Full wwPDB X-ray Structure Validation Report (i)

Sep 17, 2023 – 04:34 AM EDT

PDB ID	:	4TSM
Title	:	MBP-fusion protein of PilA1 from C. difficile R20291 residues 26-166
Authors	:	Piepenbrink, K.H.; Sundberg, E.J.
Deposited on	:	2014-06-19
Resolution	:	1.90 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 (i)) were used in the production of this report:

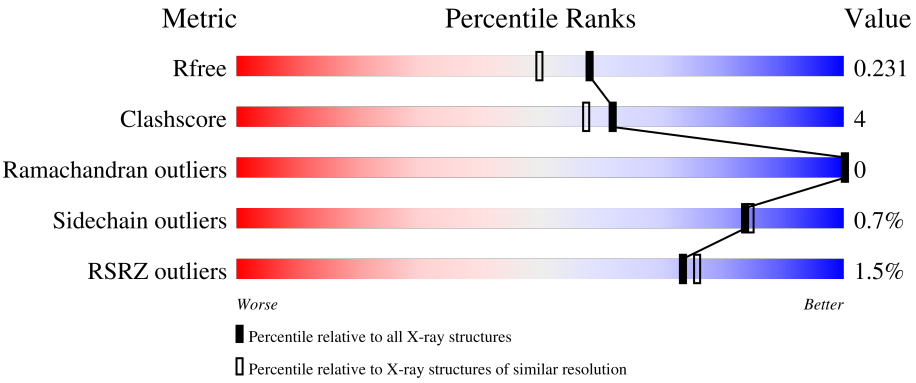
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	520	2% 88% 8% ·
1	B	520	2% 92% 6% ·
1	C	520	% 89% 9% ·
2	D	4	50% 50%
2	E	4	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	4	50% 50%

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
3	TMO	A	1201	-	X	X	-
3	TMO	A	1202	-	X	-	-
3	TMO	A	1203	-	X	-	-
3	TMO	A	1204	-	X	-	-
3	TMO	A	1205	-	X	-	-
3	TMO	A	1206	-	X	-	-
3	TMO	A	1207	-	X	-	-
3	TMO	A	1208	-	X	-	-
3	TMO	B	1201	-	X	-	-
3	TMO	B	1202	-	X	-	-
3	TMO	B	1203	-	X	-	-
3	TMO	B	1204	-	X	-	-
3	TMO	B	1205	-	X	-	-
3	TMO	C	1201	-	X	-	-
3	TMO	C	1202	-	X	X	-
3	TMO	C	1203	-	X	X	-
3	TMO	C	1204	-	X	-	-
3	TMO	C	1205	-	X	-	-
3	TMO	C	1206	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12717 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 maltose-binding protein, pilin chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	505	Total	C	N	O	S	0	2	0
			3861	2471	624	758	8			
1	B	512	Total	C	N	O	S	0	3	0
			3914	2503	633	768	10			
1	C	512	Total	C	N	O	S	0	4	0
			3915	2502	632	771	10			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP D8A942
A	82	ALA	ASP	engineered mutation	UNP D8A942
A	83	ALA	LYS	engineered mutation	UNP D8A942
A	172	ALA	GLU	engineered mutation	UNP D8A942
A	173	ALA	ASN	engineered mutation	UNP D8A942
A	239	ALA	LYS	engineered mutation	UNP D8A942
A	362	ALA	LYS	engineered mutation	UNP D8A942
A	363	ALA	ASP	engineered mutation	UNP D8A942
A	367	ASN	-	linker	UNP D8A942
A	368	ALA	-	linker	UNP D8A942
A	369	ALA	-	linker	UNP D8A942
A	370	ALA	-	linker	UNP D8A942
A	1165	GLY	-	expression tag	UNP C9YRY2
A	1166	SER	-	expression tag	UNP C9YRY2
A	1167	LEU	-	expression tag	UNP C9YRY2
A	1168	GLU	-	expression tag	UNP C9YRY2
A	1169	HIS	-	expression tag	UNP C9YRY2
A	1170	HIS	-	expression tag	UNP C9YRY2
A	1171	HIS	-	expression tag	UNP C9YRY2
A	1172	HIS	-	expression tag	UNP C9YRY2
A	1173	HIS	-	expression tag	UNP C9YRY2
A	1174	HIS	-	expression tag	UNP C9YRY2
B	0	MET	-	initiating methionine	UNP D8A942

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	82	ALA	ASP	engineered mutation	UNP D8A942
B	83	ALA	LYS	engineered mutation	UNP D8A942
B	172	ALA	GLU	engineered mutation	UNP D8A942
B	173	ALA	ASN	engineered mutation	UNP D8A942
B	239	ALA	LYS	engineered mutation	UNP D8A942
B	362	ALA	LYS	engineered mutation	UNP D8A942
B	363	ALA	ASP	engineered mutation	UNP D8A942
B	367	ASN	-	linker	UNP D8A942
B	368	ALA	-	linker	UNP D8A942
B	369	ALA	-	linker	UNP D8A942
B	370	ALA	-	linker	UNP D8A942
B	1165	GLY	-	expression tag	UNP C9YRY2
B	1166	SER	-	expression tag	UNP C9YRY2
B	1167	LEU	-	expression tag	UNP C9YRY2
B	1168	GLU	-	expression tag	UNP C9YRY2
B	1169	HIS	-	expression tag	UNP C9YRY2
B	1170	HIS	-	expression tag	UNP C9YRY2
B	1171	HIS	-	expression tag	UNP C9YRY2
B	1172	HIS	-	expression tag	UNP C9YRY2
B	1173	HIS	-	expression tag	UNP C9YRY2
B	1174	HIS	-	expression tag	UNP C9YRY2
C	0	MET	-	initiating methionine	UNP D8A942
C	82	ALA	ASP	engineered mutation	UNP D8A942
C	83	ALA	LYS	engineered mutation	UNP D8A942
C	172	ALA	GLU	engineered mutation	UNP D8A942
C	173	ALA	ASN	engineered mutation	UNP D8A942
C	239	ALA	LYS	engineered mutation	UNP D8A942
C	362	ALA	LYS	engineered mutation	UNP D8A942
C	363	ALA	ASP	engineered mutation	UNP D8A942
C	367	ASN	-	linker	UNP D8A942
C	368	ALA	-	linker	UNP D8A942
C	369	ALA	-	linker	UNP D8A942
C	370	ALA	-	linker	UNP D8A942
C	1165	GLY	-	expression tag	UNP C9YRY2
C	1166	SER	-	expression tag	UNP C9YRY2
C	1167	LEU	-	expression tag	UNP C9YRY2
C	1168	GLU	-	expression tag	UNP C9YRY2
C	1169	HIS	-	expression tag	UNP C9YRY2
C	1170	HIS	-	expression tag	UNP C9YRY2
C	1171	HIS	-	expression tag	UNP C9YRY2
C	1172	HIS	-	expression tag	UNP C9YRY2
C	1173	HIS	-	expression tag	UNP C9YRY2

Continued on next page...

