Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 09:49 PM BST

PDB ID	:	2W7Y
Title	:	Structure of a Streptococcus pneumoniae solute-binding protein in complex with the blood group A-trisaccharide.
Authors	:	Higgins, M.A.; Abbott, D.W.; Boulanger, M.J.; Boraston, A.B.
Deposited on	:	2009-01-06
Resolution	:	2.35 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:

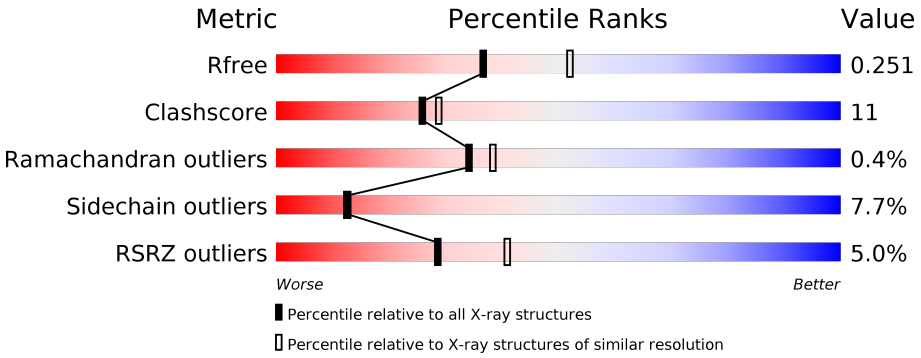
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	430	2% 73% 14% 10%
1	B	430	7% 73% 14% 10%
2	C	3	33% 67%
2	D	3	100%

2 Entry composition

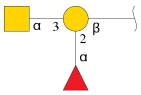
There are 4 unique types of molecules in this entry. The entry contains 6450 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROBABLE SUGAR ABC TRANSPORTER, SUGAR-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	Se	0	0	0
			2983	1883	497	594	9			
1	B	389	Total	C	N	O	Se	0	0	0
			2983	1883	497	594	9			

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			36	20	1	15			
2	D	3	Total	C	N	O	0	0	0
			36	20	1	15			

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	I	0	0
			1	1		
3	A	1	Total	I	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	215	Total	O	0	0
			215	215		

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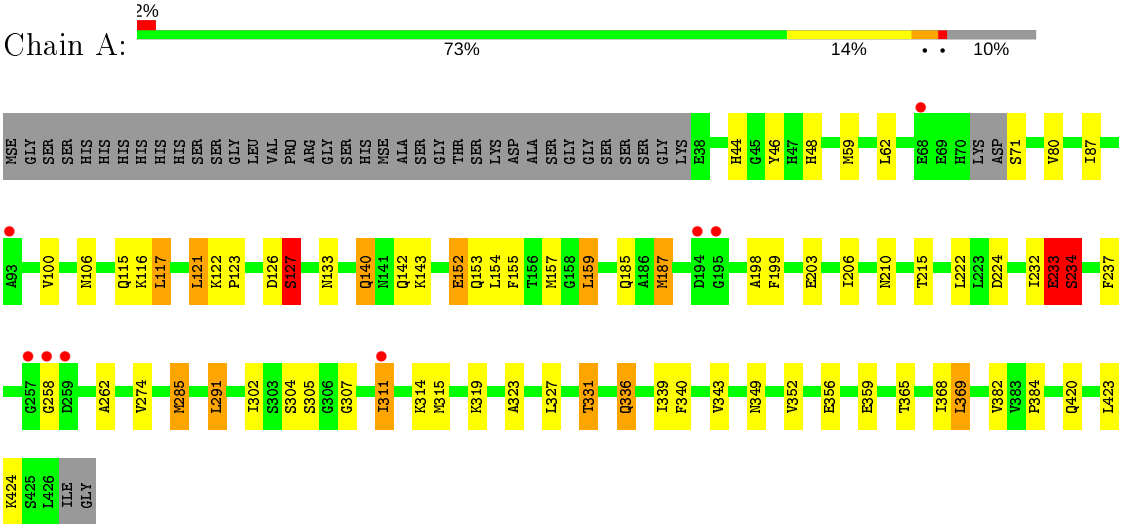
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	195	Total	O	0	0
			195	195		

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.

