



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:49 PM UTC

PDB ID : 5U73 / pdb_00005u73
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 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
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

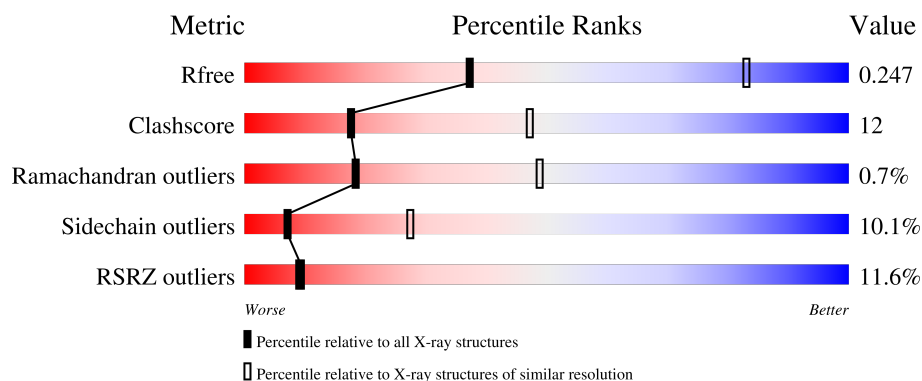
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1434 (3.38-3.30)
Clashscore	190562	1479 (3.38-3.30)
Ramachandran outliers	187476	1456 (3.38-3.30)
Sidechain outliers	187428	1455 (3.38-3.30)
RSRZ outliers	180081	1434 (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 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	1278	8% 46% 21% • 30%
2	B	2	50% 50%
3	C	3	100%
3	D	3	100%

2 Entry composition [i](#)

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:

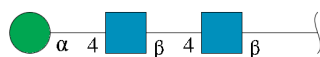
Chain	Residue	Modelled	Actual	Comment	Reference
A	642	ILE	MET	conflict	UNP O15118

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



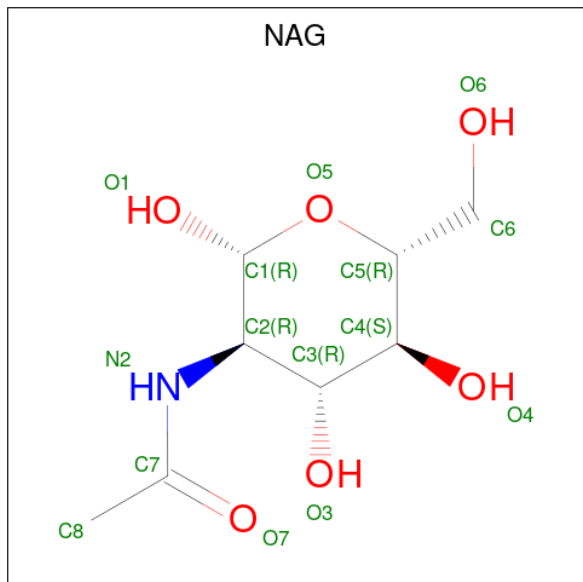
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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.

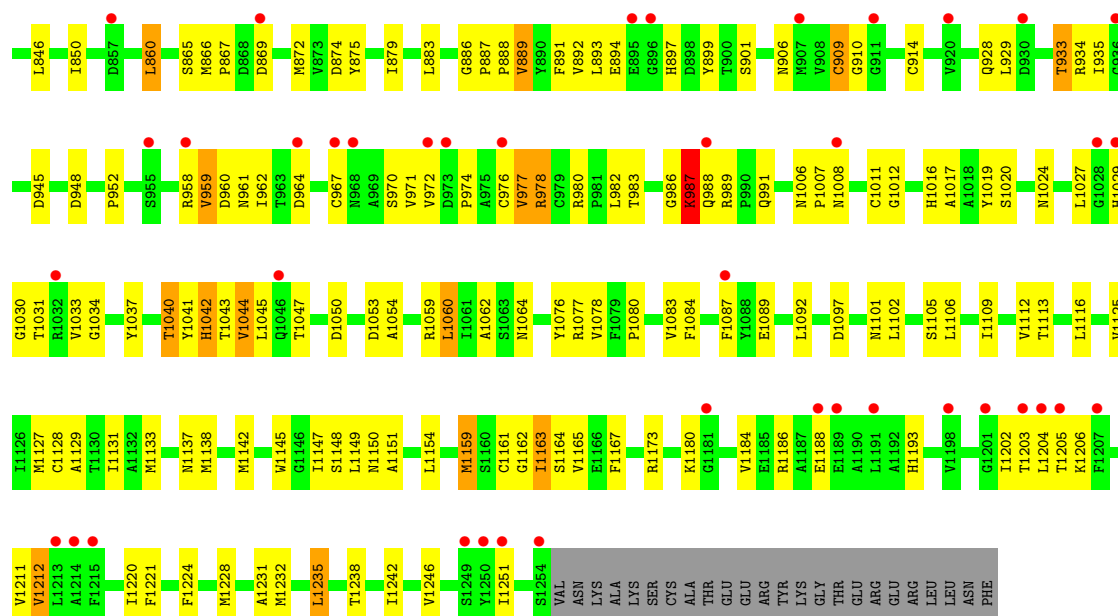


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



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

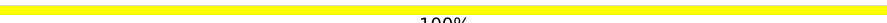


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:  50%

MAG1
MAG2

- 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:  100%

MAG1
MAG2
MAN3

- 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:  100%

MAG1
MAG2
MAN3

4 Data and refinement statistics

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) 51.4 (41.15-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.45 (at 3.32Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.233 , 0.258 0.231 , 0.247	Depositor DCC
R_{free} test set	874 reflections (2.50%)	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 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

