



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 15, 2024 – 12:13 PM EST

PDB ID : 5U74
Title : Structure of human Niemann-Pick C1 protein
Authors : Li, X.
Deposited on : 2016-12-11
Resolution : 3.33 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.21
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

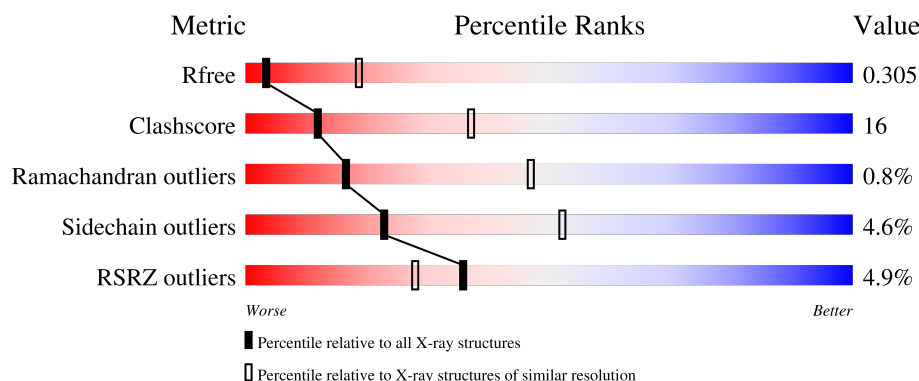
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.33 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}	164625	1325 (3.38-3.30)
Clashscore	180529	1376 (3.38-3.30)
Ramachandran outliers	177936	1376 (3.38-3.30)
Sidechain outliers	177891	1375 (3.38-3.30)
RSRZ outliers	164620	1325 (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	 3% 45% 24% 30%
2	B	2	 50% 50%
3	C	3	 33% 67%
4	D	3	 67% 33%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7311 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	900	Total	C	N	O	S	0	3	0
			7081	4604	1144	1287	46			

There is a discrepancy between the modelled and reference sequences:

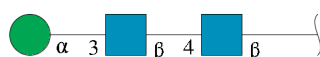
Chain	Residue	Modelled	Actual	Comment	Reference
A	642	ILE	MET	conflict	UNP O15118

- 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			

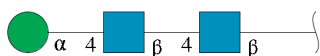
- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

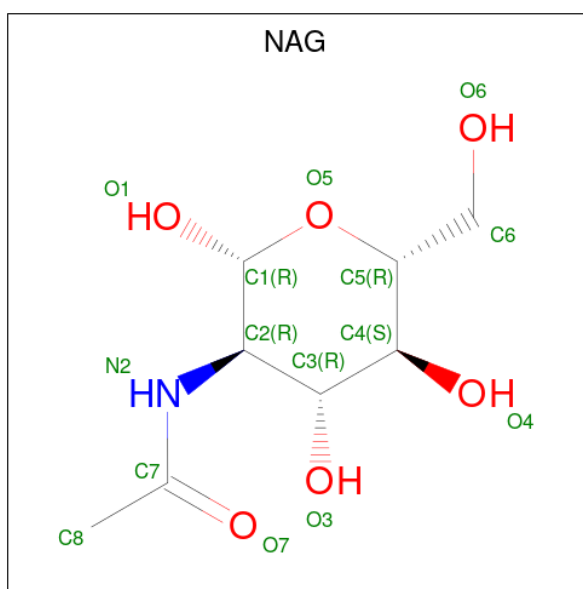
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-

beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



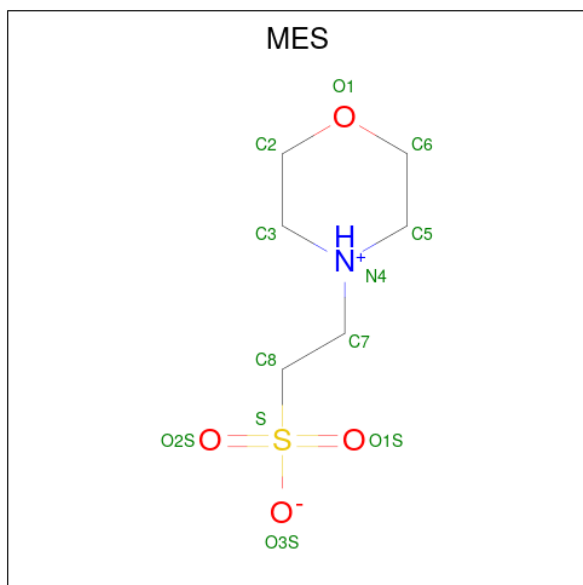
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).