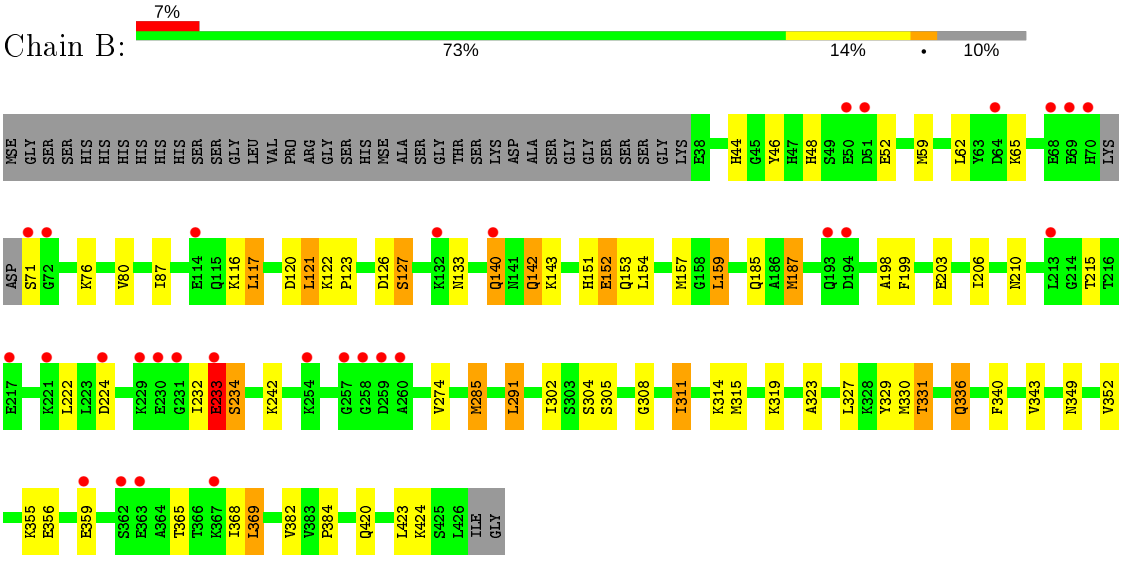
• Molecule 1: PROBABLE SUGAR ABC TRANSPORTER, SUGAR-BINDING PROTEIN

Chain A:



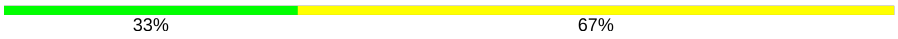
• Molecule 1: PROBABLE SUGAR ABC TRANSPORTER, SUGAR-BINDING PROTEIN

Chain B:



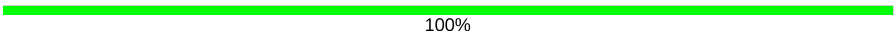
• Molecule 2: alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose

Chain C:



• Molecule 2: alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	36.99Å 104.90Å 97.70Å 90.00° 89.95° 90.00°	Depositor
Resolution (Å)	97.59 – 2.35 29.48 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (97.59-2.35) 99.8 (29.48-2.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.28 (at 2.36Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.213 , 0.263 0.227 , 0.251	Depositor DCC
R_{free} test set	1569 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	26.4	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 8.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.186 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6450	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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: A2G, IOD, GAL, FUC

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	0.50	1/3029 (0.0%)	0.59	3/4078 (0.1%)
1	B	0.45	3/3029 (0.1%)	0.57	2/4078 (0.0%)
All	All	0.48	4/6058 (0.1%)	0.58	5/8156 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	SER	CB-OG	16.98	1.64	1.42
1	B	127	SER	CB-OG	12.45	1.58	1.42
1	B	142	GLN	CD-NE2	5.80	1.47	1.32
1	B	142	GLN	CD-OE1	5.61	1.36	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	127	SER	N-CA-C	-10.26	83.30	111.00
1	B	159	LEU	CA-CB-CG	6.23	129.64	115.30
1	A	159	LEU	CA-CB-CG	5.95	128.99	115.30
1	B	233	GLU	N-CA-C	5.44	125.69	111.00
1	A	233	GLU	N-CA-C	5.14	124.88	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	ASP	Peptide
1	A	233	GLU	Peptide
1	B	126	ASP	Peptide
1	B	233	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2983	0	2930	67	0
1	B	2983	0	2930	58	0
2	C	36	0	32	1	0
2	D	36	0	32	0	0
3	A	1	0	0	1	0
3	B	1	0	0	1	0
4	A	215	0	0	8	0
4	B	195	0	0	10	0
All	All	6450	0	5924	126	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 11.

