Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 05:06 PM BST

PDB ID	:	5KKB
Title	:	Structure of mouse Golgi alpha-1,2-mannosidase IA and Man9GlcNAc2-PA complex
Authors	:	Xiang, Y.; Moremen, K.W.
Deposited on	:	2016-06-21
Resolution	:	1.77 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

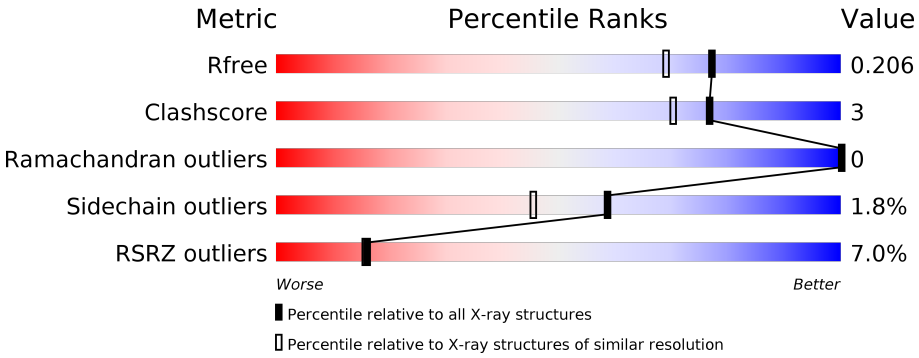
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.77 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	469	6% 93% 7%
1	B	469	8% 92% 8%
2	C	9	11% 89%
2	D	9	22% 78%

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	1PS	A	712	-	-	-	X
5	1PS	B	711	-	-	X	X

2 Entry composition

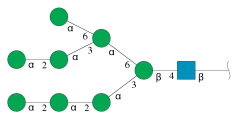
There are 7 unique types of molecules in this entry. The entry contains 8514 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Mannosyl-oligosaccharide 1,2-alpha-mannosidase IA.

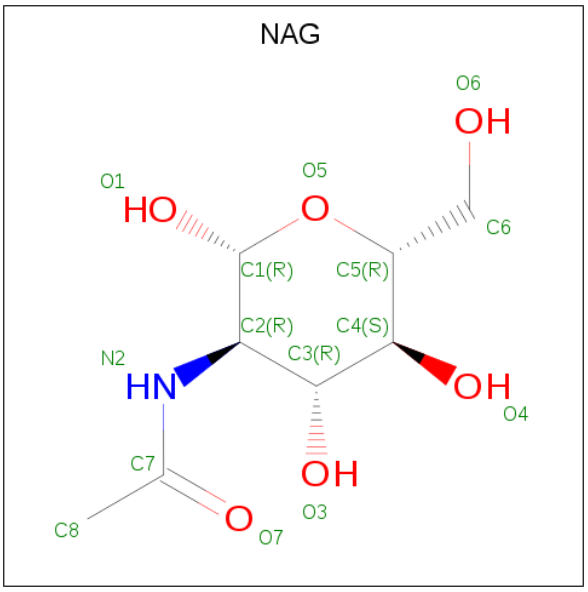
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	469	Total	C	N	O	S	0	5	0
			3820	2468	645	689	18			
1	B	469	Total	C	N	O	S	0	6	0
			3815	2470	639	688	18			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	0	0	0
			103	56	1	46			
2	D	9	Total	C	N	O	0	0	0
			103	56	1	46			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

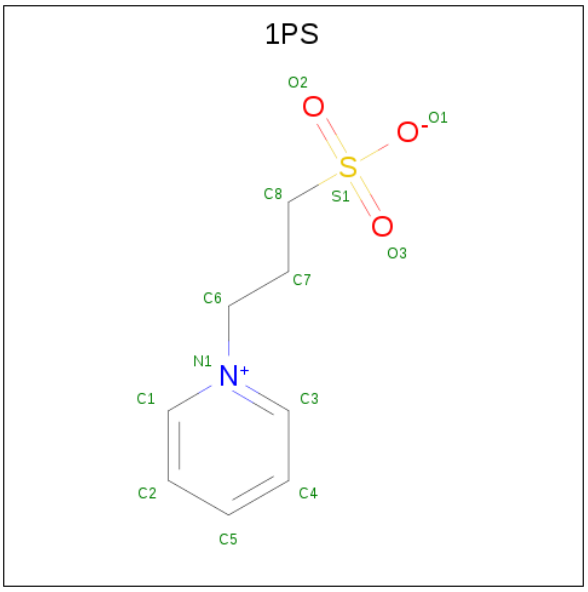


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is LANTHANUM (III) ION (three-letter code: LA) (formula: La).