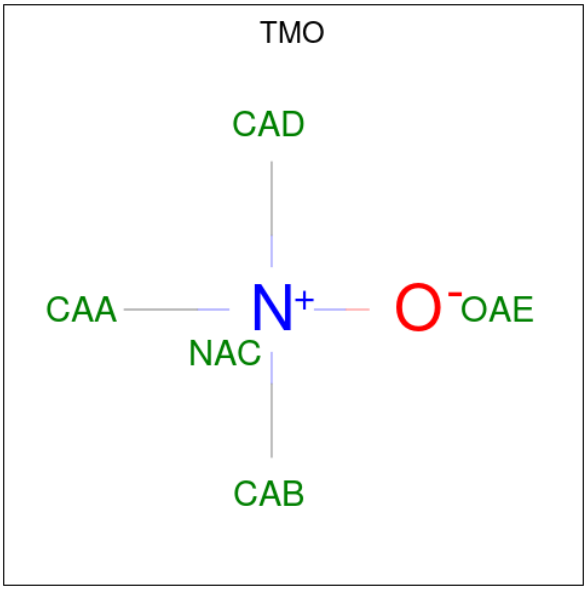
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1174	HIS	-	expression tag	UNP C9YRY2

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	D	4	Total C O 45 24 21	0	0	0
2	E	4	Total C O 45 24 21	0	0	0
2	F	4	Total C O 45 24 21	0	0	0

- Molecule 3 is trimethylamine oxide (three-letter code: TMO) (formula: C_3H_9NO).



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

Continued on next page...

Continued from previous page...

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

- Molecule 4 is water.

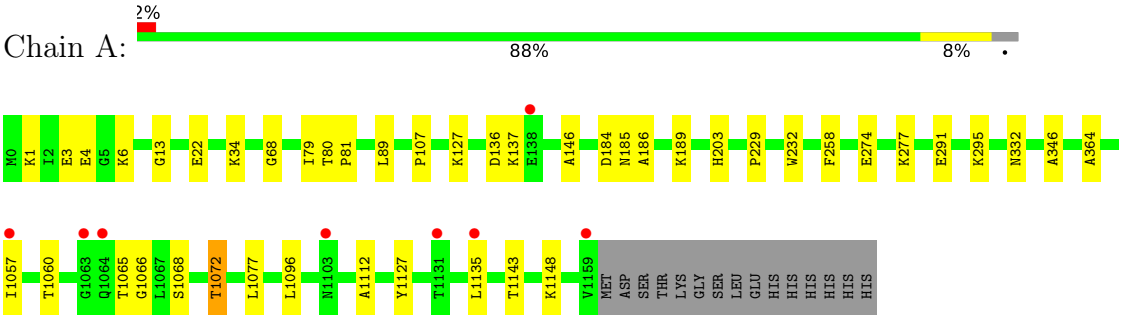
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	257	Total O 257 257	0	0
4	B	261	Total O 261 261	0	0
4	C	279	Total O 279 279	0	0

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.

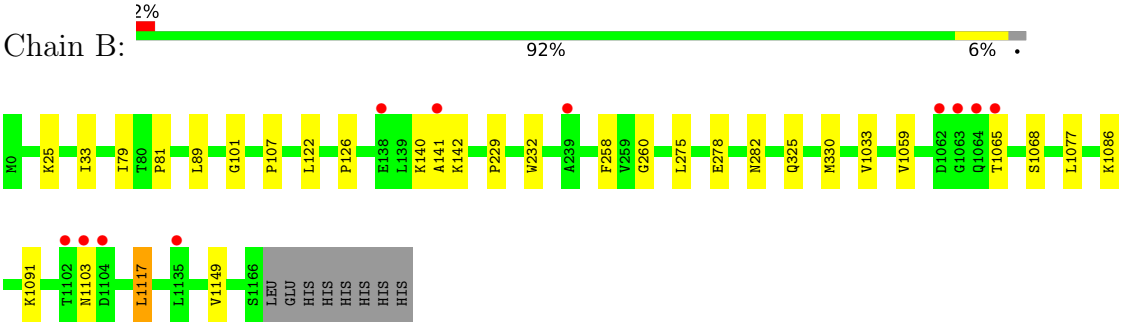
• Molecule 1: maltose-binding protein, pilin chimera

Chain A:



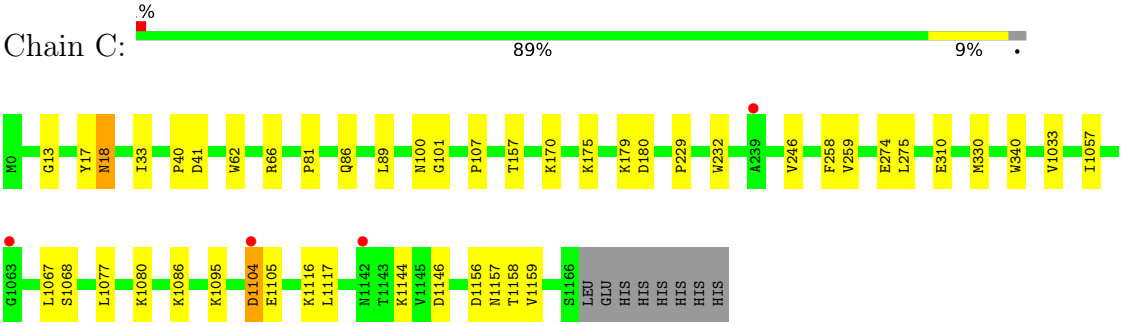
• Molecule 1: maltose-binding protein, pilin chimera

Chain B:



• Molecule 1: maltose-binding protein, pilin chimera

Chain C:

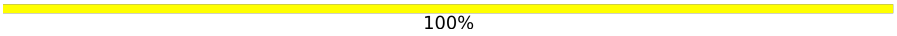


• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain D:

• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain E:



• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	143.95Å 79.37Å 164.75Å 90.00° 90.23° 90.00°	Depositor
Resolution (Å)	38.58 – 1.90 38.58 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (38.58-1.90) 84.9 (38.58-1.90)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 1.89Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.197 , 0.233 0.196 , 0.231	Depositor DCC
R_{free} test set	1999 reflections (1.43%)	wwPDB-VP
Wilson B-factor (Å^2)	19.2	Xtriage
Anisotropy	0.643	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 44.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.017 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.017 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.089 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.107 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.023 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12717	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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: TMO, 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	0.40	0/3947	0.54	0/5366
1	B	0.39	0/4003	0.55	0/5438
1	C	0.40	0/4007	0.56	0/5445
All	All	0.40	0/11957	0.55	0/16249

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	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	18	ASN	Sidechain

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	3861	0	3858	38	0
1	B	3914	0	3920	22	0
1	C	3915	0	3914	42	0
2	D	45	0	39	1	0
2	E	45	0	39	0	0
2	F	45	0	39	2	0
3	A	40	0	72	16	0
3	B	25	0	45	3	0
3	C	30	0	54	9	0
4	A	257	0	0	9	1
4	B	261	0	0	5	2
4	C	279	0	0	7	2
All	All	12717	0	11980	106	3

