Full wwPDB X-ray Structure Validation Report (i)

Oct 25, 2022 – 10:29 pm BST

PDB ID	:	7QM2
Title	:	Crystal structure of the PP1/PTG/beta-cyclodextrin ternary complex
Authors	:	Semrau, M.S.; Storici, P.; Lolli, G.
Deposited on	:	2021-12-20
Resolution	:	2.69 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

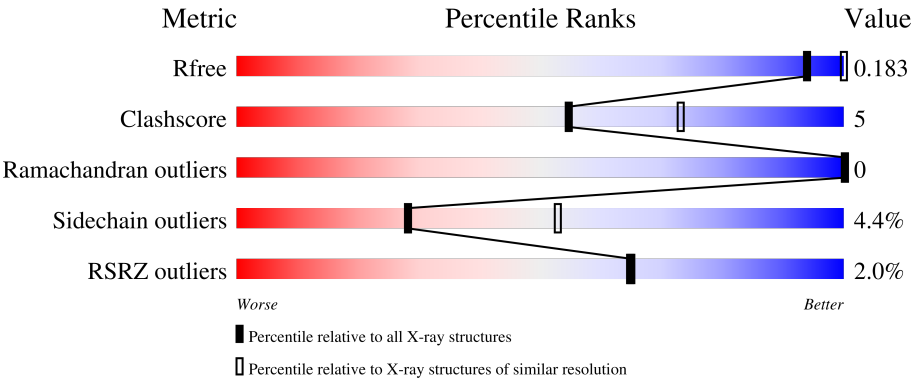
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.69 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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

Mol	Chain	Length	Quality of chain
1	A	299	84% 11% 5%
1	C	299	81% 13% 5%
2	B	200	67% 15% 18%
2	D	200	5% 62% 18% 19%
3	E	7	57% 43%

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Mol	Chain	Length	Quality of chain
3	F	7	100%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7413 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 Serine/threonine-protein phosphatase PP1-alpha catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2291	1472	380	421	18			
1	C	284	Total	C	N	O	S	0	0	0
			2291	1472	380	421	18			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	-	expression tag	UNP P62136
A	3	HIS	-	expression tag	UNP P62136
A	4	MET	-	expression tag	UNP P62136
A	5	GLY	-	expression tag	UNP P62136
A	6	SER	-	expression tag	UNP P62136
C	2	GLY	-	expression tag	UNP P62136
C	3	HIS	-	expression tag	UNP P62136
C	4	MET	-	expression tag	UNP P62136
C	5	GLY	-	expression tag	UNP P62136
C	6	SER	-	expression tag	UNP P62136

- Molecule 2 is a protein called Protein phosphatase 1 regulatory subunit 3C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	165	Total	C	N	O	S	0	0	0
			1338	857	222	254	5			
2	D	162	Total	C	N	O	S	0	0	0
			1320	844	220	251	5			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	65	GLY	-	expression tag	UNP Q9UQK1

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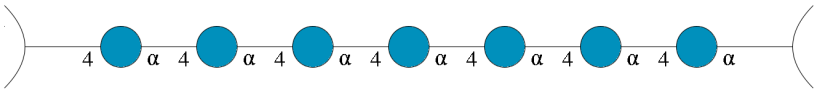
Chain	Residue	Modelled	Actual	Comment	Reference
B	66	PRO	-	expression tag	UNP Q9UQK1
B	67	LEU	-	expression tag	UNP Q9UQK1
B	68	GLY	-	expression tag	UNP Q9UQK1
B	69	SER	-	expression tag	UNP Q9UQK1
D	65	GLY	-	expression tag	UNP Q9UQK1
D	66	PRO	-	expression tag	UNP Q9UQK1
D	67	LEU	-	expression tag	UNP Q9UQK1
D	68	GLY	-	expression tag	UNP Q9UQK1
D	69	SER	-	expression tag	UNP Q9UQK1

- Molecule 3 is an oligosaccharide called Cycloheptakis-(1-4)-(alpha-D-glucopyranose).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	E	7	Total C O 77 42 35	0	0	0
3	F	7	Total C O 77 42 35	0	0	0

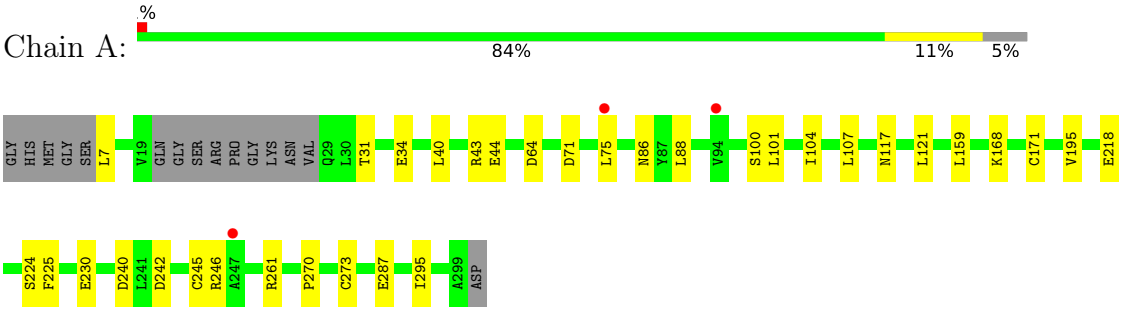
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total O 4 4	0	0
4	B	4	Total O 4 4	0	0
4	C	6	Total O 6 6	0	0
4	D	5	Total O 5 5	0	0

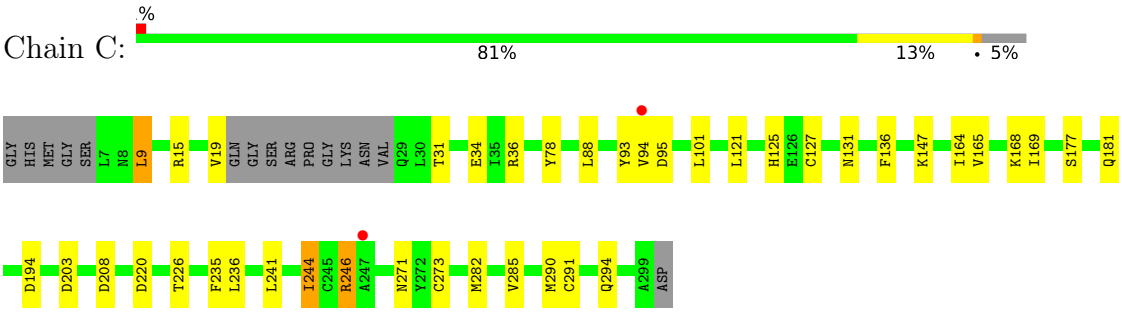
3 Residue-property plots (i)

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.