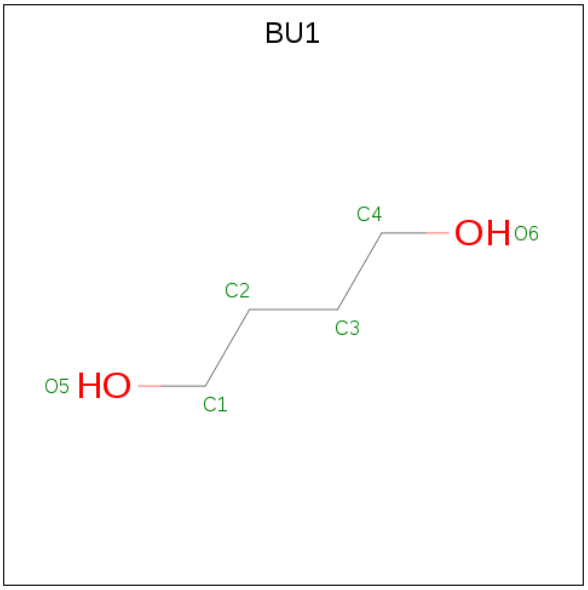
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total La 1 1	0	0
4	A	1	Total La 1 1	0	0

- Molecule 5 is 3-PYRIDINIUM-1-YLPROPANE-1-SULFONATE (three-letter code: 1PS) (formula: $C_8H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
5	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 6 is 1,4-BUTANEDIOL (three-letter code: BU1) (formula: $C_4H_{10}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	O		0	0
			6	4	2			

- Molecule 7 is water.

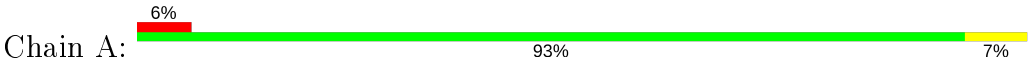
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	305	Total O 305 305	0	0
7	B	306	Total O 306 306	0	0

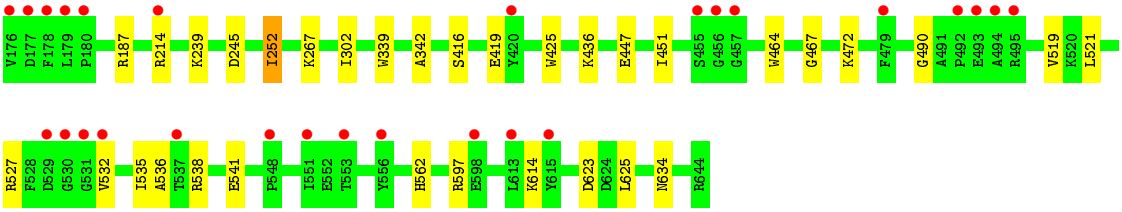
3 Residue-property plots (i)

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: Mannosyl-oligosaccharide 1,2-alpha-mannosidase IA

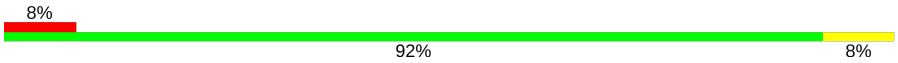
Chain A:

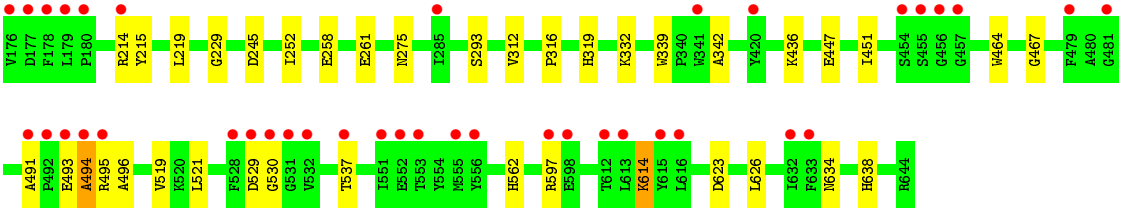




• Molecule 1: Mannosyl-oligosaccharide 1,2-alpha-mannosidase IA

Chain B:



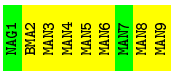


• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:


NAG1
BMA2
MAN3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	94.95Å 131.49Å 87.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.84 – 1.77 41.76 – 1.77	Depositor EDS
% Data completeness (in resolution range)	94.8 (39.84-1.77) 91.3 (41.76-1.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.66 (at 1.77Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.161 , 0.191 0.180 , 0.206	Depositor DCC
R_{free} test set	1999 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å^2)	18.2	Xtriage
Anisotropy	1.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8514	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 82.82 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5372e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, LA, BU1, 1PS, 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	0.38	0/3928	0.54	0/5315
1	B	0.38	0/3926	0.54	0/5315
All	All	0.38	0/7854	0.54	0/10630

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	B	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	B	494	ALA	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3820	0	3731	17	0
1	B	3815	0	3735	24	0
2	C	103	0	85	0	0
2	D	103	0	85	0	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	13	0	11	2	0
5	B	13	0	11	7	0
6	B	6	0	10	1	0
7	A	305	0	0	3	0
7	B	306	0	0	2	0
All	All	8514	0	7694	46	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 3.

