



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 03:07 AM BST

PDB ID : 5OJ2
Title : Crystal structure of the chicken MDGA1 ectodomain
Authors : Elegheert, J.; Clayton, A.J.; Aricescu, A.R.
Deposited on : 2017-07-20
Resolution : 3.20 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

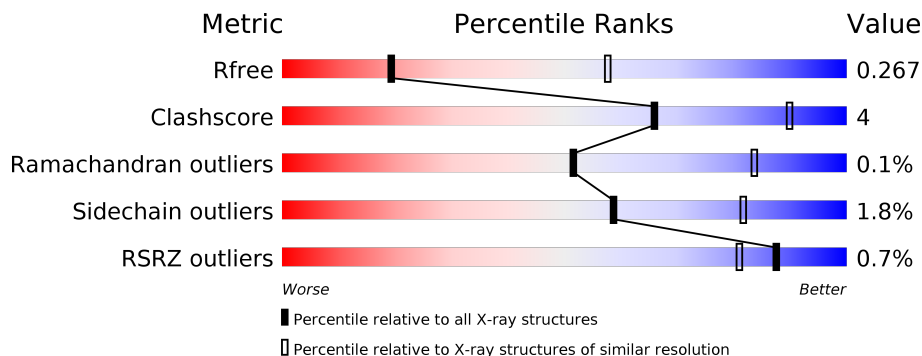
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 $\leq 5\%$. 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	910	
1	B	910	
2	C	3	
3	D	4	

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
4	NAG	B	1011	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11087 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 MAM domain-containing glycosylphosphatidylinositol anchor protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	691	5384	3396	930	1031	16	11	0	0	0
1	B	692	5404	3412	935	1030	16	11	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	LYS	ARG	conflict	UNP Q0WYX8
A	920	GLY	-	expression tag	UNP Q0WYX8
A	921	THR	-	expression tag	UNP Q0WYX8
A	922	LYS	-	expression tag	UNP Q0WYX8
A	923	HIS	-	expression tag	UNP Q0WYX8
A	924	HIS	-	expression tag	UNP Q0WYX8
A	925	HIS	-	expression tag	UNP Q0WYX8
A	926	HIS	-	expression tag	UNP Q0WYX8
A	927	HIS	-	expression tag	UNP Q0WYX8
A	928	HIS	-	expression tag	UNP Q0WYX8
B	120	LYS	ARG	engineered mutation	UNP Q0WYX8
B	920	GLY	-	expression tag	UNP Q0WYX8
B	921	THR	-	expression tag	UNP Q0WYX8
B	922	LYS	-	expression tag	UNP Q0WYX8
B	923	HIS	-	expression tag	UNP Q0WYX8
B	924	HIS	-	expression tag	UNP Q0WYX8
B	925	HIS	-	expression tag	UNP Q0WYX8
B	926	HIS	-	expression tag	UNP Q0WYX8
B	927	HIS	-	expression tag	UNP Q0WYX8
B	928	HIS	-	expression tag	UNP Q0WYX8