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 (106) 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:274:GLU:H	3:A:1201:TMO:HAA	1.43	0.83
1:B:101:GLY:H	3:B:1201:TMO:HABA	1.42	0.81
1:B:79:ILE:HG22	1:B:81:PRO:HD3	1.62	0.81
1:A:79:ILE:HD12	1:A:81:PRO:HD3	1.62	0.80
1:C:41:ASP:H	3:C:1203:TMO:HAB	1.47	0.78
1:C:274:GLU:H	3:C:1202:TMO:HADB	1.48	0.78
1:B:278:GLU:OE2	1:B:282:ASN:ND2	2.18	0.74
1:B:142:LYS:O	4:B:1542:HOH:O	2.11	0.68
1:B:1065:THR:O	4:B:1524:HOH:O	2.11	0.67
1:A:3[A]:GLU:OE1	4:A:1526:HOH:O	2.14	0.65
1:C:17:TYR:CD1	1:C:18:ASN:ND2	2.65	0.65
3:A:1201:TMO:HADB	1:C:179:LYS:NZ	2.13	0.63
1:A:1057:ILE:HD11	1:A:1096:LEU:HB2	1.82	0.62
4:C:1573:HOH:O	2:F:4:GLC:O4	2.16	0.61
1:B:1033:VAL:HG13	1:B:1117:LEU:HD13	1.81	0.61
1:B:325:GLN:OE1	4:B:1400:HOH:O	2.16	0.61
1:C:1104:ASP:HB3	1:C:1105:GLU:HG3	1.84	0.60
1:A:1065:THR:OG1	1:A:1066:GLY:N	2.33	0.59
1:C:1116:LYS:NZ	4:C:1510:HOH:O	2.22	0.59
1:C:157:THR:HG23	4:C:1534:HOH:O	2.02	0.59
1:A:137:LYS:HE2	1:A:203:HIS:HE1	1.67	0.59
1:B:101:GLY:N	3:B:1201:TMO:HABA	2.16	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:GLY:H	3:B:1201:TMO:CAB	2.14	0.57
1:C:274:GLU:H	3:C:1202:TMO:CAD	2.16	0.56
1:A:4[B]:GLU:OE1	1:C:179:LYS:HB2	2.06	0.55
1:A:1148:LYS:HD3	4:A:1303:HOH:O	2.07	0.54
1:A:137:LYS:HE2	1:A:203:HIS:CE1	2.42	0.54
1:A:291:GLU:OE2	1:A:295:LYS:HE2	2.07	0.54
1:A:274:GLU:H	3:A:1201:TMO:CAA	2.14	0.54
1:C:62:TRP:CD1	1:C:66:ARG:HG2	2.42	0.54
1:B:25:LYS:NZ	4:B:1548:HOH:O	2.38	0.54
1:A:184:ASP:O	1:A:189:LYS:NZ	2.41	0.54
1:A:1112:ALA:HB1	3:A:1207:TMO:HADB	1.90	0.52
1:A:186:ALA:N	3:A:1206:TMO:OAE	2.42	0.52
1:A:277:LYS:NZ	4:A:1545:HOH:O	2.42	0.51
1:B:1103:ASN:OD1	1:B:1149:VAL:HG23	2.11	0.51
3:C:1202:TMO:HAD	4:C:1357:HOH:O	2.09	0.51
3:A:1201:TMO:HADB	1:C:179:LYS:HZ3	1.74	0.50
1:C:33:ILE:HD13	1:C:275:LEU:HD22	1.93	0.50
1:B:1068:SER:HA	1:B:1077:LEU:HD21	1.94	0.50
1:C:17:TYR:CE1	1:C:18:ASN:ND2	2.80	0.50
1:C:1144:LYS:HE3	1:C:1146[A]:ASP:OD2	2.12	0.49
1:B:260:GLY:HA2	1:B:330:MET:HE2	1.95	0.49
1:C:18:ASN:HD22	1:C:18:ASN:N	2.11	0.49
1:B:89:LEU:HD23	1:B:107:PRO:HG2	1.95	0.49
1:C:41:ASP:N	3:C:1203:TMO:HAB	2.23	0.48
1:C:89:LEU:HD23	1:C:107:PRO:HG2	1.95	0.48
1:A:1068:SER:HA	1:A:1077:LEU:HD21	1.95	0.48
1:A:80:THR:OG1	4:A:1545:HOH:O	2.21	0.47
1:C:1033:VAL:HG13	1:C:1117:LEU:HD13	1.96	0.47
1:A:1060:THR:HG21	1:A:1065:THR:HA	1.96	0.47
3:A:1207:TMO:HABA	4:A:1510:HOH:O	2.14	0.47
1:C:41:ASP:H	3:C:1203:TMO:CAB	2.23	0.47
1:B:33:ILE:HD12	1:B:275:LEU:HD22	1.97	0.46
1:C:175:LYS:NZ	4:C:1577:HOH:O	2.49	0.46
3:A:1201:TMO:HADB	1:C:179:LYS:HZ1	1.81	0.46
1:C:229:PRO:HA	1:C:232:TRP:CE2	2.51	0.46
1:B:122:LEU:HD21	1:B:126:PRO:HD3	1.96	0.46
3:A:1201:TMO:HABA	4:A:1503:HOH:O	2.15	0.46
1:B:1059:VAL:HG11	1:B:1091:LYS:HG3	1.98	0.46
1:A:185:ASN:HB2	3:A:1206:TMO:HABA	1.98	0.46
3:A:1201:TMO:HAAA	4:A:1367:HOH:O	2.15	0.46
1:A:6:LYS:HD2	1:A:34:LYS:HD3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LYS:CD	1:A:34:LYS:HD3	2.47	0.45
1:C:1157:ASN:OD1	1:C:1159:VAL:HG22	2.17	0.45
1:A:137:LYS:HA	1:A:137:LYS:HD3	1.67	0.44
1:A:1127:TYR:CE1	1:A:1135:LEU:HD13	2.52	0.44
1:C:310:GLU:OE1	4:C:1301:HOH:O	2.21	0.44
1:C:1095:LYS:HG2	1:C:1156:ASP:O	2.16	0.44
1:A:89:LEU:HD23	1:A:107:PRO:HG2	2.00	0.44
1:A:3[B]:GLU:OE2	1:B:141:ALA:HA	2.18	0.43
1:C:18:ASN:ND2	1:C:18:ASN:N	2.66	0.43
1:A:1:LYS:HG3	3:A:1208:TMO:HABA	2.01	0.43
1:C:170:LYS:HD2	1:C:180:ASP:OD2	2.19	0.43
1:C:1067:LEU:HB2	1:C:1077:LEU:HD22	1.99	0.43
1:C:66:ARG:HD3	2:F:3:GLC:O2	2.19	0.43
1:A:79:ILE:HD12	1:A:81:PRO:CD	2.41	0.43
1:B:33:ILE:CD1	1:B:275:LEU:HD13	2.49	0.43
3:A:1208:TMO:HAD	1:C:101:GLY:HA2	2.01	0.43
1:C:274:GLU:N	3:C:1202:TMO:HADB	2.26	0.43
1:A:136:ASP:HA	1:A:146:ALA:HB2	2.01	0.42
1:C:40:PRO:HA	3:C:1203:TMO:HAD	2.01	0.42
1:A:68:GLY:HA3	1:A:332:ASN:O	2.19	0.42
1:C:13:GLY:HA3	3:C:1205:TMO:HAD	2.01	0.42
1:C:1080:LYS:HG2	1:C:1086:LYS:HG2	2.01	0.42
1:C:1068:SER:HA	1:C:1077:LEU:HD11	2.01	0.42
1:B:1086:LYS:HD3	4:B:1556:HOH:O	2.19	0.42
1:C:330:MET:CE	1:C:340:TRP:HZ2	2.32	0.42
1:A:22:GLU:HG2	4:A:1548:HOH:O	2.20	0.42
1:A:229:PRO:HA	1:A:232:TRP:CE2	2.55	0.42
1:A:346:ALA:HB2	1:A:364:ALA:HB2	2.00	0.42
2:D:3:GLC:H62	2:D:4:GLC:H5	2.02	0.42
1:A:1072:THR:HB	4:A:1437:HOH:O	2.20	0.41
1:C:330:MET:HE3	1:C:340:TRP:HZ2	1.84	0.41
1:A:13:GLY:HA3	3:A:1203:TMO:HADB	2.01	0.41
1:A:1:LYS:HG2	1:C:100:ASN:HA	2.02	0.41
1:C:330:MET:CE	1:C:340:TRP:HE1	2.33	0.41
1:C:259:VAL:O	1:C:330:MET:HG3	2.20	0.41
1:C:81:PRO:HG2	1:C:86:GLN:HG2	2.03	0.41
1:A:127:LYS:HA	1:A:127:LYS:HD2	1.89	0.40
1:B:229:PRO:HA	1:B:232:TRP:CE2	2.56	0.40
1:A:1112:ALA:CB	3:A:1207:TMO:HADB	2.52	0.40
3:A:1205:TMO:HAB	4:C:1389:HOH:O	2.20	0.40
1:B:140:LYS:C	1:B:142:LYS:H	2.25	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1057:ILE:CD1	1:C:1158:THR:HB	2.51	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1324:HOH:O	4:C:1377:HOH:O[2_758]	2.11	0.09
4:A:1346:HOH:O	4:C:1350:HOH:O[2_757]	2.13	0.07
4:B:1362:HOH:O	4:B:1365:HOH:O[4_758]	2.15	0.05

