Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 09:49 AM EDT

PDB ID	:	1YO8
Title	:	Structure of the C-terminal domain of human thrombospondin-2
Authors	:	Carlson, C.B.; Bernstein, D.A.; Annis, D.S.; Misenheimer, T.M.; Hannah, B.A.; Mosher, D.F.; Keck, J.L.
Deposited on	:	2005-01-26
Resolution	:	2.60 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 (i) 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 (i)) were used in the production of this report:

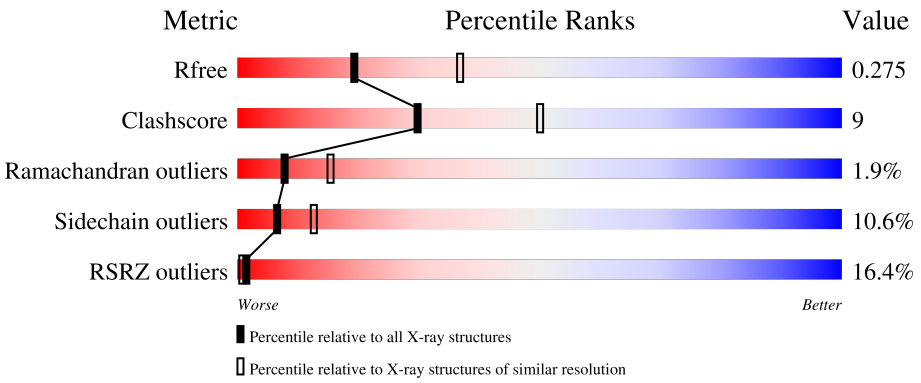
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	634	16%, 71%, 23%, • •
2	B	3	100%
3	C	2	50%, 50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	1	-	-	-	X
2	NAG	B	2	-	-	-	X
2	MAN	B	3	X	-	-	-
3	NAG	C	2	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5085 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.

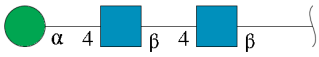
- Molecule 1 is a protein called thrombospondin-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	621	4844	2949	837	1017	36	5	0	0	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	548	ALA	-	cloning artifact	UNP P35442
A	549	ASP	-	cloning artifact	UNP P35442
A	550	PRO	-	cloning artifact	UNP P35442
A	675	MSE	MET	modified residue	UNP P35442
A	964	MSE	MET	modified residue	UNP P35442
A	1041	MSE	MET	modified residue	UNP P35442
A	1134	MSE	MET	modified residue	UNP P35442
A	1159	MSE	MET	modified residue	UNP P35442
A	1173	ALA	-	expression tag	UNP P35442
A	1174	ALA	-	expression tag	UNP P35442
A	1175	GLY	-	expression tag	UNP P35442
A	1176	HIS	-	expression tag	UNP P35442
A	1177	HIS	-	expression tag	UNP P35442
A	1178	HIS	-	expression tag	UNP P35442
A	1179	HIS	-	expression tag	UNP P35442
A	1180	HIS	-	expression tag	UNP P35442
A	1181	HIS	-	expression tag	UNP P35442

- Molecule 2 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.

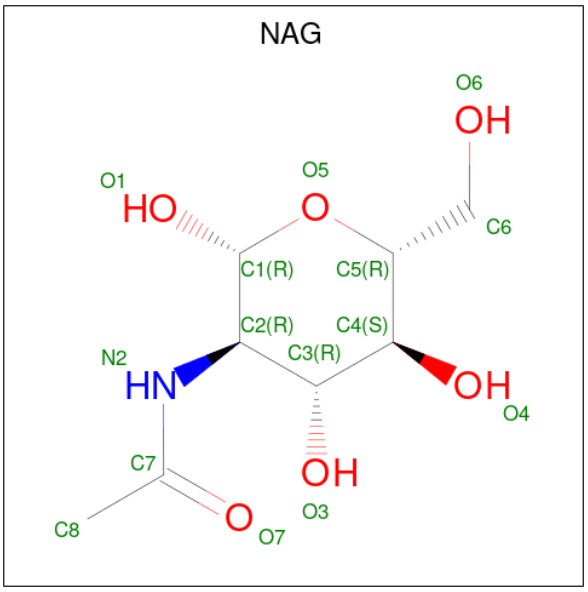


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	39	22	2	15	0	0	0

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

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

- 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
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	A	1	14	8	1	5	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	A	30	30	30	0	0

- Molecule 6 is water.

