wwPDB X-ray Structure Validation Summary Report (i)

Dec 3, 2020 – 09:10 am GMT

PDB ID	:	6Z32
Title	:	Human cation-independent mannose 6-phosphate/IGF2 receptor domains 7-11
Authors	:	Bochel, A.J.; Williams, C.; McCoy, A.J.; Hoppe, H.; Winter, A.J.; Nicholls, R.D.; Harlos, K.; Jones, Y.E.; Berger, I.; Hassan, B.; Crump, M.P.
Deposited on	:	2020-05-19
Resolution	:	3.47 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see references (1)) were used in the production of this report:

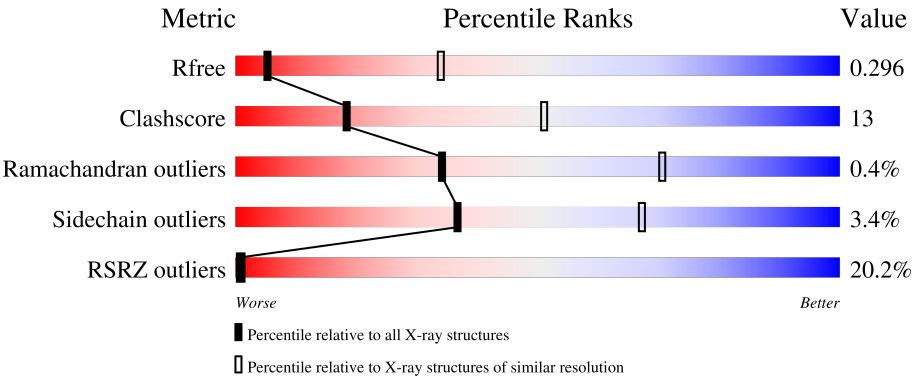
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 3.47 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	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)

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	737	19% 70% 21% · 7%
1	B	737	18% 70% 19% · 10%
2	C	6	67% 33%
2	D	6	83% 17%

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	C	2	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10549 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 Cation-independent mannose-6-phosphate receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	686	Total	C	N	O	S	0	0	0
			5257	3312	887	1011	47			
1	B	665	Total	C	N	O	S	0	0	0
			5101	3212	858	984	47			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	913	GLU	-	expression tag	UNP P11717
A	914	THR	-	expression tag	UNP P11717
A	915	GLY	-	expression tag	UNP P11717
A	916	GLN	-	expression tag	UNP P11717
A	917	LEU	-	expression tag	UNP P11717
A	918	LYS	-	expression tag	UNP P11717
A	919	HIS	-	expression tag	UNP P11717
A	920	HIS	-	expression tag	UNP P11717
A	921	HIS	-	expression tag	UNP P11717
A	922	HIS	-	expression tag	UNP P11717
A	923	HIS	-	expression tag	UNP P11717
A	924	HIS	-	expression tag	UNP P11717
A	925	GLU	-	expression tag	UNP P11717
A	926	PHE	-	expression tag	UNP P11717
A	1619	GLY	ARG	variant	UNP P11717
B	913	GLU	-	expression tag	UNP P11717
B	914	THR	-	expression tag	UNP P11717
B	915	GLY	-	expression tag	UNP P11717
B	916	GLN	-	expression tag	UNP P11717
B	917	LEU	-	expression tag	UNP P11717
B	918	LYS	-	expression tag	UNP P11717
B	919	HIS	-	expression tag	UNP P11717
B	920	HIS	-	expression tag	UNP P11717
B	921	HIS	-	expression tag	UNP P11717
B	922	HIS	-	expression tag	UNP P11717

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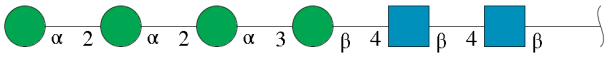
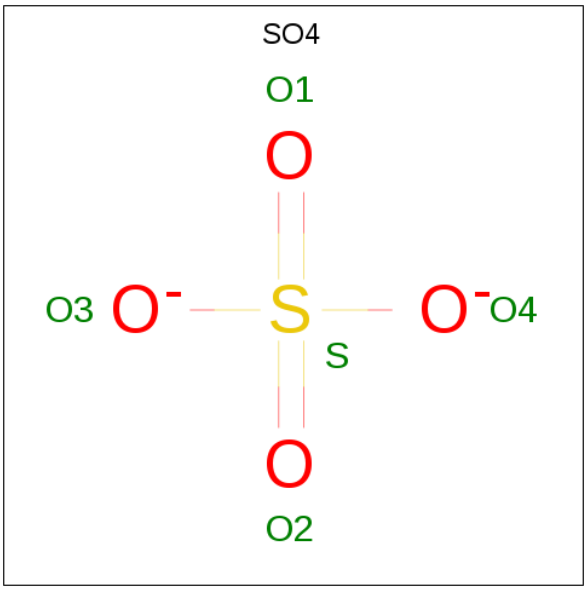
Chain	Residue	Modelled	Actual	Comment	Reference
B	923	HIS	-	expression tag	UNP P11717
B	924	HIS	-	expression tag	UNP P11717
B	925	GLU	-	expression tag	UNP P11717
B	926	PHE	-	expression tag	UNP P11717
B	1619	GLY	ARG	variant	UNP P11717