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



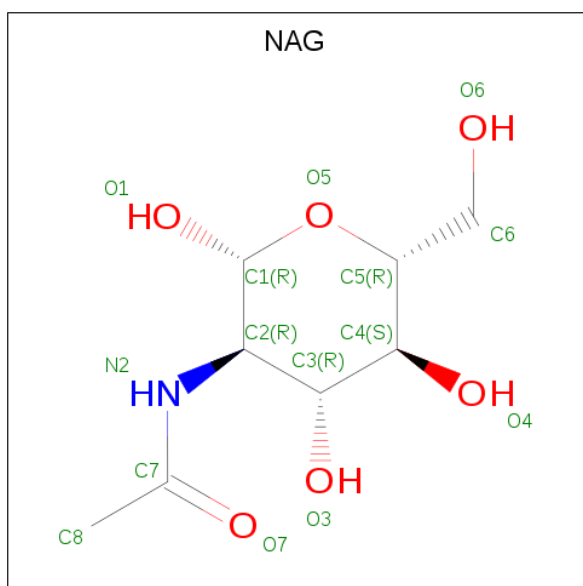
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	3	39	22	2	15	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos e-(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			
3	D	4	50	28	2	20	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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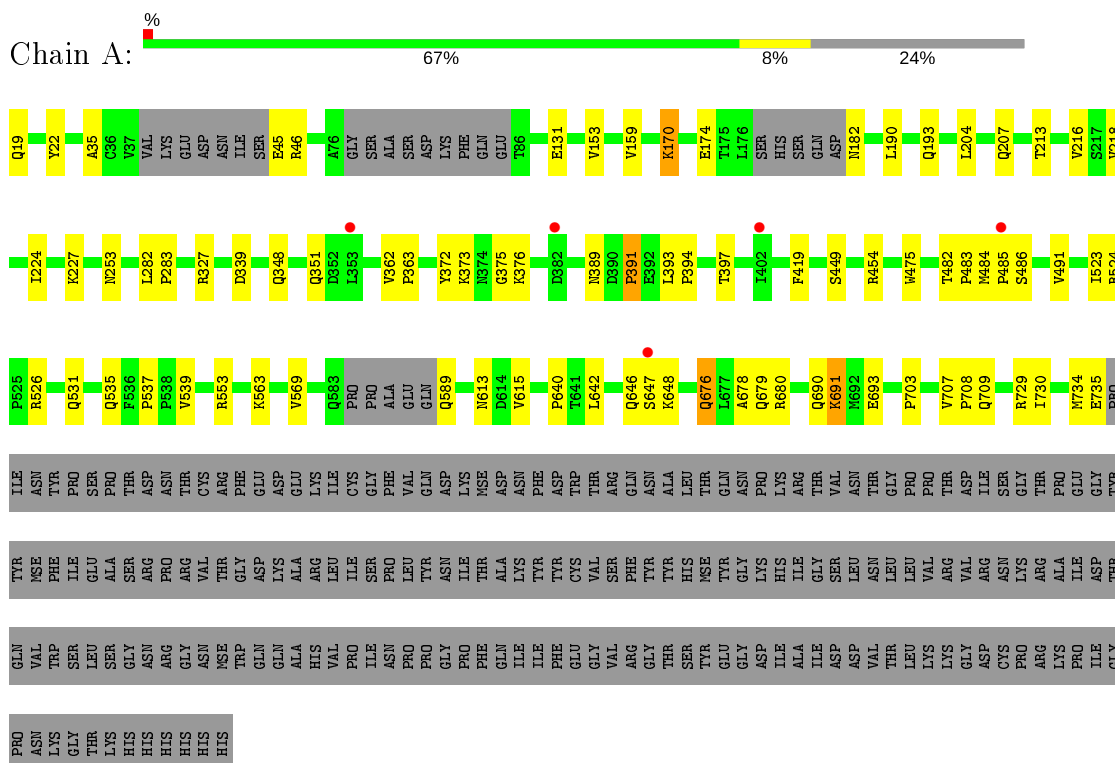
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	B	1	Total 14	C 8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

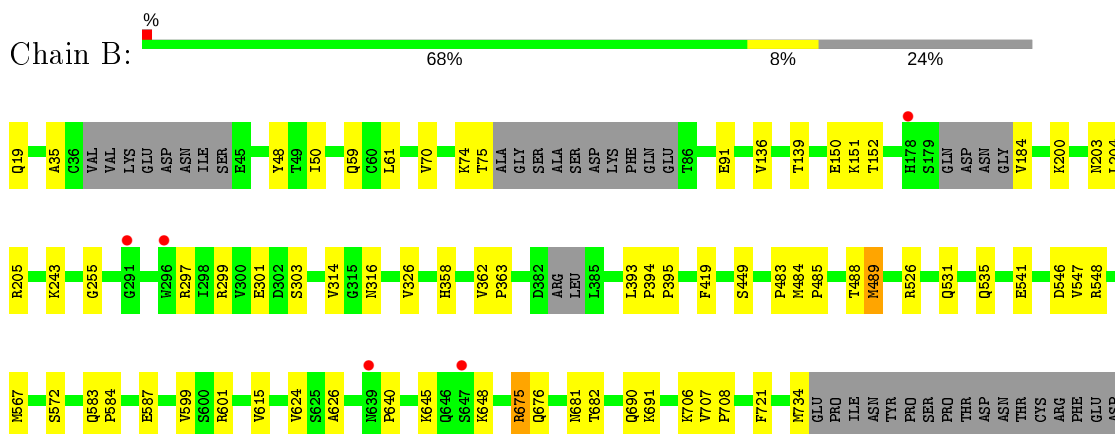
3 Residue-property plots [i](#)

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

- Molecule 1: MAM domain-containing glycosylphosphatidylinositol anchor protein 1



- Molecule 1: MAM domain-containing glycosylphosphatidylinositol anchor protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.18Å 109.04Å 208.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.65 – 3.20 96.65 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (96.65-3.20) 99.9 (96.65-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 3.19Å)	Xtrriage
Refinement program	PHENIX (dev_2044)	Depositor
R, R_{free}	0.214 , 0.251 0.228 , 0.267	Depositor DCC
R_{free} test set	2029 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	94.6	Xtrriage
Anisotropy	0.196	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 58.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11087	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: BMA, NAG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/5484	0.45	0/7452
1	B	0.25	0/5507	0.45	0/7481
All	All	0.25	0/10991	0.45	0/14933

There are no bond length outliers.