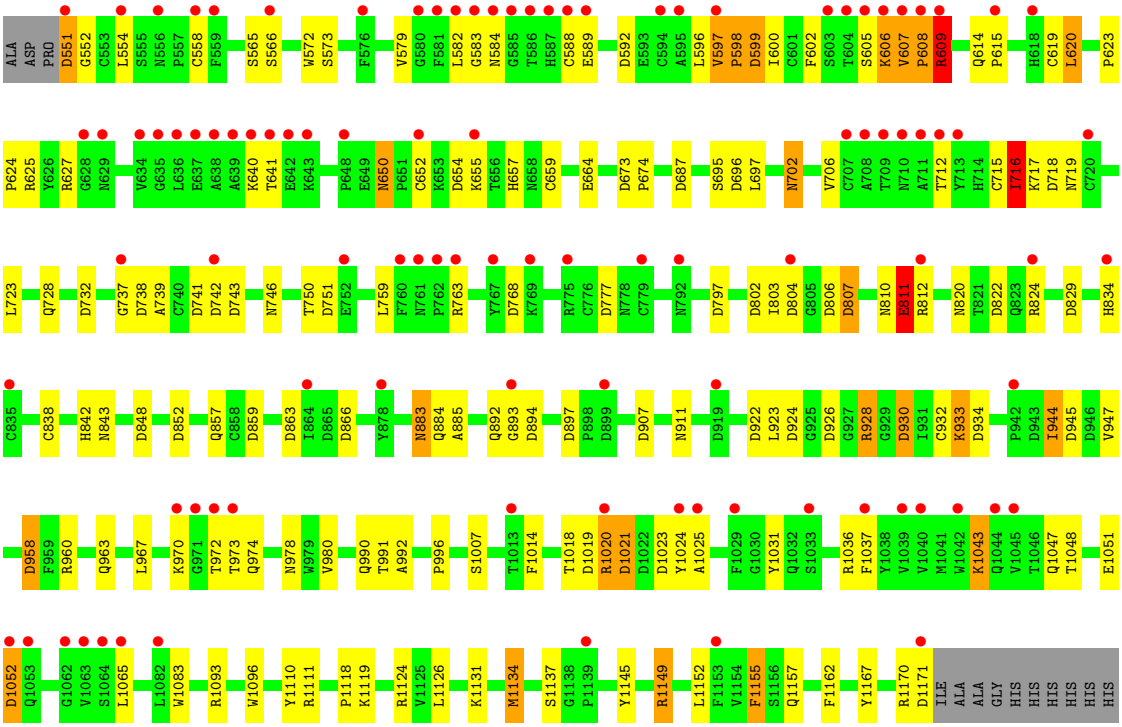
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	116	116	116	0	0

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.

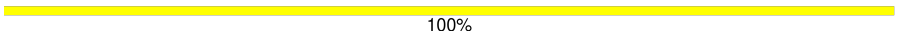
• Molecule 1: thrombospondin-2

Chain A:



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

Chain B:



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

Chain C:

NAG1
NAG2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	93.44Å 121.59Å 155.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 26.86 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.0 (20.00-2.60) 94.9 (26.86-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.59 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.218 , 0.284 0.216 , 0.275	Depositor DCC
R_{free} test set	2575 reflections (9.85%)	wwPDB-VP
Wilson B-factor (Å^2)	41.8	Xtriage
Anisotropy	0.803	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 67.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5085	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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 (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.57	0/4962	0.87	27/6755 (0.4%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	696	ASP	CB-CG-OD2	6.86	124.47	118.30
1	A	866	ASP	CB-CG-OD2	6.72	124.35	118.30
1	A	738	ASP	CB-CG-OD2	6.51	124.16	118.30
1	A	797	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	718	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	958	ASP	CB-CG-OD2	5.86	123.57	118.30
1	A	924	ASP	CB-CG-OD2	5.72	123.44	118.30
1	A	945	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	930	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	592	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	848	ASP	CB-CG-OD2	5.56	123.31	118.30
1	A	926	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	654	ASP	CB-CG-OD2	5.32	123.08	118.30
1	A	852	ASP	CB-CG-OD2	5.30	123.08	118.30
1	A	1171	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	863	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	777	ASP	CB-CG-OD2	5.28	123.06	118.30
1	A	802	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	804	ASP	CB-CG-OD2	5.23	123.00	118.30
1	A	934	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	768	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	687	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	551	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	599	ASP	CB-CG-OD2	5.13	122.92	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	859	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	732	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	907	ASP	CB-CG-OD2	5.06	122.85	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4844	0	4248	87	0
2	B	39	0	34	0	0
3	C	28	0	25	0	0
4	A	28	0	26	5	0
5	A	30	0	0	0	0
6	A	116	0	0	1	0
All	All	5085	0	4333	87	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 9.

