Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 07:10 AM EDT

PDB ID	:	6E0W
Title	:	Crystal structure of the colanidase tailspike protein gp150 of Phage Phi92 complexed with one repeating unit of colanic acid
Authors	:	Plattner, M.; Browning, C.; Gerardy-Schahn, R.; Shneider, M.M.; Leiman, P.G.; Schwarzer, D.
Deposited on	:	2018-07-07
Resolution	:	1.80 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

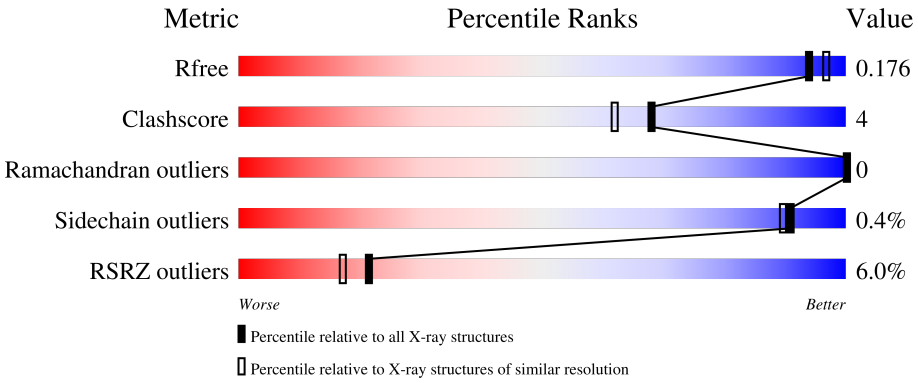
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	626	5% 89% 7% .
1	B	626	6% 88% 8% .
2	C	5	80% 20%
2	D	5	100%

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	SO4	B	906	-	-	X	-
5	HLA	A	906	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 10586 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 Bacteriophage Phi92 gp150.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	602	Total	C	N	O	S	0	4	0
			4590	2878	779	907	26			
1	B	602	Total	C	N	O	S	0	6	0
			4605	2886	781	912	26			

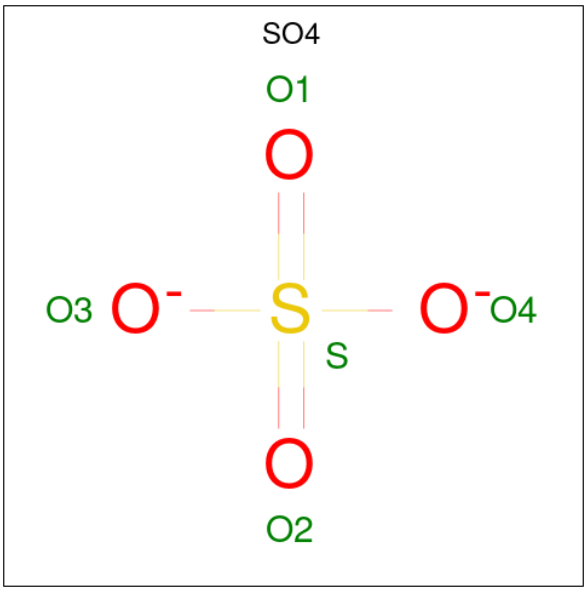
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	179	SER	-	expression tag	UNP I7I026
B	179	SER	-	expression tag	UNP I7I026

- Molecule 2 is an oligosaccharide called beta-D-glucopyranuronic acid-(1-3)-alpha-D-galactopyranose-(1-3)-alpha-L-fucopyranose-(1-4)-alpha-L-fucopyranose-(1-3)-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	5	Total	C	O	0	0	0
			55	30	25			
2	D	5	Total	C	O	0	0	0
			55	30	25			