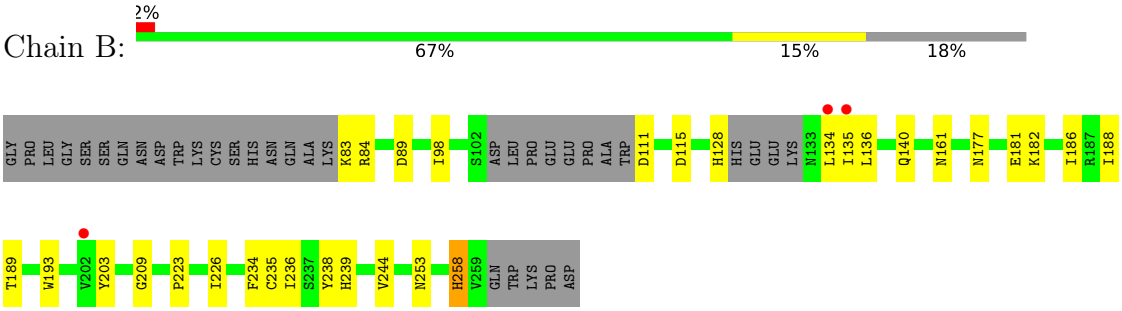
• Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit



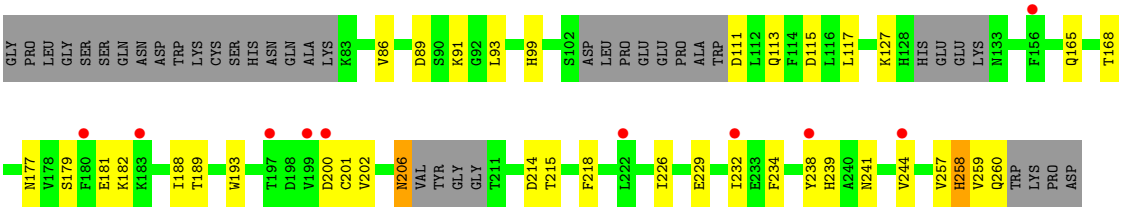
• Molecule 1: Serine/threonine-protein phosphatase PP1-alpha catalytic subunit



• Molecule 2: Protein phosphatase 1 regulatory subunit 3C

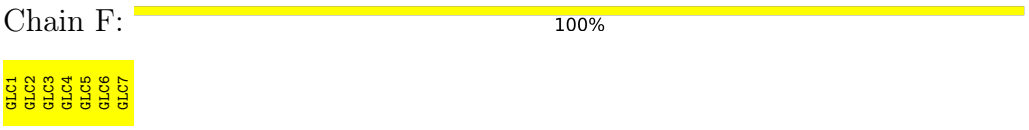


• Molecule 2: Protein phosphatase 1 regulatory subunit 3C



• Molecule 3: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)

• Molecule 3: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	153.60Å 153.60Å 285.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	52.29 – 2.69 120.59 – 2.69	Depositor EDS
% Data completeness (in resolution range)	65.3 (52.29-2.69) 65.3 (120.59-2.69)	Depositor EDS
R_{merge}	0.36	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.11.1	Depositor
R, R_{free}	0.177 , 0.213 0.178 , 0.183	Depositor DCC
R_{free} test set	1812 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	65.3	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7413	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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: GLC

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	0.54	0/2343	0.66	0/3165
1	C	0.53	1/2343 (0.0%)	0.68	1/3165 (0.0%)
2	B	0.42	0/1368	0.66	0/1853
2	D	0.45	0/1348	0.62	0/1824
All	All	0.50	1/7402 (0.0%)	0.66	1/10007 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	127	CYS	CB-SG	-5.99	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	194	ASP	CB-CA-C	-6.70	97.00	110.40

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	2291	0	2250	17	0
1	C	2291	0	2250	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1338	0	1295	24	0
2	D	1320	0	1278	17	0
3	E	77	0	63	5	0
3	F	77	0	63	0	0
4	A	4	0	0	0	0
4	B	4	0	0	1	0
4	C	6	0	0	0	0
4	D	5	0	0	1	0
All	All	7413	0	7199	76	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 5.