There are no bond angle outliers.

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	5384	0	5351	50	0
1	B	5404	0	5391	42	0
2	C	39	0	34	0	0
3	D	50	0	43	0	0
4	A	112	0	104	0	0
4	B	98	0	91	0	0
All	All	11087	0	11014	88	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 4.

All (88) 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:680:ARG:NH2	1:B:584:PRO:O	2.13	0.80
1:B:572:SER:N	1:B:587:GLU:OE2	2.19	0.73
1:B:19:GLN:OE1	1:B:19:GLN:N	2.31	0.63
1:B:546:ASP:OD1	1:B:548:ARG:NE	2.33	0.61
1:A:174:GLU:N	1:A:174:GLU:OE1	2.35	0.59
1:A:648:LYS:O	1:A:707:VAL:N	2.37	0.57
1:A:613:ASN:OD1	1:A:615:VAL:N	2.34	0.57
1:A:373:LYS:N	1:A:375:GLY:O	2.34	0.56
1:B:601:ARG:HD2	1:B:721:PHE:CE1	2.43	0.54
1:B:690:GLN:N	1:B:690:GLN:OE1	2.42	0.52
1:B:299:ARG:NE	1:B:301:GLU:OE2	2.42	0.51
1:B:488:THR:OG1	1:B:489:MSE:N	2.44	0.51
1:A:363:PRO:HG2	1:A:419:PHE:CZ	2.45	0.51
1:A:207:GLN:OE1	1:A:207:GLN:N	2.42	0.51
1:A:170:LYS:HG3	1:A:213:THR:HG23	1.93	0.50
1:A:348:GLN:NE2	1:A:351:GLN:OE1	2.42	0.50
1:A:19:GLN:O	1:A:19:GLN:HG2	2.10	0.50
1:B:393:LEU:HB3	1:B:394:PRO:CD	2.42	0.49
1:A:391:PRO:HG2	1:A:393:LEU:HG	1.94	0.49
1:A:393:LEU:HB3	1:A:394:PRO:CD	2.42	0.49
1:A:676:GLN:HG2	1:A:679:GLN:HG2	1.94	0.49
1:A:642:LEU:O	1:A:642:LEU:HD12	2.12	0.48
1:B:707:VAL:CG1	1:B:708:PRO:HD3	2.43	0.48
1:B:70:VAL:HG21	1:B:91:GLU:HA	1.95	0.48
1:B:74:LYS:O	1:B:75:THR:HB	2.12	0.48
1:B:675:ARG:HG3	1:B:682:THR:HG22	1.94	0.48
1:A:539:VAL:HG22	1:A:563:LYS:HB2	1.96	0.48
1:A:537:PRO:HA	1:A:613:ASN:HD21	1.80	0.47
1:A:253:ASN:OD1	1:A:327:ARG:NH1	2.47	0.47
1:A:535:GLN:HB3	1:A:615:VAL:HG21	1.97	0.47
1:B:583:GLN:CB	1:B:584:PRO:CD	2.93	0.47
1:A:708:PRO:HG2	1:A:709:GLN:HG3	1.96	0.46
1:B:449:SER:O	1:B:531:GLN:N	2.46	0.46
1:B:681:ASN:OD1	1:B:682:THR:N	2.49	0.46
1:B:363:PRO:HG2	1:B:419:PHE:CZ	2.51	0.45
1:A:676:GLN:HG3	1:A:678:ALA:H	1.81	0.45
1:A:190:LEU:HD21	1:B:316:ASN:OD1	2.17	0.45
1:A:372:TYR:CD1	1:A:376:LYS:CB	3.00	0.45
1:A:475:TRP:HB2	1:A:491:VAL:CG2	2.47	0.45
1:B:184:VAL:N	1:B:200:LYS:O	2.49	0.45
1:A:218:VAL:HG11	1:A:224:ILE:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:VAL:O	1:A:569:VAL:HG23	2.16	0.44
1:A:131:GLU:HG2	1:A:227:LYS:HD3	1.99	0.44
1:B:151:LYS:HD3	1:B:204:LEU:HD23	1.99	0.44
1:A:282:LEU:HB2	1:A:283:PRO:HD3	2.00	0.44