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

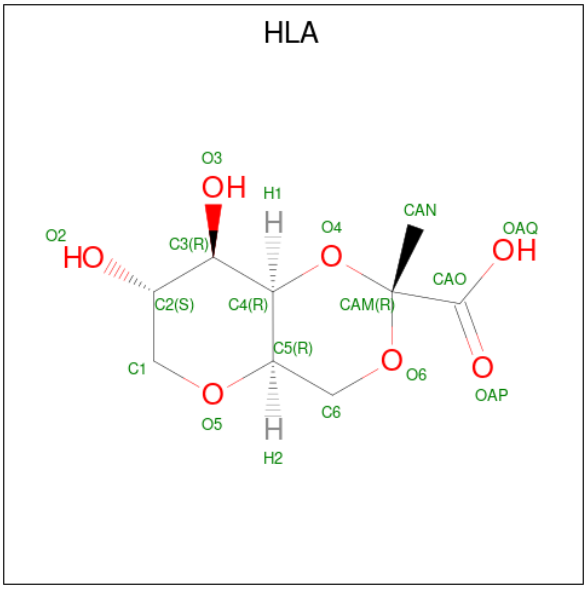


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

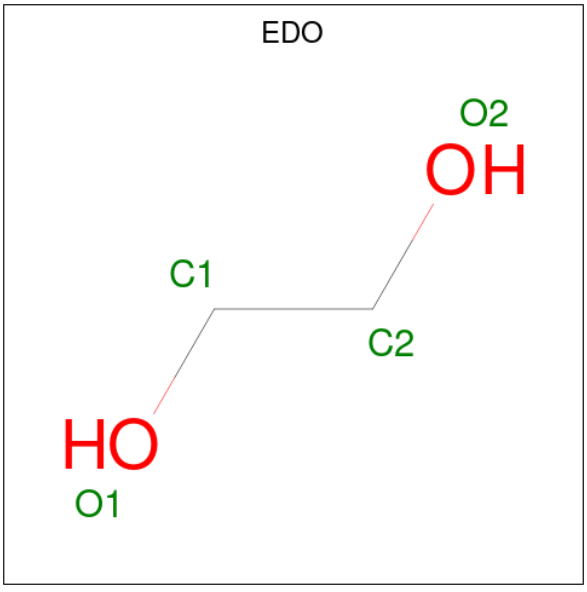
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	2	Total Mg 2 2	0	0

- Molecule 5 is 1,5-anhydro-4,6-O-[(1R)-1-carboxyethylidene]-D-galactitol (three-letter code: HLA) (formula: $C_9H_{14}O_7$).



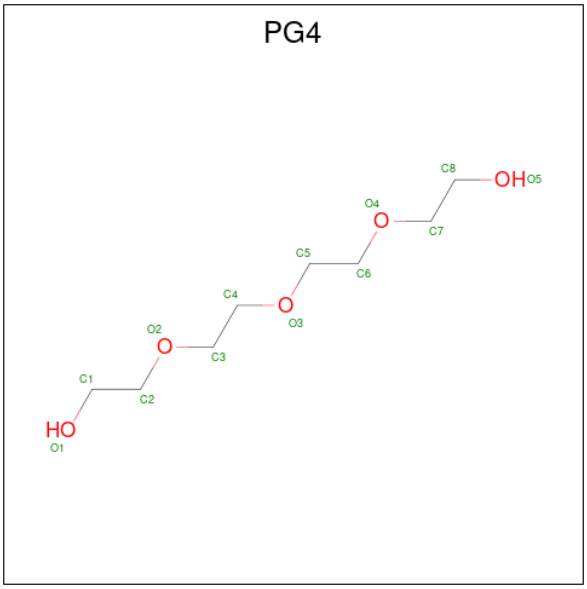
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 16 9 7	0	0
5	B	1	Total C O 16 9 7	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 4 2 2	0	0

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 13 8 5	0	0

- Molecule 8 is water.

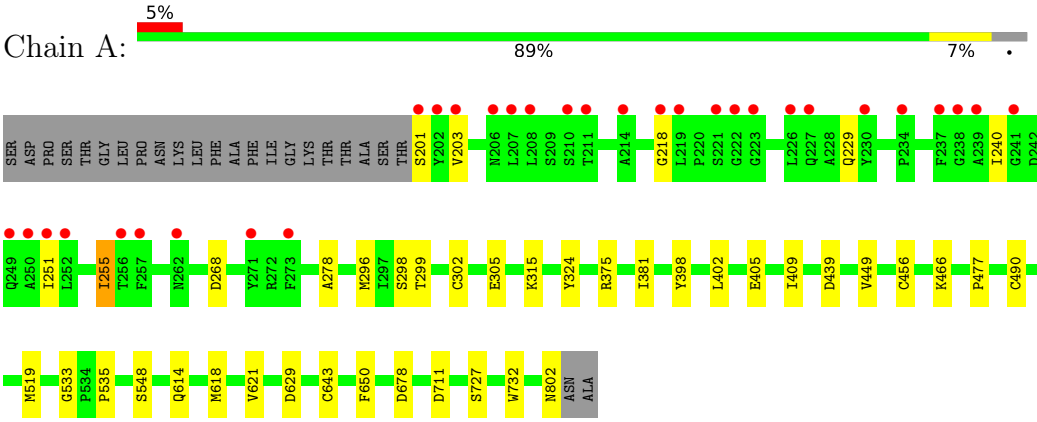
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	604	Total O 604 604	0	0
8	B	575	Total O 575 575	0	0

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.