All (87) 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:597:VAL:HB	1:A:598:PRO:CD	1.90	1.02
1:A:597:VAL:HB	1:A:598:PRO:HD3	1.03	0.99
1:A:597:VAL:CB	1:A:598:PRO:HD3	1.93	0.97
1:A:719:ASN:H	1:A:728:GLN:HE22	1.25	0.83
1:A:608:PRO:O	1:A:609:ARG:HB2	1.79	0.81
1:A:810:ASN:O	1:A:811:GLU:HB3	1.83	0.78
1:A:751:ASP:HB3	6:A:1320:HOH:O	1.85	0.75
1:A:978:ASN:H	1:A:990:GLN:HE21	1.35	0.74
1:A:1110:TYR:CE2	1:A:1134:MSE:HE3	2.23	0.73
1:A:606:LYS:HB3	1:A:608:PRO:HD2	1.71	0.71
1:A:572:TRP:NE1	4:A:6:NAG:H82	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:TRP:CD1	4:A:6:NAG:C8	2.78	0.66
1:A:972:THR:C	1:A:974:GLN:H	1.99	0.66
1:A:883:ASN:HD22	1:A:884:GLN:N	1.95	0.64
1:A:572:TRP:HE1	4:A:6:NAG:H82	1.63	0.64
1:A:607:VAL:H	1:A:608:PRO:CD	2.11	0.64
1:A:978:ASN:H	1:A:990:GLN:NE2	1.95	0.63
1:A:1024:TYR:HB2	1:A:1155:PHE:HB3	1.80	0.63
1:A:883:ASN:ND2	1:A:885:ALA:H	1.97	0.63
1:A:958:ASP:OD1	1:A:960:ARG:HB2	2.00	0.61
1:A:607:VAL:H	1:A:608:PRO:HD3	1.65	0.61
1:A:883:ASN:HD22	1:A:883:ASN:C	2.04	0.61
1:A:607:VAL:N	1:A:608:PRO:CD	2.65	0.60
1:A:695:SER:HB3	1:A:702:ASN:HD21	1.66	0.60
1:A:1124:ARG:CZ	1:A:1126:LEU:HD21	2.32	0.60
1:A:715:CYS:O	1:A:716:ILE:HB	2.03	0.59
1:A:978:ASN:N	1:A:990:GLN:HE21	2.01	0.59
1:A:614:GLN:HB2	1:A:615:PRO:HD3	1.84	0.58
1:A:810:ASN:O	1:A:811:GLU:CB	2.52	0.57
1:A:990:GLN:NE2	1:A:992:ALA:H	2.03	0.57
1:A:552:GLY:O	4:A:6:NAG:H83	2.05	0.56
1:A:602:PHE:O	1:A:609:ARG:HG3	2.06	0.55
1:A:572:TRP:CD1	4:A:6:NAG:H82	2.41	0.55
1:A:719:ASN:N	1:A:728:GLN:HE22	2.01	0.55
1:A:1152:LEU:HD13	1:A:1162:PHE:CG	2.42	0.53
1:A:928:ARG:NH1	1:A:932:CYS:O	2.38	0.53
1:A:990:GLN:HE22	1:A:992:ALA:H	1.55	0.53
1:A:609:ARG:NH2	1:A:623:PRO:HB3	2.25	0.52
1:A:582:LEU:N	1:A:589:GLU:O	2.42	0.51
1:A:883:ASN:HD22	1:A:885:ALA:H	1.57	0.51
1:A:650:ASN:HD21	1:A:652:CYS:HB2	1.75	0.51
1:A:657:HIS:HD2	1:A:659:CYS:H	1.59	0.51
1:A:1036:ARG:HB3	1:A:1145:TYR:CE2	2.47	0.50
1:A:1043:LYS:HZ1	1:A:1047:GLN:HB3	1.76	0.50
1:A:763:ARG:HG3	1:A:763:ARG:HH11	1.77	0.50
1:A:582:LEU:HG	1:A:583:GLY:H	1.76	0.49
1:A:1043:LYS:NZ	1:A:1047:GLN:HB3	2.28	0.49
1:A:609:ARG:HH11	1:A:620:LEU:HB3	1.78	0.48
1:A:972:THR:C	1:A:974:GLN:N	2.62	0.48
1:A:719:ASN:H	1:A:728:GLN:NE2	2.04	0.48
1:A:829:ASP:HB3	1:A:842:HIS:CD2	2.48	0.48
1:A:820:ASN:HB3	1:A:834:HIS:HD2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:PRO:HG2	1:A:600:ILE:HG13	1.96	0.47
1:A:715:CYS:O	1:A:716:ILE:CB	2.63	0.47
1:A:1152:LEU:HD13	1:A:1162:PHE:CB	2.44	0.47
1:A:723:LEU:HD23	1:A:739:ALA:HB1	1.96	0.47
1:A:650:ASN:C	1:A:650:ASN:HD22	2.17	0.47
1:A:843:ASN:HB3	1:A:857:GLN:HG3	1.96	0.47
1:A:1052:ASP:OD1	1:A:1052:ASP:N	2.43	0.47
1:A:1023:ASP:HA	1:A:1043:LYS:HE2	1.96	0.46
1:A:1124:ARG:NH2	1:A:1126:LEU:HD21	2.30	0.46
1:A:1018:THR:OG1	1:A:1020:ARG:HG2	2.16	0.46
1:A:737:GLY:O	1:A:741:ASP:HB2	2.16	0.46
1:A:624:PRO:O	1:A:625:ARG:HB2	2.16	0.45
1:A:674:PRO:HD2	1:A:944:ILE:HG23	1.99	0.45
1:A:1021:ASP:HB3	1:A:1157:GLN:OE1	2.16	0.45
1:A:1031:TYR:HA	1:A:1037:PHE:HB3	1.98	0.45
1:A:697:LEU:HD13	1:A:1111:ARG:HB2	1.99	0.45
1:A:1096:TRP:CE2	1:A:1137:SER:HA	2.51	0.45
1:A:803:ILE:HG23	1:A:810:ASN:HD21	1.82	0.44
1:A:947:VAL:HB	1:A:1167:TYR:O	2.18	0.44
1:A:963:GLN:OE1	1:A:1149:ARG:NH2	2.37	0.43
1:A:743:ASP:OD2	1:A:746:ASN:HA	2.19	0.43
1:A:609:ARG:HD3	1:A:609:ARG:HA	1.85	0.42
1:A:922:ASP:HA	1:A:930:ASP:OD1	2.19	0.42
1:A:673:ASP:OD2	1:A:933:LYS:O	2.38	0.41
1:A:657:HIS:CD2	1:A:659:CYS:HB2	2.56	0.41
1:A:806:ASP:O	1:A:807:ASP:HB2	2.19	0.41
1:A:1110:TYR:CE2	1:A:1134:MSE:CE	3.00	0.41
1:A:892:GLN:HB3	1:A:897:ASP:HB2	2.03	0.41
1:A:893:GLY:O	1:A:894:ASP:C	2.59	0.41
1:A:1007:SER:HA	1:A:1118:PRO:HD2	2.03	0.41
1:A:1014:PHE:CE2	1:A:1025:ALA:HB3	2.55	0.41
1:A:1043:LYS:HE3	1:A:1083:TRP:CZ2	2.56	0.41
1:A:673:ASP:HA	1:A:674:PRO:HA	1.86	0.40
1:A:944:ILE:H	1:A:944:ILE:HG13	1.50	0.40
1:A:996:PRO:HD3	1:A:1155:PHE:CE2	2.57	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	619/634 (98%)	550 (89%)	57 (9%)	12 (2%)	8 15