All (76) 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)
2:D:182:LYS:HB3	2:D:238:TYR:HE1	1.59	0.66
2:B:223:PRO:HD2	2:B:226:ILE:HD11	1.81	0.62
2:B:188:ILE:HG13	2:B:234:PHE:HB3	1.81	0.61
2:D:188:ILE:HG13	2:D:234:PHE:HB3	1.83	0.61
1:A:261:ARG:NH1	2:B:89:ASP:OD2	2.33	0.59
2:B:258:HIS:H	2:B:258:HIS:CD2	2.19	0.59
1:A:88:LEU:HD11	1:A:121:LEU:HD13	1.86	0.56
2:B:186:ILE:HD12	2:B:236:ILE:HG12	1.87	0.56
2:B:177:ASN:ND2	3:E:5:GLC:O2	2.34	0.56
2:D:179:SER:HB2	2:D:241:ASN:HB2	1.87	0.55
1:C:78:TYR:CZ	2:D:99:HIS:HB2	2.42	0.55
1:A:31:THR:HG23	1:A:34:GLU:H	1.71	0.54
1:C:131:ASN:HB2	1:C:136:PHE:HB3	1.90	0.54
1:A:242:ASP:OD2	2:B:84:ARG:HG3	2.09	0.53
1:A:287:GLU:OE1	2:B:83:LYS:NZ	2.42	0.52
2:D:177:ASN:ND2	2:D:214:ASP:OD2	2.41	0.52
1:A:86:ASN:OD1	1:A:117:ASN:HB3	2.10	0.52
2:B:235:CYS:HB3	2:B:253:ASN:ND2	2.24	0.52
2:B:182:LYS:HB3	2:B:238:TYR:HE2	1.75	0.51
1:A:71:ASP:OD2	1:A:270:PRO:HD2	2.10	0.51
2:D:259:VAL:HG12	2:D:260:GLN:H	1.74	0.51
3:E:6:GLC:H3	3:E:7:GLC:O2	2.10	0.51
1:C:15:ARG:NH1	1:C:34:GLU:OE2	2.42	0.50
2:B:203:TYR:CE2	3:E:5:GLC:H61	2.47	0.49
1:A:295:ILE:HB	2:B:98:ILE:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:GLY:H	1:C:181:GLN:HG3	1.79	0.47
1:A:44:GLU:HG2	2:B:135:ILE:CD1	2.45	0.47
2:B:111:ASP:N	4:B:303:HOH:O	2.46	0.47
1:C:15:ARG:HH12	1:C:34:GLU:CD	2.18	0.47
1:C:177:SER:HB2	1:C:203:ASP:HB2	1.97	0.46
2:B:235:CYS:HB3	2:B:253:ASN:HD22	1.80	0.46
1:C:282:MET:HE3	1:C:282:MET:HB3	1.77	0.46
2:B:239:HIS:CD2	2:B:244:VAL:HG22	2.50	0.46
1:C:235:PHE:HD2	1:C:244:ILE:HD11	1.80	0.46
2:B:140:GLN:OE1	2:B:161:ASN:ND2	2.44	0.45
2:B:182:LYS:NZ	3:E:5:GLC:H3	2.31	0.45
2:D:257:VAL:HG12	2:D:258:HIS:H	1.82	0.45
1:A:100:SER:O	1:A:104:ILE:HG22	2.16	0.45
1:C:165:VAL:CG1	1:C:169:ILE:HB	2.46	0.45
2:D:165:GLN:O	2:D:168:THR:HG22	2.15	0.45
1:C:285:VAL:HG22	1:C:291:CYS:SG	2.56	0.45
2:D:111:ASP:N	4:D:303:HOH:O	2.49	0.45
2:D:226:ILE:HG21	2:D:232:ILE:HD11	1.99	0.44
1:A:168:LYS:HA	1:A:168:LYS:HD3	1.74	0.44
1:A:171:CYS:HA	1:A:245:CYS:O	2.18	0.44
1:A:44:GLU:HG2	2:B:135:ILE:HD11	2.00	0.44
1:C:236:LEU:HD21	1:C:244:ILE:HD12	1.99	0.43
2:D:239:HIS:CD2	2:D:244:VAL:HG22	2.52	0.43
2:B:134:LEU:HD23	2:B:258:HIS:HA	2.00	0.43
1:A:224:SER:OG	1:A:225:PHE:N	2.50	0.43
2:B:258:HIS:CD2	2:B:258:HIS:N	2.86	0.43
1:C:93:TYR:HB2	1:C:94:VAL:HG13	1.99	0.43
1:C:246:ARG:HD3	1:C:246:ARG:C	2.39	0.43
1:C:282:MET:HE3	1:C:294:GLN:HB2	2.00	0.43
3:E:5:GLC:H62	3:E:6:GLC:O5	2.19	0.43
2:D:206:ASN:HD22	2:D:206:ASN:HA	1.73	0.43
1:C:165:VAL:HG13	1:C:169:ILE:HB	2.01	0.42
2:D:201:CYS:SG	2:D:218:PHE:HB3	2.59	0.42
1:C:164:ILE:HA	1:C:169:ILE:O	2.19	0.42
2:D:91:LYS:O	2:D:93:LEU:HD12	2.19	0.42
1:A:40:LEU:HA	1:A:40:LEU:HD23	1.73	0.42
1:C:88:LEU:HD11	1:C:121:LEU:HG	2.02	0.42
1:C:290:MET:HA	2:D:86:VAL:O	2.20	0.41
1:A:101:LEU:HD23	1:A:101:LEU:HA	1.85	0.41
2:D:189:THR:HG21	2:D:193:TRP:CD2	2.56	0.41
2:D:226:ILE:HD13	2:D:226:ILE:HA	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ASP:OD1	1:A:64:ASP:N	2.54	0.41
1:C:36:ARG:NH2	1:C:147:LYS:HE2	2.35	0.41
2:B:189:THR:HG21	2:B:193:TRP:CE2	2.56	0.41
1:C:9:LEU:HD23	1:C:9:LEU:HA	1.82	0.41
1:C:168:LYS:HA	1:C:168:LYS:HD3	1.78	0.40
1:C:36:ARG:HH22	1:C:147:LYS:HE2	1.87	0.40
2:B:181:GLU:HG3	2:B:181:GLU:O	2.21	0.40
1:C:95:ASP:HB2	1:C:125:HIS:ND1	2.36	0.40
1:C:101:LEU:HD23	1:C:101:LEU:HA	1.84	0.40
1:C:208:ASP:O	1:C:226:THR:HA	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	280/299 (94%)	262 (94%)	18 (6%)	0	100	100
1	C	280/299 (94%)	264 (94%)	16 (6%)	0	100	100
2	B	159/200 (80%)	152 (96%)	7 (4%)	0	100	100
2	D	154/200 (77%)	147 (96%)	7 (4%)	0	100	100
All	All	873/998 (88%)	825 (94%)	48 (6%)	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	251/262 (96%)	240 (96%)	11 (4%)	28	53
1	C	251/262 (96%)	242 (96%)	9 (4%)	35	61
2	B	154/185 (83%)	150 (97%)	4 (3%)	46	73
2	D	153/185 (83%)	141 (92%)	12 (8%)	12	27
All	All	809/894 (90%)	773 (96%)	36 (4%)	28	53