All (126) 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:127:SER:CB	1:A:127:SER:OG	1.64	1.44
1:B:285:MSE:HG3	1:B:291:LEU:HD13	1.33	1.07
1:A:285:MSE:HG3	1:A:291:LEU:HD13	1.31	1.07
1:A:100:VAL:HG13	4:A:2144:HOH:O	1.67	0.93
1:A:285:MSE:HG3	1:A:291:LEU:CD1	2.05	0.87
1:A:258:GLY:HA3	4:A:2117:HOH:O	1.77	0.84
1:A:262:ALA:HB3	4:A:2117:HOH:O	1.79	0.82
1:B:285:MSE:HG3	1:B:291:LEU:CD1	2.10	0.82
1:B:123:PRO:O	1:B:127:SER:CB	2.29	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:PRO:O	1:A:127:SER:HB3	1.81	0.80
1:A:122:LYS:HE3	1:A:142:GLN:NE2	1.96	0.80
1:A:123:PRO:O	1:A:127:SER:CB	2.30	0.79
1:A:133:ASN:HB3	1:A:331:THR:HG23	1.66	0.78
1:A:311:ILE:HG21	4:A:2152:HOH:O	1.82	0.78
1:B:157:MSE:HE3	1:B:302:ILE:HD13	1.64	0.77
1:B:133:ASN:HB3	1:B:331:THR:HG23	1.67	0.76
3:B:1427:IOD:I	4:B:2008:HOH:O	2.72	0.76
1:B:123:PRO:O	1:B:127:SER:HB2	1.86	0.75
1:A:285:MSE:CG	1:A:291:LEU:HD13	2.12	0.75
4:A:2214:HOH:O	2:C:1:GAL:H1	1.87	0.75
1:B:199:PHE:HB3	1:B:274:VAL:HG13	1.68	0.74
1:B:71:SER:HB3	4:B:2022:HOH:O	1.87	0.74
1:A:157:MSE:HE3	1:A:302:ILE:HD13	1.68	0.74
1:A:199:PHE:HB3	1:A:274:VAL:HG13	1.68	0.73
1:B:285:MSE:O	1:B:291:LEU:HD11	1.89	0.73
1:B:285:MSE:CG	1:B:291:LEU:HD13	2.15	0.71
1:A:285:MSE:O	1:A:291:LEU:HD11	1.91	0.70
1:B:133:ASN:HB3	1:B:331:THR:CG2	2.22	0.70
1:A:133:ASN:HB3	1:A:331:THR:CG2	2.23	0.69
3:A:1427:IOD:I	4:A:2061:HOH:O	2.86	0.64
1:B:140:GLN:HE22	1:B:305:SER:H	1.48	0.62
1:B:336:GLN:HB3	1:B:352:VAL:HG21	1.81	0.61
1:A:140:GLN:HE22	1:A:305:SER:H	1.49	0.60
1:A:336:GLN:HB3	1:A:352:VAL:HG21	1.82	0.60
1:A:336:GLN:HG2	1:A:349:ASN:CB	2.33	0.59
1:B:123:PRO:O	1:B:127:SER:HB3	2.03	0.58
1:A:187:MSE:HE2	1:A:198:ALA:HB1	1.86	0.58
1:B:311:ILE:HD12	1:B:323:ALA:HB3	1.85	0.58
1:A:59:MSE:CE	1:A:153:GLN:OE1	2.52	0.57
1:B:187:MSE:HE2	1:B:198:ALA:HB1	1.87	0.57
1:B:336:GLN:HG2	1:B:349:ASN:CB	2.35	0.57
1:A:314:LYS:HE2	1:B:120:ASP:OD2	2.05	0.56
1:A:311:ILE:HD12	1:A:323:ALA:HB3	1.87	0.56
1:B:187:MSE:HG3	1:B:198:ALA:HB1	1.88	0.56
1:B:355:LYS:HE2	4:B:2160:HOH:O	2.04	0.55
1:A:127:SER:CB	1:A:127:SER:HG	2.08	0.55
1:A:122:LYS:HE3	1:A:142:GLN:HE21	1.70	0.55
1:B:233:GLU:HG2	1:B:233:GLU:O	2.05	0.55
1:A:44:HIS:HD2	1:A:46:TYR:H	1.54	0.54
1:A:59:MSE:HE1	1:A:153:GLN:OE1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:HIS:HD2	1:B:46:TYR:H	1.55	0.54
1:A:187:MSE:HG3	1:A:198:ALA:HB1	1.90	0.53
1:B:59:MSE:HE2	1:B:343:VAL:HG11	1.89	0.53
1:A:127:SER:CA	1:A:127:SER:OG	2.52	0.53
1:B:311:ILE:HD12	1:B:323:ALA:CB	2.38	0.53
1:A:123:PRO:O	1:A:127:SER:HB2	2.05	0.52
1:A:311:ILE:HD12	1:A:323:ALA:CB	2.38	0.52
1:B:59:MSE:CE	1:B:153:GLN:OE1	2.57	0.52
1:A:59:MSE:HE2	1:A:343:VAL:HG11	1.91	0.52
1:A:115:GLN:HE21	1:B:123:PRO:HB3	1.75	0.51
1:B:65:LYS:HE2	1:B:329:TYR:OH	2.09	0.51
1:A:233:GLU:HG2	1:A:233:GLU:O	2.10	0.51
1:A:336:GLN:HG2	1:A:349:ASN:HB2	1.91	0.51
1:B:336:GLN:HG2	1:B:349:ASN:HB2	1.91	0.49
1:B:59:MSE:HE1	1:B:153:GLN:OE1	2.12	0.49