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	597	VAL
1	A	598	PRO
1	A	609	ARG
1	A	716	ILE
1	A	584	ASN
1	A	608	PRO
1	A	706	VAL
1	A	811	GLU
1	A	973	THR
1	A	558	CYS
1	A	970	LYS
1	A	607	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	540/544 (99%)	483 (89%)	57 (11%)	6 12

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	551	ASP
1	A	554	LEU
1	A	565	SER
1	A	566	SER
1	A	573	SER
1	A	579	VAL
1	A	588	CYS
1	A	596	LEU
1	A	599	ASP
1	A	605	SER
1	A	606	LYS
1	A	609	ARG
1	A	619	CYS
1	A	620	LEU
1	A	627	ARG
1	A	640	LYS
1	A	641	THR
1	A	650	ASN
1	A	655	LYS
1	A	664	GLU
1	A	702	ASN
1	A	712	THR
1	A	716	ILE
1	A	717	LYS
1	A	742	ASP
1	A	750	THR
1	A	759	LEU
1	A	807	ASP
1	A	811	GLU
1	A	812	ARG
1	A	822	ASP
1	A	824	ARG
1	A	838	CYS
1	A	883	ASN
1	A	911	ASN
1	A	923	LEU
1	A	928	ARG
1	A	933	LYS
1	A	944	ILE
1	A	967	LEU
1	A	980	VAL
1	A	991	THR
1	A	1019	ASP

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Mol	Chain	Res	Type
1	A	1020	ARG
1	A	1021	ASP
1	A	1043	LYS
1	A	1048	THR
1	A	1051	GLU
1	A	1052	ASP
1	A	1065	LEU
1	A	1093	ARG
1	A	1119	LYS
1	A	1131	LYS
1	A	1134	MSE
1	A	1149	ARG
1	A	1155	PHE
1	A	1170	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	650	ASN
1	A	657	HIS
1	A	728	GLN
1	A	834	HIS
1	A	842	HIS
1	A	883	ASN
1	A	911	ASN
1	A	990	GLN
1	A	1091	GLN
1	A	1113	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