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	43	ARG
1	A	75	LEU
1	A	107	LEU
1	A	159	LEU
1	A	195	VAL
1	A	218	GLU
1	A	230	GLU
1	A	240	ASP
1	A	246	ARG
1	A	273	CYS
2	B	115	ASP
2	B	128	HIS
2	B	136	LEU
2	B	258	HIS
1	C	9	LEU
1	C	19	VAL
1	C	31	THR
1	C	220	ASP
1	C	241	LEU
1	C	244	ILE
1	C	246	ARG
1	C	271	ASN
1	C	273	CYS
2	D	89	ASP
2	D	113	GLN
2	D	115	ASP
2	D	117	LEU
2	D	127	LYS
2	D	181	GLU

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Mol	Chain	Res	Type
2	D	200	ASP
2	D	202	VAL
2	D	206	ASN
2	D	215	THR
2	D	229	GLU
2	D	258	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	68	GLN
2	B	133	ASN
2	B	177	ASN
2	B	185	GLN
2	B	239	HIS
2	B	253	ASN
2	B	258	HIS
1	C	66	HIS
1	C	68	GLN
1	C	294	GLN
2	D	120	ASN
2	D	128	HIS
2	D	133	ASN
2	D	155	ASN
2	D	206	ASN
2	D	239	HIS
2	D	258	HIS

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

14 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	$\#\|Z\| > 2$
3	GLC	E	1	3	11,11,12	1.04	0	15,15,17	1.12	1 (6%)
3	GLC	E	2	3	11,11,12	1.24	1 (9%)	15,15,17	1.94	4 (26%)
3	GLC	E	3	3	11,11,12	0.85	0	15,15,17	1.66	2 (13%)
3	GLC	E	4	3	11,11,12	1.29	2 (18%)	15,15,17	1.44	2 (13%)
3	GLC	E	5	3	11,11,12	0.78	0	15,15,17	2.82	7 (46%)
3	GLC	E	6	3	11,11,12	1.39	2 (18%)	15,15,17	3.40	7 (46%)
3	GLC	E	7	3	11,11,12	1.07	0	15,15,17	2.17	4 (26%)
3	GLC	F	1	3	11,11,12	1.24	2 (18%)	15,15,17	2.58	9 (60%)
3	GLC	F	2	3	11,11,12	1.32	3 (27%)	15,15,17	1.26	2 (13%)
3	GLC	F	3	3	11,11,12	0.86	0	15,15,17	1.21	2 (13%)
3	GLC	F	4	3	11,11,12	1.64	3 (27%)	15,15,17	2.46	6 (40%)
3	GLC	F	5	3	11,11,12	0.84	0	15,15,17	1.37	4 (26%)
3	GLC	F	6	3	11,11,12	1.23	1 (9%)	15,15,17	1.67	4 (26%)
3	GLC	F	7	3	11,11,12	1.05	1 (9%)	15,15,17	1.08	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
3	GLC	E	1	3	-	1/2/19/22	0/1/1/1
3	GLC	E	2	3	-	0/2/19/22	0/1/1/1
3	GLC	E	3	3	-	2/2/19/22	0/1/1/1
3	GLC	E	4	3	-	1/2/19/22	0/1/1/1
3	GLC	E	5	3	-	0/2/19/22	0/1/1/1
3	GLC	E	6	3	-	1/2/19/22	0/1/1/1
3	GLC	E	7	3	-	2/2/19/22	0/1/1/1
3	GLC	F	1	3	-	1/2/19/22	0/1/1/1
3	GLC	F	2	3	-	0/2/19/22	0/1/1/1
3	GLC	F	3	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLC	F	4	3	-	0/2/19/22	0/1/1/1
3	GLC	F	5	3	-	0/2/19/22	0/1/1/1
3	GLC	F	6	3	-	2/2/19/22	0/1/1/1
3	GLC	F	7	3	-	2/2/19/22	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	4	GLC	O4-C4	3.00	1.50	1.43
3	F	4	GLC	C1-C2	2.98	1.59	1.52
3	E	2	GLC	C1-C2	2.76	1.58	1.52
3	F	1	GLC	C1-C2	2.63	1.58	1.52
3	E	4	GLC	C1-C2	2.55	1.58	1.52
3	F	2	GLC	C1-C2	2.52	1.57	1.52
3	E	6	GLC	C1-C2	2.42	1.57	1.52
3	F	1	GLC	C2-C3	2.27	1.55	1.52
3	F	4	GLC	O2-C2	-2.20	1.38	1.43
3	F	2	GLC	C2-C3	2.16	1.55	1.52
3	F	7	GLC	C1-C2	2.09	1.57	1.52
3	F	6	GLC	C1-C2	2.09	1.57	1.52
3	E	6	GLC	O2-C2	-2.02	1.39	1.43
3	E	4	GLC	O4-C4	2.02	1.47	1.43
3	F	2	GLC	O2-C2	-2.00	1.39	1.43