1:A:327:LEU:O	1:A:331:THR:HB	2.13	0.48
1:A:122:LYS:HD2	1:A:142:GLN:HE21	1.78	0.48
1:B:327:LEU:O	1:B:331:THR:HB	2.13	0.48
1:A:340:PHE:CE1	1:A:369:LEU:HD13	2.49	0.48
1:B:140:GLN:NE2	1:B:305:SER:H	2.10	0.48
1:A:122:LYS:CE	1:A:142:GLN:NE2	2.74	0.47
1:A:339:ILE:O	1:A:343:VAL:O	2.32	0.47
1:A:140:GLN:NE2	1:A:305:SER:H	2.11	0.47
1:B:121:LEU:HD11	1:B:311:ILE:HG23	1.97	0.46
1:B:80:VAL:HG11	1:B:87:ILE:HD13	1.96	0.46
1:B:122:LYS:HE3	1:B:142:GLN:NE2	2.31	0.45
1:B:304:SER:HB3	1:B:384:PRO:HA	1.97	0.45
1:A:140:GLN:HE22	1:A:304:SER:HB2	1.81	0.45
1:A:187:MSE:HA	1:A:187:MSE:HE3	1.99	0.45
1:A:117:LEU:HD12	1:A:314:LYS:HZ3	1.81	0.45
1:A:315:MSE:HB3	1:A:319:LYS:HG3	1.98	0.45
1:B:330:MSE:HE3	4:B:2148:HOH:O	2.16	0.45
1:A:336:GLN:HG2	1:A:349:ASN:HB3	1.99	0.45
1:A:122:LYS:HE3	1:A:142:GLN:HE22	1.76	0.45
1:B:140:GLN:HE22	1:B:304:SER:HB2	1.81	0.45
1:B:117:LEU:HD12	1:B:314:LYS:HZ3	1.82	0.45
1:A:121:LEU:HD11	1:A:311:ILE:HG23	1.98	0.45
1:A:356:GLU:O	1:A:359:GLU:HB2	2.17	0.44
1:B:76:LYS:HB2	4:B:2023:HOH:O	2.17	0.44
1:A:185:GLN:NE2	4:A:2078:HOH:O	2.49	0.44
1:B:340:PHE:CE1	1:B:369:LEU:HD13	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:VAL:HG11	1:A:87:ILE:CD1	2.47	0.44
1:B:152:GLU:OE2	4:B:2061:HOH:O	2.20	0.44
1:B:203:GLU:O	1:B:206:ILE:HG22	2.17	0.44
1:A:365:THR:O	1:A:369:LEU:HB2	2.18	0.44
1:A:420:GLN:O	1:A:424:LYS:HD2	2.18	0.44
1:A:80:VAL:HG11	1:A:87:ILE:HD13	2.00	0.44
1:B:315:MSE:HB3	1:B:319:LYS:HG3	1.99	0.44
1:A:304:SER:HB3	1:A:384:PRO:HA	1.99	0.44
1:A:232:ILE:O	1:A:232:ILE:HG22	2.17	0.44
1:B:157:MSE:HE3	1:B:302:ILE:CD1	2.42	0.44
1:B:185:GLN:NE2	4:B:2083:HOH:O	2.50	0.43
1:B:356:GLU:O	1:B:359:GLU:HB2	2.17	0.43
1:B:420:GLN:O	1:B:424:LYS:HD2	2.19	0.43
1:A:203:GLU:O	1:A:206:ILE:HG22	2.18	0.43
1:B:187:MSE:HA	1:B:187:MSE:HE3	2.01	0.43
1:B:331:THR:HG22	4:B:2147:HOH:O	2.19	0.43
1:B:365:THR:O	1:B:369:LEU:HB2	2.19	0.43
1:B:48:HIS:HB3	1:B:52:GLU:HG3	2.00	0.43
1:B:80:VAL:HG11	1:B:87:ILE:CD1	2.47	0.43
1:A:59:MSE:HE3	1:A:153:GLN:OE1	2.17	0.42
1:A:155:PHE:HE2	1:A:157:MSE:CE	2.33	0.42
1:A:48:HIS:H	1:A:48:HIS:CD2	2.37	0.42
1:A:122:LYS:CE	1:A:142:GLN:HE21	2.33	0.42
1:B:336:GLN:HG2	1:B:349:ASN:HB3	2.02	0.42
1:B:48:HIS:H	1:B:48:HIS:CD2	2.38	0.42
1:B:291:LEU:HB3	4:B:2067:HOH:O	2.19	0.42
1:A:117:LEU:HD12	1:A:314:LYS:NZ	2.35	0.42
1:A:152:GLU:H	1:A:152:GLU:HG3	1.55	0.42
1:A:234:SER:OG	1:A:237:PHE:HB2	2.19	0.42
1:B:232:ILE:HG22	1:B:232:ILE:O	2.19	0.42
1:B:151:HIS:HA	1:B:308:GLY:HA3	2.03	0.41
1:A:157:MSE:HE3	1:A:302:ILE:CD1	2.44	0.41
1:B:242:LYS:HE2	4:B:2103:HOH:O	2.20	0.41
1:A:106:ASN:O	1:A:307:GLY:HA3	2.20	0.41
1:A:71:SER:HB3	4:A:2019:HOH:O	2.22	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	385/430 (90%)	375 (97%)	8 (2%)	2 (0%)	29	32
1	B	385/430 (90%)	374 (97%)	10 (3%)	1 (0%)	41	47
All	All	770/860 (90%)	749 (97%)	18 (2%)	3 (0%)	34	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	SER
1	B	234	SER
1	A	127	SER