5 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	0.76	1 (7%)	17,19,21	1.29	1 (5%)
2	NAG	B	2	2	14,14,15	0.65	0	17,19,21	0.95	1 (5%)
2	MAN	B	3	2	11,11,12	0.63	0	15,15,17	1.83	3 (20%)
3	NAG	C	1	1,3	14,14,15	0.71	0	17,19,21	1.14	1 (5%)
3	NAG	C	2	3	14,14,15	0.50	0	17,19,21	0.70	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1
2	MAN	B	3	2	1/1/4/5	0/2/19/22	0/1/1/1
3	NAG	C	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	C1-C2	2.24	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3	MAN	C1-O5-C5	5.16	119.10	112.19
2	B	1	NAG	C1-O5-C5	4.09	117.67	112.19
2	B	3	MAN	C1-C2-C3	4.05	115.54	109.64
3	C	1	NAG	C4-C3-C2	3.08	115.53	111.02
2	B	2	NAG	O5-C1-C2	-2.47	107.47	111.29
2	B	3	MAN	O5-C1-C2	2.04	115.65	110.79

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	3	MAN	C1

All (16) torsion outliers are listed below:

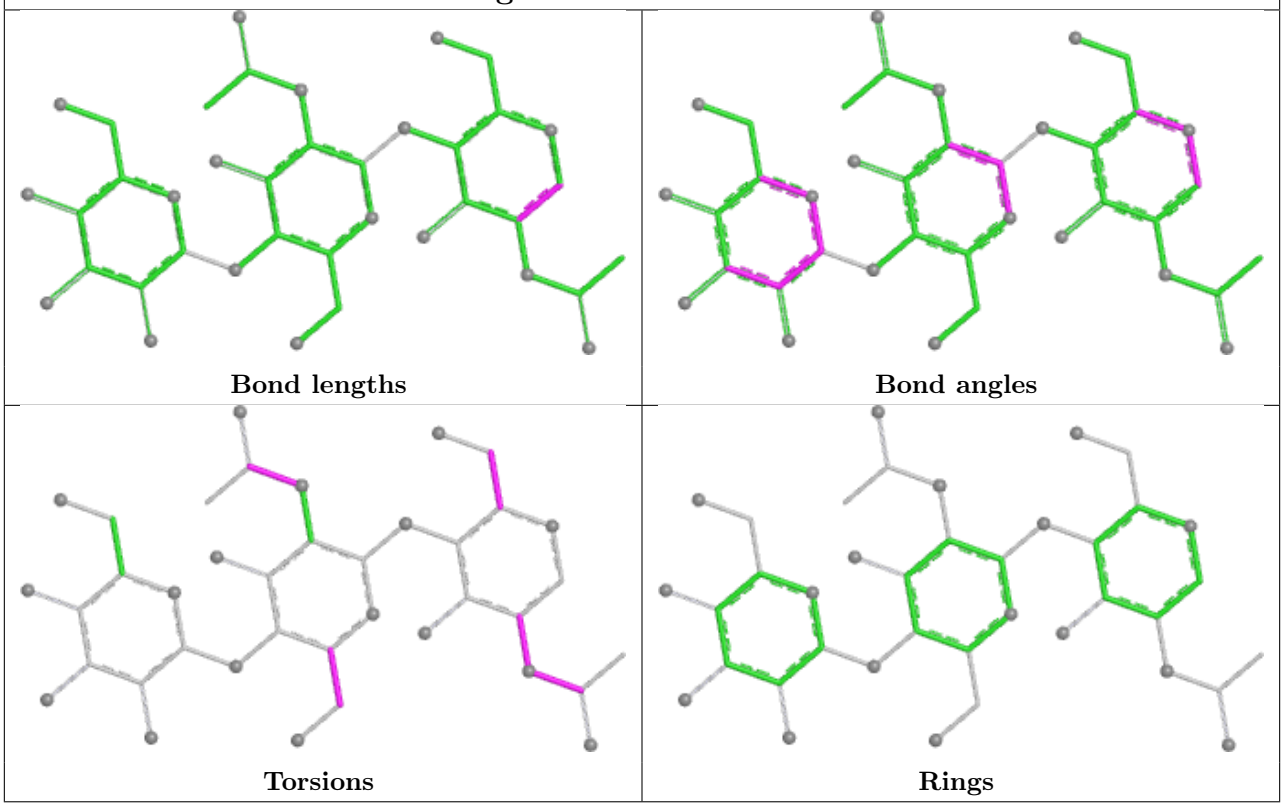
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
3	C	1	NAG	C8-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
3	C	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	1	NAG	C3-C2-N2-C7

There are no ring outliers.