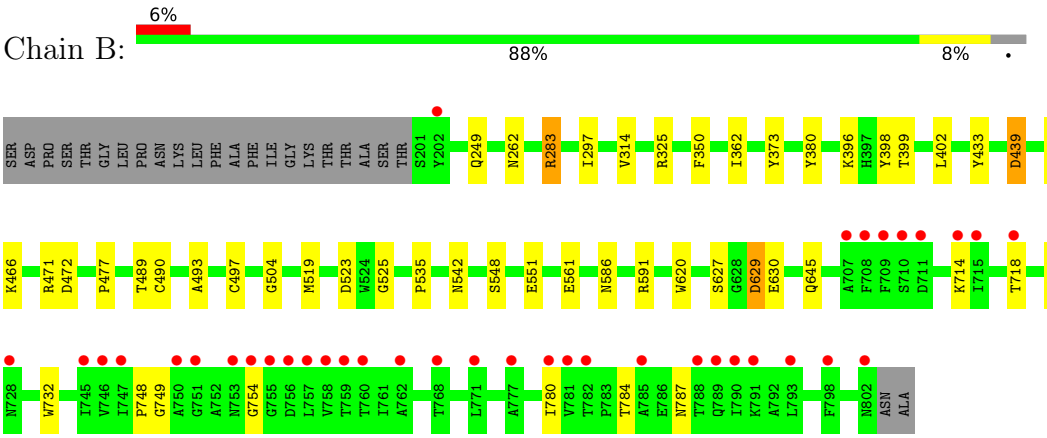
• Molecule 1: Bacteriophage Phi92 gp150

Chain A:



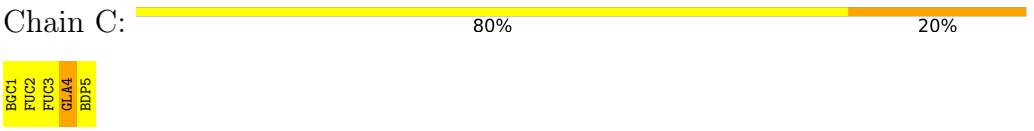
• Molecule 1: Bacteriophage Phi92 gp150

Chain B:



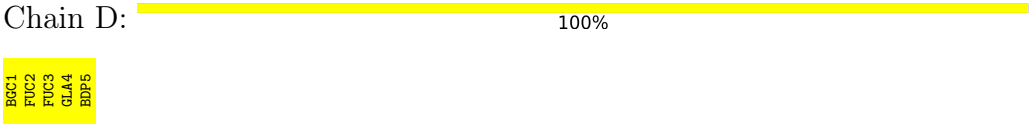
• Molecule 2: beta-D-glucopyranuronic acid-(1-3)-alpha-D-galactopyranose-(1-3)-alpha-L-fucopyranose-(1-4)-alpha-L-fucopyranose-(1-3)-beta-D-glucopyranose

Chain C:



• Molecule 2: beta-D-glucopyranuronic acid-(1-3)-alpha-D-galactopyranose-(1-3)-alpha-L-fucopyranose-(1-4)-alpha-L-fucopyranose-(1-3)-beta-D-glucopyranose

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	117.62Å 117.62Å 308.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	61.46 – 1.80 96.72 – 1.80	Depositor EDS
% Data completeness (in resolution range)	95.6 (61.46-1.80) 99.4 (96.72-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 1.81Å)	Xtriage
Refinement program	PHENIX (dev_3092: ???)	Depositor
R, R_{free}	0.153 , 0.176 0.153 , 0.176	Depositor DCC
R_{free} test set	2852 reflections (1.95%)	wwPDB-VP
Wilson B-factor (Å^2)	29.5	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 52.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.068 for -h-k,k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	10586	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: BDP, EDO, SO4, GLA, MG, FUC, BGC, HLA, PG4