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	320/343 (93%)	295 (92%)	25 (8%)	12	12
1	B	320/343 (93%)	296 (92%)	24 (8%)	13	13
All	All	640/686 (93%)	591 (92%)	49 (8%)	13	12

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	LEU
1	A	116	LYS
1	A	117	LEU

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Mol	Chain	Res	Type
1	A	121	LEU
1	A	127	SER
1	A	140	GLN
1	A	143	LYS
1	A	152	GLU
1	A	154	LEU
1	A	159	LEU
1	A	187	MSE
1	A	210	ASN
1	A	215	THR
1	A	222	LEU
1	A	224	ASP
1	A	234	SER
1	A	285	MSE
1	A	291	LEU
1	A	311	ILE
1	A	331	THR
1	A	336	GLN
1	A	368	ILE
1	A	369	LEU
1	A	382	VAL
1	A	423	LEU
1	B	62	LEU
1	B	116	LYS
1	B	117	LEU
1	B	121	LEU
1	B	140	GLN
1	B	143	LYS
1	B	152	GLU
1	B	154	LEU
1	B	159	LEU
1	B	187	MSE
1	B	210	ASN
1	B	215	THR
1	B	222	LEU
1	B	224	ASP
1	B	234	SER
1	B	285	MSE
1	B	291	LEU
1	B	311	ILE
1	B	331	THR
1	B	336	GLN

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Mol	Chain	Res	Type
1	B	368	ILE
1	B	369	LEU
1	B	382	VAL
1	B	423	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	81	ASN
1	A	115	GLN
1	A	140	GLN
1	A	142	GLN
1	A	185	GLN
1	A	255	ASN
1	A	268	GLN
1	A	400	ASN
1	A	414	GLN
1	B	44	HIS
1	B	48	HIS
1	B	70	HIS
1	B	81	ASN
1	B	106	ASN
1	B	140	GLN
1	B	142	GLN
1	B	185	GLN
1	B	268	GLN
1	B	400	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

6 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	GAL	C	1	2	12,12,12	0.58	0	17,17,17	0.62	0
2	FUC	C	2	2	10,10,11	0.62	0	14,14,16	0.72	0
2	A2G	C	3	2	14,14,15	0.83	1 (7%)	17,19,21	1.08	2 (11%)
2	GAL	D	1	2	12,12,12	0.56	0	17,17,17	0.79	0
2	FUC	D	2	2	10,10,11	0.55	0	14,14,16	0.77	0
2	A2G	D	3	2	14,14,15	0.90	0	17,19,21	0.89	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	GAL	C	1	2	-	1/2/22/22	0/1/1/1
2	FUC	C	2	2	-	-	0/1/1/1
2	A2G	C	3	2	-	0/6/23/26	0/1/1/1
2	GAL	D	1	2	-	0/2/22/22	0/1/1/1
2	FUC	D	2	2	-	-	0/1/1/1
2	A2G	D	3	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	A2G	O5-C5	2.32	1.48	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3	A2G	O5-C1-C2	-2.21	107.79	111.29
2	C	3	A2G	C1-O5-C5	2.10	115.04	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