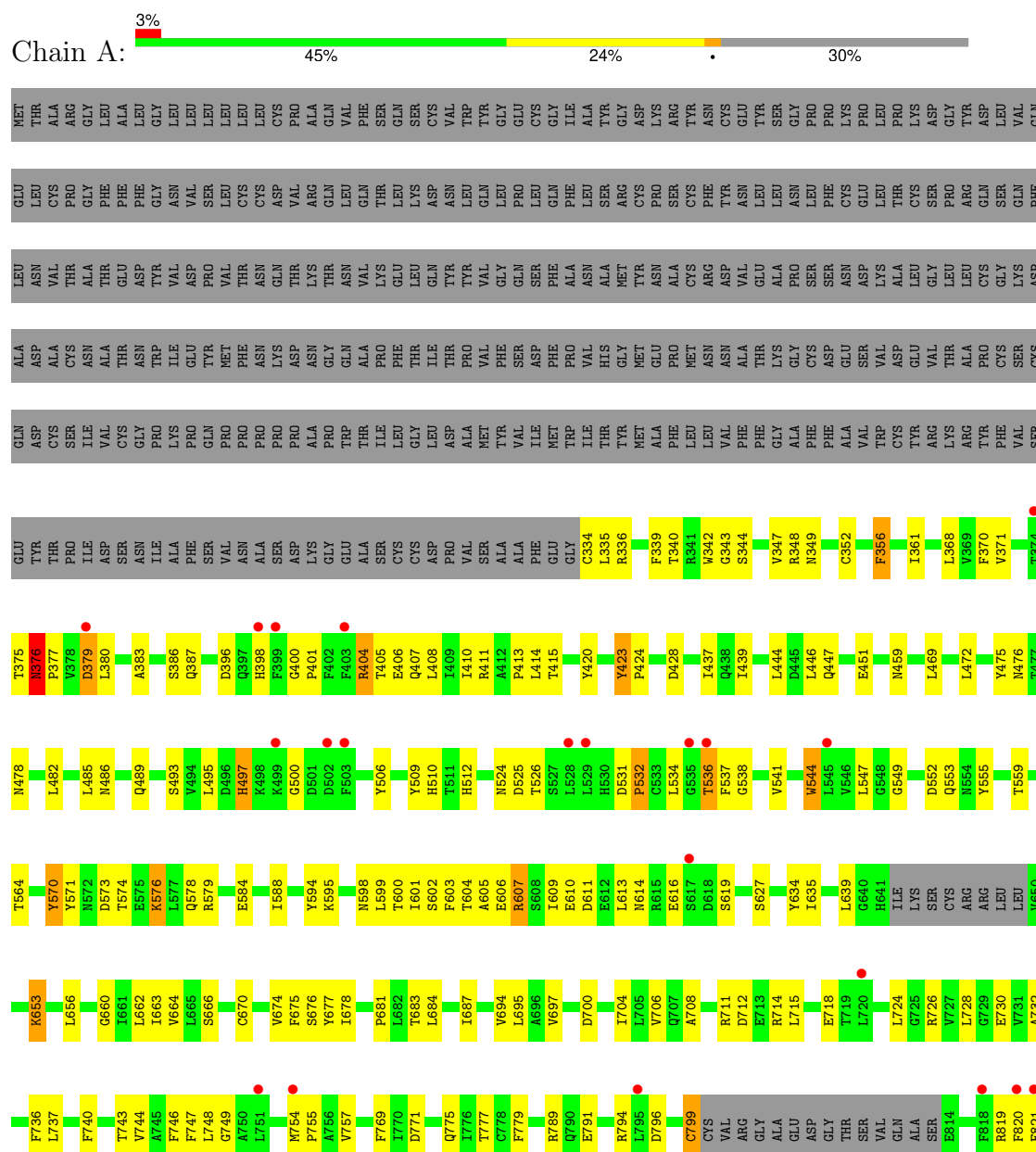


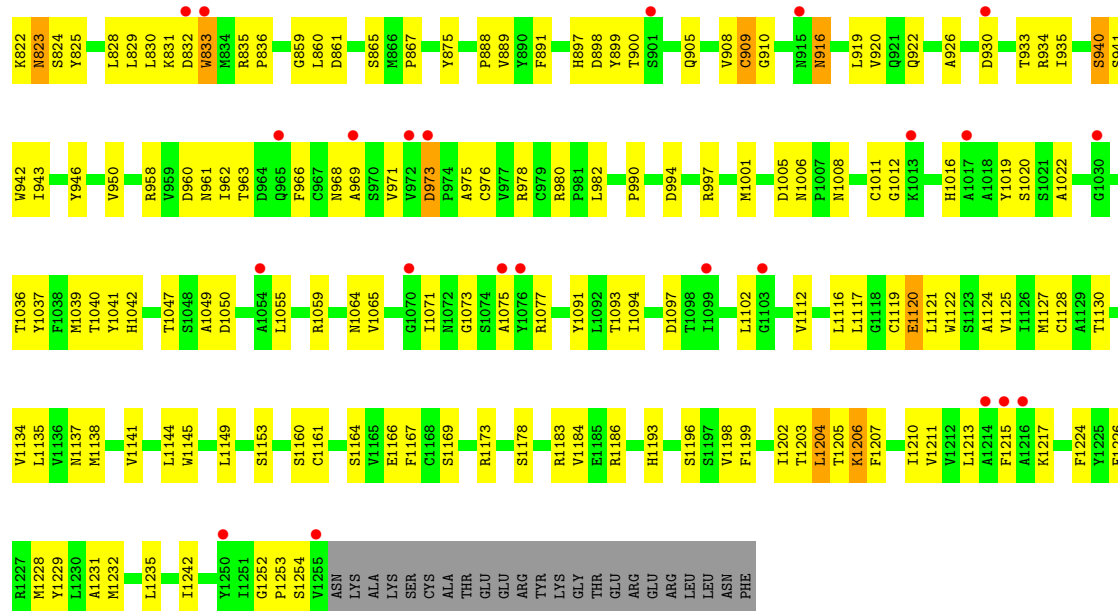
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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: Niemann-Pick C1 protein





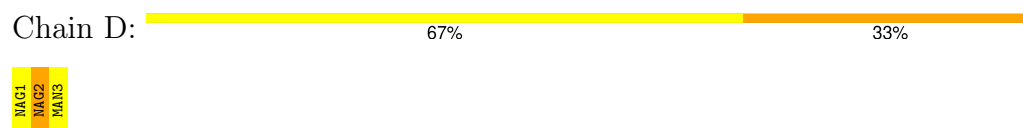
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 4: 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	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	174.87Å 222.12Å 107.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.92 – 3.33 67.92 – 3.33	Depositor EDS
% Data completeness (in resolution range)	96.1 (67.92-3.33) 96.0 (67.92-3.33)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.246 , 0.299 0.251 , 0.305	Depositor DCC
R_{free} test set	2704 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	102.6	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 65.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7311	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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, MES, NAG

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	0.30	0/7259	0.48	1/9879 (0.0%)

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.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	973	ASP	CB-CG-OD1	7.47	125.03	118.30

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	7081	0	6994	221	0
2	B	28	0	25	1	0
3	C	39	0	34	1	0
4	D	39	0	34	2	0
5	A	112	0	102	5	0
6	A	12	0	12	1	0
All	All	7311	0	7201	225	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 16.