All (46) 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:B:623:ASP:H	6:B:713:BU1:H22	1.31	0.96
5:B:711:1PS:H2	7:B:943:HOH:O	1.84	0.77
1:A:267:LYS:HG2	1:A:302:ILE:HG12	1.73	0.69
1:B:316:PRO:HD3	5:B:711:1PS:O1	1.98	0.64
1:B:530:GLY:O	7:B:801:HOH:O	2.16	0.63
1:A:519:VAL:HG23	1:A:521:LEU:H	1.72	0.53
1:B:252[B]:ILE:HD11	1:B:614:LYS:HG3	1.90	0.53
1:B:519:VAL:HG23	1:B:521:LEU:H	1.74	0.52
1:B:219:LEU:HD13	1:B:229:GLY:HA3	1.91	0.52
1:B:562:HIS:NE2	1:B:623:ASP:OD2	2.43	0.51
1:B:319:HIS:ND1	5:B:711:1PS:H5	2.26	0.50
1:B:275:ASN:OD1	1:B:332:LYS:HD2	2.12	0.50
5:A:712:1PS:H4	7:A:901:HOH:O	2.11	0.49
1:B:464:TRP:CE2	1:B:467:GLY:HA2	2.48	0.49
1:B:447:GLU:HG2	1:B:451:ILE:HD12	1.95	0.49
1:A:464:TRP:CE2	1:A:467:GLY:HA2	2.48	0.49
1:A:252:ILE:HD11	1:A:625:LEU:HG	1.95	0.48
1:B:494:ALA:HA	1:B:496:ALA:H	1.78	0.48
1:B:252[A]:ILE:CD1	1:B:626:LEU:HD11	2.44	0.48
1:B:493:GLU:HA	1:B:494:ALA:HA	1.60	0.47
1:B:214:ARG:HG2	1:B:215:TYR:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:HIS:NE2	1:A:623:ASP:OD2	2.47	0.47
5:B:711:1PS:O1	5:B:711:1PS:H61	2.14	0.46
1:B:562:HIS:CE1	1:B:623:ASP:OD2	2.69	0.46
1:B:339:TRP:HB2	1:B:342:ALA:HB2	1.97	0.46
1:A:532:VAL:HB	1:A:535:ILE:HD13	1.98	0.45
1:B:312:VAL:HG13	5:B:711:1PS:O3	2.17	0.45
1:A:267:LYS:HE2	1:A:302:ILE:HG21	1.98	0.45
1:A:536:ALA:HB1	1:A:541[A]:GLU:HG3	1.99	0.44
1:B:258:GLU:O	1:B:261:GLU:HG2	2.18	0.44
5:A:712:1PS:H61	7:A:845:HOH:O	2.17	0.44
1:B:493:GLU:HB2	1:B:496:ALA:HB2	1.99	0.44
1:A:447:GLU:HG2	1:A:451:ILE:HD12	1.99	0.43
1:A:472:LYS:HD3	1:A:527:ARG:CZ	2.48	0.43
5:B:711:1PS:H71	5:B:711:1PS:H3	1.77	0.43
1:A:425:TRP:HH2	1:A:490:GLY:HA3	1.85	0.42
1:B:319:HIS:HB2	5:B:711:1PS:H5	2.01	0.42
1:B:436:LYS:NZ	1:B:491:ALA:HB3	2.35	0.42
1:A:562:HIS:CE1	1:A:623:ASP:OD2	2.72	0.42
1:A:416:SER:HA	1:A:419:GLU:HB3	2.02	0.41
1:B:562:HIS:HE2	1:B:623:ASP:CG	2.22	0.41
1:A:425:TRP:CD1	1:A:436:LYS:HB2	2.56	0.41
1:A:339:TRP:HB2	1:A:342:ALA:HB2	2.03	0.41
1:A:538:ARG:O	1:A:541[A]:GLU:HG2	2.21	0.41
1:A:239:LYS:NZ	7:A:805:HOH:O	2.43	0.40
1:B:293[B]:SER:OG	1:B:638:HIS:HB3	2.21	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	472/469 (101%)	459 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	473/469 (101%)	460 (97%)	13 (3%)	0	100 100
All	All	945/938 (101%)	919 (97%)	26 (3%)	0	100 100

There are no Ramachandran outliers to report.

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	397/392 (101%)	390 (98%)	7 (2%)	59 45
1	B	398/392 (102%)	391 (98%)	7 (2%)	59 45
All	All	795/784 (101%)	781 (98%)	14 (2%)	59 45

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187	ARG
1	A	214	ARG
1	A	245	ASP
1	A	252	ILE
1	A	597	ARG
1	A	614	LYS
1	A	634	ASN
1	B	245	ASP
1	B	495	ARG
1	B	529	ASP
1	B	537	THR
1	B	597	ARG
1	B	614	LYS
1	B	634	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

18 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	C	1	2	15,15,15	0.19	0	21,21,21	0.21	0
2	BMA	C	2	2	11,11,12	0.95	1 (9%)	15,15,17	1.03	0
2	MAN	C	3	2	11,11,12	0.80	0	15,15,17	1.05	1 (6%)
2	MAN	C	4	2	11,11,12	0.93	0	15,15,17	1.01	2 (13%)
2	MAN	C	5	2,4	11,11,12	1.11	1 (9%)	15,15,17	2.00	3 (20%)
2	MAN	C	6	2	11,11,12	0.81	1 (9%)	15,15,17	1.06	1 (6%)
2	MAN	C	7	2	11,11,12	0.86	0	15,15,17	1.02	1 (6%)
2	MAN	C	8	2	11,11,12	0.86	0	15,15,17	0.90	1 (6%)
2	MAN	C	9	2	11,11,12	0.83	0	15,15,17	1.02	1 (6%)
2	NAG	D	1	2	15,15,15	0.22	0	21,21,21	0.40	0
2	BMA	D	2	2	11,11,12	1.10	1 (9%)	15,15,17	1.17	2 (13%)
2	MAN	D	3	2	11,11,12	1.09	0	15,15,17	0.94	1 (6%)
2	MAN	D	4	2	11,11,12	1.11	2 (18%)	15,15,17	1.13	2 (13%)
2	MAN	D	5	2,4	11,11,12	1.23	1 (9%)	15,15,17	2.03	4 (26%)
2	MAN	D	6	2	11,11,12	0.67	0	15,15,17	1.00	1 (6%)
2	MAN	D	7	2	11,11,12	0.86	0	15,15,17	1.07	0
2	MAN	D	8	2	11,11,12	0.75	0	15,15,17	0.91	1 (6%)
2	MAN	D	9	2	11,11,12	0.86	0	15,15,17	1.02	2 (13%)