1:B:59:GLN:HG2	1:B:61:LEU:CD1	2.48	0.44
1:A:389:ASN:O	1:A:397:THR:O	2.35	0.44
1:A:613:ASN:OD1	1:A:615:VAL:HB	2.17	0.44
1:A:523:ILE:HG22	1:A:524:ARG:N	2.33	0.43
1:A:589:GLN:O	1:A:589:GLN:HG3	2.18	0.43
1:A:676:GLN:HE22	1:A:709:GLN:CD	2.22	0.43
1:A:35:ALA:HB3	1:B:483:PRO:HG3	2.00	0.43
1:B:136:VAL:O	1:B:314:VAL:HA	2.18	0.42
1:A:449:SER:O	1:A:531:GLN:N	2.50	0.42
1:B:484:MSE:HB3	1:B:485:PRO:HD2	2.01	0.42
1:A:707:VAL:CG1	1:A:708:PRO:HD3	2.49	0.42
1:B:535:GLN:HB3	1:B:615:VAL:HG21	1.99	0.42
1:A:362:VAL:HB	1:A:363:PRO:HD3	2.02	0.42
1:A:486:SER:OG	1:A:491:VAL:HG12	2.20	0.42
1:B:70:VAL:CG2	1:B:91:GLU:HA	2.49	0.42
1:A:45:GLU:HG2	1:A:46:ARG:HG2	2.02	0.42
1:B:547:VAL:CG1	1:B:624:VAL:HG22	2.50	0.42
1:A:159:VAL:HG11	1:A:216:VAL:HG21	2.02	0.41
1:A:640:PRO:HG3	1:A:734:MSE:HB3	2.01	0.41
1:A:19:GLN:HB2	1:A:22:TYR:CD2	2.55	0.41
1:A:218:VAL:O	1:A:218:VAL:HG22	2.20	0.41
1:A:484:MSE:HB3	1:A:485:PRO:HD2	2.02	0.41
1:A:153:VAL:HG22	1:A:204:LEU:HD13	2.02	0.41
1:B:362:VAL:HB	1:B:363:PRO:HD3	2.02	0.41
1:A:646:GLN:O	1:A:647:SER:OG	2.31	0.41
1:B:150:GLU:HG3	1:B:203:ASN:OD1	2.21	0.41
1:A:483:PRO:HG3	1:B:35:ALA:H	1.85	0.41
1:B:151:LYS:HD3	1:B:204:LEU:CD2	2.51	0.41
1:B:303:SER:OG	1:B:326:VAL:HG12	2.20	0.41
1:B:599:VAL:HG13	1:B:599:VAL:O	2.21	0.41
1:A:690:GLN:HG2	1:A:691:LYS:N	2.36	0.41
1:B:203:ASN:ND2	1:B:205:ARG:NH2	2.69	0.41
1:B:48:TYR:CE2	1:B:50:ILE:HG21	2.55	0.41
1:B:567:MSE:O	1:B:567:MSE:HG3	2.21	0.41
1:B:626:ALA:HB3	1:B:721:PHE:CD1	2.56	0.41
1:B:74:LYS:O	1:B:75:THR:CB	2.69	0.41
1:A:393:LEU:HB3	1:A:394:PRO:HD2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:GLN:O	1:A:193:GLN:HG3	2.21	0.40
1:B:255:GLY:O	1:B:297:ARG:HA	2.20	0.40
1:B:640:PRO:HG3	1:B:734:MSE:HB2	2.04	0.40
1:A:729:ARG:HG2	1:A:730:ILE:N	2.37	0.40
1:B:139:THR:N	1:B:152:THR:O	2.54	0.40
1:B:358:HIS:CE1	1:B:395:PRO:O	2.75	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	681/910 (75%)	627 (92%)	53 (8%)	1 (0%)	51 83
1	B	682/910 (75%)	632 (93%)	50 (7%)	0	100 100
All	All	1363/1820 (75%)	1259 (92%)	103 (8%)	1 (0%)	51 83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	391	PRO

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	608/795 (76%)	596 (98%)	12 (2%)	55	80
1	B	612/795 (77%)	602 (98%)	10 (2%)	62	84
All	All	1220/1590 (77%)	1198 (98%)	22 (2%)	59	82