All (225) 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	1.80	0.81
1:A:771:ASP:O	1:A:775:GLN:HB2	1.82	0.79
1:A:371:VAL:HB	1:A:676:SER:HB2	1.66	0.78
1:A:410:ILE:HD11	1:A:599:LEU:HD13	1.66	0.76
1:A:405:THR:H	1:A:606:GLU:HG3	1.51	0.75
1:A:1183:ARG:NH2	1:A:1252:GLY:O	2.20	0.75
1:A:684:LEU:HD12	1:A:687:ILE:HD12	1.68	0.73
1:A:958:ARG:NH1	1:A:968:ASN:O	2.23	0.72
1:A:616:GLU:HB2	1:A:867:PRO:HG3	1.72	0.71
1:A:401:PRO:HG3	1:A:570:TYR:H	1.55	0.71
1:A:376:ASN:H	1:A:377:PRO:HD2	1.57	0.70
1:A:401:PRO:HG3	1:A:570:TYR:N	2.08	0.68
1:A:1073[A]:GLY:O	1:A:1075:ALA:N	2.21	0.68
1:A:610:GLU:O	1:A:614:ASN:ND2	2.27	0.67
1:A:1011:CYS:SG	1:A:1012:GLY:N	2.63	0.67
1:A:1122:TRP:HA	1:A:1125:VAL:HG12	1.76	0.67
1:A:820:PHE:O	1:A:823:ASN:ND2	2.28	0.67
1:A:1186:ARG:NH2	1:A:1253:PRO:O	2.26	0.67
1:A:1206:LYS:NZ	1:A:1210:ILE:HD11	2.10	0.67
1:A:472:LEU:HD11	1:A:537:PHE:HD2	1.60	0.66
1:A:916:ASN:OD1	5:A:1305:NAG:N2	2.29	0.65
1:A:376:ASN:H	1:A:377:PRO:CD	2.10	0.64
1:A:789:ARG:NH1	1:A:796:ASP:O	2.30	0.63
1:A:958:ARG:HH21	1:A:973:ASP:HB3	1.62	0.63
1:A:375:THR:HB	1:A:681:PRO:HB2	1.81	0.63
1:A:664:VAL:HG11	1:A:695:LEU:HA	1.80	0.63
1:A:919:LEU:HD13	1:A:1065:VAL:HG11	1.79	0.63
1:A:1153:SER:HA	1:A:1228:MET:HE1	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:961:ASN:HB2	1:A:975:ALA:O	1.99	0.62
1:A:888:PRO:HA	1:A:1041:TYR:HA	1.82	0.62
1:A:613:LEU:HD21	6:A:1309:MES:H22	1.81	0.62
1:A:664:VAL:HG13	1:A:694:VAL:HG12	1.81	0.62
1:A:1121:LEU:O	1:A:1124:ALA:N	2.32	0.62
1:A:822:LYS:HG3	1:A:1196:SER:HB3	1.81	0.62
1:A:973:ASP:HB2	1:A:976:CYS:HB2	1.80	0.61
1:A:1199:PHE:HA	1:A:1202:ILE:HD12	1.81	0.61
1:A:820:PHE:HA	1:A:823:ASN:HD22	1.66	0.61
1:A:387:GLN:OE1	1:A:1059:ARG:NH1	2.33	0.61
1:A:536:THR:HG23	2:B:1:NAG:HN2	1.66	0.61
1:A:1047:THR:HG22	1:A:1049:ALA:H	1.66	0.61
1:A:547:LEU:HD13	1:A:555:TYR:HB3	1.82	0.61
1:A:909:CYS:SG	1:A:910:GLY:N	2.73	0.61
1:A:635:ILE:HD11	1:A:1204:LEU:HD13	1.83	0.60
5:A:1308:NAG:H83	5:A:1308:NAG:H3	1.83	0.60
1:A:829:LEU:HD21	1:A:1242:ILE:HA	1.84	0.59
1:A:1178:SER:HB3	1:A:1186:ARG:HD2	1.83	0.59
1:A:1117:LEU:HD11	1:A:1173:ARG:HA	1.83	0.59
1:A:406:GLU:HA	1:A:604:THR:O	2.03	0.59
1:A:413:PRO:HG3	1:A:600:THR:HG23	1.83	0.59
1:A:714:ARG:NH2	1:A:791:GLU:OE2	2.28	0.59
1:A:574:THR:O	1:A:578:GLN:NE2	2.32	0.58
1:A:1006:ASN:O	1:A:1008:ASN:ND2	2.36	0.58
1:A:744:VAL:HG11	1:A:1112:VAL:HG21	1.86	0.58
1:A:524:ASN:HA	1:A:531:ASP:O	2.03	0.57
1:A:934:ARG:NH2	1:A:1050:ASP:OD1	2.37	0.57
1:A:1231:ALA:O	1:A:1235:LEU:CB	2.52	0.57
1:A:737:LEU:HD13	1:A:1116:LEU:HD12	1.86	0.57
1:A:712:ASP:OD1	1:A:726:ARG:NH2	2.37	0.57
1:A:1102:LEU:HD13	1:A:1135:LEU:HD13	1.86	0.57
1:A:536:THR:O	1:A:538:GLY:N	2.37	0.57
1:A:700:ASP:O	1:A:704:ILE:HG12	2.05	0.57
1:A:601:ILE:HD12	1:A:601:ILE:O	2.05	0.56
1:A:489:GLN:NE2	1:A:532:PRO:O	2.39	0.56
1:A:775:GLN:O	1:A:779:PHE:HB3	2.06	0.56
1:A:352:CYS:O	1:A:356:PHE:HB2	2.06	0.56
1:A:859:GLY:HA2	1:A:1091:TYR:CE1	2.40	0.56
1:A:619:SER:HB2	1:A:1217:LYS:HB2	1.88	0.55
3:C:2:NAG:H62	3:C:3:MAN:H2	1.87	0.55
1:A:829:LEU:HD11	1:A:1242:ILE:HG23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1016:HIS:HA	1:A:1020:SER:HB3	1.89	0.54
1:A:344:SER:OG	1:A:348:ARG:NH2	2.38	0.54
1:A:1186:ARG:HH22	1:A:1254:SER:HA	1.73	0.53
1:A:459:ASN:OD1	5:A:1302:NAG:N2	2.42	0.53
1:A:1094:ILE:CG2	1:A:1149:LEU:HD22	2.39	0.53
1:A:663:ILE:HD13	1:A:779:PHE:HB2	1.91	0.53
1:A:714:ARG:HG3	1:A:718:GLU:HB3	1.91	0.53
1:A:493:SER:O	1:A:497:HIS:ND1	2.39	0.53
1:A:718:GLU:OE1	1:A:726:ARG:NH1	2.42	0.53
1:A:423:TYR:HB3	1:A:424:PRO:HD3	1.91	0.52
1:A:576:LYS:O	1:A:579:ARG:HG2	2.09	0.52
1:A:1055:LEU:HD11	1:A:1059:ARG:HE	1.75	0.52
1:A:525:ASP:OD1	1:A:526:THR:N	2.42	0.52
1:A:933:THR:O	1:A:935:ILE:N	2.39	0.52
1:A:754:MET:O	1:A:757:VAL:HG12	2.10	0.52
1:A:660:GLY:HA2	1:A:663:ILE:HD12	1.92	0.52
1:A:940:SER:O	1:A:940:SER:OG	2.18	0.52
1:A:789:ARG:HD3	1:A:796:ASP:HA	1.92	0.52
1:A:820:PHE:CA	1:A:823:ASN:HD22	2.23	0.52
1:A:404:ARG:NH1	1:A:584:GLU:OE2	2.40	0.51
1:A:413:PRO:HG2	1:A:414:LEU:HD13	1.91	0.51
1:A:926:ALA:O	1:A:933:THR:OG1	2.29	0.51
1:A:446:LEU:HD12	1:A:594:TYR:CE1	2.46	0.51
1:A:1206:LYS:HZ2	1:A:1210:ILE:HD11	1.76	0.50
1:A:534:LEU:HD22	1:A:537:PHE:HE1	1.77	0.50
1:A:1164:SER:HA	1:A:1167:PHE:HD2	1.76	0.50
1:A:1213:LEU:HB3	1:A:1226:PHE:CE1	2.46	0.50
1:A:376:ASN:N	1:A:377:PRO:HD2	2.24	0.50
1:A:512:HIS:HD2	1:A:525:ASP:OD2	1.95	0.50
1:A:396:ASP:HA	1:A:400:GLY:O	2.11	0.50
1:A:408:LEU:HA	1:A:602:SER:O	2.12	0.50
1:A:966:PHE:HB2	1:A:1001:MET:HE3	1.93	0.50
1:A:406:GLU:N	1:A:406:GLU:OE1	2.45	0.50
1:A:1040:THR:OG1	1:A:1041:TYR:N	2.45	0.50
1:A:714:ARG:HD2	1:A:718:GLU:O	2.12	0.49
1:A:830:LEU:HD13	1:A:1184:VAL:CG1	2.42	0.49
1:A:835:ARG:HB2	1:A:836:PRO:HD3	1.93	0.49
1:A:552:ASP:OD1	1:A:553:GLN:N	2.45	0.49
1:A:830:LEU:HD13	1:A:1184:VAL:HG13	1.94	0.49
1:A:420:TYR:HB2	1:A:510:HIS:CD2	2.47	0.49
1:A:472:LEU:HD11	1:A:537:PHE:CD2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1005:ASP:OD1	1:A:1006:ASN:N	2.45	0.49
1:A:407:GLN:O	1:A:603:PHE:HA	2.13	0.49