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: 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	0.14	0/7221	0.38	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 [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	7044	0	6960	177	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	178	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 (178) 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:552:ASP:CG	3:D:2:NAG:H62	2.13	0.73
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: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:1109:ILE:O	1:A:1113:THR:OG1	2.15	0.63
1:A:394:TYR:O	1:A:397:GLN:HG3	1.98	0.63
1:A:692:PHE:CD2	1:A:1159:MET:HE1	2.34	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:609:ILE:HG13	1:A:872:MET:HE2	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:711:ARG:CB	1:A:819:ARG:HH12	2.15	0.59
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:754:MET:HE1	1:A:1151:ALA:HA	1.85	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:692:PHE:HD2	1:A:1159:MET:HE1	1.68	0.57
1:A:537:PHE:CE1	1:A:1017:ALA:HB1	2.38	0.57
1:A:711:ARG:HB3	1:A:819:ARG:NH1	2.18	0.57
1:A:1180:LYS:HB2	1:A:1186:ARG:HG3	1.86	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:960:ASP:OD1	1:A:961:ASN:N	2.39	0.54
1:A:1142:MET:HG2	1:A:1147:ILE:HD11	1.89	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:1212:VAL:HG13	1:A:1221:PHE:HE2	1.72	0.54
1:A:746:PHE:CZ	1:A:1162:GLY:HA3	2.43	0.54
1:A:933:THR:O	1:A:933:THR:OG1	2.24	0.54
1:A:513:PHE:HD1	1:A:514:LEU:HD12	1.73	0.54
1:A:1161:CYS:SG	1:A:1162:GLY:N	2.81	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:HG2	1:A:372:ARG:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:482:LEU:HB2	1:A:564:THR:HB	1.95	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:HD12	1:A:1220:ILE:H	1.79	0.48
1:A:1238:THR:O	1:A:1242:ILE:HB	2.14	0.48
1:A:375:THR:HG23	1:A:380:LEU:HD11	1.96	0.47
1:A:865:SER:HA	1:A:1220:ILE:HD11	1.94	0.47
1:A:1138:MET:HE1	1:A:1232:MET:HA	1.96	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:1040:THR:OG1	1:A:1041:TYR:N	2.47	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:739:SER:O	1:A:743:THR:HG23	2.16	0.46
1:A:1029:HIS:N	1:A:1030:GLY:HA2	2.28	0.46
1:A:1159:MET:HE2	1:A:1163:ILE:HD12	1.96	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:693:LEU:HB2	1:A:1159:MET:HE3	1.98	0.45
1:A:846:LEU:O	1:A:850:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG13	1:A:678:ILE:H	1.62	0.44
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:1044:VAL:HG23	1:A:1045:LEU:H	1.83	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:680:LEU:HD12	1:A:681:PRO:HD2	1.99	0.44
1:A:1084:PHE:HA	1:A:1087:PHE:HD2	1.82	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:1138:MET:HE2	1:A:1138:MET:HB2	1.87	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:462:VAL:HG21	1:A:579:ARG:HG3	2.00	0.43
1:A:515:TYR:CE2	1:A:525:ASP:HA	2.54	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:945:ASP:OD2	1:A:1019:TYR:OH	2.33	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:HD13	1:A:860:LEU:HA	1.88	0.42
1:A:1006:ASN:HB3	1:A:1007:PRO:HD2	2.01	0.42
1:A:1159:MET:SD	1:A:1232:MET:HE1	2.60	0.42
1:A:347:VAL:HG11	1:A:720:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:349:ASN:O	1:A:349:ASN:ND2	2.50	0.41
1:A:974:PRO:O	4:A:1306:NAG:H82	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
1:A:1059:ARG:O	1:A:1062:ALA:HB3	2.20	0.41
1:A:562:VAL:HG21	1:A:883:LEU:HD13	2.03	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:1102:LEU:O	1:A:1105:SER:HB2	2.21	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: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:889:VAL:HG23	1:A:1040:THR:HG23	2.04	0.40
1:A:978:ARG:H	1:A:978:ARG:HG2	1.70	0.40
1:A:1127:MET:HE2	1:A:1127:MET:HB3	1.93	0.40
1:A:1184:VAL:O	1:A:1188:GLU:HG3	2.21	0.40
1:A:696:ALA:O	1:A:699:VAL:HG12	2.22	0.40
1:A:431:PHE:HD2	1:A:435:LEU:HB3	1.85	0.40
1:A:754:MET:HE2	1:A:1154:LEU:HD23	2.03	0.40
1:A:1148:SER:HB2	1:A:1150:ASN:ND2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	892/1278 (70%)	788 (88%)	98 (11%)	6 (1%)	18	49