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	C	1	2	-	0/6/26/26	0/1/1/1
2	BMA	C	2	2	-	0/2/19/22	0/1/1/1
2	MAN	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2,4	-	0/2/19/22	0/1/1/1
2	MAN	C	6	2	-	0/2/19/22	0/1/1/1
2	MAN	C	7	2	-	2/2/19/22	0/1/1/1
2	MAN	C	8	2	-	0/2/19/22	0/1/1/1
2	MAN	C	9	2	-	0/2/19/22	0/1/1/1
2	NAG	D	1	2	-	0/6/26/26	0/1/1/1
2	BMA	D	2	2	-	0/2/19/22	0/1/1/1
2	MAN	D	3	2	-	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1
2	MAN	D	5	2,4	-	0/2/19/22	0/1/1/1
2	MAN	D	6	2	-	0/2/19/22	0/1/1/1
2	MAN	D	7	2	-	2/2/19/22	0/1/1/1
2	MAN	D	8	2	-	0/2/19/22	0/1/1/1
2	MAN	D	9	2	-	0/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	5	MAN	O5-C5	2.69	1.48	1.43
2	D	5	MAN	O5-C5	2.59	1.48	1.43
2	D	2	BMA	C1-C2	2.40	1.57	1.52
2	D	4	MAN	C2-C3	2.28	1.55	1.52
2	C	2	BMA	C1-C2	2.17	1.57	1.52
2	D	4	MAN	O5-C5	2.10	1.47	1.43
2	C	6	MAN	O5-C1	-2.09	1.40	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	5	MAN	C1-O5-C5	5.43	119.55	112.19
2	D	5	MAN	C1-O5-C5	5.43	119.54	112.19
2	C	5	MAN	O5-C5-C6	3.84	113.22	107.20
2	D	5	MAN	O5-C5-C6	3.69	112.99	107.20
2	C	3	MAN	O2-C2-C3	-2.94	104.25	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	9	MAN	C1-O5-C5	2.77	115.95	112.19
2	D	5	MAN	O5-C1-C2	2.77	115.05	110.77
2	D	9	MAN	C1-O5-C5	2.72	115.87	112.19
2	C	6	MAN	O2-C2-C3	-2.72	104.70	110.14
2	D	5	MAN	O2-C2-C3	-2.69	104.75	110.14
2	D	4	MAN	C1-O5-C5	2.68	115.82	112.19
2	D	4	MAN	O2-C2-C3	-2.67	104.79	110.14
2	C	4	MAN	C1-O5-C5	2.53	115.62	112.19
2	D	6	MAN	O2-C2-C3	-2.40	105.33	110.14
2	D	3	MAN	O2-C2-C3	-2.36	105.40	110.14
2	C	5	MAN	O5-C1-C2	2.31	114.33	110.77
2	D	2	BMA	O2-C2-C1	2.22	113.70	109.15
2	D	2	BMA	O2-C2-C3	-2.18	105.77	110.14
2	D	8	MAN	O2-C2-C3	-2.16	105.81	110.14
2	C	7	MAN	C1-O5-C5	2.13	115.07	112.19
2	C	4	MAN	O2-C2-C3	-2.12	105.90	110.14
2	D	9	MAN	O2-C2-C3	-2.07	105.99	110.14
2	C	8	MAN	C1-O5-C5	2.03	114.95	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

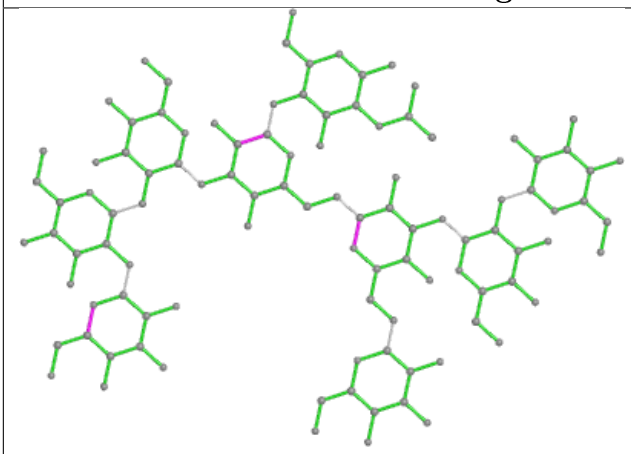
Mol	Chain	Res	Type	Atoms
2	C	7	MAN	O5-C5-C6-O6
2	D	7	MAN	O5-C5-C6-O6
2	C	7	MAN	C4-C5-C6-O6
2	D	7	MAN	C4-C5-C6-O6

There are no ring outliers.