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	LYS
1	A	182	ASN
1	A	339	ASP
1	A	454	ARG
1	A	482	THR
1	A	526	ARG
1	A	553	ARG
1	A	676	GLN
1	A	691	LYS
1	A	693	GLU
1	A	703	PRO
1	A	735	GLU
1	B	243	LYS
1	B	489	MSE
1	B	526	ARG
1	B	541	GLU
1	B	645	LYS
1	B	648	LYS
1	B	675	ARG
1	B	676	GLN
1	B	691	LYS
1	B	706	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	676	GLN

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](#)

7 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	1,2	14,14,15	0.22	0	17,19,21	0.50	0
2	NAG	C	2	2	14,14,15	0.42	0	17,19,21	0.47	0
2	BMA	C	3	2	11,11,12	0.55	0	15,15,17	0.83	0
3	NAG	D	1	1,3	14,14,15	0.18	0	17,19,21	0.56	0
3	NAG	D	2	3	14,14,15	0.24	0	17,19,21	0.43	0
3	BMA	D	3	3	11,11,12	0.74	0	15,15,17	1.52	4 (26%)
3	MAN	D	4	3	11,11,12	1.04	1 (9%)	15,15,17	0.84	1 (6%)

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	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4	MAN	O5-C1	-2.68	1.39	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3	BMA	C1-C2-C3	-2.91	106.09	109.67
3	D	3	BMA	C3-C4-C5	-2.54	105.70	110.24
3	D	3	BMA	O3-C3-C2	2.53	114.83	109.99
3	D	4	MAN	O2-C2-C3	-2.27	105.59	110.14
3	D	3	BMA	O3-C3-C4	2.22	115.49	110.35

There are no chirality outliers.

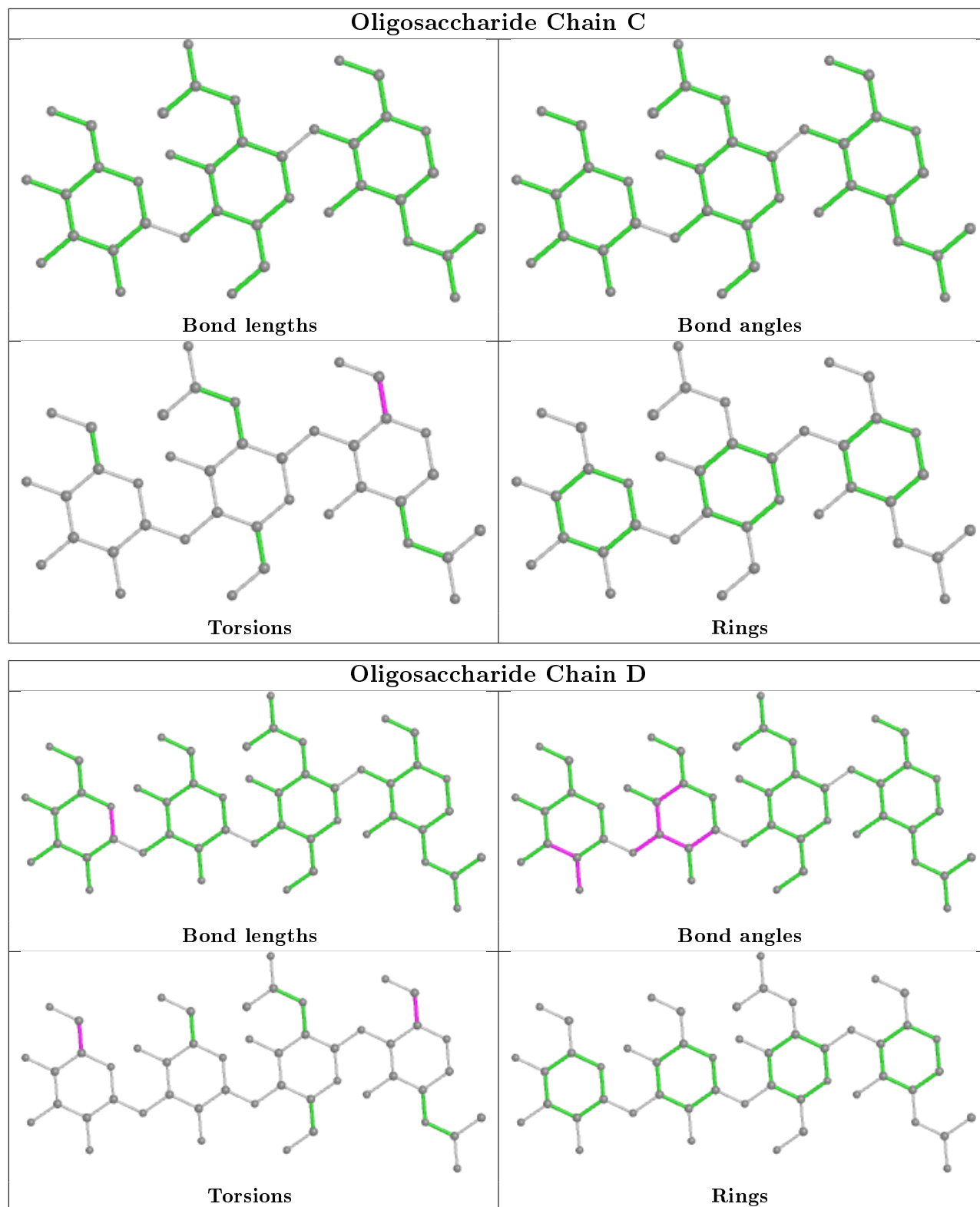
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	4	MAN	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
3	D	4	MAN	C4-C5-C6-O6
3	D	1	NAG	O5-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.