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	505/520 (97%)	496 (98%)	9 (2%)	0	100	100
1	B	513/520 (99%)	503 (98%)	10 (2%)	0	100	100
1	C	514/520 (99%)	505 (98%)	9 (2%)	0	100	100
All	All	1532/1560 (98%)	1504 (98%)	28 (2%)	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	406/418 (97%)	403 (99%)	3 (1%)	84	84
1	B	413/418 (99%)	411 (100%)	2 (0%)	88	89
1	C	414/418 (99%)	411 (99%)	3 (1%)	84	84
All	All	1233/1254 (98%)	1225 (99%)	8 (1%)	84	87

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	PHE
1	A	1072	THR
1	A	1143	THR
1	B	258	PHE
1	B	1117	LEU
1	C	246	VAL
1	C	258	PHE
1	C	1104	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	241	ASN
1	B	325	GLN
1	B	1064	GLN
1	C	18	ASN

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	GLC	D	1	2	12,12,12	1.99	3 (25%)	17,17,17	0.87	0
2	GLC	D	2	2	11,11,12	2.68	4 (36%)	15,15,17	0.98	1 (6%)
2	GLC	D	3	2	11,11,12	2.66	3 (27%)	15,15,17	1.17	2 (13%)
2	GLC	D	4	2	11,11,12	2.55	6 (54%)	15,15,17	1.27	2 (13%)
2	GLC	E	1	2	12,12,12	2.02	5 (41%)	17,17,17	0.92	0
2	GLC	E	2	2	11,11,12	2.76	3 (27%)	15,15,17	1.13	1 (6%)
2	GLC	E	3	2	11,11,12	2.58	3 (27%)	15,15,17	1.40	2 (13%)
2	GLC	E	4	2	11,11,12	2.72	5 (45%)	15,15,17	1.70	3 (20%)
2	GLC	F	1	2	12,12,12	2.02	2 (16%)	17,17,17	0.66	0
2	GLC	F	2	2	11,11,12	2.71	3 (27%)	15,15,17	0.98	0
2	GLC	F	3	2	11,11,12	2.59	3 (27%)	15,15,17	1.31	2 (13%)
2	GLC	F	4	2	11,11,12	2.95	4 (36%)	15,15,17	2.19	6 (40%)

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	GLC	D	1	2	-	0/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	GLC	D	3	2	-	0/2/19/22	0/1/1/1
2	GLC	D	4	2	-	0/2/19/22	0/1/1/1
2	GLC	E	1	2	-	0/2/22/22	0/1/1/1
2	GLC	E	2	2	-	0/2/19/22	0/1/1/1
2	GLC	E	3	2	-	0/2/19/22	0/1/1/1
2	GLC	E	4	2	-	2/2/19/22	0/1/1/1
2	GLC	F	1	2	-	0/2/22/22	0/1/1/1
2	GLC	F	2	2	-	0/2/19/22	0/1/1/1
2	GLC	F	3	2	-	0/2/19/22	0/1/1/1
2	GLC	F	4	2	-	1/2/19/22	0/1/1/1

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	GLC	O5-C5	7.03	1.57	1.43
2	E	2	GLC	O5-C5	6.85	1.57	1.43
2	F	3	GLC	O5-C5	6.67	1.56	1.43
2	E	3	GLC	O5-C5	6.55	1.56	1.43
2	D	2	GLC	O5-C5	6.42	1.56	1.43
2	F	2	GLC	O5-C5	6.42	1.56	1.43
2	F	4	GLC	O5-C5	6.27	1.56	1.43
2	E	4	GLC	O5-C5	5.48	1.54	1.43
2	D	4	GLC	O5-C5	4.93	1.53	1.43
2	D	1	GLC	O5-C5	4.21	1.54	1.44
2	E	1	GLC	O5-C5	4.19	1.54	1.44
2	F	1	GLC	O5-C5	4.17	1.54	1.44
2	E	2	GLC	C6-C5	-4.08	1.38	1.51
2	F	4	GLC	O5-C1	4.03	1.50	1.43
2	F	4	GLC	C2-C3	-3.92	1.46	1.52
2	D	2	GLC	C6-C5	-3.91	1.38	1.51
2	F	2	GLC	C6-C5	-3.90	1.38	1.51
2	E	4	GLC	C2-C3	-3.85	1.46	1.52
2	E	4	GLC	O5-C1	3.57	1.49	1.43
2	D	4	GLC	O2-C2	3.56	1.50	1.43
2	D	4	GLC	O5-C1	3.39	1.49	1.43
2	F	4	GLC	O2-C2	3.37	1.50	1.43
2	E	3	GLC	O5-C1	3.36	1.49	1.43
2	D	1	GLC	C6-C5	-3.33	1.40	1.51
2	E	4	GLC	O2-C2	3.32	1.50	1.43
2	F	1	GLC	C6-C5	-3.24	1.41	1.51
2	F	3	GLC	O5-C1	3.12	1.48	1.43
2	E	1	GLC	C6-C5	-3.09	1.41	1.51
2	D	3	GLC	C6-C5	-2.95	1.42	1.51
2	D	4	GLC	C2-C3	-2.92	1.48	1.52
2	F	3	GLC	C6-C5	-2.85	1.42	1.51
2	D	3	GLC	O5-C1	2.82	1.48	1.43
2	F	2	GLC	O5-C1	2.60	1.47	1.43
2	E	3	GLC	C6-C5	-2.54	1.43	1.51
2	D	2	GLC	O5-C1	2.44	1.47	1.43
2	E	1	GLC	O5-C1	2.33	1.48	1.42
2	D	1	GLC	O2-C2	2.31	1.48	1.43
2	D	4	GLC	O3-C3	2.20	1.48	1.43
2	E	2	GLC	O5-C1	2.19	1.47	1.43
2	D	4	GLC	C6-C5	-2.18	1.44	1.51
2	E	1	GLC	C3-C2	-2.17	1.46	1.52
2	E	1	GLC	O2-C2	2.14	1.48	1.43
2	D	2	GLC	C1-C2	-2.13	1.47	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	4	GLC	C1-C2	-2.07	1.47	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	4	GLC	C1-O5-C5	4.99	118.95	112.19
2	F	4	GLC	C1-O5-C5	4.91	118.84	112.19
2	F	4	GLC	C6-C5-C4	-3.83	104.02	113.00
2	E	3	GLC	O4-C4-C5	-2.94	102.00	109.30
2	F	3	GLC	C1-C2-C3	2.88	113.20	109.67
2	F	4	GLC	O5-C1-C2	2.81	115.10	110.77
2	E	2	GLC	O5-C1-C2	-2.79	106.46	110.77
2	D	4	GLC	O5-C5-C4	-2.79	104.04	110.83
2	F	4	GLC	C3-C4-C5	2.71	115.07	110.24
2	D	4	GLC	C1-C2-C3	2.69	112.97	109.67
2	F	4	GLC	O3-C3-C4	-2.47	104.64	110.35
2	F	4	GLC	C1-C2-C3	2.45	112.68	109.67
2	D	3	GLC	C1-C2-C3	2.36	112.56	109.67
2	E	4	GLC	C6-C5-C4	-2.31	107.60	113.00
2	D	3	GLC	O4-C4-C5	-2.15	103.96	109.30
2	D	2	GLC	O2-C2-C1	-2.10	104.85	109.15
2	F	3	GLC	O4-C4-C5	-2.08	104.13	109.30
2	E	3	GLC	O5-C5-C4	-2.02	105.91	110.83
2	E	4	GLC	O3-C3-C4	-2.01	105.70	110.35