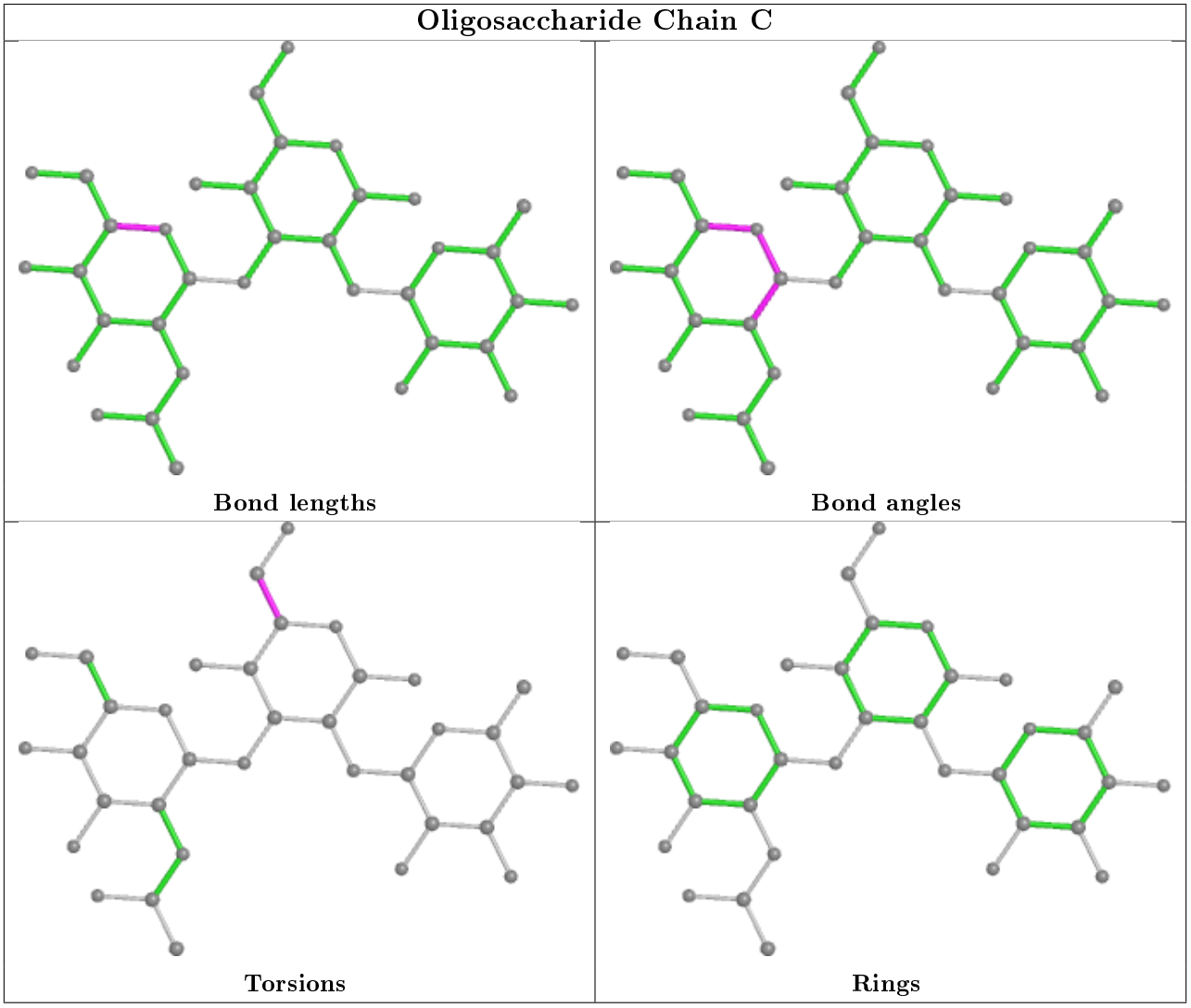
Mol	Chain	Res	Type	Atoms
2	C	1	GAL	C4-C5-C6-O6

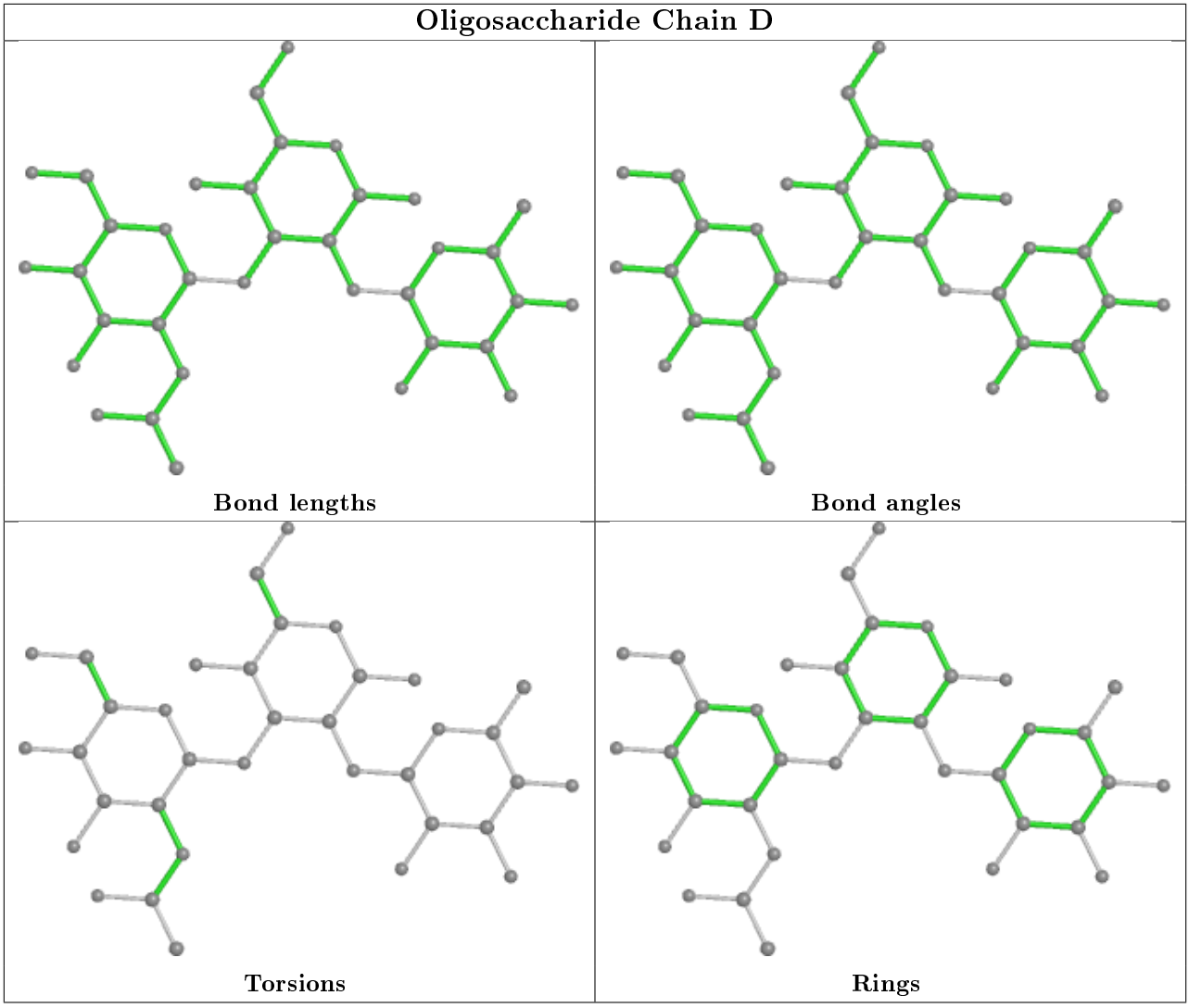
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	GAL	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.