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
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%)	703 (90%)	79 (10%)	7 27

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	349	ASN
1	A	358	LEU
1	A	374	THR
1	A	379	ASP
1	A	397	GLN
1	A	405	THR
1	A	429	VAL
1	A	460	GLU
1	A	485	LEU
1	A	498	LYS
1	A	499	LYS
1	A	505	VAL
1	A	528	LEU
1	A	545	LEU
1	A	557	ASN
1	A	598	ASN
1	A	600	THR
1	A	606	GLU
1	A	607	ARG

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Mol	Chain	Res	Type
1	A	611	ASP
1	A	623	THR
1	A	633	LEU
1	A	656	LEU
1	A	674	VAL
1	A	677	TYR
1	A	682	LEU
1	A	685	ILE
1	A	715	LEU
1	A	716	GLN
1	A	720	LEU
1	A	728	LEU
1	A	731	VAL
1	A	754	MET
1	A	775	GLN
1	A	776	ILE
1	A	798	PHE
1	A	823	ASN
1	A	830	LEU
1	A	860	LEU
1	A	869	ASP
1	A	874	ASP
1	A	889	VAL
1	A	909	CYS
1	A	928	GLN
1	A	929	LEU
1	A	933	THR
1	A	948	ASP
1	A	959	VAL
1	A	962	ILE
1	A	970	SER
1	A	977	VAL
1	A	978	ARG
1	A	982	LEU
1	A	987	LYS
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

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Mol	Chain	Res	Type
1	A	1053	ASP
1	A	1060	LEU
1	A	1077	ARG
1	A	1083	VAL
1	A	1092	LEU
1	A	1116	LEU
1	A	1131	ILE
1	A	1145	TRP
1	A	1149	LEU
1	A	1159	MET
1	A	1163	ILE
1	A	1165	VAL
1	A	1193	HIS
1	A	1206	LYS
1	A	1211	VAL
1	A	1212	VAL
1	A	1235	LEU
1	A	1251	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	447	GLN
1	A	490	ASN
1	A	578	GLN
1	A	593	ASN
1	A	716	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	2,1	14,14,15	0.94	1 (7%)	17,19,21	0.87	1 (5%)
2	NAG	B	2	2	14,14,15	0.34	0	17,19,21	0.60	0
3	NAG	C	1	3,1	14,14,15	0.88	1 (7%)	17,19,21	0.74	1 (5%)
3	NAG	C	2	3	14,14,15	1.25	2 (14%)	17,19,21	1.28	1 (5%)
3	MAN	C	3	3	11,11,12	1.69	3 (27%)	15,15,17	1.58	4 (26%)
3	NAG	D	1	3,1	14,14,15	0.96	2 (14%)	17,19,21	0.81	0
3	NAG	D	2	3	14,14,15	1.12	2 (14%)	17,19,21	1.48	2 (11%)
3	MAN	D	3	3	11,11,12	1.67	2 (18%)	15,15,17	1.78	4 (26%)

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	2,1	-	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	3,1	-	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	3,1	-	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 (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	MAN	C1-C2	4.02	1.61	1.52
3	D	3	MAN	O5-C5	3.70	1.50	1.43
3	C	2	NAG	C1-C2	3.65	1.57	1.52
3	D	3	MAN	C4-C5	3.30	1.60	1.53
3	D	2	NAG	O5-C1	3.07	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	C1-C2	2.87	1.56	1.52
3	C	2	NAG	O5-C1	2.77	1.48	1.43
3	D	2	NAG	C1-C2	2.70	1.56	1.52
3	C	3	MAN	O5-C5	2.65	1.48	1.43
3	D	1	NAG	C1-C2	2.52	1.55	1.52
3	C	1	NAG	C1-C2	2.51	1.55	1.52
3	D	1	NAG	O5-C1	2.43	1.47	1.43
3	C	3	MAN	C4-C5	2.19	1.57	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	NAG	O4-C4-C5	-5.03	96.93	109.32
3	C	2	NAG	O4-C4-C5	-4.92	97.21	109.32
3	D	3	MAN	C1-C2-C3	-3.96	103.88	109.64
3	C	3	MAN	O2-C2-C1	3.36	116.93	109.22
3	D	3	MAN	C1-O5-C5	3.19	116.46	112.19
2	B	1	NAG	C1-O5-C5	3.15	116.41	112.19
3	D	2	NAG	C1-O5-C5	2.86	116.01	112.19
3	C	3	MAN	O2-C2-C3	-2.68	104.59	110.15
3	C	3	MAN	C1-O5-C5	2.60	115.68	112.19
3	C	3	MAN	C1-C2-C3	-2.57	105.90	109.64
3	D	3	MAN	C3-C4-C5	2.54	114.83	110.23
3	C	1	NAG	C1-O5-C5	2.17	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:

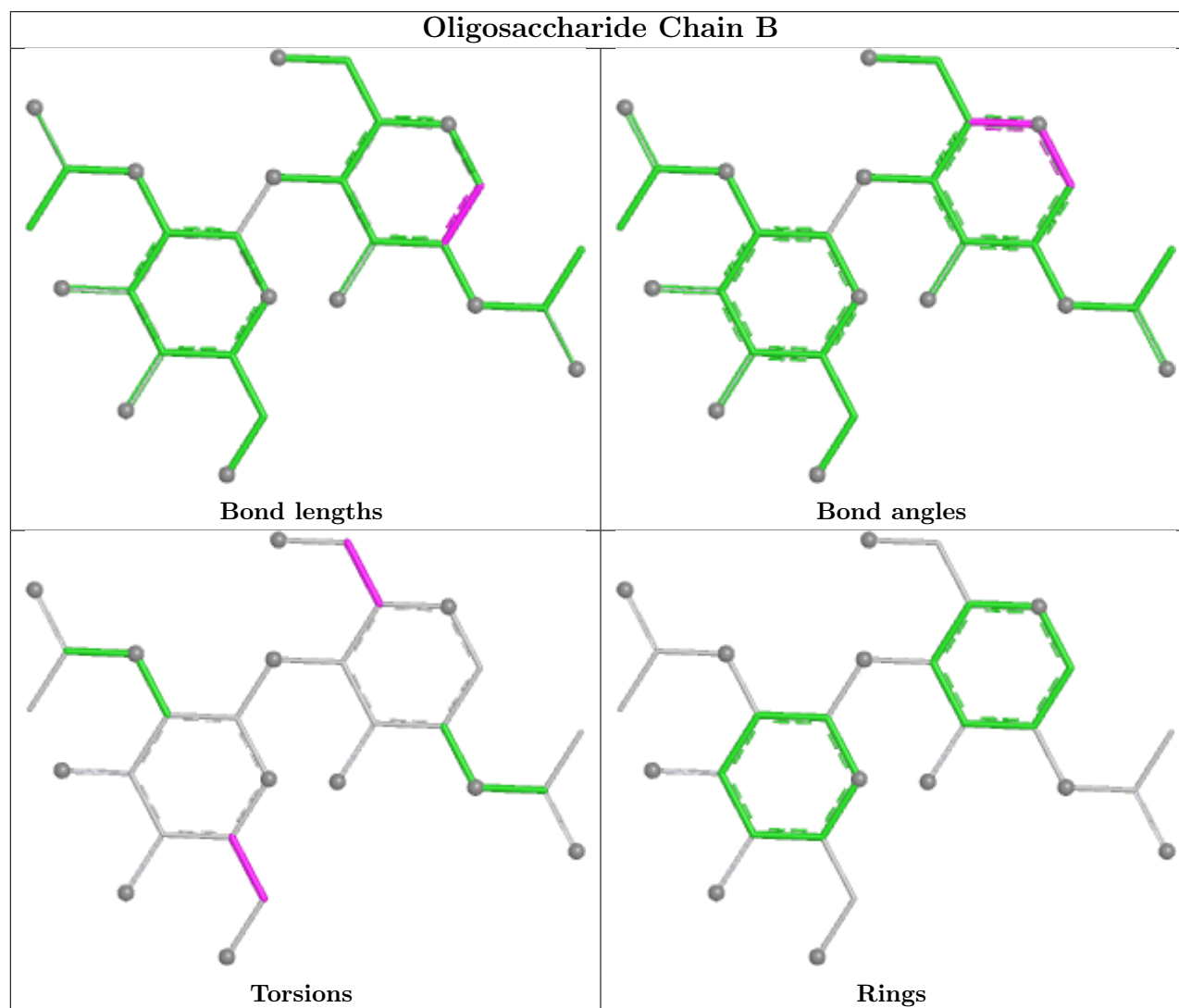
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	3	MAN	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6