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	4	GLC	O5-C5-C6-O6
2	E	4	GLC	C4-C5-C6-O6
2	F	4	GLC	C4-C5-C6-O6

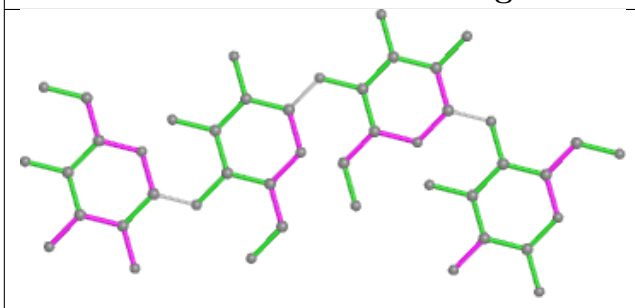
There are no ring outliers.

4 monomers are involved in 3 short contacts:

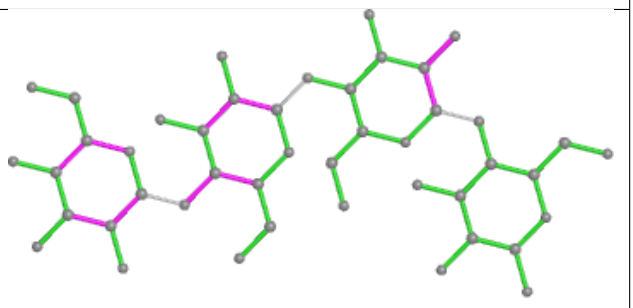
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	4	GLC	1	0
2	F	3	GLC	1	0
2	D	3	GLC	1	0
2	F	4	GLC	1	0