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



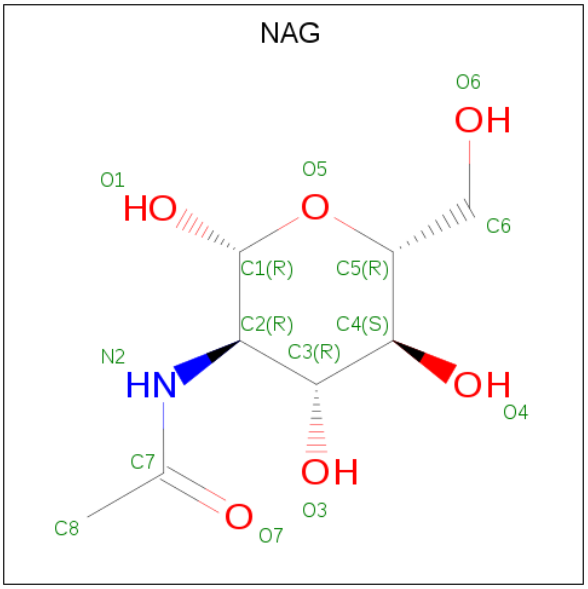
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	C	6	Total C N O 72 40 2 30	0	0	0
2	D	6	Total C N O 72 40 2 30	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0

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



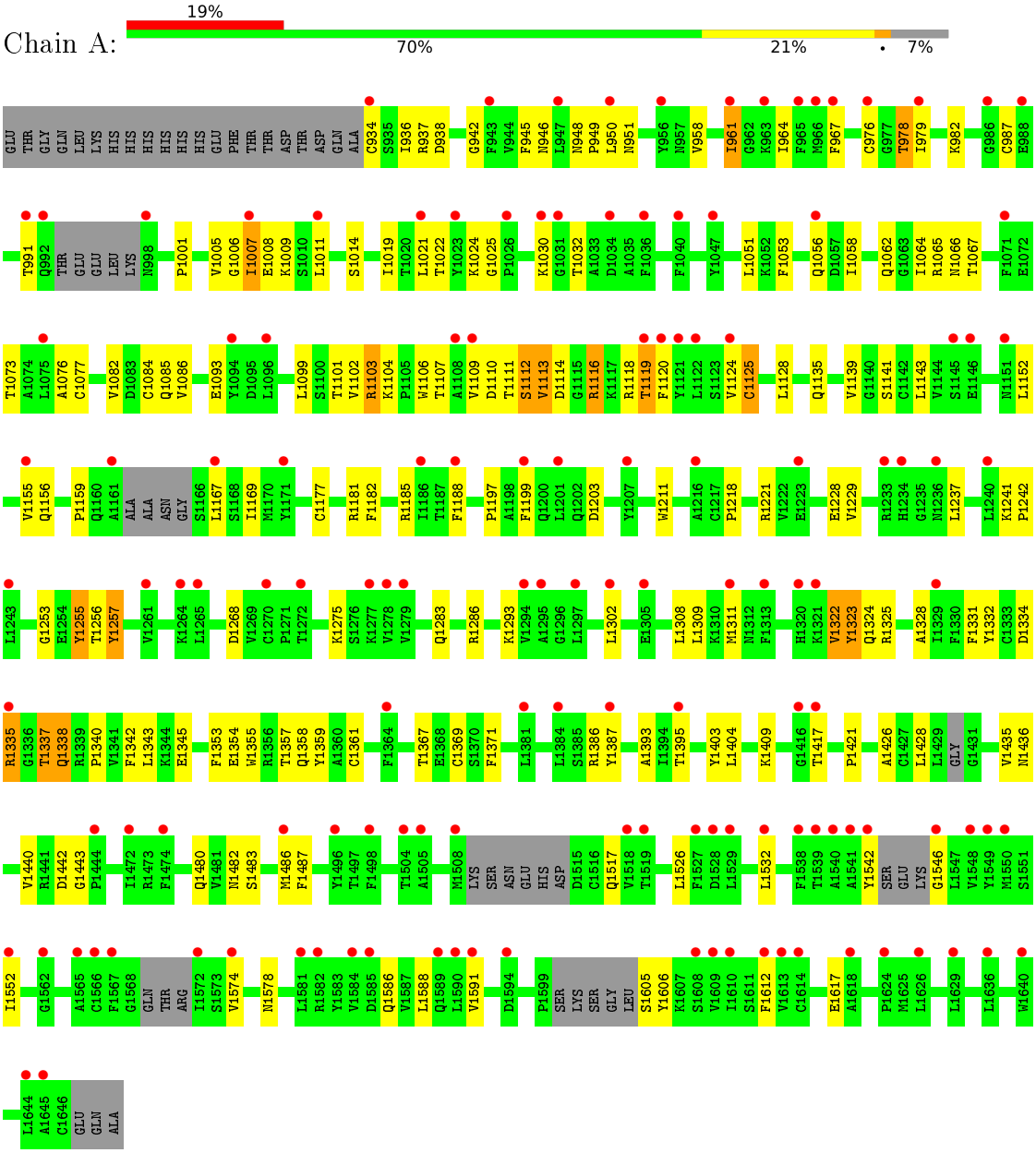
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots (i)