1:A:980:ARG:NH1	1:A:990:PRO:HA	2.29	0.48
1:A:544:TRP:NE1	1:A:555:TYR:OH	2.45	0.48
1:A:973:ASP:CB	1:A:976:CYS:HB2	2.42	0.48
1:A:380:LEU:O	1:A:755:PRO:HG2	2.14	0.48
1:A:994:ASP:HA	1:A:997:ARG:HB3	1.95	0.48
1:A:406:GLU:HG3	1:A:605:ALA:HA	1.94	0.48
1:A:746:PHE:O	1:A:749:GLY:N	2.47	0.48
1:A:820:PHE:C	1:A:823:ASN:HD22	2.16	0.48
1:A:524:ASN:OD1	5:A:1303:NAG:N2	2.46	0.48
1:A:1224:PHE:O	1:A:1228:MET:HB2	2.14	0.48
1:A:342:TRP:CH2	1:A:777:THR:HG22	2.48	0.47
1:A:835:ARG:HE	1:A:835:ARG:HB3	1.41	0.47
1:A:728:LEU:HD13	1:A:732:ALA:HB2	1.96	0.47
1:A:978:ARG:HH12	1:A:982:LEU:HD22	1.79	0.47
1:A:335:LEU:HB3	1:A:339:PHE:CE2	2.50	0.47
1:A:674:VAL:O	1:A:678:ILE:HG13	2.15	0.47
1:A:1204:LEU:H	1:A:1204:LEU:HD23	1.79	0.47
1:A:607:ARG:NH1	1:A:611:ASP:OD2	2.48	0.47
1:A:744:VAL:O	1:A:748:LEU:HB2	2.15	0.47
1:A:958:ARG:HH12	1:A:969:ALA:HA	1.80	0.47
1:A:634:TYR:CD2	1:A:1204:LEU:HB3	2.49	0.47
1:A:570:TYR:CZ	1:A:576:LYS:HB2	2.51	0.46
1:A:946:TYR:O	1:A:950:VAL:HG23	2.16	0.46
1:A:486:ASN:HB3	1:A:541:VAL:HG21	1.97	0.46
1:A:398:HIS:HE1	1:A:1037:TYR:HD2	1.63	0.46
1:A:588:ILE:HG23	1:A:603:PHE:HE2	1.80	0.46
1:A:860:LEU:HD13	1:A:861:ASP:N	2.30	0.46
1:A:1204:LEU:HG	1:A:1205:THR:N	2.31	0.46
1:A:407:GLN:OE1	1:A:875:TYR:OH	2.33	0.46
1:A:1137:ASN:HB2	1:A:1235:LEU:HD21	1.97	0.46
1:A:336:ARG:O	1:A:340:THR:OG1	2.27	0.46
1:A:889:VAL:HG11	1:A:1042:HIS:CE1	2.51	0.46
1:A:447:GLN:O	1:A:451:GLU:HB2	2.15	0.45
1:A:743:THR:HG21	1:A:769:PHE:HB2	1.97	0.45
1:A:376:ASN:N	1:A:377:PRO:CD	2.79	0.45
1:A:570:TYR:OH	1:A:576:LYS:HB2	2.17	0.45
1:A:962:ILE:HD12	1:A:963:THR:N	2.31	0.45
1:A:343:GLY:O	1:A:347:VAL:HG23	2.16	0.45
1:A:344:SER:O	1:A:348:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:905:GLN:HG2	1:A:943:ILE:HD11	1.99	0.45
1:A:1093:THR:OG1	1:A:1097:ASP:OD2	2.27	0.45
1:A:704:ILE:O	1:A:708:ALA:HB2	2.16	0.45
1:A:728:LEU:O	1:A:732:ALA:CB	2.64	0.45
1:A:437:ILE:HB	1:A:509:TYR:CE2	2.52	0.45
1:A:860:LEU:HD11	1:A:865:SER:HB3	1.99	0.45
1:A:482:LEU:HB2	1:A:564:THR:HB	1.99	0.45
1:A:1121:LEU:H	1:A:1121:LEU:HD22	1.81	0.45
1:A:1206:LYS:HZ1	1:A:1210:ILE:HD11	1.80	0.45
1:A:339:PHE:O	1:A:728:LEU:HD12	2.17	0.45
1:A:415:THR:HG21	1:A:439:ILE:HD11	1.98	0.45
1:A:683:THR:O	1:A:687:ILE:HG13	2.17	0.45
1:A:1127:MET:SD	1:A:1169:SER:HA	2.57	0.45
1:A:697:VAL:HG22	1:A:1166:GLU:HG3	1.98	0.44
1:A:831:LYS:O	1:A:833:TRP:N	2.49	0.44
1:A:1203:THR:O	1:A:1207:PHE:HB2	2.16	0.44
1:A:728:LEU:O	1:A:732:ALA:HB2	2.18	0.44
1:A:1112:VAL:O	1:A:1116:LEU:HB3	2.18	0.44
1:A:1141:VAL:HG11	1:A:1231:ALA:HB2	1.98	0.44
1:A:1130:THR:O	1:A:1134:VAL:HG23	2.18	0.44
1:A:411:ARG:HG3	1:A:600:THR:OG1	2.18	0.43
1:A:1198:VAL:O	1:A:1202:ILE:HG13	2.18	0.43
1:A:711:ARG:CZ	1:A:819:ARG:HD3	2.48	0.43
1:A:1019:TYR:HA	1:A:1022:ALA:HB3	2.00	0.43
1:A:639:LEU:HD22	1:A:706:VAL:HG11	1.99	0.43
1:A:824:SER:O	1:A:828:LEU:HG	2.18	0.43
1:A:922:GLN:NE2	5:A:1308:NAG:O7	2.51	0.43
4:D:2:NAG:C7	4:D:2:NAG:O4	2.67	0.43
4:D:2:NAG:O4	4:D:2:NAG:O7	2.36	0.43
1:A:370:PHE:CD1	1:A:370:PHE:C	2.92	0.43
1:A:375:THR:HB	1:A:681:PRO:CB	2.47	0.43
1:A:653:LYS:HD2	1:A:653:LYS:N	2.34	0.43
1:A:1229:TYR:HA	1:A:1232:MET:SD	2.59	0.43
1:A:398:HIS:CE1	1:A:1037:TYR:HD2	2.37	0.43
1:A:662:LEU:O	1:A:666:SER:OG	2.20	0.43
1:A:897:HIS:HB3	1:A:899:TYR:CE2	2.54	0.43
1:A:960:ASP:HA	1:A:976:CYS:HA	2.01	0.43
1:A:371:VAL:HG21	1:A:676:SER:O	2.19	0.43
1:A:820:PHE:HA	1:A:823:ASN:ND2	2.33	0.43
1:A:1138:MET:HB2	1:A:1138:MET:HE2	1.47	0.43
1:A:469:LEU:HD23	1:A:469:LEU:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:942:TRP:CZ2	1:A:1036:THR:HG21	2.53	0.42
1:A:379:ASP:OD1	1:A:379:ASP:N	2.52	0.42
1:A:1037:TYR:HE1	1:A:1039:MET:HB2	1.85	0.42
1:A:347:VAL:HG22	1:A:724:LEU:HD23	2.01	0.42
1:A:413:PRO:HD2	1:A:598:ASN:O	2.20	0.42
1:A:971:VAL:HG13	1:A:973:ASP:H	1.84	0.42
1:A:908:VAL:O	1:A:920:VAL:HG22	2.20	0.42
1:A:794:ARG:HB3	1:A:799:CYS:HB2	2.02	0.42
1:A:500:GLY:HA2	1:A:506:TYR:CE2	2.54	0.42
1:A:383:ALA:HB3	1:A:386:SER:HB3	2.01	0.42
1:A:609:ILE:O	1:A:613:LEU:HB2	2.19	0.42
1:A:361:ILE:HA	1:A:670:CYS:SG	2.60	0.42
1:A:444:LEU:HD13	1:A:485:LEU:HD23	2.01	0.41
1:A:476:ASN:OD1	1:A:478:ASN:HB2	2.21	0.41
1:A:920:VAL:HG11	1:A:941:SER:HB3	2.02	0.41
1:A:1119:CYS:HB3	1:A:1120:GLU:H	1.53	0.41
1:A:398:HIS:HE1	1:A:1037:TYR:CD2	2.38	0.41
1:A:715:LEU:HB2	1:A:718:GLU:HB2	2.01	0.41
1:A:825:TYR:OH	1:A:1242:ILE:HG12	2.20	0.41
1:A:627:SER:HA	1:A:1211:VAL:HG11	2.02	0.41
1:A:898:ASP:O	1:A:900:THR:N	2.45	0.41
1:A:930:ASP:N	1:A:930:ASP:OD1	2.45	0.41
1:A:1071[B]:ILE:O	1:A:1073[B]:GLY:N	2.44	0.41
1:A:437:ILE:HG13	1:A:495:LEU:HD21	2.02	0.40
1:A:736:PHE:O	1:A:740:PHE:HB2	2.21	0.40
1:A:1206:LYS:HE3	1:A:1206:LYS:HB3	1.83	0.40
1:A:891:PHE:O	1:A:1037:TYR:HA	2.22	0.40
1:A:1160:SER:HA	1:A:1232:MET:HE2	2.03	0.40
1:A:534:LEU:HD23	1:A:534:LEU:HA	1.98	0.40
1:A:819:ARG:HA	1:A:819:ARG:HD2	1.78	0.40
1:A:726:ARG:O	1:A:730:GLU:HG3	2.22	0.40
1:A:549:GLY:HA3	1:A:559:THR:OG1	2.21	0.40
1:A:819:ARG:HH12	1:A:1193:HIS:CE1	2.40	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	897/1278 (70%)	774 (86%)	116 (13%)	7 (1%)	16	47