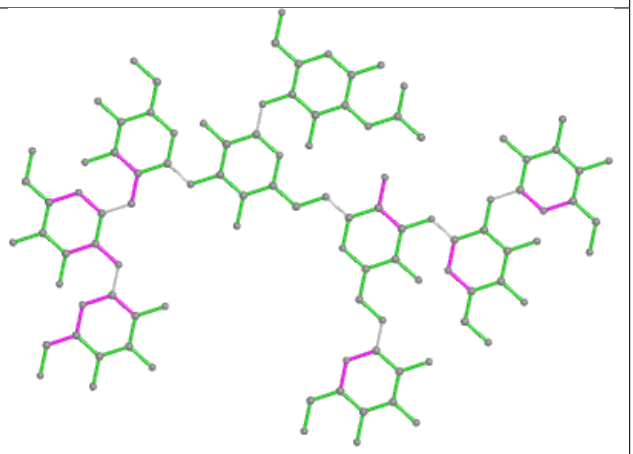
No monomer is involved in short contacts.

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

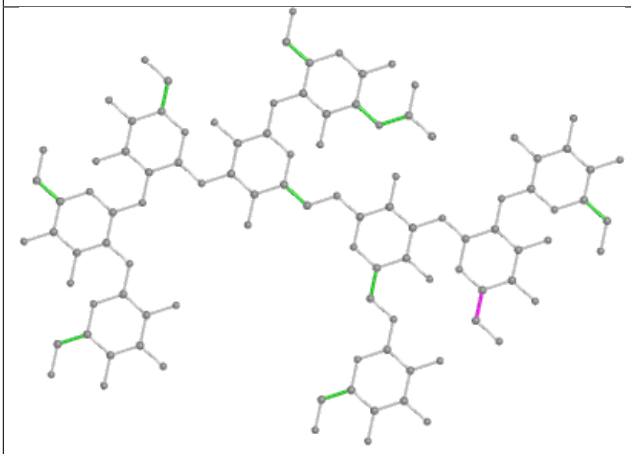
Oligosaccharide Chain C



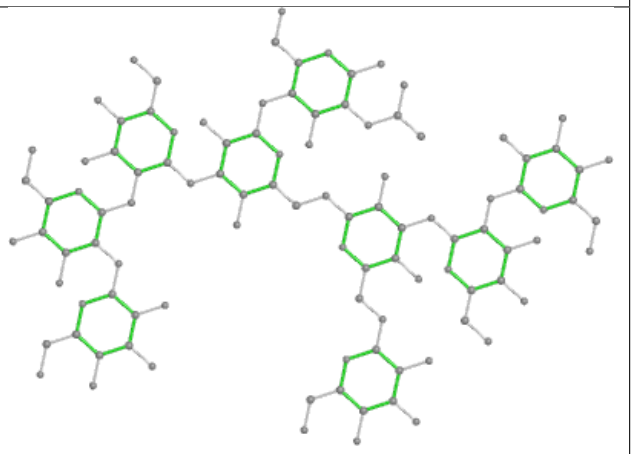
Bond lengths



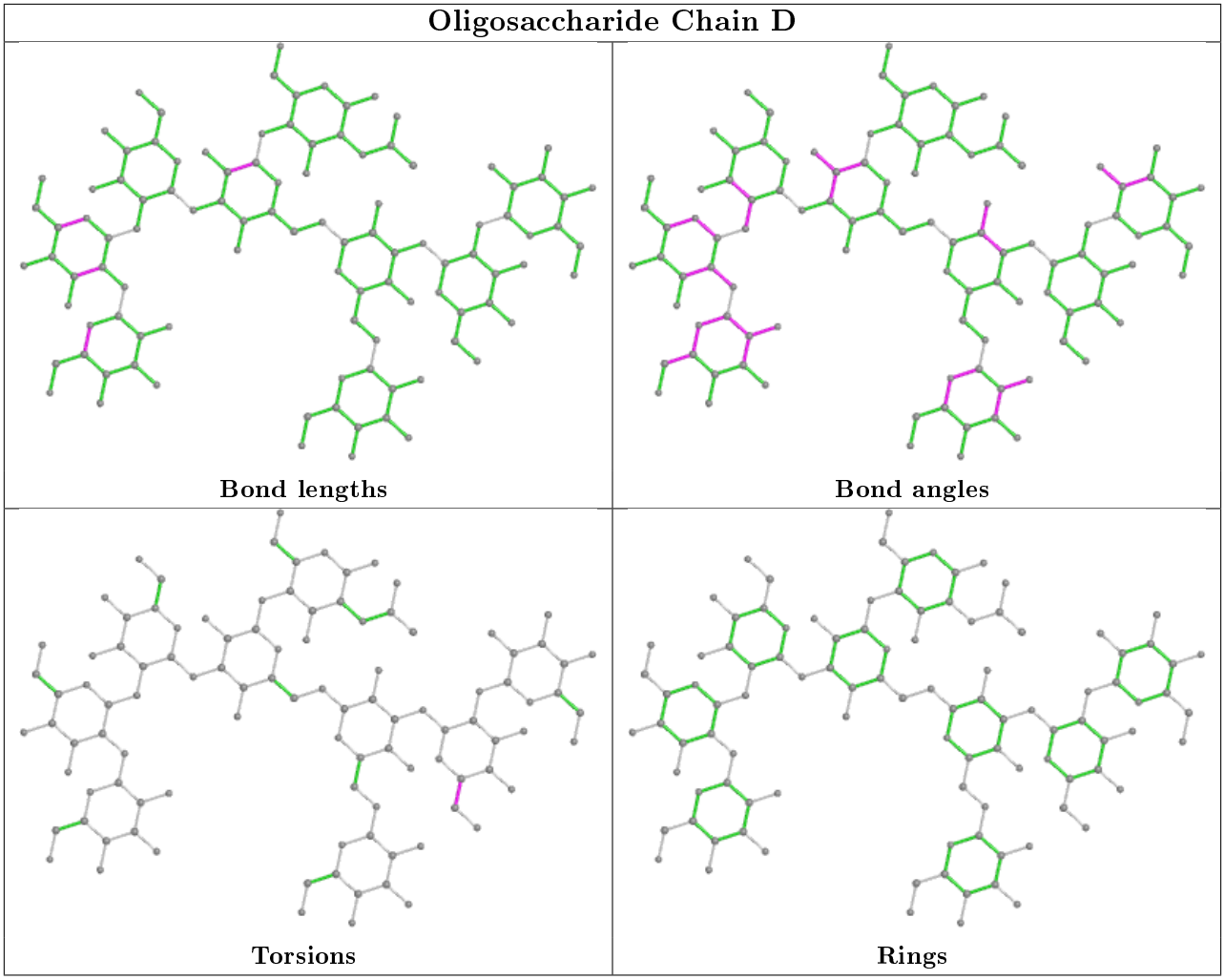
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
5	1PS	A	712	-	13,13,13	1.50	3 (23%)	17,17,17	1.73	4 (23%)
5	1PS	B	711	-	13,13,13	1.35	2 (15%)	17,17,17	2.37	6 (35%)
3	NAG	B	710	1	14,14,15	0.19	0	17,19,21	0.51	0
3	NAG	A	710	1	14,14,15	0.24	0	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	BU1	B	713	-	5,5,5	0.32	0	4,4,4	0.62	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
5	1PS	A	712	-	-	1/7/7/7	0/1/1/1
5	1PS	B	711	-	-	5/7/7/7	0/1/1/1
3	NAG	B	710	1	-	0/6/23/26	0/1/1/1
3	NAG	A	710	1	-	0/6/23/26	0/1/1/1
6	BU1	B	713	-	-	0/3/3/3	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	712	1PS	C8-S1	3.46	1.82	1.77
5	B	711	1PS	C8-S1	3.01	1.81	1.77
5	A	712	1PS	O3-S1	2.48	1.52	1.45
5	B	711	1PS	O2-S1	2.33	1.51	1.45
5	A	712	1PS	O2-S1	2.21	1.51	1.45