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	0.68	2/4688 (0.0%)	0.70	0/6376
1	B	0.74	2/4703 (0.0%)	0.72	3/6397 (0.0%)
All	All	0.71	4/9391 (0.0%)	0.71	3/12773 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	373	TYR	CD1-CE1	6.97	1.49	1.39
1	B	380	TYR	CD1-CE1	6.24	1.48	1.39
1	A	650	PHE	CE2-CZ	5.46	1.47	1.37
1	A	621	VAL	CB-CG1	5.01	1.63	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	283	ARG	NE-CZ-NH1	-8.85	115.88	120.30
1	B	523	ASP	CB-CG-OD1	5.71	123.44	118.30
1	B	325	ARG	NE-CZ-NH2	-5.41	117.60	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4590	0	4396	31	0
1	B	4605	0	4405	35	0
2	C	55	0	44	1	0
2	D	55	0	44	0	0
3	A	20	0	0	0	0
3	B	30	0	0	0	7
4	A	1	0	0	0	0
4	B	2	0	0	0	0
5	A	16	0	0	1	0
5	B	16	0	0	0	0
6	B	4	0	6	1	0
7	B	13	0	18	1	0
8	A	604	0	0	13	6
8	B	575	0	0	15	1
All	All	10586	0	8913	69	13

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 (69) 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:678:ASP:OD2	8:A:1001:HOH:O	1.98	0.81
1:A:203:VAL:O	8:A:1002:HOH:O	2.00	0.80
1:B:561:GLU:OE1	8:B:1001:HOH:O	2.03	0.75
1:A:439:ASP:HB3	8:A:1019:HOH:O	1.88	0.73
1:B:262:ASN:OD1	8:B:1002:HOH:O	2.08	0.72
1:A:315:LYS:NZ	5:A:906:HLA:O2	2.24	0.71
1:A:201:SER:N	8:A:1008:HOH:O	2.25	0.69
1:B:748:PRO:O	8:B:1003:HOH:O	2.10	0.69
1:A:268:ASP:O	8:A:1003:HOH:O	2.10	0.68
1:A:439:ASP:OD1	1:A:466:LYS:NZ	2.29	0.65
1:B:472:ASP:OD2	8:B:1004:HOH:O	2.15	0.64
1:B:714:LYS:HD2	1:B:787:ASN:HB3	1.80	0.64
1:B:439:ASP:OD2	1:B:466:LYS:NZ	2.32	0.63
1:B:551:GLU:OE2	8:B:1005:HOH:O	2.16	0.59
7:B:910:PG4:H22	8:B:1432:HOH:O	2.03	0.57
1:A:296:MET:CE	1:A:298:SER:HB3	2.36	0.56
1:A:218:GLY:O	8:A:1005:HOH:O	2.18	0.55
1:B:749:GLY:HA2	1:B:754:GLY:O	2.09	0.53
1:B:466:LYS:NZ	8:B:1021:HOH:O	2.43	0.51
1:B:718:THR:CG2	1:B:784:THR:H	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:909:EDO:O2	8:B:1006:HOH:O	2.18	0.51
1:B:249:GLN:NE2	8:B:1023:HOH:O	2.44	0.50
1:B:283:ARG:HD2	8:B:1033:HOH:O	2.12	0.49
1:A:490[A]:CYS:SG	1:A:493:ALA:HB2	2.52	0.49
1:A:229:GLN:NE2	8:A:1020:HOH:O	2.46	0.49
1:A:727:SER:HB2	1:A:732:TRP:CE2	2.48	0.48
1:A:456:CYS:O	1:A:477:PRO:HA	2.15	0.47
1:B:586:ASN:ND2	8:B:1014:HOH:O	2.37	0.47
1:A:240:ILE:HG13	1:A:245:THR:HG21	1.97	0.47
1:A:519:MET:HB2	1:A:548:SER:HB3	1.96	0.47
1:A:278:ALA:HA	1:A:298:SER:OG	2.15	0.47
1:B:727:SER:HB2	1:B:732:TRP:CE2	2.50	0.46
1:A:375:ARG:NH1	8:A:1015:HOH:O	2.43	0.46
8:A:1004:HOH:O	2:C:4:GLA:O2	2.17	0.46
1:B:497:CYS:O	1:B:535:PRO:HA	2.16	0.45
1:B:629:ASP:OD1	1:B:629:ASP:N	2.50	0.45
1:A:711:ASP:OD1	8:A:1006:HOH:O	2.21	0.45
1:B:396:LYS:NZ	8:B:1030:HOH:O	2.47	0.45
1:B:456:CYS:O	1:B:477:PRO:HA	2.17	0.45
1:A:614:GLN:NE2	8:A:1024:HOH:O	2.49	0.45
1:B:471:ARG:HD2	8:B:1079:HOH:O	2.17	0.45
1:A:802:ASN:ND2	8:A:1023:HOH:O	2.47	0.44
1:B:444:ARG:HA	1:B:466:LYS:O	2.17	0.44
1:B:433:TYR:CD1	1:B:525:GLY:HA3	2.52	0.44
1:B:350:PHE:CE1	1:B:362:ILE:HD11	2.52	0.43
1:B:591:ARG:N	1:B:591:ARG:HD2	2.32	0.43
1:A:398:TYR:CG	1:A:402:LEU:HB2	2.54	0.43
1:A:496:GLY:HA2	1:A:533:GLY:O	2.18	0.43
1:B:399[B]:THR:HG23	8:B:1013:HOH:O	2.18	0.43
1:A:299:THR:HB	1:A:302:CYS:HB2	1.99	0.43
1:A:381:ILE:O	1:A:409:ILE:HA	2.18	0.43
1:B:714:LYS:HB3	1:B:787:ASN:HA	2.01	0.43
1:B:519:MET:HB2	1:B:548:SER:HB3	2.00	0.42
1:A:629:ASP:HB2	8:A:1144:HOH:O	2.19	0.42
1:B:398:TYR:CG	1:B:402:LEU:HB2	2.54	0.42
1:B:489:THR:O	1:B:490[A]:CYS:HB3	2.19	0.42
1:A:497:CYS:O	1:A:535:PRO:HA	2.19	0.42
1:A:618:MET:O	1:A:643:CYS:HA	2.20	0.42
1:A:251:ILE:O	1:A:255:ILE:HD13	2.20	0.42
1:A:296:MET:HE3	1:A:298:SER:HB3	2.00	0.42
1:A:305:GLU:HA	1:A:324:TYR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:GLU:HA	1:A:449:VAL:O	2.21	0.41
1:B:718:THR:OG1	1:B:780:ILE:HG13	2.21	0.41
1:B:504:GLY:HA2	1:B:542:ASN:O	2.21	0.41
1:B:620:TRP:O	1:B:645:GLN:HA	2.21	0.41
1:B:283:ARG:NH1	8:B:1002:HOH:O	2.43	0.41
1:B:297:ILE:O	1:B:314:VAL:HA	2.21	0.40
1:B:490[A]:CYS:SG	1:B:493:ALA:HB2	2.61	0.40
1:B:627:SER:O	1:B:630:GLU:HG2	2.22	0.40

