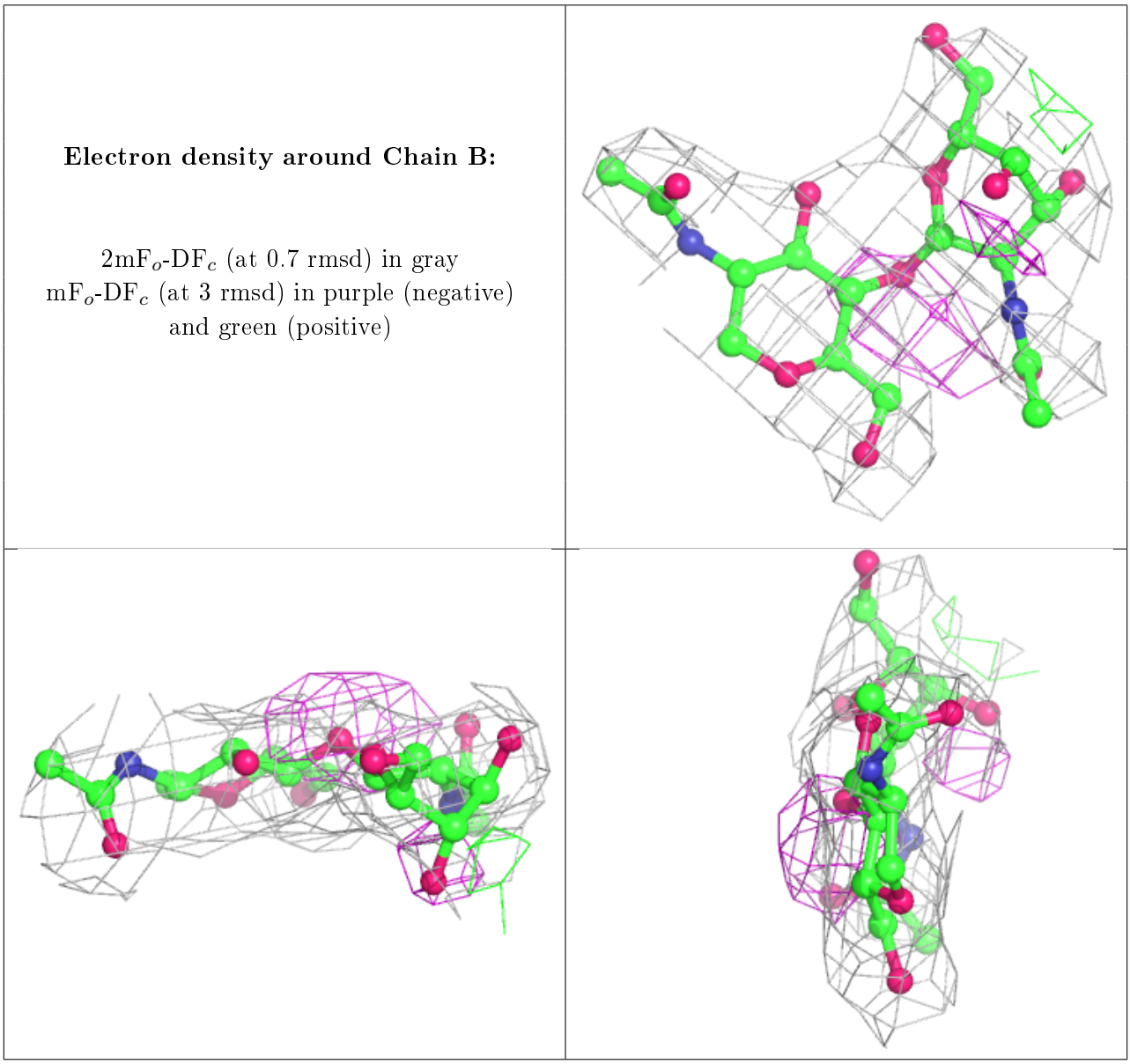
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	MAN	D	3	11/12	0.25	0.59	108,118,127,127	0
3	NAG	D	2	14/15	0.83	0.63	107,113,118,121	0
3	MAN	C	3	11/12	0.86	0.33	48,63,73,77	0
2	NAG	B	1	14/15	0.87	0.25	28,50,62,72	0
2	NAG	B	2	14/15	0.88	0.42	77,86,91,100	0
3	NAG	D	1	14/15	0.92	0.43	37,78,88,99	0
3	NAG	C	1	14/15	0.92	0.20	34,48,57,60	0
3	NAG	C	2	14/15	0.94	0.32	35,58,65,68	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.