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	711	1PS	O1-S1-C8	5.99	115.45	105.77
5	A	712	1PS	O3-S1-C8	4.68	112.56	106.92
5	B	711	1PS	O1-S1-O2	-4.38	100.58	111.27
5	B	711	1PS	O2-S1-C8	4.10	111.85	106.92
5	A	712	1PS	O2-S1-C8	3.40	111.01	106.92
5	A	712	1PS	O3-S1-O2	-3.24	102.72	113.95
5	B	711	1PS	C7-C8-S1	-2.57	109.31	113.25
5	B	711	1PS	C7-C6-N1	-2.30	105.27	111.64
5	B	711	1PS	C1-C2-C5	2.29	122.27	118.85
5	A	712	1PS	O1-S1-C8	2.02	109.03	105.77

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	711	1PS	C7-C8-S1-O1
5	B	711	1PS	C7-C6-N1-C3
5	B	711	1PS	C7-C6-N1-C1
5	B	711	1PS	C7-C8-S1-O2
5	B	711	1PS	C7-C8-S1-O3
5	A	712	1PS	N1-C6-C7-C8

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	712	1PS	2	0
5	B	711	1PS	7	0
6	B	713	BU1	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	469/469 (100%)	0.34	27 (5%)	23	22	14, 25, 50, 114	1 (0%)
1	B	469/469 (100%)	0.52	39 (8%)	11	11	14, 26, 51, 116	0
All	All	938/938 (100%)	0.43	66 (7%)	16	16	14, 26, 51, 116	1 (0%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	491	ALA	13.1
1	A	531	GLY	11.1
1	A	532	VAL	9.7
1	A	494	ALA	8.6
1	B	531	GLY	8.5
1	B	532	VAL	7.1
1	B	177	ASP	5.9
1	B	494	ALA	5.7
1	B	492	PRO	5.4
1	B	178	PHE	5.2
1	B	493	GLU	5.1
1	A	530	GLY	4.8
1	A	179	LEU	4.8
1	A	492	PRO	4.7
1	B	179	LEU	4.7
1	A	177	ASP	4.2
1	A	176	VAL	4.0
1	A	493	GLU	4.0
1	A	456	GLY	3.6
1	B	556	TYR	3.4
1	A	178	PHE	3.4
1	B	528	PHE	3.4
1	B	176	VAL	3.3
1	A	455	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	457	GLY	3.1
1	B	530	GLY	3.0
1	B	633	PHE	3.0
1	B	180	PRO	3.0
1	A	598	GLU	2.9
1	B	598	GLU	2.9
1	A	180	PRO	2.8
1	B	341	TRP	2.8
1	B	456	GLY	2.8
1	B	597	ARG	2.7
1	A	548	PRO	2.7
1	B	455	SER	2.7
1	B	615	TYR	2.7
1	B	613	LEU	2.7
1	A	615	TYR	2.7
1	A	556	TYR	2.6
1	B	479	PHE	2.6
1	A	551	ILE	2.6
1	A	613	LEU	2.5
1	A	457	GLY	2.5
1	B	537	THR	2.5
1	B	555[A]	MET	2.5
1	A	537	THR	2.5
1	B	616	LEU	2.5
1	A	495	ARG	2.5
1	B	529	ASP	2.5
1	A	214	ARG	2.4
1	B	214	ARG	2.4
1	B	285	ILE	2.4
1	B	420	TYR	2.4
1	A	420	TYR	2.3
1	A	553	THR	2.3
1	A	479	PHE	2.3
1	B	553	THR	2.2
1	A	529	ASP	2.2
1	B	551	ILE	2.2
1	B	454	SER	2.1
1	B	612	THR	2.1
1	B	552	GLU	2.1
1	B	632	ILE	2.1
1	B	481	GLY	2.1
1	B	495	ARG	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)