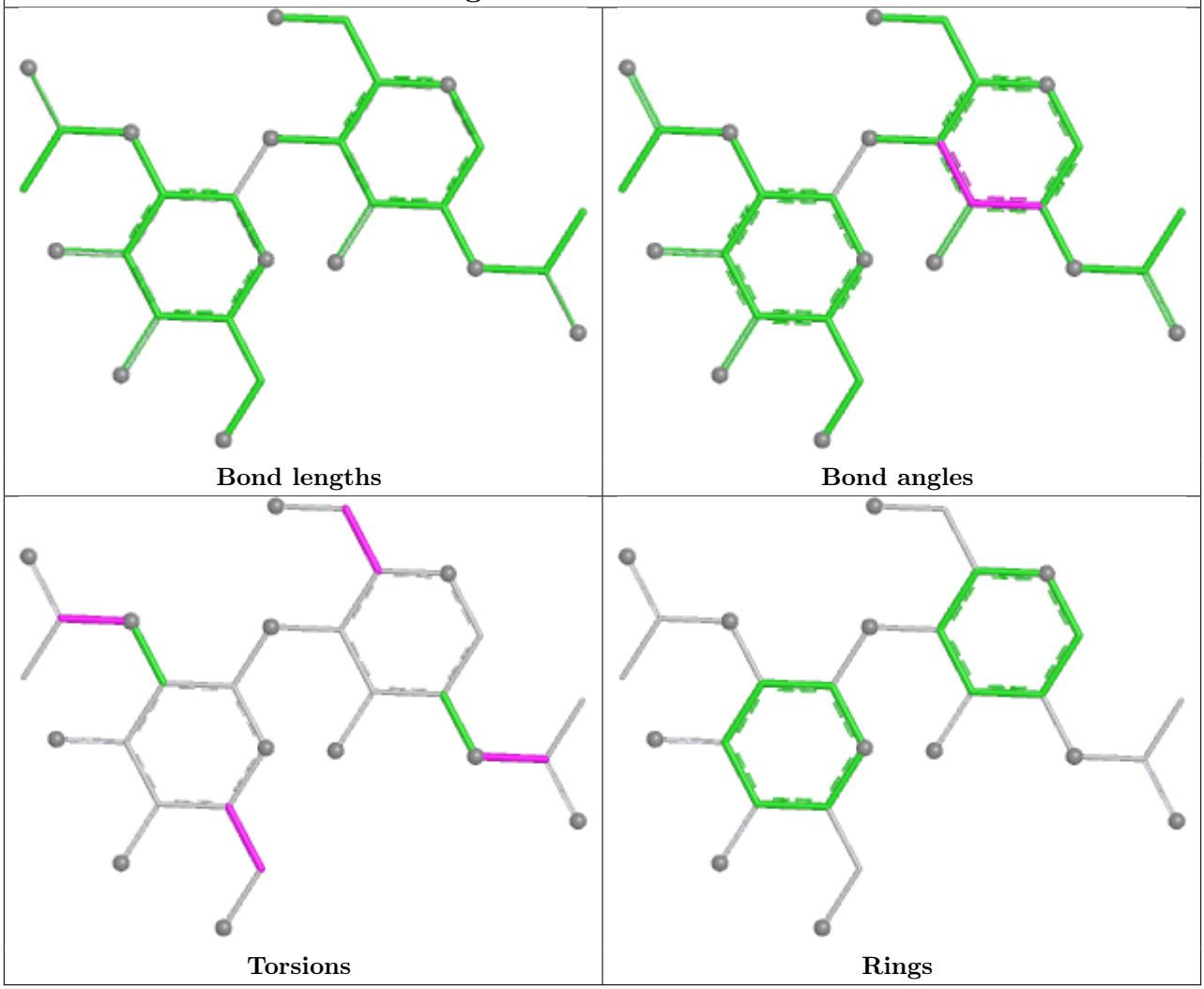
No monomer is involved in short contacts.

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

Oligosaccharide Chain B



Oligosaccharide Chain C



5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 30 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	7	1	14,14,15	0.61	0	17,19,21	1.21	2 (11%)
4	NAG	A	6	1	14,14,15	0.67	0	17,19,21	0.96	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	7	1	-	3/6/23/26	0/1/1/1
4	NAG	A	6	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	7	NAG	C1-O5-C5	3.73	117.18	112.19
4	A	7	NAG	O5-C1-C2	-2.08	108.07	111.29