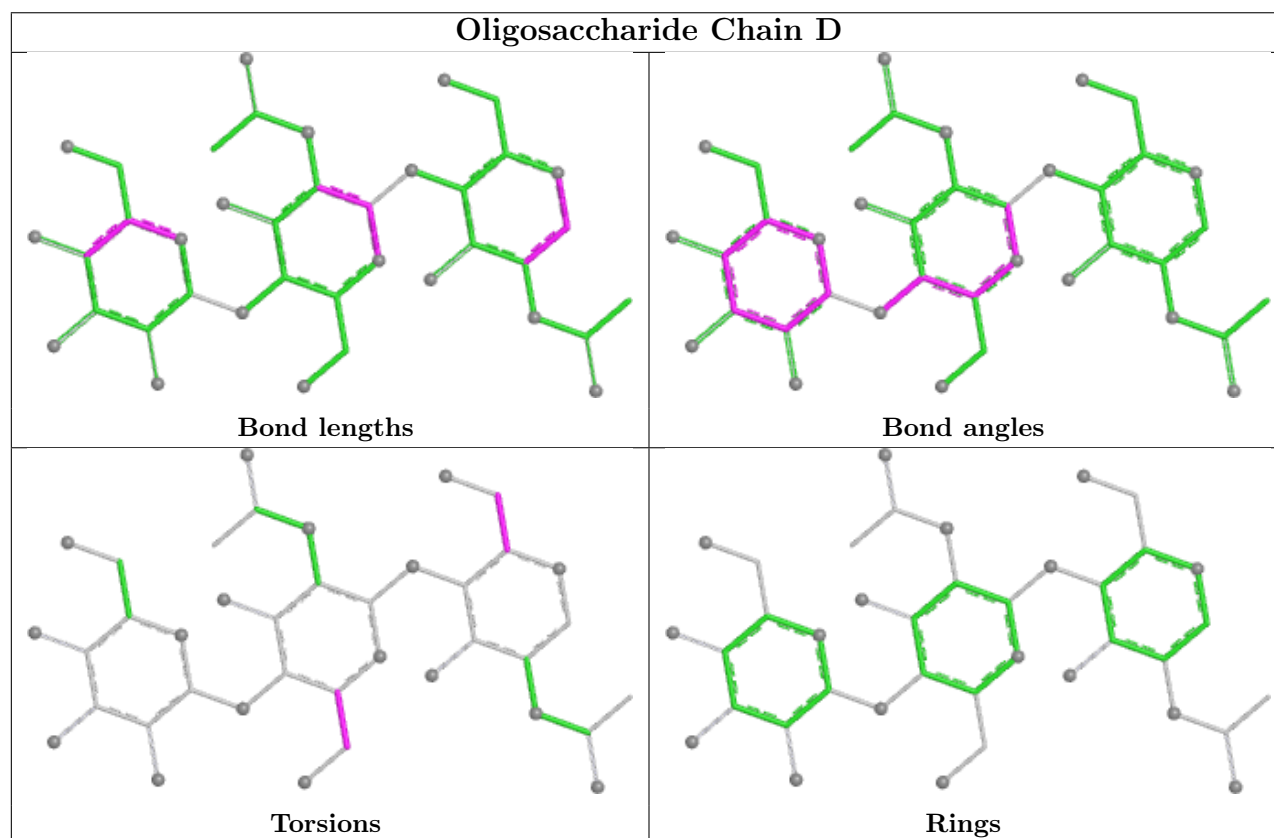
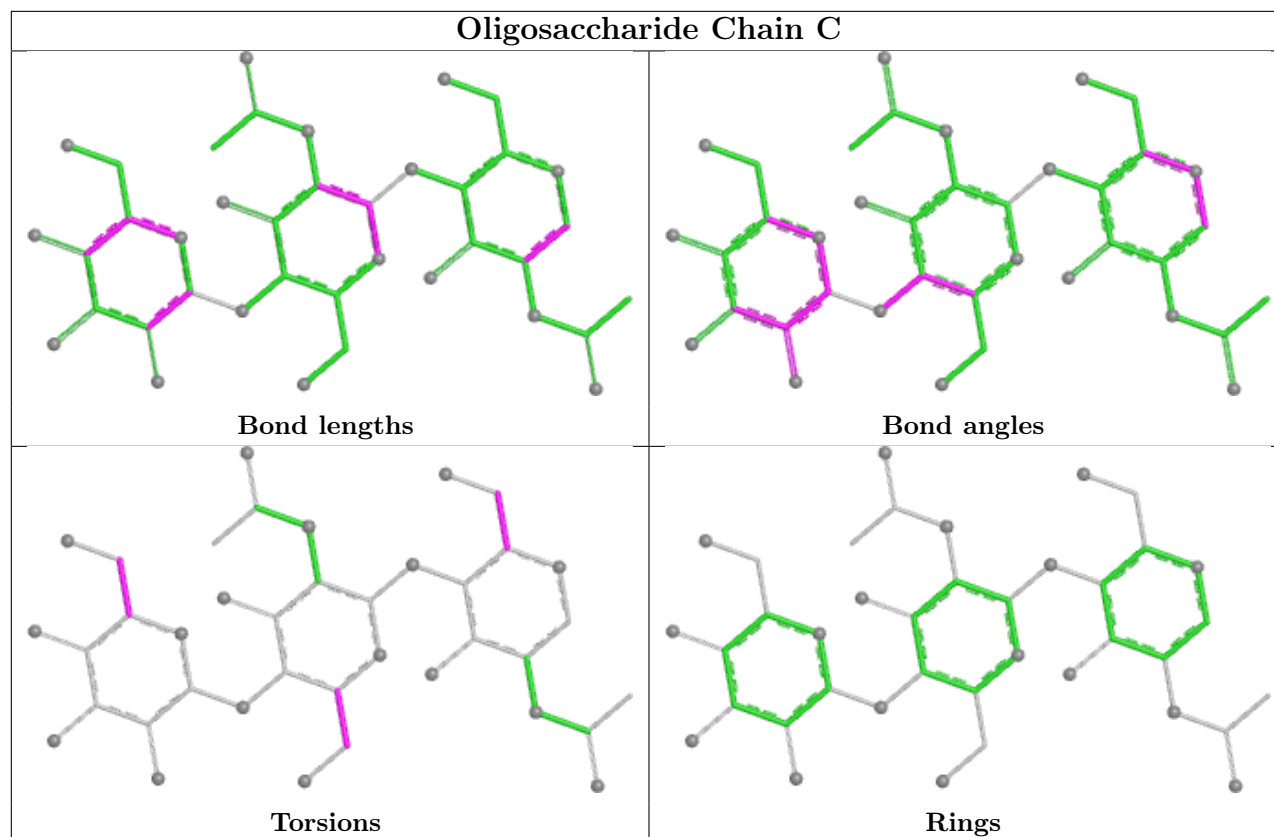
There are no ring outliers.