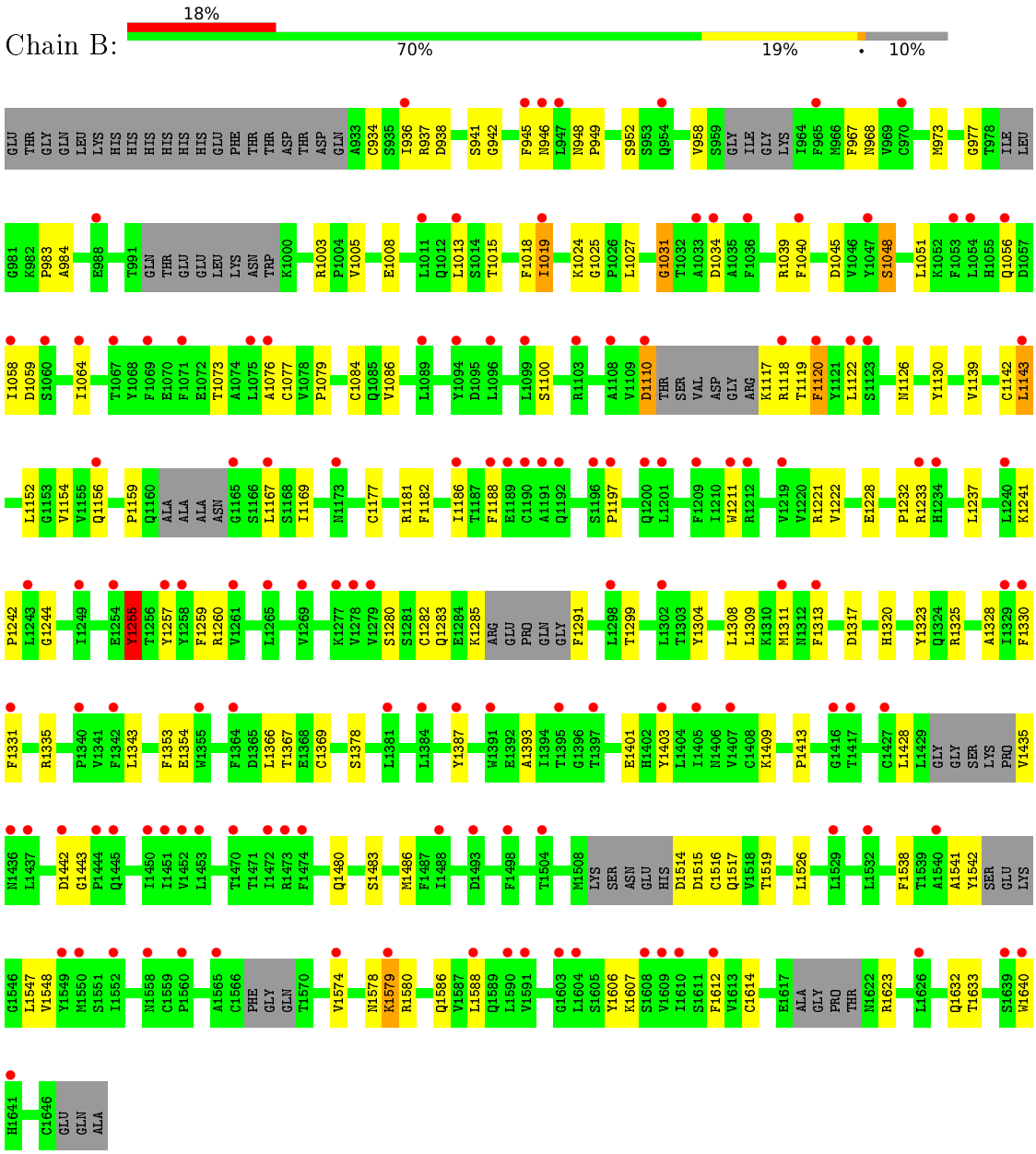
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Cation-independent mannose-6-phosphate receptor