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	6	GLC	C1-O5-C5	8.10	123.17	112.19
3	E	5	GLC	C1-C2-C3	6.31	117.42	109.67
3	E	6	GLC	C1-C2-C3	5.54	116.48	109.67
3	F	1	GLC	C1-C2-C3	5.28	116.16	109.67
3	E	7	GLC	C1-C2-C3	5.20	116.06	109.67
3	F	4	GLC	O4-C4-C5	5.19	122.18	109.30
3	E	2	GLC	C1-C2-C3	4.85	115.63	109.67
3	E	5	GLC	C2-C3-C4	4.78	119.17	110.89
3	E	6	GLC	O5-C1-C2	4.45	117.64	110.77
3	F	4	GLC	C2-C3-C4	-4.39	103.31	110.89
3	E	7	GLC	C2-C3-C4	4.00	117.82	110.89
3	E	3	GLC	C1-O5-C5	3.98	117.58	112.19
3	E	6	GLC	C2-C3-C4	3.94	117.71	110.89
3	F	1	GLC	C2-C3-C4	3.91	117.67	110.89
3	F	6	GLC	C1-O5-C5	3.88	117.45	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	4	GLC	C1-O5-C5	3.87	117.43	112.19
3	E	4	GLC	C1-O5-C5	3.80	117.35	112.19
3	E	5	GLC	O4-C4-C3	-3.78	101.62	110.35
3	E	5	GLC	C1-O5-C5	3.76	117.28	112.19
3	F	1	GLC	C3-C4-C5	3.59	116.64	110.24
3	E	6	GLC	C3-C4-C5	3.46	116.40	110.24
3	F	2	GLC	C1-C2-C3	3.39	113.83	109.67
3	E	3	GLC	O5-C1-C2	3.23	115.75	110.77
3	F	4	GLC	O4-C4-C3	3.09	117.48	110.35
3	F	1	GLC	O5-C5-C6	3.05	111.99	107.20
3	E	2	GLC	C2-C3-C4	3.03	116.14	110.89
3	E	2	GLC	O4-C4-C3	-3.02	103.37	110.35
3	F	4	GLC	O5-C1-C2	2.99	115.38	110.77
3	E	6	GLC	O5-C5-C4	2.94	117.98	110.83
3	E	6	GLC	C6-C5-C4	-2.90	106.20	113.00
3	F	1	GLC	C1-O5-C5	2.84	116.04	112.19
3	E	7	GLC	O2-C2-C3	-2.80	104.53	110.14
3	F	3	GLC	O4-C4-C3	-2.73	104.03	110.35
3	E	7	GLC	O3-C3-C2	-2.72	104.79	109.99
3	E	5	GLC	C3-C4-C5	2.65	114.96	110.24
3	E	5	GLC	O2-C2-C3	-2.56	105.01	110.14
3	F	5	GLC	O2-C2-C3	-2.56	105.02	110.14
3	F	5	GLC	O2-C2-C1	2.55	114.38	109.15
3	F	6	GLC	O5-C1-C2	2.48	114.60	110.77
3	E	1	GLC	C1-C2-C3	2.45	112.67	109.67
3	F	1	GLC	C6-C5-C4	-2.42	107.33	113.00
3	E	4	GLC	O5-C5-C4	2.34	116.53	110.83
3	F	6	GLC	O5-C5-C4	2.32	116.47	110.83
3	E	2	GLC	O2-C2-C3	-2.32	105.50	110.14
3	F	6	GLC	C3-C4-C5	2.31	114.36	110.24
3	F	3	GLC	C1-O5-C5	2.24	115.23	112.19
3	F	2	GLC	C2-C3-C4	2.23	114.76	110.89
3	F	5	GLC	O4-C4-C3	-2.23	105.19	110.35
3	F	1	GLC	O2-C2-C3	-2.22	105.70	110.14
3	F	5	GLC	O5-C1-C2	2.21	114.19	110.77
3	E	5	GLC	C6-C5-C4	-2.21	107.82	113.00
3	F	4	GLC	O3-C3-C4	2.09	115.17	110.35
3	F	1	GLC	O2-C2-C1	2.07	113.39	109.15
3	F	1	GLC	O5-C1-C2	2.02	113.89	110.77
3	F	7	GLC	O5-C5-C4	2.00	115.70	110.83

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	7	GLC	O5-C5-C6-O6
3	F	7	GLC	O5-C5-C6-O6
3	E	3	GLC	O5-C5-C6-O6
3	F	6	GLC	C4-C5-C6-O6
3	E	3	GLC	C4-C5-C6-O6
3	E	4	GLC	O5-C5-C6-O6
3	E	7	GLC	C4-C5-C6-O6
3	F	6	GLC	O5-C5-C6-O6
3	E	1	GLC	O5-C5-C6-O6
3	F	7	GLC	C4-C5-C6-O6
3	E	6	GLC	O5-C5-C6-O6
3	F	1	GLC	O5-C5-C6-O6

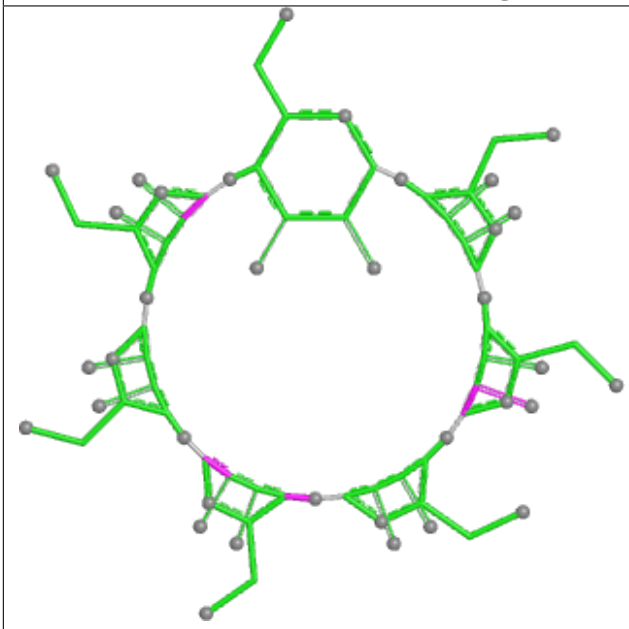
There are no ring outliers.