3 monomers are involved in 3 short contacts:

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

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





5.6 Ligand geometry

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	1302	1	14,14,15	0.27	0	17,19,21	0.48	0
4	NAG	A	1305	1	14,14,15	0.52	0	17,19,21	0.77	1 (5%)
4	NAG	A	1304	1	14,14,15	0.22	0	17,19,21	0.35	0
4	NAG	A	1301	1	14,14,15	0.25	0	17,19,21	0.41	0
4	NAG	A	1303	1	14,14,15	0.25	0	17,19,21	0.56	0
4	NAG	A	1306	1	14,14,15	0.40	0	17,19,21	0.41	0
4	NAG	A	1307	1	14,14,15	0.81	1 (7%)	17,19,21	1.15	1 (5%)
4	NAG	A	1308	1	14,14,15	0.99	1 (7%)	17,19,21	0.88	1 (5%)

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	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1308	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	1308	NAG	O5-C1	-3.29	1.38	1.43
4	A	1307	NAG	C1-C2	2.85	1.56	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1307	NAG	C1-O5-C5	4.15	117.75	112.19
4	A	1305	NAG	C1-O5-C5	2.68	115.78	112.19
4	A	1308	NAG	C3-C4-C5	2.22	114.27	110.23

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1307	NAG	O5-C5-C6-O6
4	A	1303	NAG	O5-C5-C6-O6
4	A	1304	NAG	O5-C5-C6-O6
4	A	1302	NAG	O5-C5-C6-O6
4	A	1303	NAG	C4-C5-C6-O6
4	A	1304	NAG	C4-C5-C6-O6
4	A	1307	NAG	C4-C5-C6-O6
4	A	1308	NAG	C4-C5-C6-O6
4	A	1306	NAG	O5-C5-C6-O6
4	A	1302	NAG	C4-C5-C6-O6
4	A	1308	NAG	O5-C5-C6-O6
4	A	1306	NAG	C4-C5-C6-O6
4	A	1301	NAG	C1-C2-N2-C7
4	A	1307	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	1306	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, 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	898/1278 (70%)	0.87	104 (11%) 9 9	8, 47, 93, 144	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1250	TYR	6.0
1	A	529	LEU	6.0
1	A	818	PHE	5.4
1	A	571	TYR	5.3
1	A	1215	PHE	5.0
1	A	552	ASP	4.5
1	A	833	TRP	4.4
1	A	930	ASP	4.2
1	A	972	VAL	4.1
1	A	538	GLY	4.1
1	A	816	CYS	3.9
1	A	1207	PHE	3.7
1	A	652	SER	3.7
1	A	973	ASP	3.6
1	A	791	GLU	3.6
1	A	539	GLY	3.5
1	A	640	GLY	3.5
1	A	1046	GLN	3.4
1	A	1205	THR	3.4
1	A	1214	ALA	3.4
1	A	610	GLU	3.3
1	A	911	GLY	3.3
1	A	465	GLN	3.3
1	A	869	ASP	3.3
1	A	451	GLU	3.3
1	A	797	ILE	3.3
1	A	715	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	620	ASP	3.1
1	A	817	LEU	3.1
1	A	976	CYS	3.1
1	A	606	GLU	3.1
1	A	799	CYS	3.0
1	A	1029	HIS	3.0
1	A	334	CYS	3.0
1	A	627	SER	2.9
1	A	378	VAL	2.9
1	A	1198	VAL	2.9
1	A	656	LEU	2.8
1	A	393	GLU	2.8
1	A	829	LEU	2.8
1	A	650	VAL	2.8
1	A	896	GLY	2.8
1	A	476	ASN	2.8
1	A	369	VAL	2.8
1	A	1189	GLU	2.7
1	A	1201	GLY	2.7
1	A	1254	SER	2.7
1	A	1032	ARG	2.7
1	A	335	LEU	2.7
1	A	385	SER	2.6
1	A	651	ASP	2.6
1	A	657	GLY	2.6
1	A	968	ASN	2.6
1	A	1028	GLY	2.6
1	A	1188	GLU	2.6
1	A	1203	THR	2.6
1	A	988	GLN	2.6
1	A	825	TYR	2.5
1	A	907	MET	2.5
1	A	857	ASP	2.5
1	A	619	SER	2.5
1	A	636	SER	2.5
1	A	730	GLU	2.4
1	A	494	VAL	2.4
1	A	958	ARG	2.4
1	A	487	TYR	2.4
1	A	474	PRO	2.4
1	A	784	GLY	2.4
1	A	711	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1181	GLY	2.4
1	A	967	CYS	2.4
1	A	572	ASN	2.3
1	A	1204	LEU	2.3
1	A	544	TRP	2.3
1	A	814	GLU	2.3
1	A	700	ASP	2.3
1	A	653	LYS	2.3
1	A	570	TYR	2.2
1	A	445	ASP	2.2
1	A	380	LEU	2.2
1	A	469	LEU	2.2
1	A	830	LEU	2.2
1	A	895	GLU	2.2
1	A	936	GLY	2.2
1	A	786	ASP	2.2
1	A	964	ASP	2.2
1	A	955	SER	2.2
1	A	1087	PHE	2.2
1	A	421	GLN	2.1
1	A	483	SER	2.1
1	A	1249	SER	2.1
1	A	569	ASN	2.1
1	A	1008	ASN	2.1
1	A	502	ASP	2.1
1	A	1213	LEU	2.1
1	A	400	GLY	2.1
1	A	527	SER	2.1
1	A	828	LEU	2.0
1	A	1191	LEU	2.0
1	A	708	ALA	2.0
1	A	713	GLU	2.0
1	A	1251	ILE	2.0
1	A	593	ASN	2.0
1	A	920	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