5.6 Ligand geometry [i](#)

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1008	1	14,14,15	0.37	0	17,19,21	0.58	0
4	NAG	A	1003	1	14,14,15	0.20	0	17,19,21	0.38	0
4	NAG	B	1002	1	14,14,15	0.26	0	17,19,21	0.38	0
4	NAG	A	1007	1	14,14,15	0.30	0	17,19,21	0.46	0
4	NAG	B	1009	1	14,14,15	0.27	0	17,19,21	0.41	0
4	NAG	A	1010	1	14,14,15	0.18	0	17,19,21	0.59	0
4	NAG	B	1010	1	14,14,15	0.21	0	17,19,21	0.62	1 (5%)
4	NAG	B	1003	1	14,14,15	0.20	0	17,19,21	0.39	0
4	NAG	B	1008	1	14,14,15	0.51	0	17,19,21	0.51	0
4	NAG	B	1011	1	14,14,15	0.39	0	17,19,21	0.43	0
4	NAG	A	1002	1	14,14,15	0.18	0	17,19,21	0.54	0
4	NAG	A	1001	1	14,14,15	0.19	0	17,19,21	0.52	0
4	NAG	A	1009	1	14,14,15	0.20	0	17,19,21	0.55	0
4	NAG	B	1001	1	14,14,15	0.27	0	17,19,21	0.44	0
4	NAG	A	1011	1	14,14,15	0.20	0	17,19,21	0.48	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	1008	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1003	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1002	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1007	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1009	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1010	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1010	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1003	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1008	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1011	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1002	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1001	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1009	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1001	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1011	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1010	NAG	C1-O5-C5	2.13	115.08	112.19

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1009	NAG	O5-C5-C6-O6
4	A	1009	NAG	O5-C5-C6-O6
4	B	1008	NAG	O5-C5-C6-O6
4	A	1009	NAG	C4-C5-C6-O6
4	B	1008	NAG	C4-C5-C6-O6
4	B	1009	NAG	C4-C5-C6-O6
4	A	1007	NAG	O5-C5-C6-O6
4	A	1008	NAG	O5-C5-C6-O6
4	A	1002	NAG	O5-C5-C6-O6
4	A	1007	NAG	C4-C5-C6-O6
4	A	1008	NAG	C1-C2-N2-C7
4	B	1011	NAG	O5-C5-C6-O6
4	A	1001	NAG	O5-C5-C6-O6
4	A	1002	NAG	C4-C5-C6-O6
4	A	1008	NAG	C3-C2-N2-C7
4	A	1008	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	680/910 (74%)	0.00	5 (0%) 87 81	47, 100, 156, 304	0
1	B	681/910 (74%)	0.02	5 (0%) 87 81	48, 102, 151, 215	0
All	All	1361/1820 (74%)	0.01	10 (0%) 87 81	47, 101, 154, 304	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	647	SER	3.4
1	A	402	ILE	3.0
1	A	647	SER	2.9
1	B	639	ASN	2.7
1	B	178	HIS	2.6
1	A	382	ASP	2.4
1	B	291	GLY	2.4
1	B	296	TRP	2.3
1	A	353	LEU	2.2
1	A	485	PRO	2.0