3 monomers are involved in 5 short contacts:

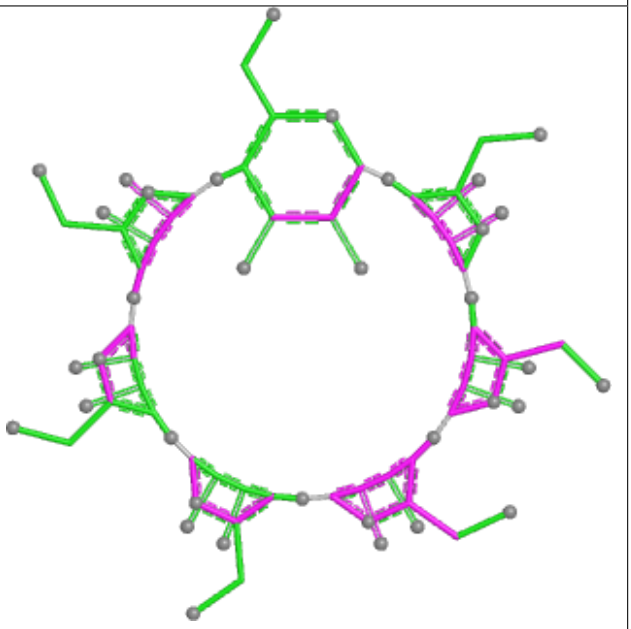
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	7	GLC	1	0
3	E	5	GLC	4	0
3	E	6	GLC	2	0