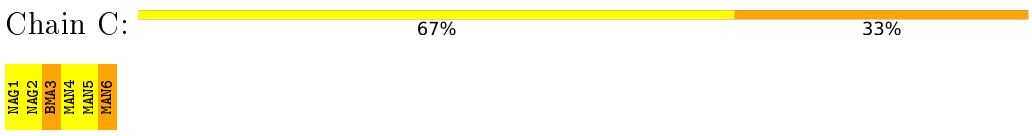
Chain A:



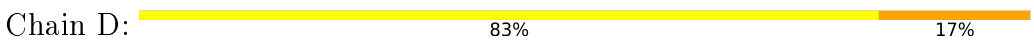
- Molecule 1: Cation-independent mannose-6-phosphate receptor



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



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




NAG1
NAG2
BMA3
MAN4
MAN5
MAN6

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	139.20Å 139.20Å 234.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.72 – 3.47 98.43 – 3.47	Depositor EDS
% Data completeness (in resolution range)	98.5 (89.72-3.47) 98.6 (98.43-3.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.261 , 0.300 0.270 , 0.296	Depositor DCC
R_{free} test set	1493 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	157.7	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 184.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10549	wwPDB-VP
Average B, all atoms (Å^2)	197.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	0.69	0/5379	0.87	2/7300 (0.0%)
1	B	0.69	0/5213	0.85	5/7067 (0.1%)
All	All	0.69	0/10592	0.86	7/14367 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1255	TYR	CA-CB-CG	5.99	124.78	113.40
1	B	1120	PHE	CB-CA-C	-5.75	98.91	110.40
1	B	1110	ASP	CB-CA-C	5.67	121.73	110.40
1	B	1118	ARG	N-CA-CB	5.49	120.48	110.60
1	A	1065	ARG	NE-CZ-NH2	5.44	123.02	120.30

There are no chirality outliers.

There are no planarity outliers.

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	5257	0	5051	165	0
1	B	5101	0	4894	128	0
2	C	72	0	61	10	0
2	D	72	0	61	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	0	1	0
4	A	14	0	13	0	0
4	B	28	0	26	1	0
All	All	10549	0	10106	275	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 13.

The worst 5 of 275 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:1102:VAL:HG21	1:A:1106:TRP:CZ2	1.74	1.20
1:A:979:ILE:HG21	1:A:1007:ILE:CD1	1.74	1.18
1:A:976:CYS:HB3	1:A:1001:PRO:HB3	1.22	1.16
1:B:1120:PHE:CE1	1:B:1143:LEU:HD12	1.82	1.14
1:A:1338:GLN:HB3	1:B:1130:TYR:CZ	1.81	1.14

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	670/737 (91%)	632 (94%)	34 (5%)	4 (1%)	25 63
1	B	641/737 (87%)	607 (95%)	33 (5%)	1 (0%)	47 80
All	All	1311/1474 (89%)	1239 (94%)	67 (5%)	5 (0%)	34 70

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1253	GLY

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Mol	Chain	Res	Type
1	A	1113	VAL
1	A	1125	CYS
1	B	1031	GLY
1	A	961	ILE

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	589/632 (93%)	564 (96%)	25 (4%)	30	61
1	B	574/632 (91%)	560 (98%)	14 (2%)	49	75
All	All	1163/1264 (92%)	1124 (97%)	39 (3%)	37	67

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1322	VAL
1	A	1361	CYS
1	B	1516	CYS
1	A	1335	ARG
1	A	1337	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1586	GLN
1	B	1586	GLN
1	B	1202	GLN
1	A	1358	GLN
1	B	1056	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)

12 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	1.01	1 (7%)	17,19,21	3.16	8 (47%)
2	NAG	C	2	2	14,14,15	0.32	0	17,19,21	0.74	0
2	BMA	C	3	2	11,11,12	2.11	6 (54%)	15,15,17	2.79	10 (66%)
2	MAN	C	4	2	11,11,12	0.33	0	15,15,17	1.05	1 (6%)
2	MAN	C	5	2	11,11,12	1.87	3 (27%)	15,15,17	2.45	5 (33%)
2	MAN	C	6	2	11,11,12	1.77	2 (18%)	15,15,17	2.86	7 (46%)
2	NAG	D	1	1,2	14,14,15	1.29	1 (7%)	17,19,21	3.33	6 (35%)
2	NAG	D	2	2	14,14,15	0.86	0	17,19,21	2.47	9 (52%)
2	BMA	D	3	2	11,11,12	0.25	0	15,15,17	0.84	0
2	MAN	D	4	2	11,11,12	1.98	4 (36%)	15,15,17	2.12	5 (33%)
2	MAN	D	5	2	11,11,12	1.22	3 (27%)	15,15,17	3.16	10 (66%)
2	MAN	D	6	2	11,11,12	2.02	5 (45%)	15,15,17	3.15	9 (60%)