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

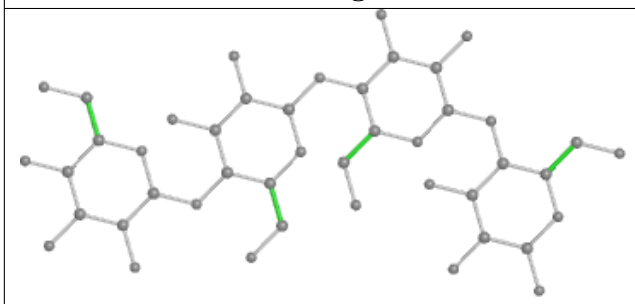
Oligosaccharide Chain D



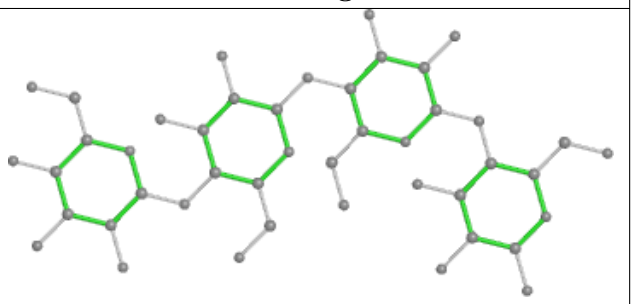
Bond lengths



Bond angles

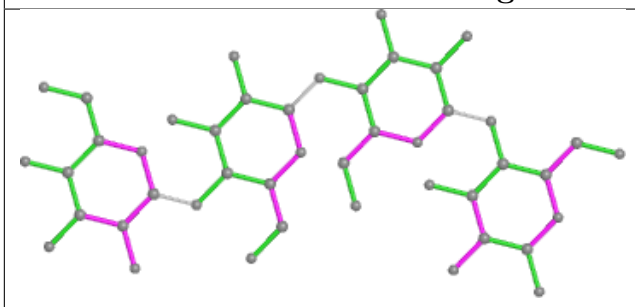


Torsions

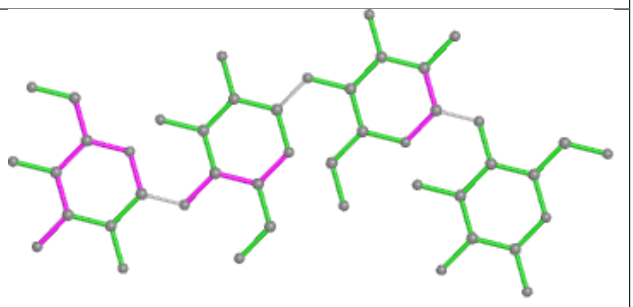


Rings

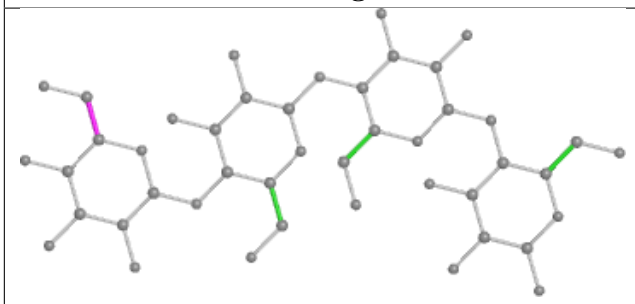
Oligosaccharide Chain E



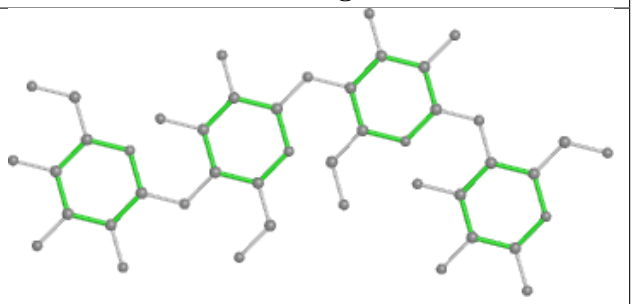
Bond lengths



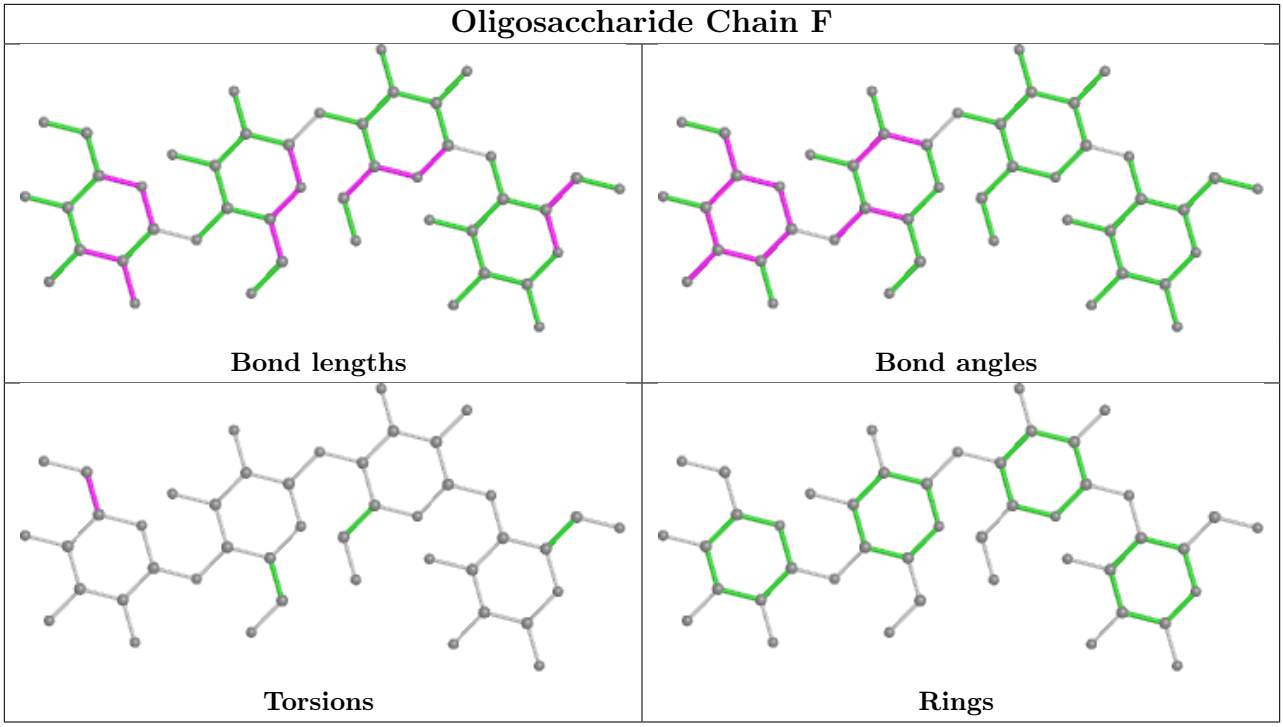
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

19 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	$\#\|Z\| > 2$
3	TMO	A	1202	-	4,4,4	4.28	4 (100%)	6,6,6	0.26	0
3	TMO	A	1205	-	4,4,4	4.62	4 (100%)	6,6,6	0.20	0
3	TMO	C	1203	-	4,4,4	4.35	4 (100%)	6,6,6	0.24	0
3	TMO	C	1202	-	4,4,4	5.08	4 (100%)	6,6,6	0.41	0
3	TMO	A	1201	-	4,4,4	5.49	4 (100%)	6,6,6	0.61	0
3	TMO	B	1203	-	4,4,4	4.04	4 (100%)	6,6,6	0.33	0
3	TMO	B	1205	-	4,4,4	4.78	4 (100%)	6,6,6	0.33	0
3	TMO	A	1208	-	4,4,4	4.75	4 (100%)	6,6,6	0.32	0
3	TMO	C	1201	-	4,4,4	4.67	4 (100%)	6,6,6	0.31	0
3	TMO	A	1207	-	4,4,4	4.11	4 (100%)	6,6,6	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	TMO	A	1203	-	4,4,4	3.87	4 (100%)	6,6,6	0.29	0
3	TMO	C	1204	-	4,4,4	4.55	4 (100%)	6,6,6	0.29	0
3	TMO	B	1204	-	4,4,4	4.27	4 (100%)	6,6,6	0.22	0
3	TMO	A	1206	-	4,4,4	4.15	4 (100%)	6,6,6	0.17	0
3	TMO	C	1206	-	4,4,4	3.99	4 (100%)	6,6,6	0.22	0
3	TMO	A	1204	-	4,4,4	3.95	4 (100%)	6,6,6	0.30	0
3	TMO	B	1202	-	4,4,4	4.69	4 (100%)	6,6,6	0.28	0
3	TMO	C	1205	-	4,4,4	4.09	4 (100%)	6,6,6	0.38	0
3	TMO	B	1201	-	4,4,4	4.63	4 (100%)	6,6,6	0.30	0