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

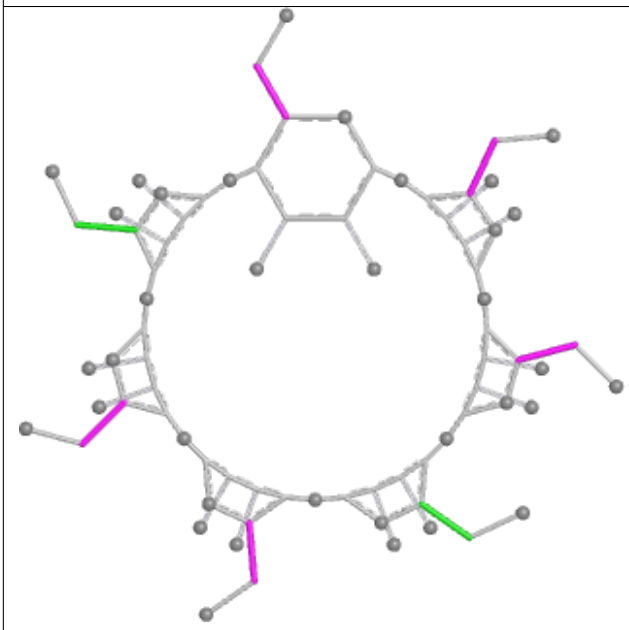
Oligosaccharide Chain E



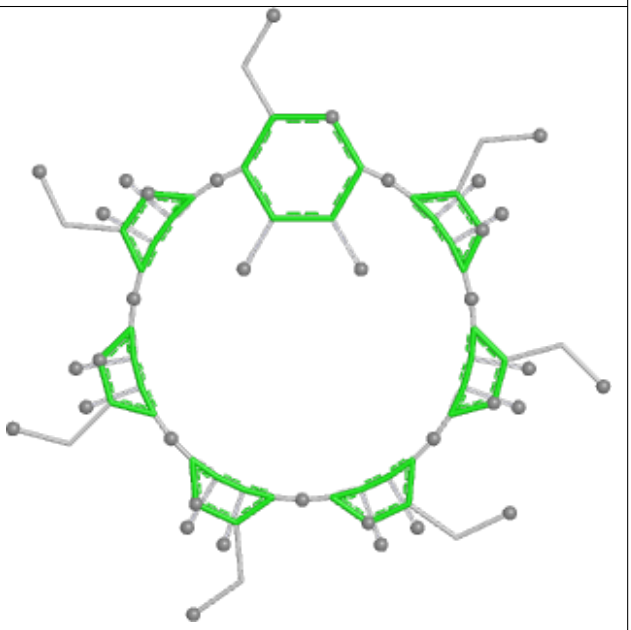
Bond lengths



Bond angles

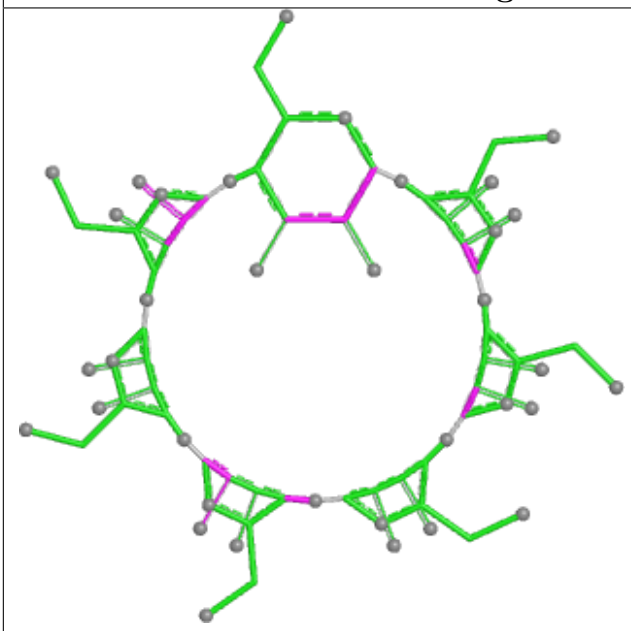


Torsions

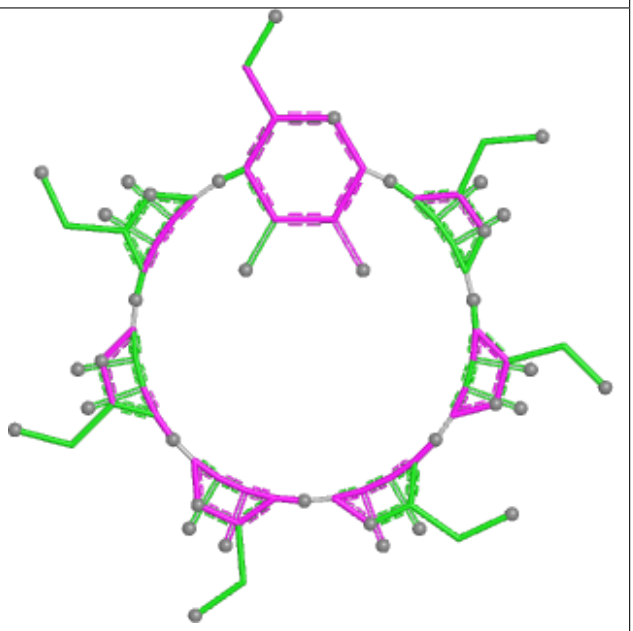


Rings

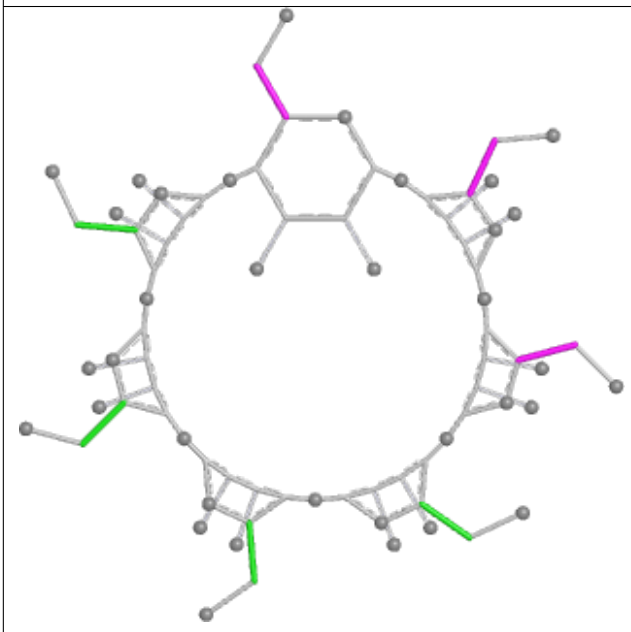
Oligosaccharide Chain F



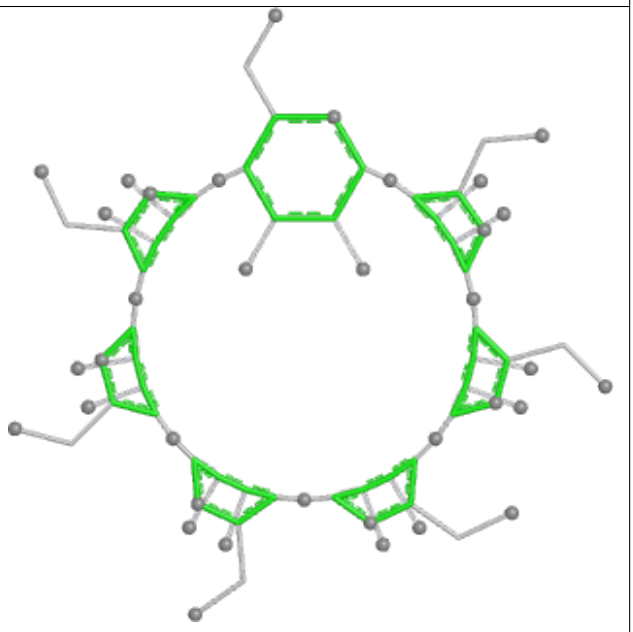
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	284/299 (94%)	0.48	3 (1%)	80	81	32, 50, 80, 102	0
1	C	284/299 (94%)	0.43	2 (0%)	87	88	36, 54, 82, 114	0
2	B	165/200 (82%)	0.54	3 (1%)	68	69	43, 66, 99, 115	0
2	D	162/200 (81%)	0.67	10 (6%)	20	18	48, 75, 113, 142	0
All	All	895/998 (89%)	0.51	18 (2%)	65	65	32, 59, 97, 142	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	222	LEU	4.2
2	B	134	LEU	3.6
2	D	244	VAL	2.9
2	D	180	PHE	2.8
2	D	199	VAL	2.7
2	D	183	LYS	2.7
1	A	94	VAL	2.6
2	D	238	TYR	2.5
1	A	75	LEU	2.4
1	A	247	ALA	2.3
2	D	200	ASP	2.2
2	B	202	VAL	2.2
2	D	232	ILE	2.2
2	D	197	THR	2.1
2	B	135	ILE	2.1
1	C	247	ALA	2.1
1	C	94	VAL	2.0
2	D	156	PHE	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)

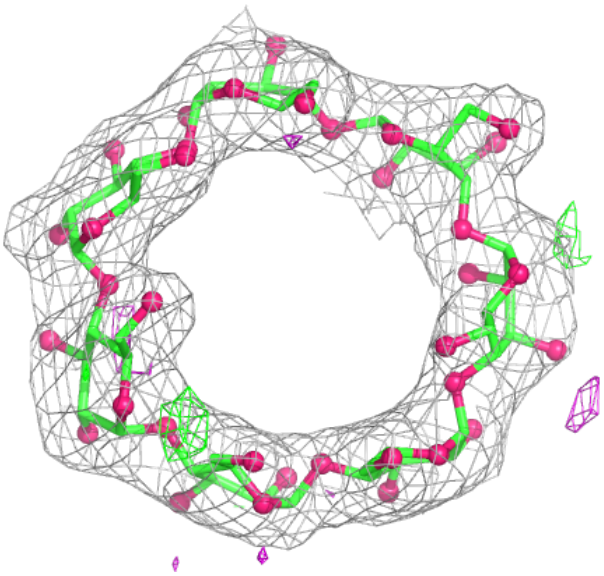
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