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	-	4/6/23/26	0/1/1/1
2	BMA	C	3	2	-	1/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	1/2/19/22	0/1/1/1

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

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	6	MAN	C2-C3	-4.34	1.46	1.52
2	D	1	NAG	O5-C1	-3.69	1.37	1.43
2	D	4	MAN	C2-C3	-3.46	1.47	1.52
2	C	3	BMA	O5-C1	-3.40	1.38	1.43
2	D	6	MAN	C2-C3	-3.31	1.47	1.52

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	NAG	C1-O5-C5	-10.04	98.59	112.19
2	C	6	MAN	O5-C1-C2	-6.91	100.10	110.77
2	C	3	BMA	C1-O5-C5	-6.84	102.93	112.19
2	D	6	MAN	C6-C5-C4	-6.60	97.55	113.00
2	C	5	MAN	C1-C2-C3	-6.50	101.68	109.67

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C1-C2-N2-C7
2	C	1	NAG	C8-C7-N2-C2
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	1	NAG	O7-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	BMA	3	0

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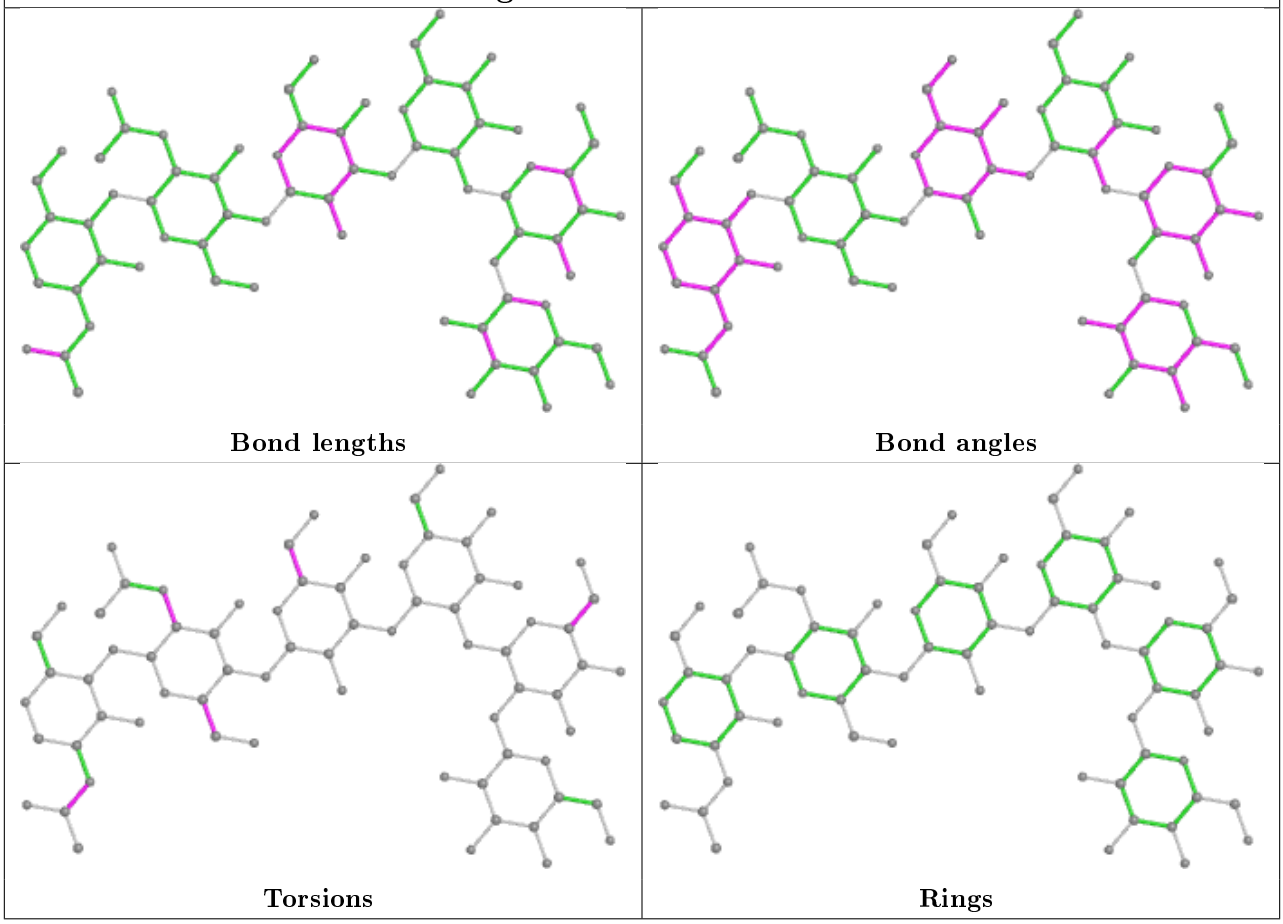
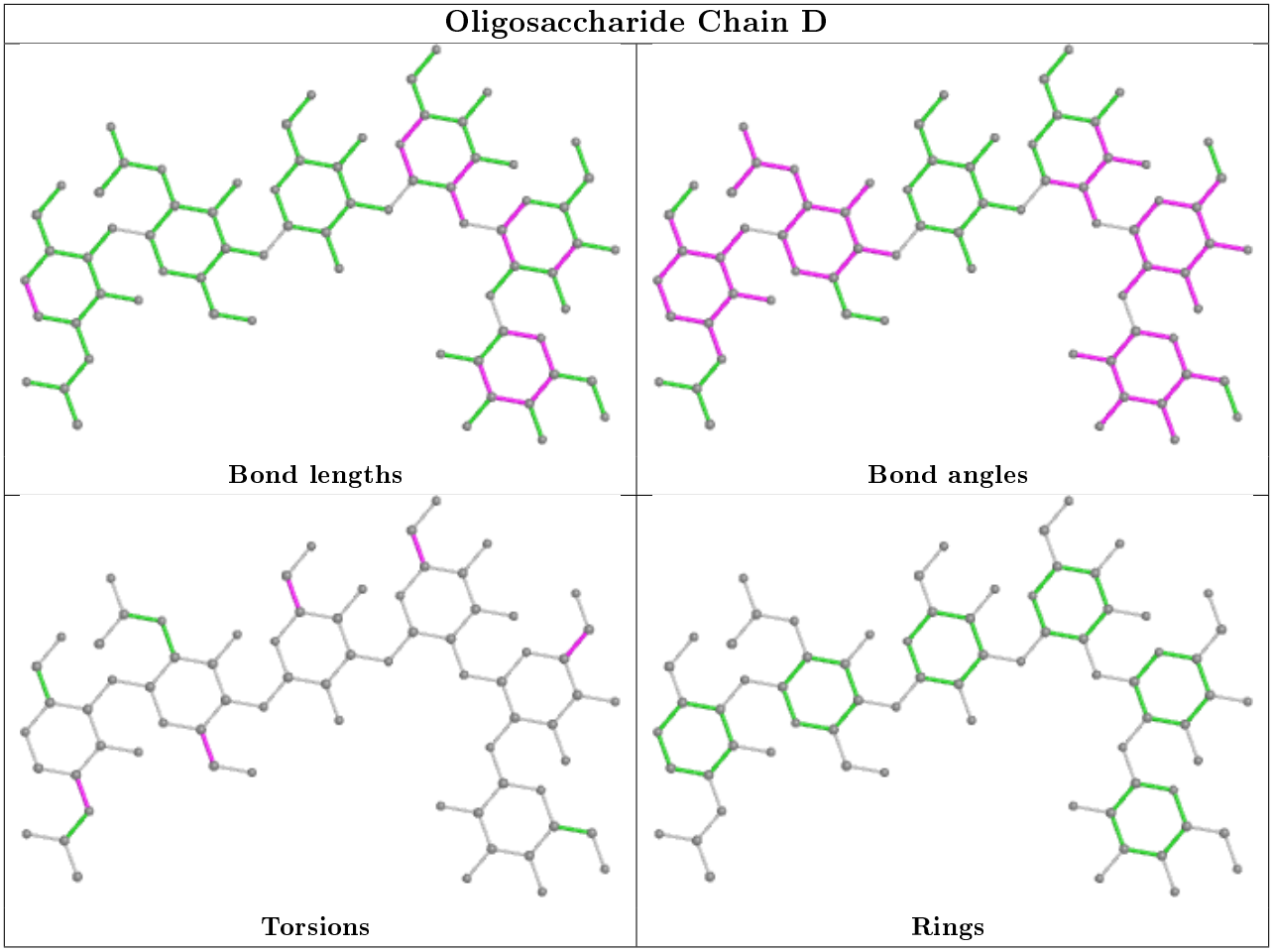
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	6	MAN	1	0
2	C	2	NAG	8	0
2	C	6	MAN	1	0
2	C	3	BMA	1	0