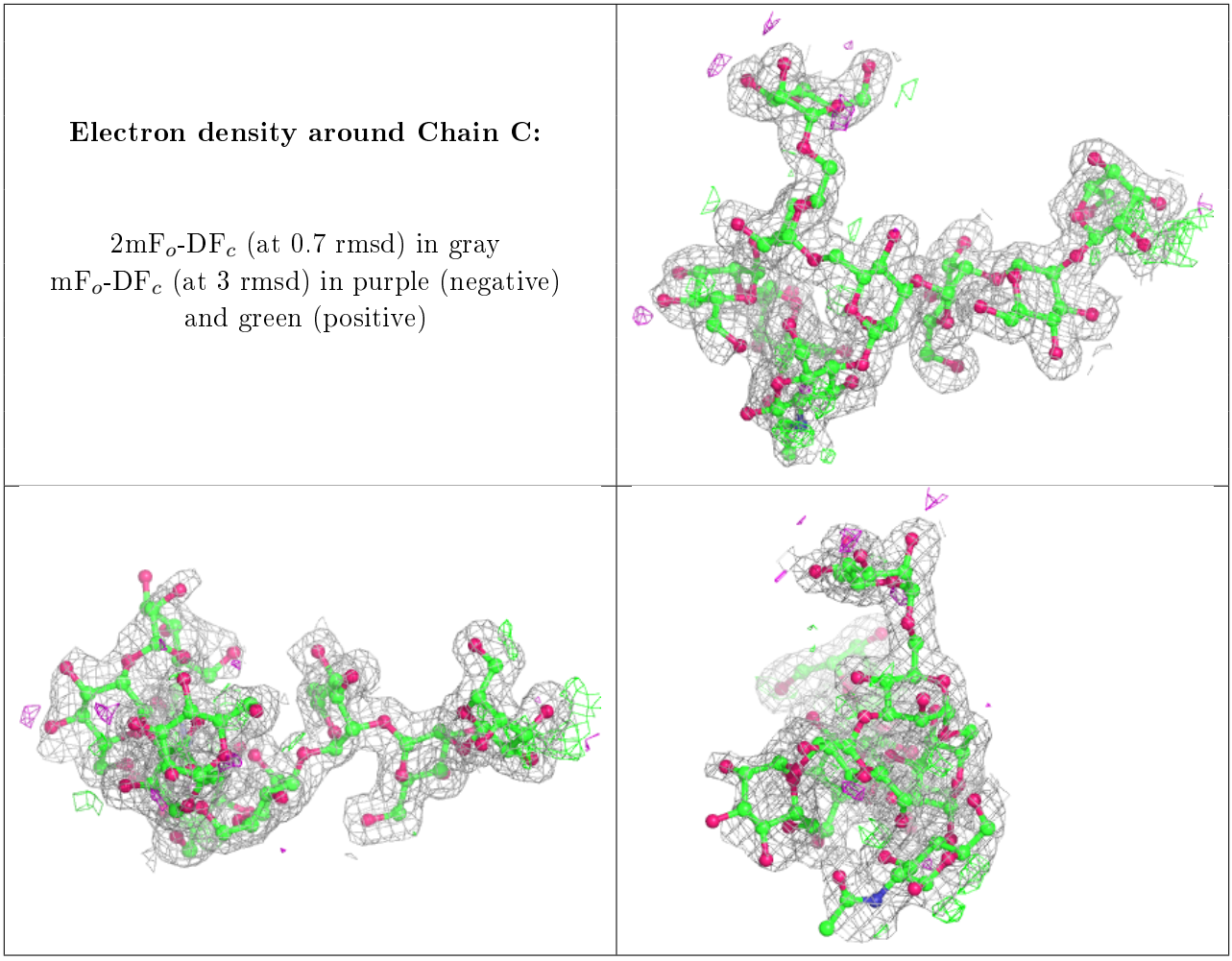
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MAN	C	8	11/12	0.77	0.22	64,66,71,75	0
2	MAN	D	7	11/12	0.84	0.15	52,58,61,62	0
2	NAG	D	1	15/15	0.85	0.17	25,38,57,66	0
2	MAN	D	8	11/12	0.86	0.20	63,69,71,72	0
2	MAN	C	7	11/12	0.87	0.15	49,58,61,64	0
2	MAN	D	9	11/12	0.89	0.12	31,37,41,45	0
2	NAG	C	1	15/15	0.90	0.14	27,40,65,67	0
2	MAN	C	9	11/12	0.90	0.15	32,39,44,44	0
2	MAN	D	5	11/12	0.93	0.16	12,16,20,23	0
2	MAN	C	6	11/12	0.94	0.12	27,31,39,41	0
2	MAN	D	6	11/12	0.94	0.12	29,33,43,45	0
2	MAN	C	5	11/12	0.94	0.18	10,15,21,24	0
2	BMA	C	2	11/12	0.96	0.06	18,22,27,28	0
2	MAN	C	3	11/12	0.96	0.08	13,17,26,32	0
2	MAN	D	3	11/12	0.97	0.07	16,18,29,29	0
2	MAN	C	4	11/12	0.98	0.15	12,15,18,18	0
2	BMA	D	2	11/12	0.98	0.06	17,20,26,26	0
2	MAN	D	4	11/12	0.98	0.14	13,15,17,18	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.