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1201	TMO	CAA-NAC	-6.98	1.39	1.48
3	C	1202	TMO	CAD-NAC	-6.38	1.39	1.48
3	B	1205	TMO	CAA-NAC	-6.01	1.40	1.48
3	A	1201	TMO	CAB-NAC	-5.43	1.41	1.48
3	C	1204	TMO	CAB-NAC	-5.33	1.41	1.48
3	A	1201	TMO	CAD-NAC	-5.22	1.41	1.48
3	B	1202	TMO	CAD-NAC	-5.21	1.41	1.48
3	A	1208	TMO	CAB-NAC	-5.15	1.41	1.48
3	A	1208	TMO	CAA-NAC	-5.10	1.41	1.48
3	B	1202	TMO	CAB-NAC	-5.06	1.41	1.48
3	B	1201	TMO	CAB-NAC	-5.05	1.41	1.48
3	C	1201	TMO	CAD-NAC	-4.86	1.41	1.48
3	C	1201	TMO	CAB-NAC	-4.86	1.41	1.48
3	C	1202	TMO	CAB-NAC	-4.84	1.41	1.48
3	B	1201	TMO	CAA-NAC	-4.76	1.42	1.48
3	A	1205	TMO	CAA-NAC	-4.73	1.42	1.48
3	B	1202	TMO	CAA-NAC	-4.73	1.42	1.48
3	A	1207	TMO	CAD-NAC	-4.70	1.42	1.48
3	C	1203	TMO	CAB-NAC	-4.69	1.42	1.48
3	A	1205	TMO	OAE-NAC	-4.68	1.36	1.42
3	C	1201	TMO	CAA-NAC	-4.63	1.42	1.48
3	A	1205	TMO	CAB-NAC	-4.62	1.42	1.48
3	A	1208	TMO	CAD-NAC	-4.57	1.42	1.48
3	A	1207	TMO	CAA-NAC	-4.52	1.42	1.48
3	C	1202	TMO	CAA-NAC	-4.47	1.42	1.48
3	B	1205	TMO	CAD-NAC	-4.47	1.42	1.48
3	A	1205	TMO	CAD-NAC	-4.46	1.42	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1201	TMO	OAE-NAC	-4.45	1.36	1.42
3	A	1202	TMO	CAB-NAC	-4.44	1.42	1.48
3	A	1202	TMO	CAA-NAC	-4.43	1.42	1.48
3	C	1203	TMO	OAE-NAC	-4.42	1.36	1.42
3	B	1204	TMO	OAE-NAC	-4.41	1.36	1.42
3	C	1205	TMO	CAD-NAC	-4.41	1.42	1.48
3	A	1204	TMO	CAD-NAC	-4.40	1.42	1.48
3	C	1202	TMO	OAE-NAC	-4.38	1.36	1.42
3	A	1206	TMO	OAE-NAC	-4.37	1.36	1.42
3	C	1204	TMO	OAE-NAC	-4.31	1.36	1.42
3	B	1204	TMO	CAB-NAC	-4.30	1.42	1.48
3	C	1204	TMO	CAA-NAC	-4.29	1.42	1.48
3	C	1201	TMO	OAE-NAC	-4.29	1.36	1.42
3	B	1204	TMO	CAD-NAC	-4.29	1.42	1.48
3	C	1205	TMO	CAA-NAC	-4.28	1.42	1.48
3	A	1202	TMO	OAE-NAC	-4.27	1.36	1.42
3	B	1205	TMO	CAB-NAC	-4.21	1.42	1.48
3	B	1201	TMO	CAD-NAC	-4.21	1.42	1.48
3	C	1206	TMO	OAE-NAC	-4.20	1.36	1.42
3	B	1205	TMO	OAE-NAC	-4.20	1.36	1.42
3	A	1206	TMO	CAB-NAC	-4.19	1.42	1.48
3	B	1203	TMO	CAB-NAC	-4.16	1.42	1.48
3	C	1204	TMO	CAD-NAC	-4.15	1.42	1.48
3	C	1203	TMO	CAD-NAC	-4.14	1.42	1.48
3	A	1208	TMO	OAE-NAC	-4.11	1.37	1.42
3	C	1203	TMO	CAA-NAC	-4.11	1.42	1.48
3	C	1205	TMO	CAB-NAC	-4.10	1.42	1.48
3	A	1206	TMO	CAD-NAC	-4.10	1.42	1.48
3	B	1203	TMO	CAD-NAC	-4.08	1.42	1.48
3	B	1203	TMO	CAA-NAC	-4.06	1.42	1.48
3	B	1204	TMO	CAA-NAC	-4.05	1.42	1.48
3	C	1206	TMO	CAD-NAC	-4.05	1.42	1.48
3	A	1204	TMO	CAA-NAC	-3.98	1.43	1.48
3	A	1202	TMO	CAD-NAC	-3.97	1.43	1.48
3	A	1203	TMO	CAA-NAC	-3.96	1.43	1.48
3	A	1203	TMO	CAD-NAC	-3.95	1.43	1.48
3	A	1206	TMO	CAA-NAC	-3.94	1.43	1.48
3	A	1207	TMO	CAB-NAC	-3.94	1.43	1.48
3	A	1203	TMO	CAB-NAC	-3.92	1.43	1.48
3	A	1201	TMO	OAE-NAC	-3.88	1.37	1.42
3	B	1203	TMO	OAE-NAC	-3.86	1.37	1.42
3	C	1206	TMO	CAB-NAC	-3.85	1.43	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1206	TMO	CAA-NAC	-3.83	1.43	1.48
3	A	1204	TMO	CAB-NAC	-3.76	1.43	1.48
3	A	1203	TMO	OAE-NAC	-3.66	1.37	1.42
3	B	1202	TMO	OAE-NAC	-3.60	1.37	1.42
3	A	1204	TMO	OAE-NAC	-3.59	1.37	1.42
3	C	1205	TMO	OAE-NAC	-3.49	1.37	1.42
3	A	1207	TMO	OAE-NAC	-3.09	1.38	1.42

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1205	TMO	1	0
3	C	1203	TMO	4	0
3	C	1202	TMO	4	0
3	A	1201	TMO	7	0
3	A	1208	TMO	2	0
3	A	1207	TMO	3	0
3	A	1203	TMO	1	0
3	A	1206	TMO	2	0
3	C	1205	TMO	1	0
3	B	1201	TMO	3	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	505/520 (97%)	-0.06	8 (1%) 72 74	15, 24, 41, 60	0
1	B	512/520 (98%)	-0.02	11 (2%) 63 66	15, 24, 41, 59	0
1	C	512/520 (98%)	-0.13	4 (0%) 86 87	14, 23, 37, 55	0
All	All	1529/1560 (98%)	-0.07	23 (1%) 73 76	14, 23, 40, 60	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1063	GLY	5.5
1	A	1063	GLY	4.7
1	B	141	ALA	3.7
1	B	1064	GLN	3.7
1	C	1104	ASP	3.7
1	B	1103	ASN	3.5
1	B	1063	GLY	3.4
1	B	1102	THR	3.2
1	A	1159	VAL	3.2
1	C	239	ALA	3.1
1	A	1135	LEU	3.1
1	C	1142	ASN	2.7
1	A	1057	ILE	2.6
1	B	1135	LEU	2.6
1	A	1064	GLN	2.4
1	B	1104	ASP	2.4
1	A	1131	THR	2.4
1	B	1065	THR	2.4
1	B	239	ALA	2.4
1	B	138	GLU	2.4
1	B	1062	ASP	2.3
1	A	138	GLU	2.2
1	A	1103	ASN	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)

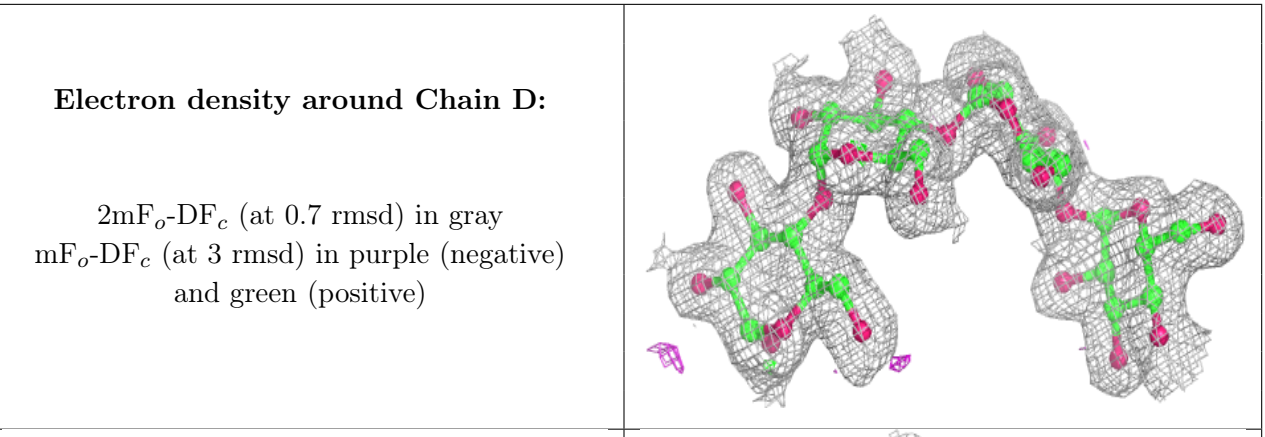
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	GLC	E	4	11/12	0.91	0.12	27,35,41,44	0
2	GLC	F	4	11/12	0.91	0.11	24,33,40,46	0
2	GLC	D	4	11/12	0.92	0.09	24,31,36,39	0
2	GLC	E	3	11/12	0.93	0.11	22,26,31,32	0
2	GLC	F	3	11/12	0.94	0.10	19,22,27,29	0
2	GLC	F	1	12/12	0.95	0.15	16,19,21,22	0
2	GLC	D	3	11/12	0.95	0.10	17,21,25,25	0
2	GLC	E	1	12/12	0.95	0.15	16,21,23,23	0
2	GLC	F	2	11/12	0.96	0.12	17,18,21,22	0
2	GLC	D	2	11/12	0.97	0.12	15,17,20,23	0
2	GLC	D	1	12/12	0.97	0.10	15,19,20,22	0
2	GLC	E	2	11/12	0.97	0.10	15,17,20,21	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.