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

Oligosaccharide Chain C





5.6 Ligand geometry (i)

4 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	1702	1	14,14,15	1.54	3 (21%)	17,19,21	1.67	4 (23%)
4	NAG	B	1702	1	14,14,15	1.29	2 (14%)	17,19,21	3.42	9 (52%)
4	NAG	B	1701	1	14,14,15	0.89	0	17,19,21	2.52	6 (35%)
3	SO4	A	1701	-	4,4,4	0.35	0	6,6,6	0.08	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	1702	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1701	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1702	1	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1702	NAG	O5-C1	-3.71	1.37	1.43
4	B	1702	NAG	O5-C5	-3.17	1.37	1.43
4	A	1702	NAG	O5-C5	-2.64	1.38	1.43
4	B	1702	NAG	C4-C5	-2.54	1.47	1.53
4	A	1702	NAG	C1-C2	-2.19	1.49	1.52

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1702	NAG	O5-C1-C2	-9.02	97.05	111.29
4	B	1701	NAG	C4-C3-C2	-6.39	101.65	111.02
4	B	1702	NAG	C4-C3-C2	-4.34	104.66	111.02
4	B	1701	NAG	O5-C5-C6	4.29	113.93	107.20
4	B	1702	NAG	C1-C2-N2	4.28	117.80	110.49

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1702	NAG	C8-C7-N2-C2
4	B	1702	NAG	O7-C7-N2-C2
4	A	1702	NAG	O5-C5-C6-O6
4	B	1701	NAG	C8-C7-N2-C2
4	B	1701	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1701	NAG	1	0
3	A	1701	SO4	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	686/737 (93%)	1.04	138 (20%)	1	1	113, 187, 275, 334	0
1	B	665/737 (90%)	1.01	135 (20%)	1	1	118, 200, 248, 294	0
All	All	1351/1474 (91%)	1.02	273 (20%)	1	1	113, 195, 266, 334	0

The worst 5 of 273 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1582	ARG	7.7
1	A	1550	MET	7.7
1	A	1612	PHE	7.4
1	A	1572	ILE	7.2
1	B	1474	PHE	6.6

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, 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	NAG	C	1	14/15	0.63	0.33	161,192,236,244	0
2	BMA	D	3	11/12	0.77	0.27	154,166,197,204	0
2	MAN	C	4	11/12	0.87	0.24	174,198,211,232	0
2	NAG	C	2	14/15	0.89	0.20	185,230,255,258	0
2	MAN	C	6	11/12	0.89	0.25	149,180,211,224	0

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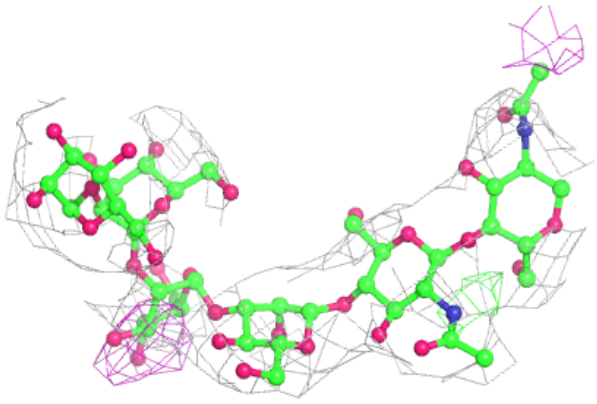
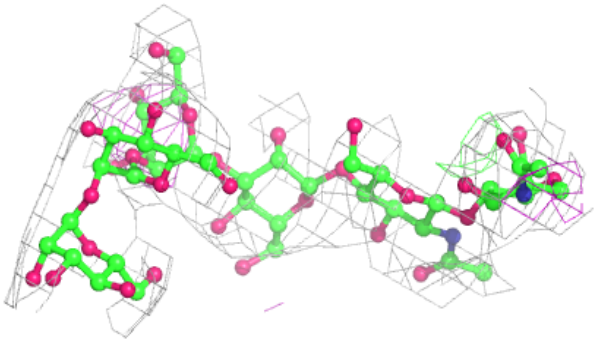
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	D	2	14/15	0.90	0.22	179,233,251,269	0
2	NAG	D	1	14/15	0.92	0.24	119,162,218,225	0
2	MAN	D	4	11/12	0.92	0.30	192,207,222,248	0
2	BMA	C	3	11/12	0.92	0.23	144,158,181,199	0
2	MAN	D	6	11/12	0.93	0.14	30,30,30,30	0
2	MAN	D	5	11/12	0.93	0.16	30,30,30,30	0
2	MAN	C	5	11/12	0.95	0.27	152,163,183,183	0