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	ASN
1	A	532	PRO
1	A	423	TYR
1	A	571	TYR
1	A	832	ASP
1	A	1120	GLU
1	A	368	LEU

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	786/1109 (71%)	750 (95%)	36 (5%)	23	52

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	334	CYS
1	A	349	ASN
1	A	356	PHE
1	A	376	ASN

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Mol	Chain	Res	Type
1	A	379	ASP
1	A	404	ARG
1	A	428	ASP
1	A	475	TYR
1	A	497	HIS
1	A	544	TRP
1	A	570	TYR
1	A	573	ASP
1	A	576	LYS
1	A	595	LYS
1	A	607	ARG
1	A	653	LYS
1	A	656	LEU
1	A	675	PHE
1	A	677	TYR
1	A	747	PHE
1	A	799	CYS
1	A	821	PHE
1	A	823	ASN
1	A	833	TRP
1	A	909	CYS
1	A	916	ASN
1	A	940	SER
1	A	1064	ASN
1	A	1077	ARG
1	A	1128	CYS
1	A	1144	LEU
1	A	1145	TRP
1	A	1161	CYS
1	A	1204	LEU
1	A	1206	LYS
1	A	1215	PHE

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

Mol	Chain	Res	Type
1	A	823	ASN
1	A	953	GLN
1	A	1006	ASN
1	A	1008	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 ⓘ

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	0.75	1 (7%)	17,19,21	0.66	1 (5%)
2	NAG	B	2	2	14,14,15	0.27	0	17,19,21	0.64	0
3	NAG	C	1	1,3	14,14,15	0.59	0	17,19,21	0.77	1 (5%)
3	NAG	C	2	3	14,14,15	0.42	0	17,19,21	1.00	1 (5%)
3	MAN	C	3	3	11,11,12	1.96	1 (9%)	15,15,17	3.27	5 (33%)
4	NAG	D	1	1,4	14,14,15	1.37	2 (14%)	17,19,21	1.69	1 (5%)
4	NAG	D	2	4	14,14,15	1.77	2 (14%)	17,19,21	1.86	4 (23%)
4	MAN	D	3	4	11,11,12	1.78	2 (18%)	15,15,17	1.95	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	-	3/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	MAN	O5-C5	5.63	1.54	1.43
4	D	2	NAG	O5-C1	5.26	1.52	1.43
4	D	1	NAG	O5-C1	4.58	1.51	1.43
4	D	3	MAN	C1-C2	4.37	1.62	1.52
4	D	2	NAG	C1-C2	3.82	1.57	1.52
4	D	3	MAN	O5-C5	2.82	1.48	1.43
2	B	1	NAG	O5-C1	2.12	1.47	1.43
4	D	1	NAG	C1-C2	2.12	1.55	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	MAN	C1-C2-C3	-7.50	98.72	109.64
4	D	1	NAG	C1-O5-C5	6.35	120.70	112.19
3	C	3	MAN	C1-O5-C5	6.30	120.64	112.19
4	D	2	NAG	C1-O5-C5	5.73	119.87	112.19
3	C	3	MAN	O3-C3-C4	5.21	122.65	110.38
3	C	3	MAN	C3-C4-C5	-4.92	101.32	110.23
4	D	3	MAN	C1-C2-C3	-3.90	103.96	109.64
4	D	3	MAN	O3-C3-C2	-3.75	102.41	110.05
4	D	3	MAN	O2-C2-C1	3.47	117.16	109.22
4	D	2	NAG	C2-N2-C7	2.89	126.77	122.90
3	C	2	NAG	C3-C4-C5	2.77	115.25	110.23
3	C	3	MAN	O3-C3-C2	2.70	115.56	110.05
4	D	3	MAN	O2-C2-C3	-2.69	104.57	110.15
3	C	1	NAG	C1-O5-C5	2.63	115.71	112.19
4	D	2	NAG	C1-C2-N2	2.62	114.56	110.43
4	D	2	NAG	O4-C4-C3	-2.35	104.84	110.38
2	B	1	NAG	C1-O5-C5	2.14	115.05	112.19

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2	NAG	C1-C2-N2-C7
4	D	1	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
4	D	3	MAN	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
4	D	3	MAN	O5-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
3	C	3	MAN	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
2	B	1	NAG	C3-C2-N2-C7