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	6	NAG	C8-C7-N2-C2
4	A	6	NAG	O7-C7-N2-C2
4	A	7	NAG	C8-C7-N2-C2
4	A	7	NAG	O7-C7-N2-C2
4	A	6	NAG	C4-C5-C6-O6
4	A	6	NAG	O5-C5-C6-O6
4	A	7	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	6	NAG	5	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	616/634 (97%)	1.21	101 (16%) 1 1	40, 61, 122, 158	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	583	GLY	13.3
1	A	972	THR	10.6
1	A	973	THR	10.3
1	A	582	LEU	9.8
1	A	641	THR	8.7
1	A	634	VAL	8.3
1	A	607	VAL	8.2
1	A	1171	ASP	7.6
1	A	588	CYS	7.5
1	A	576	PHE	6.8
1	A	709	THR	6.2
1	A	566	SER	6.0
1	A	587	HIS	5.9
1	A	712	THR	5.6
1	A	603	SER	5.2
1	A	581	PHE	4.8
1	A	589	GLU	4.8
1	A	605	SER	4.7
1	A	551	ASP	4.6
1	A	1039	VAL	4.5
1	A	595	ALA	4.4
1	A	642	GLU	4.4
1	A	584	ASN	4.3
1	A	639	ALA	4.3
1	A	971	GLY	4.3
1	A	762	PRO	4.2
1	A	835	CYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	710	ASN	4.1
1	A	636	LEU	4.0
1	A	597	VAL	4.0
1	A	1040	VAL	3.9
1	A	637	GLU	3.8
1	A	580	GLY	3.8
1	A	708	ALA	3.8
1	A	713	TYR	3.7
1	A	640	LYS	3.7
1	A	604	THR	3.5
1	A	559	PHE	3.5
1	A	608	PRO	3.5
1	A	606	LYS	3.3
1	A	761	ASN	3.3
1	A	737	GLY	3.2
1	A	1042	TRP	3.2
1	A	586	THR	3.2
1	A	760	PHE	3.1
1	A	628	GLY	3.1
1	A	775	ARG	3.1
1	A	812	ARG	3.1
1	A	707	CYS	3.1
1	A	1025	ALA	3.0
1	A	556	ASN	3.0
1	A	711	ALA	3.0
1	A	1139	PRO	2.9
1	A	629	ASN	2.9
1	A	1045	VAL	2.9
1	A	585	GLY	2.9
1	A	615	PRO	2.9
1	A	752	GLU	2.8
1	A	769	LYS	2.8
1	A	970	LYS	2.8
1	A	1153	PHE	2.8
1	A	864	ILE	2.8
1	A	763	ARG	2.8
1	A	1065	LEU	2.8
1	A	1013	THR	2.8
1	A	834	HIS	2.8
1	A	1053	GLN	2.7
1	A	609	ARG	2.7
1	A	1063	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1082	LEU	2.6
1	A	1020	ARG	2.6
1	A	792	ASN	2.6
1	A	638	ALA	2.5
1	A	742	ASP	2.5
1	A	1044	GLN	2.5
1	A	767	TYR	2.5
1	A	942	PRO	2.4
1	A	1037	PHE	2.4
1	A	804	ASP	2.4
1	A	558	CYS	2.4
1	A	618	HIS	2.4
1	A	1024	TYR	2.3
1	A	1029	PHE	2.3
1	A	1062	GLY	2.3
1	A	899	ASP	2.3
1	A	652	CYS	2.2
1	A	1052	ASP	2.2
1	A	919	ASP	2.2
1	A	893	GLY	2.2
1	A	648	PRO	2.2
1	A	655	LYS	2.1
1	A	1064	SER	2.1
1	A	635	GLY	2.1
1	A	643	LYS	2.1
1	A	554	LEU	2.1
1	A	878	TYR	2.1
1	A	594	CYS	2.1
1	A	779	CYS	2.1
1	A	824	ARG	2.0
1	A	720	CYS	2.0
1	A	1033	SER	2.0

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

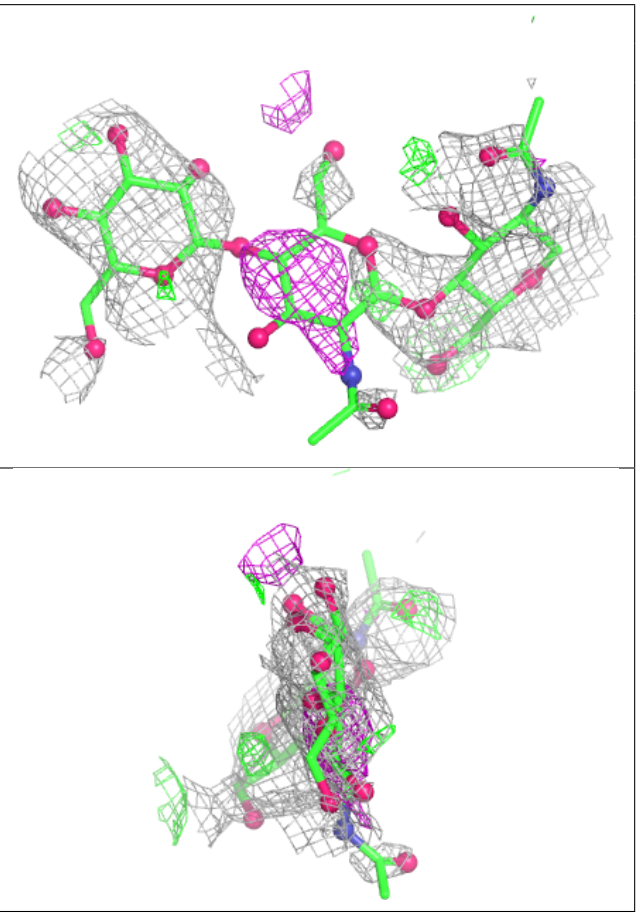
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	B	2	14/15	0.41	0.87	123,127,131,132	0
2	MAN	B	3	11/12	0.62	0.38	133,136,137,138	0
2	NAG	B	1	14/15	0.65	0.43	114,119,121,122	0
3	NAG	C	2	14/15	0.71	0.51	115,123,126,127	0
3	NAG	C	1	14/15	0.81	0.27	80,89,98,107	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.