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

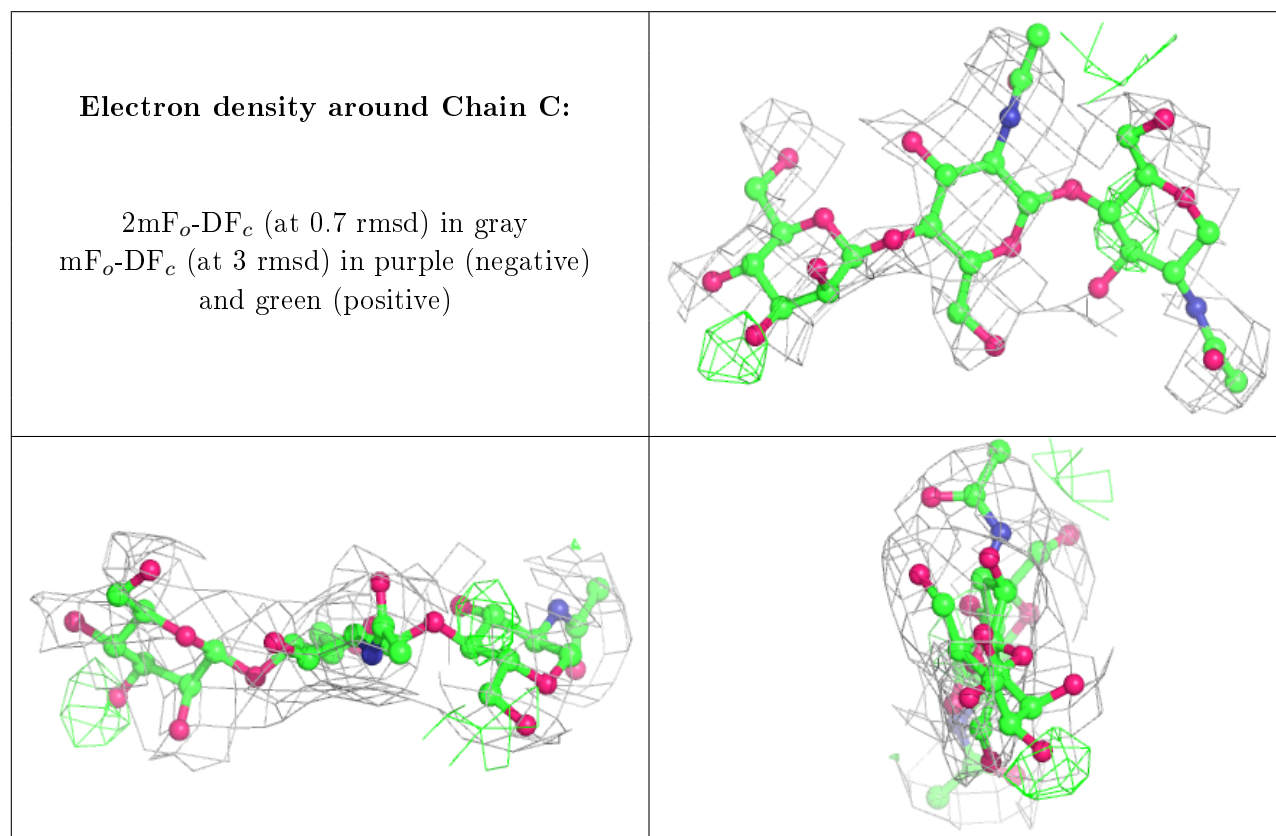
There are no non-standard protein/DNA/RNA residues in this entry.