5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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

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	380/430 (88%)	0.45	8 (2%) 63 74	23, 23, 24, 24	0
1	B	380/430 (88%)	0.64	30 (7%) 12 19	23, 23, 24, 24	0
All	All	760/860 (88%)	0.55	38 (5%) 28 41	23, 23, 24, 24	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	71	SER	4.8
1	B	257	GLY	4.7
1	B	194	ASP	4.1
1	B	233	GLU	3.6
1	B	231	GLY	3.4
1	B	68	GLU	3.3
1	B	69	GLU	3.2
1	A	258	GLY	3.2
1	B	221	LYS	3.2
1	B	229	LYS	3.1
1	B	258	GLY	3.0
1	A	257	GLY	2.9
1	A	259	ASP	2.8
1	B	51	ASP	2.8
1	B	193	GLN	2.8
1	B	254	LYS	2.7
1	B	362	SER	2.6
1	B	367	LYS	2.6
1	B	259	ASP	2.6
1	B	217	GLU	2.6
1	B	230	GLU	2.6
1	B	359	GLU	2.5
1	B	64	ASP	2.5
1	A	311	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	260	ALA	2.3
1	B	140	GLN	2.3
1	B	72	GLY	2.3
1	A	93	ALA	2.2
1	B	70	HIS	2.2
1	B	213	LEU	2.2
1	A	195	GLY	2.2
1	B	224	ASP	2.2
1	A	68	GLU	2.2
1	B	363	GLU	2.2
1	B	114	GLU	2.1
1	A	194	ASP	2.1
1	B	50	GLU	2.0
1	B	132	LYS	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)

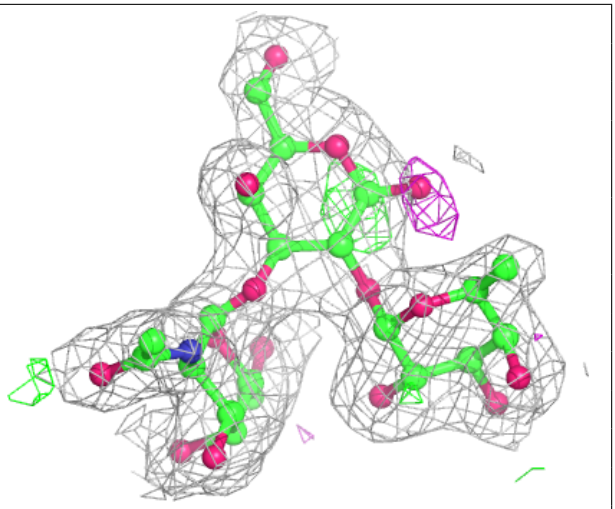
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

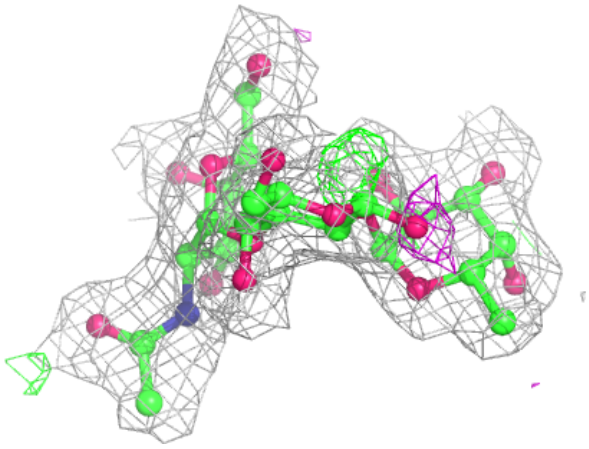
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GAL	C	1	12/12	0.86	0.17	12,16,16,20	0
2	GAL	D	1	12/12	0.89	0.17	18,19,22,22	0
2	A2G	C	3	14/15	0.93	0.12	12,14,15,15	0
2	FUC	D	2	10/11	0.94	0.13	22,22,23,23	0
2	A2G	D	3	14/15	0.94	0.12	19,19,20,20	0
2	FUC	C	2	10/11	0.95	0.12	12,14,15,16	0