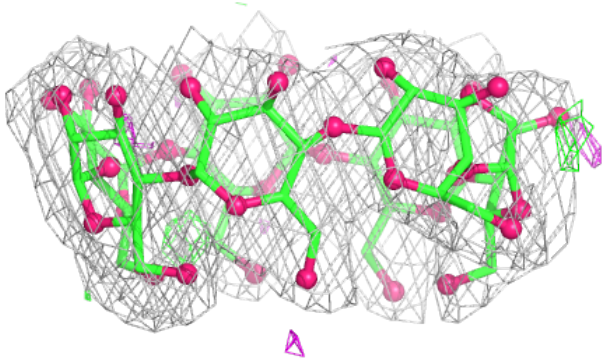
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GLC	F	1	11/12	0.88	0.18	74,95,105,106	0
3	GLC	F	4	11/12	0.93	0.17	64,74,79,91	0
3	GLC	F	7	11/12	0.93	0.12	76,82,93,94	0
3	GLC	F	5	11/12	0.94	0.17	65,82,95,95	0
3	GLC	F	2	11/12	0.94	0.16	87,98,104,104	0
3	GLC	E	2	11/12	0.95	0.16	67,72,81,87	0
3	GLC	E	3	11/12	0.95	0.12	47,59,72,78	0
3	GLC	F	3	11/12	0.95	0.11	73,82,94,95	0
3	GLC	F	6	11/12	0.96	0.15	74,81,86,87	0
3	GLC	E	6	11/12	0.96	0.18	53,74,88,107	0
3	GLC	E	4	11/12	0.97	0.13	39,60,63,65	0
3	GLC	E	5	11/12	0.97	0.15	49,64,75,82	0
3	GLC	E	7	11/12	0.98	0.17	67,73,81,90	0
3	GLC	E	1	11/12	0.98	0.17	44,52,70,75	0

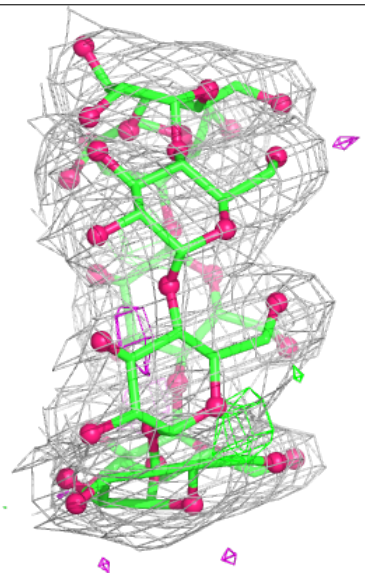
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

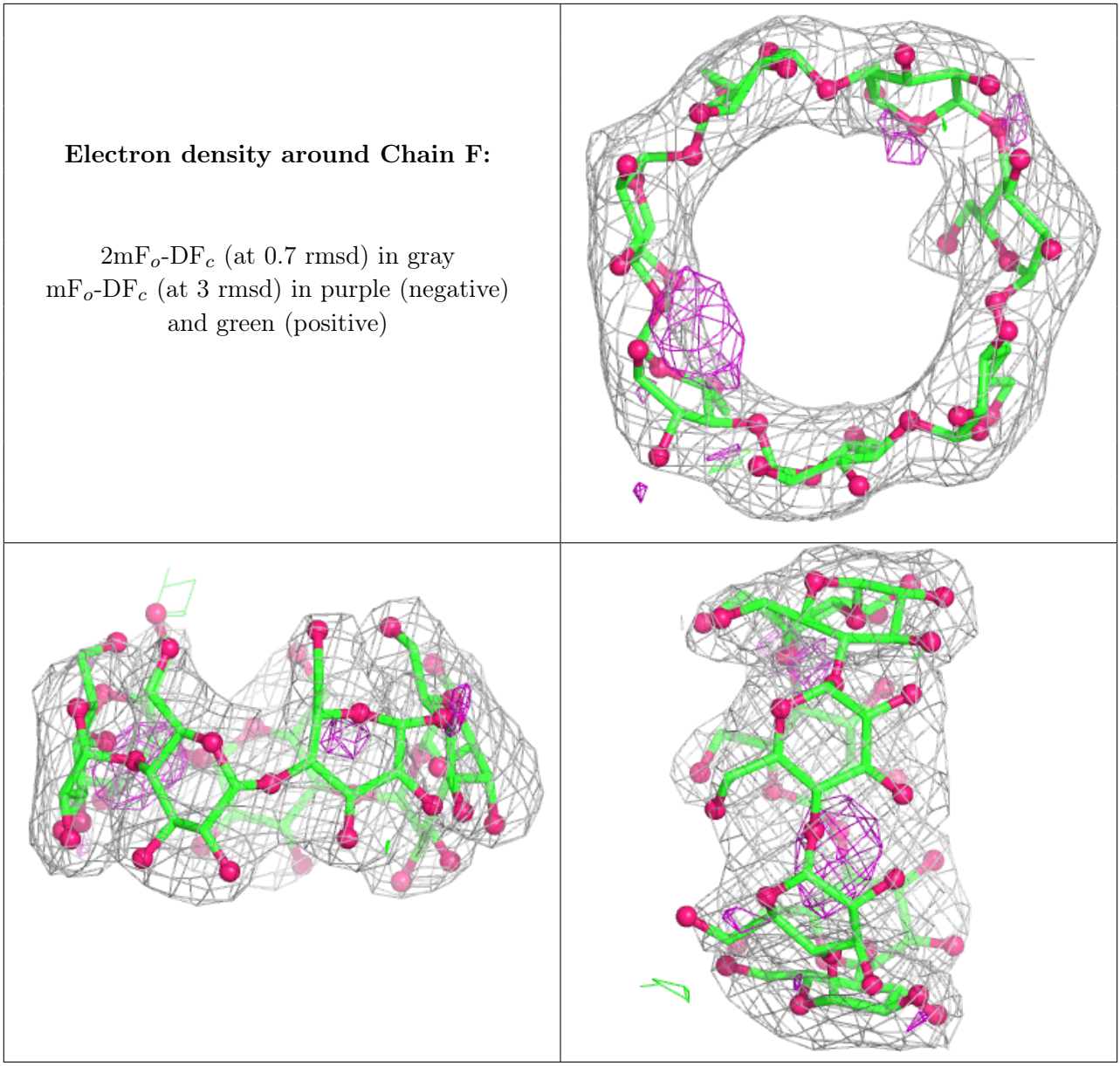






Electron density around Chain F:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.