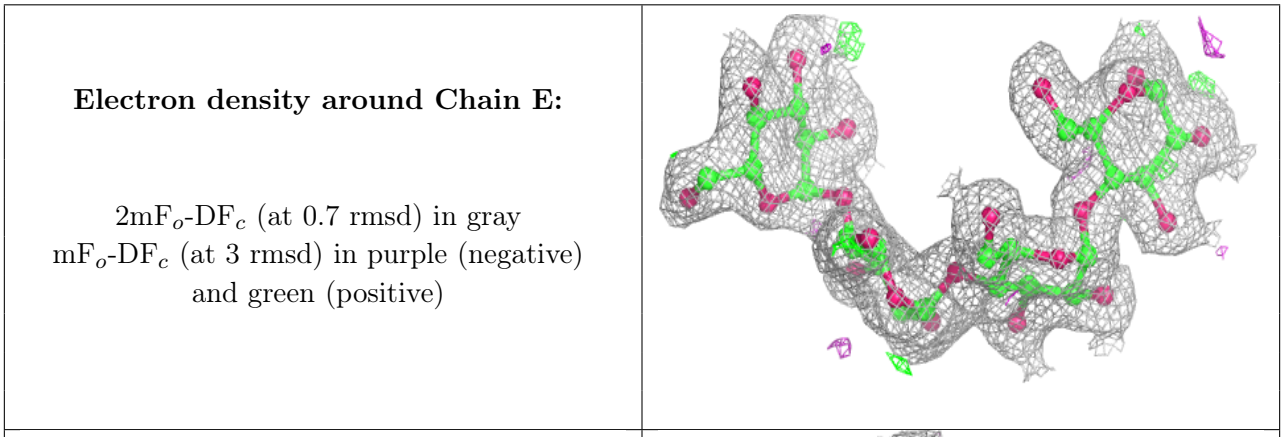
Electron density around Chain D:

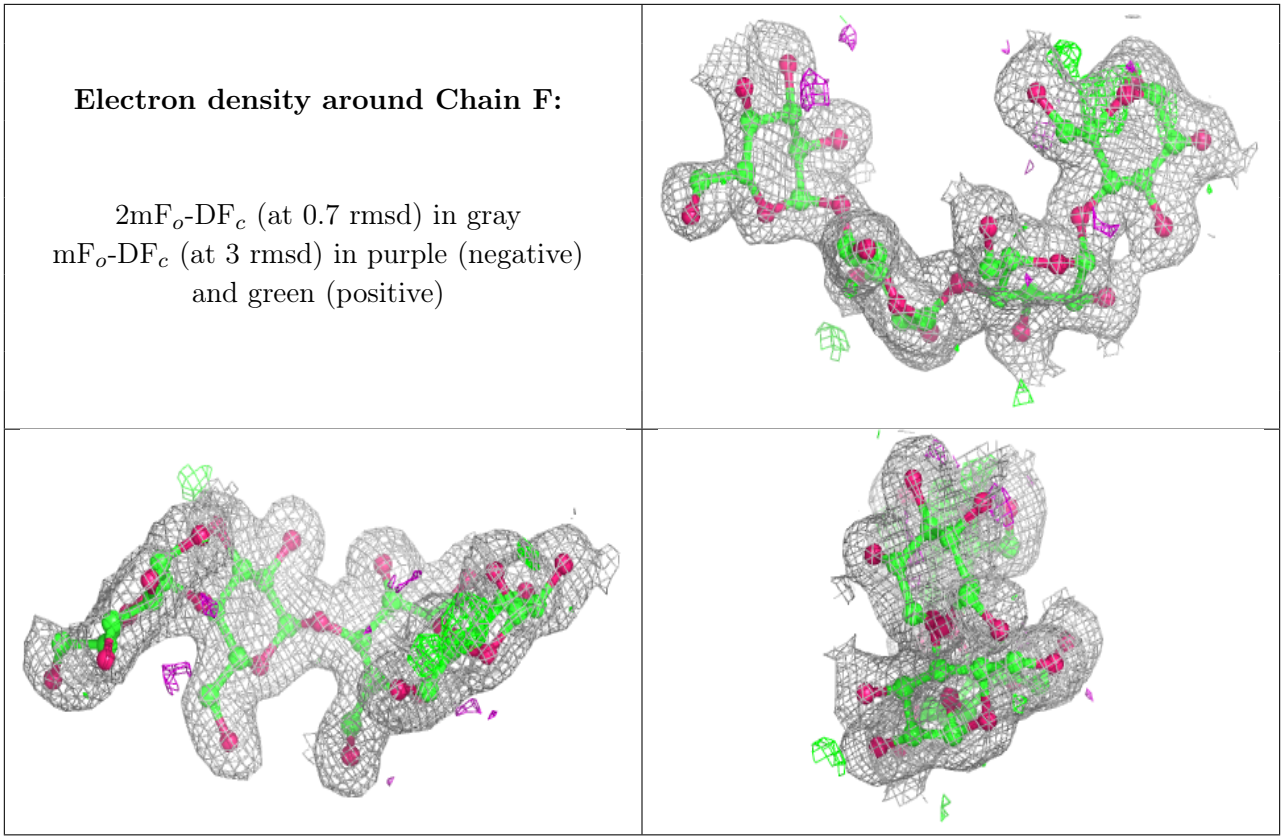
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain E:

$2mF_o$-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	TMO	A	1207	5/5	0.86	0.18	29,32,36,40	0
3	TMO	A	1204	5/5	0.89	0.26	33,34,35,37	0
3	TMO	C	1204	5/5	0.90	0.13	31,33,41,45	0
3	TMO	A	1206	5/5	0.91	0.16	40,43,50,50	0
3	TMO	C	1206	5/5	0.91	0.17	36,43,45,48	0
3	TMO	A	1203	5/5	0.93	0.15	33,33,37,39	0
3	TMO	A	1205	5/5	0.93	0.14	27,30,32,33	0
3	TMO	B	1205	5/5	0.94	0.14	31,31,32,33	0
3	TMO	A	1201	5/5	0.95	0.17	12,13,18,20	0
3	TMO	B	1201	5/5	0.95	0.13	19,21,30,40	0
3	TMO	C	1205	5/5	0.95	0.15	34,38,41,44	0
3	TMO	B	1203	5/5	0.95	0.13	28,35,37,38	0
3	TMO	C	1202	5/5	0.96	0.15	13,15,17,18	0
3	TMO	C	1201	5/5	0.97	0.14	15,19,22,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	TMO	B	1202	5/5	0.97	0.15	10,12,17,22	0
3	TMO	C	1203	5/5	0.97	0.12	23,29,40,44	0
3	TMO	A	1208	5/5	0.97	0.15	18,24,28,33	0
3	TMO	B	1204	5/5	0.97	0.12	28,31,33,36	0
3	TMO	A	1202	5/5	0.97	0.11	30,30,34,36	0

6.5 Other polymers

There are no such residues in this entry.