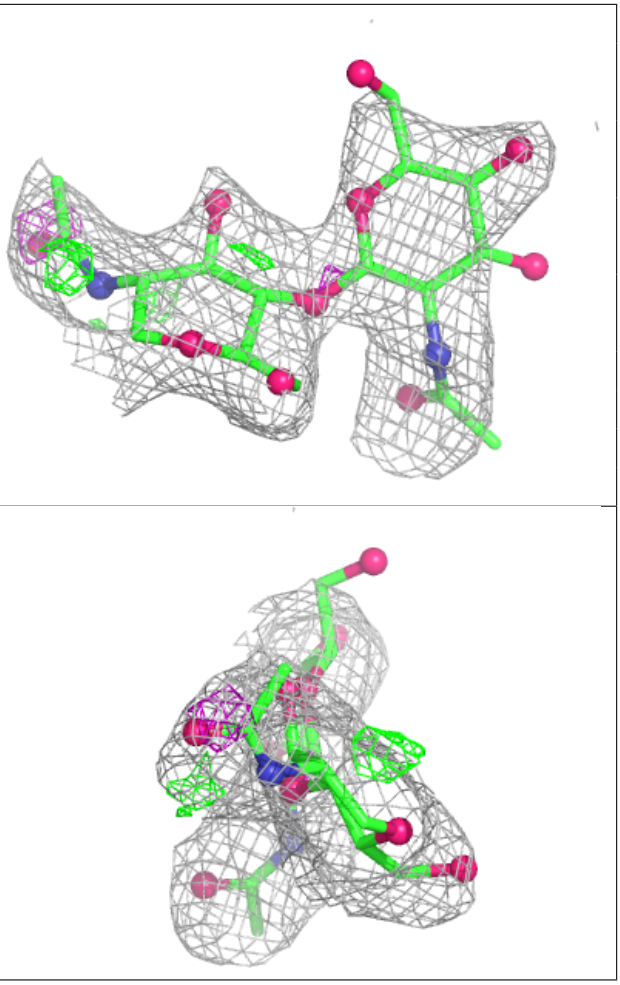
Electron density around Chain B:

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)



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	A	7	14/15	0.67	0.33	140,146,149,149	0
4	NAG	A	6	14/15	0.75	0.33	103,117,128,133	0
5	CA	A	1184	1/1	0.79	0.13	74,74,74,74	0
5	CA	A	1202	1/1	0.81	0.10	71,71,71,71	0
5	CA	A	1188	1/1	0.86	0.09	55,55,55,55	0
5	CA	A	1187	1/1	0.88	0.08	70,70,70,70	0
5	CA	A	1199	1/1	0.91	0.09	59,59,59,59	0
5	CA	A	1201	1/1	0.91	0.11	70,70,70,70	0
5	CA	A	1197	1/1	0.91	0.09	63,63,63,63	0
5	CA	A	1203	1/1	0.91	0.06	81,81,81,81	0
5	CA	A	1194	1/1	0.93	0.10	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CA	A	1206	1/1	0.93	0.11	62,62,62,62	0
5	CA	A	1207	1/1	0.93	0.07	65,65,65,65	0
5	CA	A	1208	1/1	0.93	0.10	58,58,58,58	0
5	CA	A	1210	1/1	0.93	0.13	51,51,51,51	0
5	CA	A	1205	1/1	0.94	0.15	72,72,72,72	0
5	CA	A	1211	1/1	0.94	0.06	116,116,116,116	0
5	CA	A	1182	1/1	0.95	0.07	46,46,46,46	0
5	CA	A	1186	1/1	0.95	0.14	58,58,58,58	0
5	CA	A	1200	1/1	0.96	0.05	62,62,62,62	0
5	CA	A	1209	1/1	0.96	0.14	45,45,45,45	0
5	CA	A	1204	1/1	0.97	0.13	70,70,70,70	0
5	CA	A	1189	1/1	0.97	0.07	61,61,61,61	0
5	CA	A	1192	1/1	0.97	0.10	55,55,55,55	0
5	CA	A	1183	1/1	0.97	0.08	50,50,50,50	0
5	CA	A	1196	1/1	0.98	0.11	52,52,52,52	0
5	CA	A	1193	1/1	0.98	0.07	57,57,57,57	0
5	CA	A	1198	1/1	0.98	0.10	50,50,50,50	0
5	CA	A	1191	1/1	0.98	0.07	53,53,53,53	0
5	CA	A	1190	1/1	0.99	0.11	63,63,63,63	0
5	CA	A	1195	1/1	0.99	0.11	53,53,53,53	0
5	CA	A	1185	1/1	0.99	0.13	57,57,57,57	0

6.5 Other polymers (i)

There are no such residues in this entry.