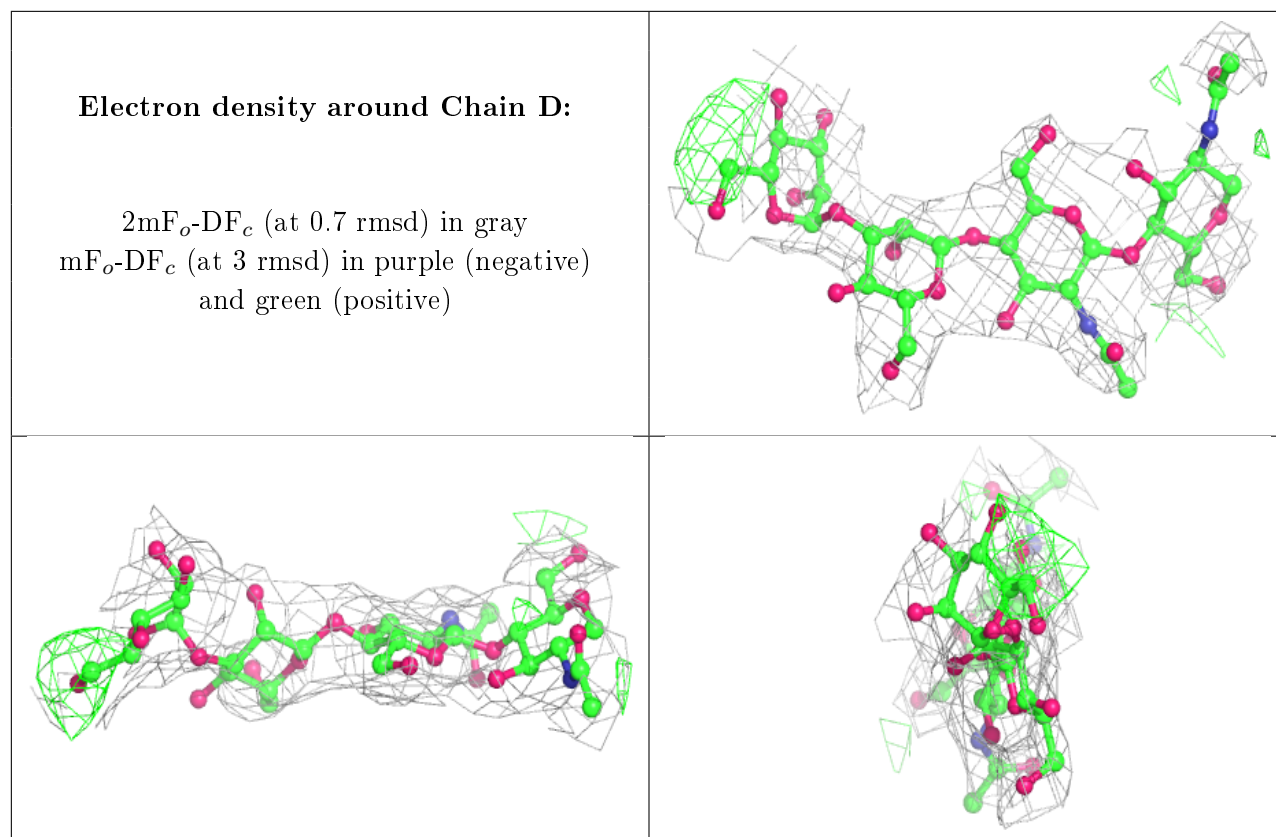
6.3 Carbohydrates [i](#)

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(\AA^2)	Q<0.9
2	BMA	C	3	11/12	0.48	0.29	163,172,181,186	0
3	MAN	D	4	11/12	0.61	0.27	216,223,228,237	0
3	BMA	D	3	11/12	0.72	0.23	173,181,193,205	0
2	NAG	C	2	14/15	0.86	0.22	124,129,138,152	0
3	NAG	D	2	14/15	0.89	0.23	128,135,150,160	0
3	NAG	D	1	14/15	0.93	0.17	83,101,111,112	0
2	NAG	C	1	14/15	0.95	0.16	92,109,118,120	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.





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	B	1011	14/15	0.80	0.48	166,192,232,253	0
4	NAG	A	1007	14/15	0.83	0.30	158,178,215,222	0
4	NAG	B	1009	14/15	0.83	0.18	130,142,164,189	0
4	NAG	B	1002	14/15	0.83	0.18	147,158,163,166	0
4	NAG	A	1002	14/15	0.83	0.27	136,148,152,157	0
4	NAG	A	1010	14/15	0.84	0.22	141,165,172,173	0
4	NAG	B	1008	14/15	0.85	0.26	170,175,212,230	0
4	NAG	B	1001	14/15	0.86	0.21	147,166,182,188	0
4	NAG	A	1001	14/15	0.87	0.20	108,114,117,120	0
4	NAG	A	1009	14/15	0.88	0.18	142,147,162,169	0
4	NAG	A	1003	14/15	0.90	0.15	109,114,119,124	0
4	NAG	B	1010	14/15	0.91	0.23	101,108,123,126	0
4	NAG	B	1003	14/15	0.92	0.23	108,116,119,120	0
4	NAG	A	1008	14/15	0.93	0.25	142,145,148,150	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	A	1011	14/15	0.93	0.21	74,78,84,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.