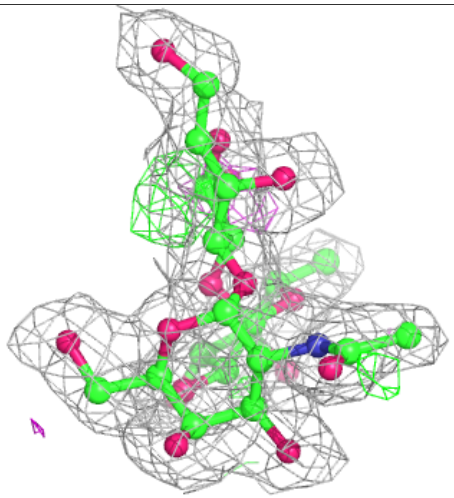
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

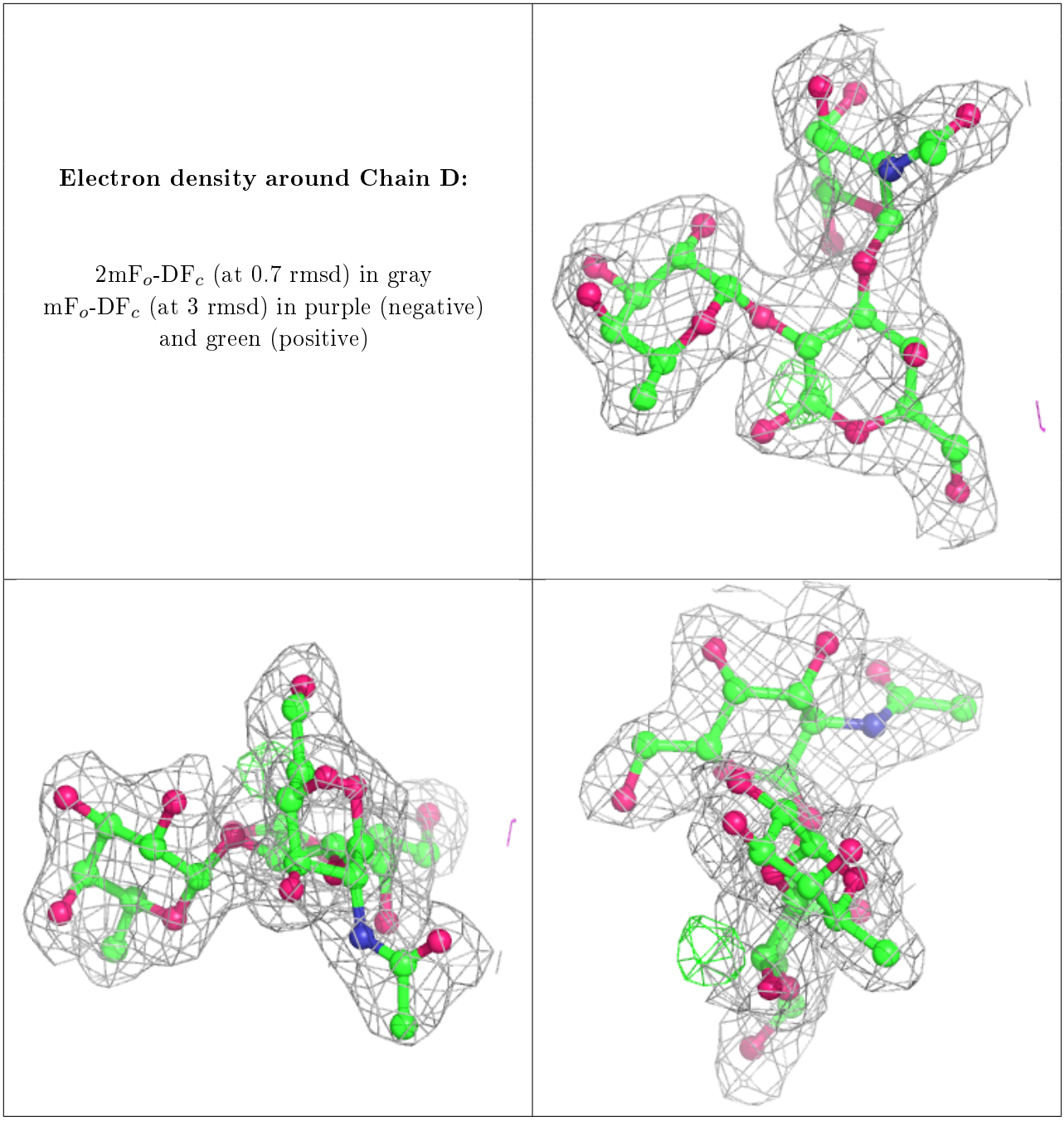






Electron density around Chain D:

$2mF_o$-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
3	IOD	A	1427	1/1	0.99	0.12	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	IOD	B	1427	1/1	1.00	0.13	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.