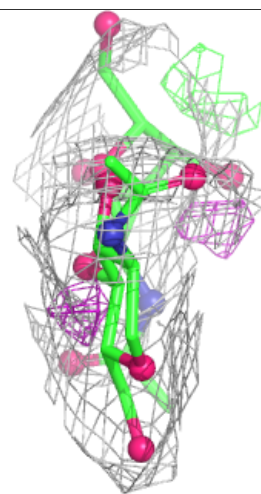
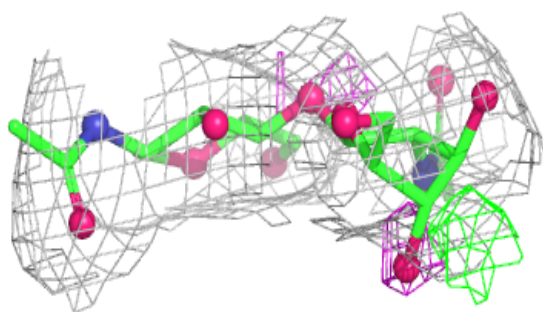
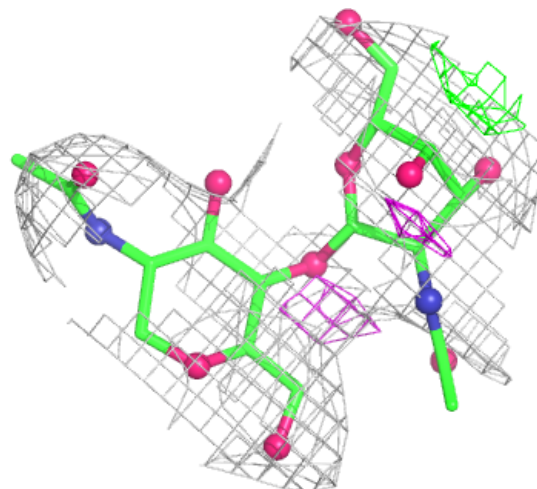
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MAN	D	3	11/12	0.46	0.29	108,118,127,127	0
3	MAN	C	3	11/12	0.56	0.17	48,63,73,77	0
2	NAG	B	2	14/15	0.74	0.19	77,86,91,100	0
3	NAG	D	2	14/15	0.77	0.18	107,113,118,121	0
3	NAG	C	2	14/15	0.84	0.13	35,58,65,68	0
3	NAG	C	1	14/15	0.84	0.13	34,48,57,60	0
2	NAG	B	1	14/15	0.88	0.12	28,50,62,72	0
3	NAG	D	1	14/15	0.91	0.10	37,78,88,99	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.

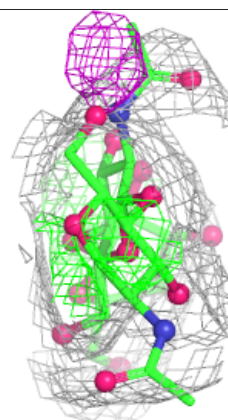
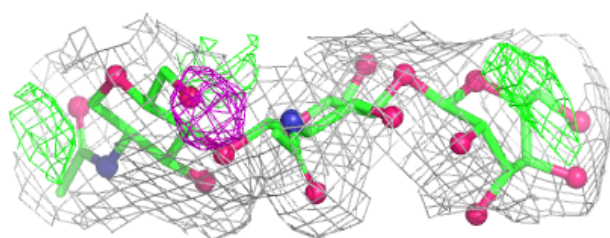
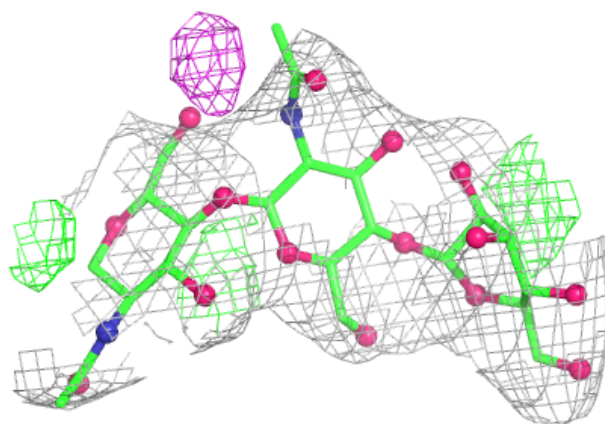
Electron density around Chain B:

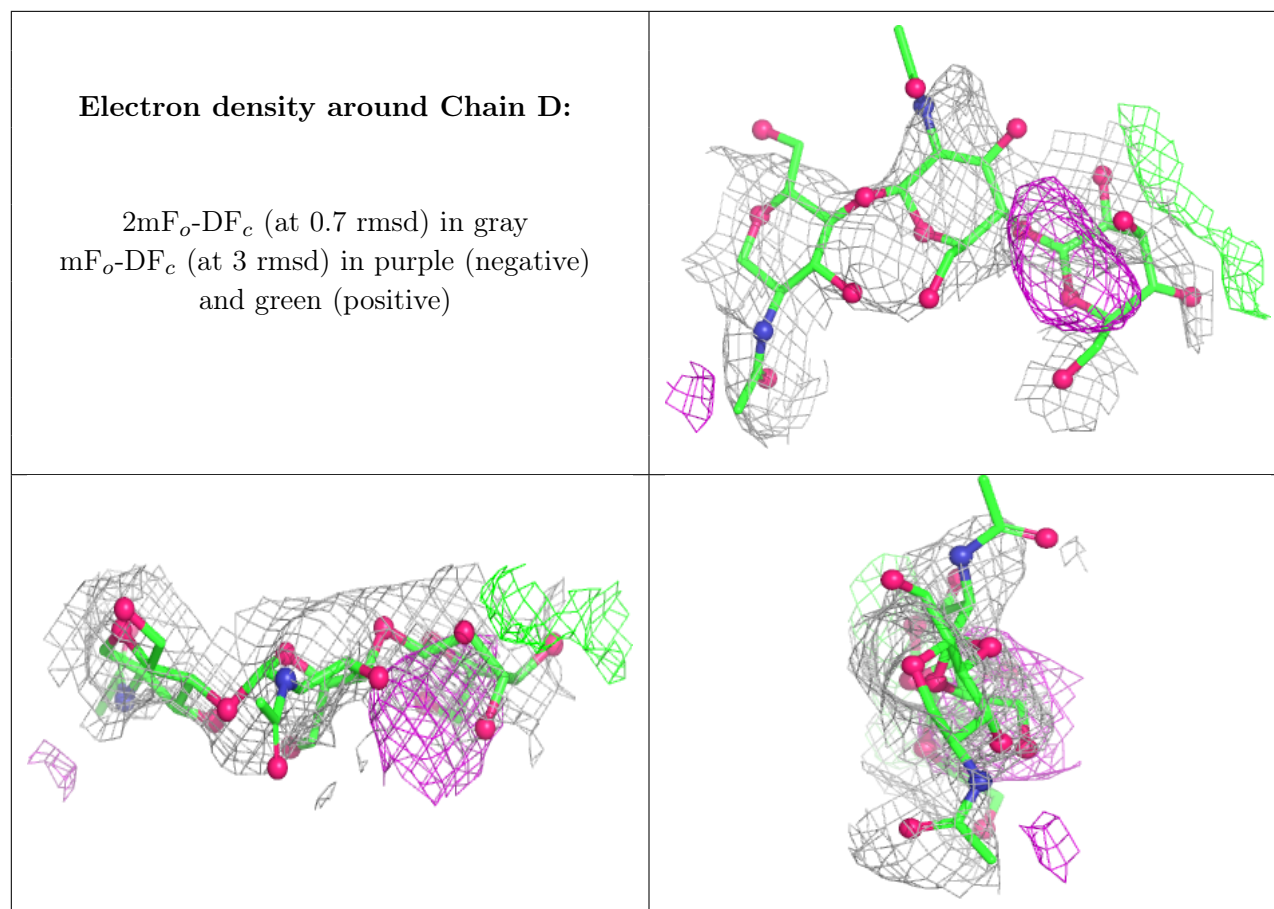
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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, 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($\text{\AA}^2$)	Q<0.9
4	NAG	A	1302	14/15	0.14	0.24	114,124,126,128	0
4	NAG	A	1301	14/15	0.61	0.18	72,83,89,90	0
4	NAG	A	1308	14/15	0.72	0.20	63,82,93,94	0
4	NAG	A	1306	14/15	0.79	0.15	70,76,93,96	0
4	NAG	A	1307	14/15	0.84	0.20	48,74,105,108	0
4	NAG	A	1305	14/15	0.84	0.15	65,91,94,94	0
4	NAG	A	1304	14/15	0.85	0.11	40,53,72,74	0
4	NAG	A	1303	14/15	0.88	0.11	62,70,87,91	0

6.5 Other polymers ⓘ

There are no such residues in this entry.