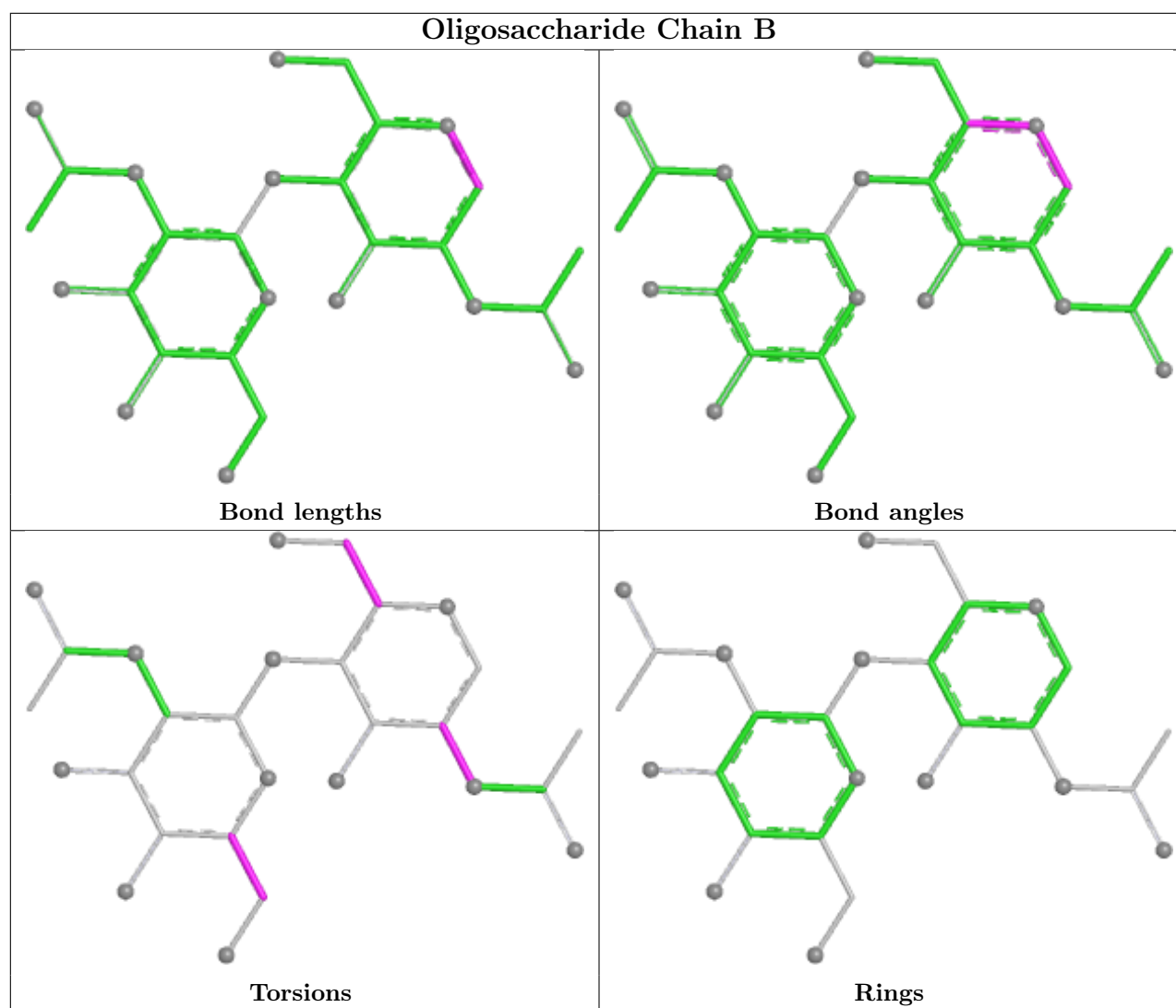
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	3	MAN	C1-C2-C3-C4-C5-O5

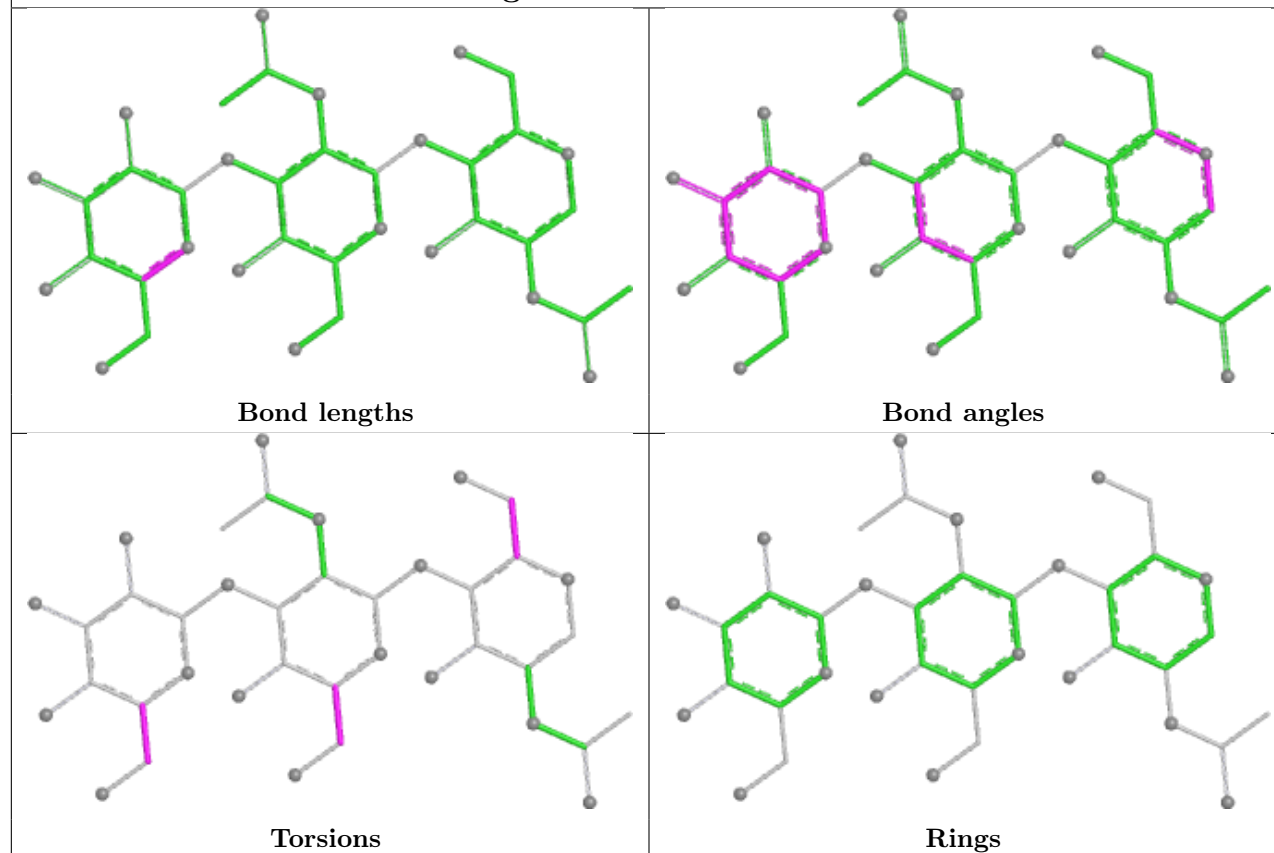
4 monomers are involved in 4 short contacts:

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

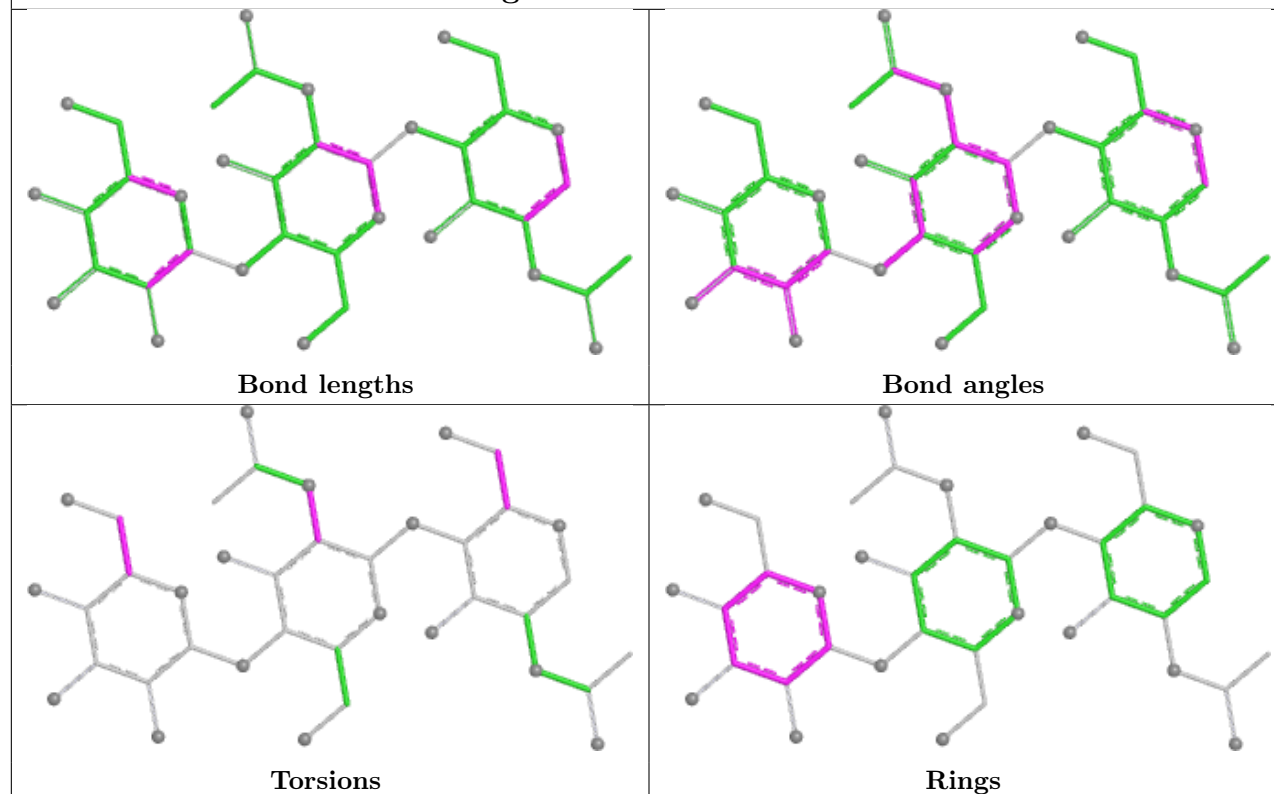
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



Oligosaccharide Chain C



Oligosaccharide Chain D



5.6 Ligand geometry

9 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$
5	NAG	A	1301	1	14,14,15	0.21	0	17,19,21	0.39	0
5	NAG	A	1308	1	14,14,15	0.62	1 (7%)	17,19,21	1.29	2 (11%)
6	MES	A	1309	-	12,12,12	2.30	1 (8%)	15,16,16	1.84	3 (20%)
5	NAG	A	1303	1	14,14,15	0.32	0	17,19,21	0.50	0
5	NAG	A	1304	1	14,14,15	0.15	0	17,19,21	0.44	0
5	NAG	A	1306	1	14,14,15	0.50	0	17,19,21	0.58	0
5	NAG	A	1302	1	14,14,15	0.38	0	17,19,21	0.54	0
5	NAG	A	1307	1	14,14,15	0.36	0	17,19,21	0.50	0
5	NAG	A	1305	1	14,14,15	0.78	2 (14%)	17,19,21	0.79	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
5	NAG	A	1301	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1308	1	-	6/6/23/26	0/1/1/1
6	MES	A	1309	-	-	5/6/14/14	0/1/1/1
5	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1306	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1305	1	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1309	MES	C8-S	-7.70	1.66	1.77
5	A	1308	NAG	C1-C2	2.15	1.55	1.52
5	A	1305	NAG	C1-C2	2.03	1.55	1.52
5	A	1305	NAG	O5-C1	2.02	1.47	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1309	MES	C5-N4-C3	4.90	119.40	108.84
5	A	1308	NAG	C2-N2-C7	4.39	128.79	122.90
5	A	1305	NAG	C1-O5-C5	2.62	115.70	112.19
5	A	1308	NAG	C1-C2-N2	2.13	113.79	110.43
6	A	1309	MES	C7-N4-C3	2.09	116.82	111.24
6	A	1309	MES	O2S-S-C8	2.06	109.84	106.73

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1309	MES	N4-C7-C8-S
5	A	1302	NAG	O5-C5-C6-O6
5	A	1304	NAG	O5-C5-C6-O6
5	A	1308	NAG	O5-C5-C6-O6
5	A	1302	NAG	C4-C5-C6-O6
5	A	1304	NAG	C4-C5-C6-O6
5	A	1308	NAG	C8-C7-N2-C2
5	A	1308	NAG	O7-C7-N2-C2
5	A	1307	NAG	O5-C5-C6-O6
5	A	1307	NAG	C4-C5-C6-O6
5	A	1305	NAG	O5-C5-C6-O6
5	A	1308	NAG	C4-C5-C6-O6
6	A	1309	MES	C8-C7-N4-C5
5	A	1305	NAG	C4-C5-C6-O6
5	A	1306	NAG	O5-C5-C6-O6
6	A	1309	MES	C7-C8-S-O3S
6	A	1309	MES	C7-C8-S-O1S
5	A	1308	NAG	C1-C2-N2-C7
5	A	1301	NAG	O5-C5-C6-O6
6	A	1309	MES	C7-C8-S-O2S
5	A	1308	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1308	NAG	2	0
6	A	1309	MES	1	0
5	A	1303	NAG	1	0
5	A	1302	NAG	1	0
5	A	1305	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	900/1278 (70%)	0.28	44 (4%)	36 28	55, 96, 142, 248	3 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	915	ASN	5.0
1	A	973	ASP	4.5
1	A	1099	ILE	4.1
1	A	535	GLY	4.0
1	A	399	PHE	3.8
1	A	930	ASP	3.8
1	A	374	THR	3.8
1	A	528	LEU	3.3
1	A	1070	GLY	3.1
1	A	972	VAL	2.9
1	A	818	PHE	2.8
1	A	821	PHE	2.8
1	A	720	LEU	2.8
1	A	1216	ALA	2.7
1	A	502	ASP	2.6
1	A	398	HIS	2.6
1	A	820	PHE	2.6
1	A	1250	TYR	2.6
1	A	1076	TYR	2.5
1	A	795	LEU	2.5
1	A	1013	LYS	2.5
1	A	1214	ALA	2.4
1	A	901	SER	2.4
1	A	1215	PHE	2.3
1	A	832	ASP	2.3
1	A	969	ALA	2.3
1	A	1103	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	529	LEU	2.3
1	A	833	TRP	2.3
1	A	536	THR	2.2
1	A	754	MET	2.2
1	A	751	LEU	2.2
1	A	403	PHE	2.2
1	A	1017	ALA	2.2
1	A	1054	ALA	2.1
1	A	503	PHE	2.1
1	A	545	LEU	2.1
1	A	965	GLN	2.1
1	A	617	SER	2.0
1	A	379	ASP	2.0
1	A	1255	VAL	2.0
1	A	499	LYS	2.0
1	A	1075	ALA	2.0
1	A	1030	GLY	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 ⓘ