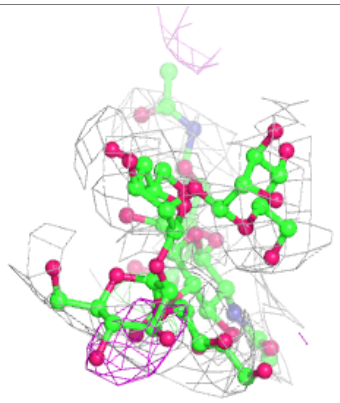
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

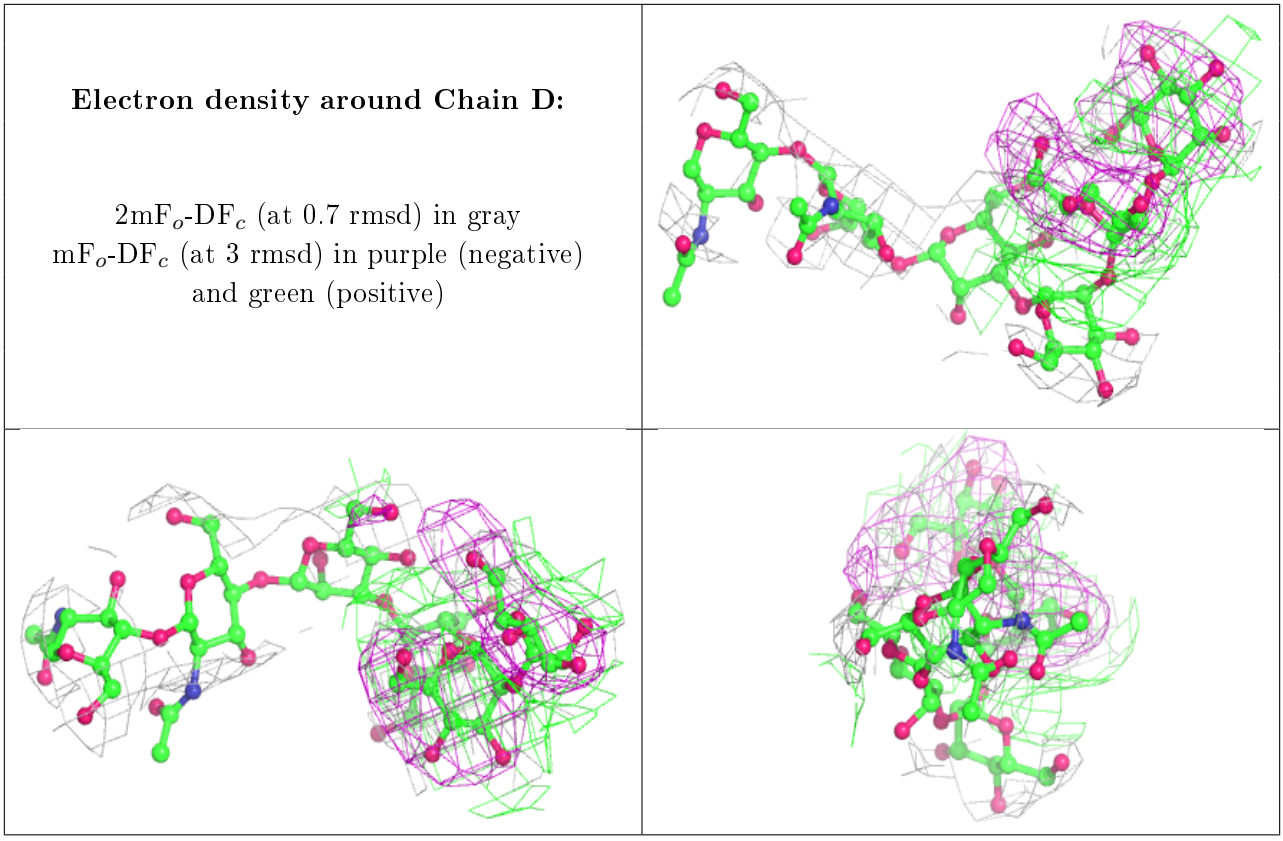






Electron density around Chain D:

$2mF_o$-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
4	NAG	B	1702	14/15	0.71	0.35	155,179,210,226	0
4	NAG	B	1701	14/15	0.75	0.31	192,209,231,234	0
4	NAG	A	1702	14/15	0.81	0.27	155,179,185,185	0
3	SO4	A	1701	5/5	0.83	0.22	157,173,190,198	0

6.5 Other polymers

There are no such residues in this entry.