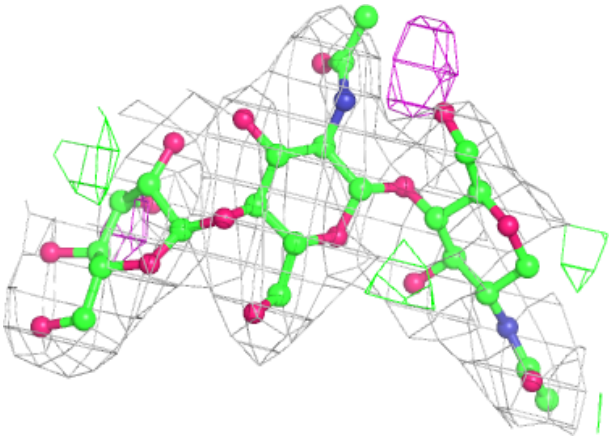
Electron density around Chain B:

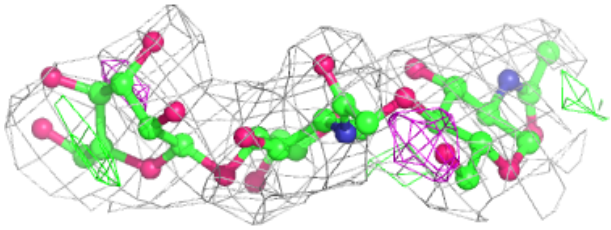
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

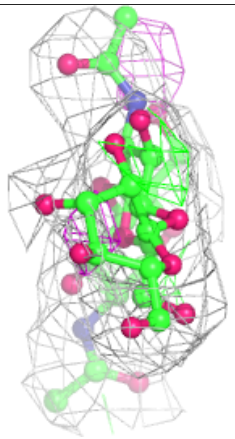


Electron density around Chain C:

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

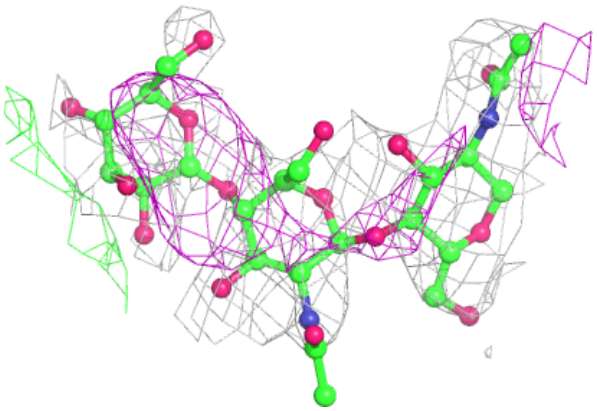


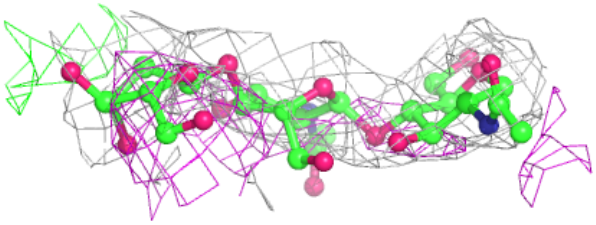


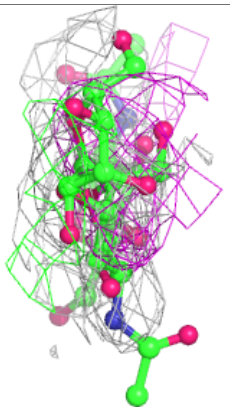


Electron density around Chain D:

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







6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
4	NAG	A	1302	14/15	0.45	0.58	114,124,126,128	0
4	NAG	A	1314	14/15	0.74	0.49	70,76,93,96	0
4	NAG	A	1316	14/15	0.80	0.34	63,82,93,94	0
4	NAG	A	1315	14/15	0.81	0.29	48,74,105,108	0
4	NAG	A	1301	14/15	0.87	0.27	72,83,89,90	0
4	NAG	A	1305	14/15	0.88	0.33	62,70,87,91	0
4	NAG	A	1310	14/15	0.90	0.37	65,91,94,94	0
4	NAG	A	1309	14/15	0.94	0.20	40,53,72,74	0

6.5 Other polymers

There are no such residues in this entry.