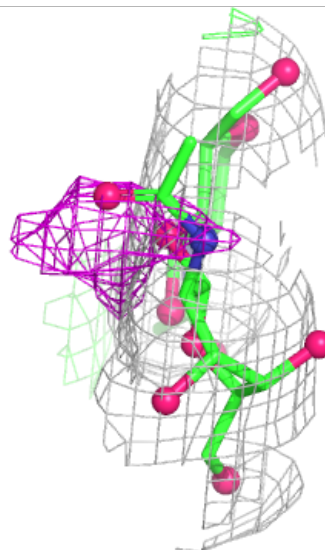
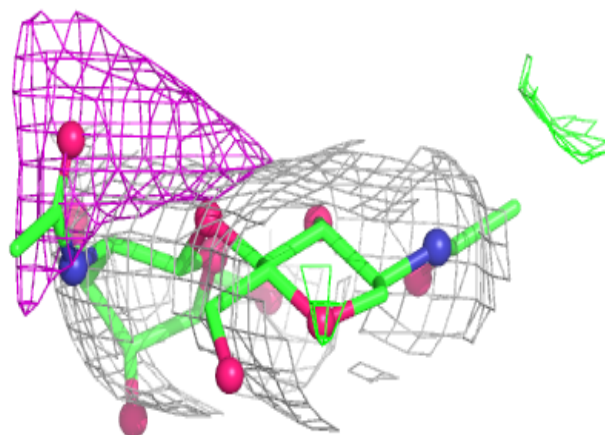
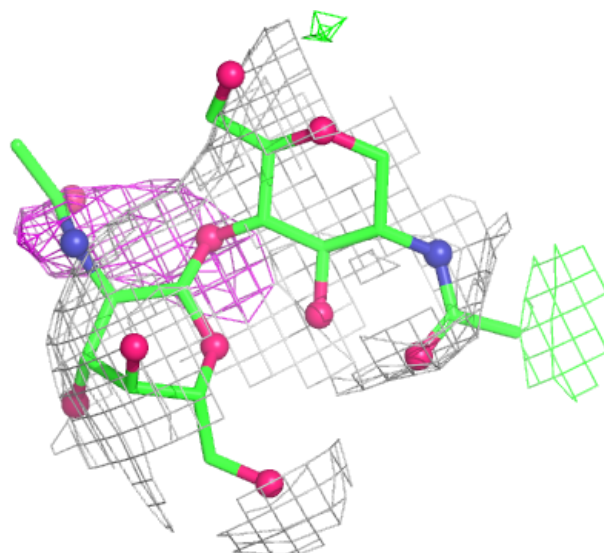
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	D	2	14/15	0.27	0.16	153,178,184,189	0
4	MAN	D	3	11/12	0.55	0.16	131,162,174,175	0
3	MAN	C	3	11/12	0.58	0.15	119,127,144,152	0
4	NAG	D	1	14/15	0.66	0.20	156,170,179,184	0
2	NAG	B	2	14/15	0.69	0.16	91,146,152,156	0
2	NAG	B	1	14/15	0.76	0.14	86,112,133,134	0
3	NAG	C	2	14/15	0.78	0.14	78,99,116,143	0
3	NAG	C	1	14/15	0.85	0.11	74,94,106,107	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.

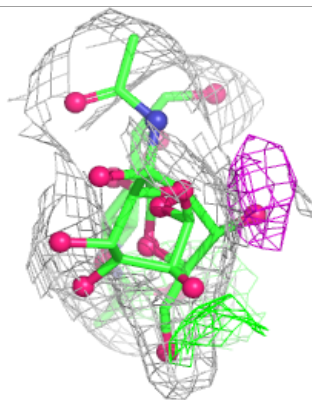
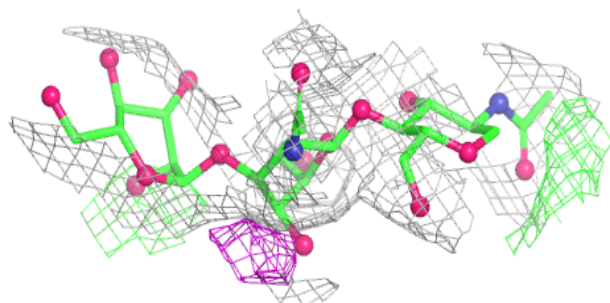
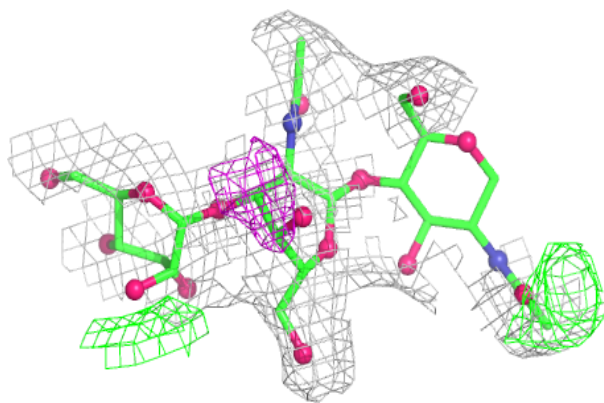
Electron density around Chain B:

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

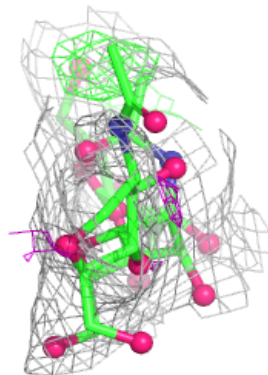
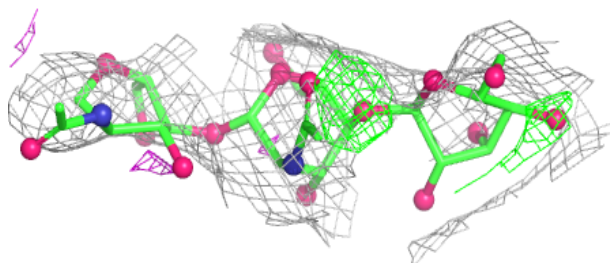
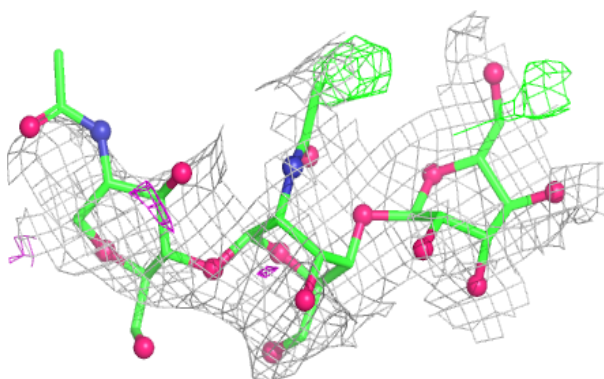


Electron density around Chain C:

$2mF_o-DF_c$ (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 [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(\AA^2)	Q<0.9
5	NAG	A	1302	14/15	0.40	0.14	168,175,181,183	0
5	NAG	A	1301	14/15	0.49	0.22	131,162,171,172	0
5	NAG	A	1303	14/15	0.50	0.15	117,142,148,149	0
5	NAG	A	1308	14/15	0.61	0.13	142,158,171,178	0
5	NAG	A	1305	14/15	0.64	0.13	123,155,166,166	0
5	NAG	A	1306	14/15	0.73	0.10	125,132,142,148	0
5	NAG	A	1307	14/15	0.75	0.17	105,136,153,153	0
5	NAG	A	1304	14/15	0.78	0.12	94,125,139,139	0
6	MES	A	1309	12/12	0.90	0.14	104,110,145,147	0

6.5 Other polymers [i](#)

There are no such residues in this entry.