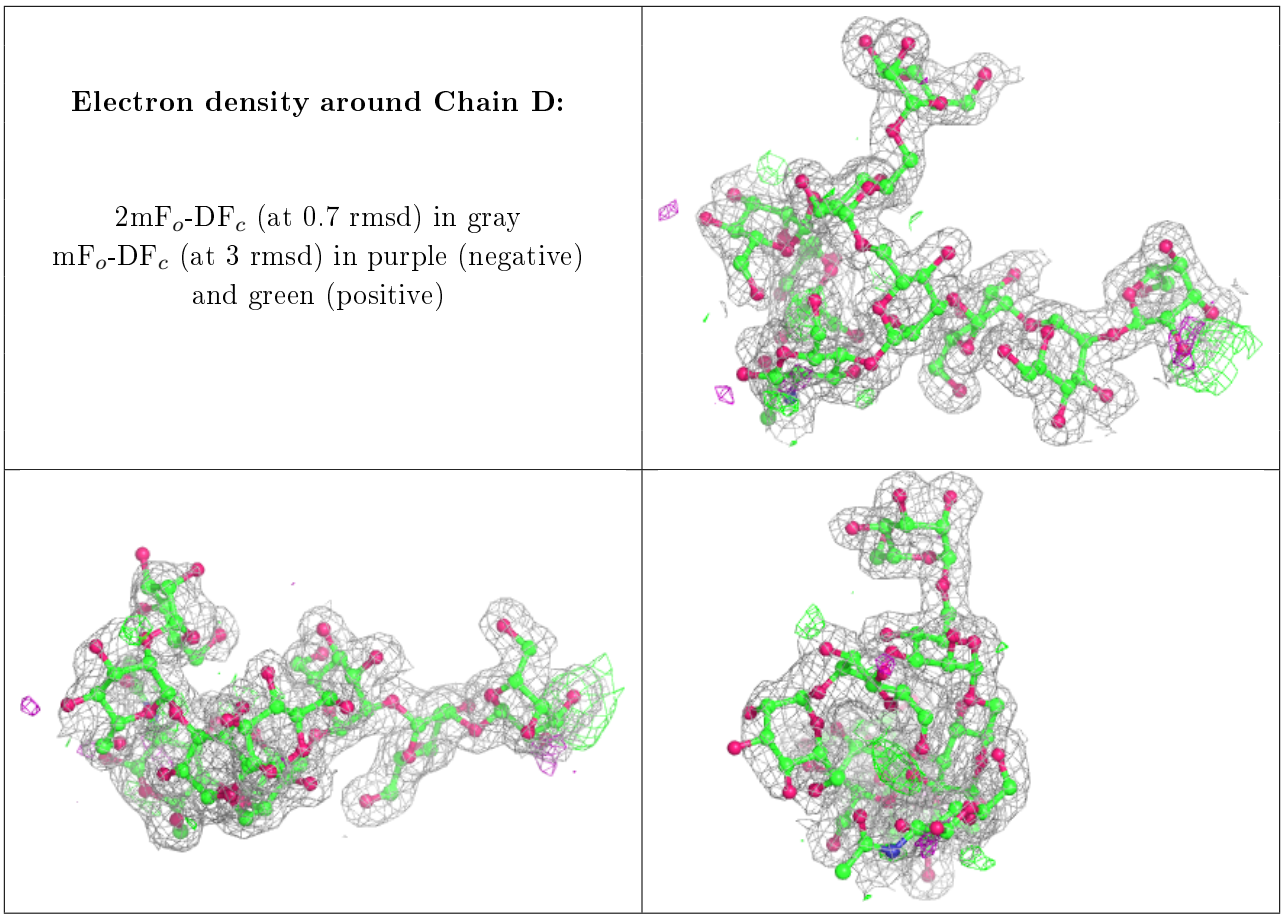
Electron density around Chain C:

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



Electron density around Chain D:

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



6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	1PS	A	712	13/13	0.53	0.44	30,43,59,61	13
5	1PS	B	711	13/13	0.70	0.43	30,37,55,57	13
3	NAG	B	710	14/15	0.86	0.20	37,52,59,62	0
6	BU1	B	713	6/6	0.87	0.12	38,44,48,55	0
3	NAG	A	710	14/15	0.88	0.19	39,51,57,60	0
4	LA	A	711	1/1	1.00	0.13	11,11,11,11	1
4	LA	B	712	1/1	1.00	0.14	11,11,11,11	1

6.5 Other polymers

There are no such residues in this entry.