All (13) 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)
3:B:906:SO4:O2	3:B:906:SO4:O4[3_455]	0.02	2.18
3:B:906:SO4:O2	3:B:906:SO4:O3[2_565]	0.03	2.17
3:B:906:SO4:O3	3:B:906:SO4:O4[2_565]	0.04	2.16
3:B:906:SO4:S	3:B:906:SO4:O1[2_565]	1.46	0.74
3:B:906:SO4:S	3:B:906:SO4:O4[2_565]	1.46	0.74
3:B:906:SO4:S	3:B:906:SO4:O3[2_565]	1.46	0.74
3:B:906:SO4:S	3:B:906:SO4:O2[2_565]	1.46	0.74
8:A:1046:HOH:O	8:A:1070:HOH:O[3_565]	1.96	0.24
8:A:1454:HOH:O	8:B:1087:HOH:O[8_554]	2.00	0.20
8:A:1297:HOH:O	8:A:1358:HOH:O[2_665]	2.05	0.15
8:A:1523:HOH:O	8:A:1544:HOH:O[3_565]	2.05	0.15
8:A:1334:HOH:O	8:A:1438:HOH:O[2_665]	2.12	0.08
8:A:1414:HOH:O	8:A:1419:HOH:O[3_565]	2.12	0.08

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	604/626 (96%)	580 (96%)	24 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	606/626 (97%)	582 (96%)	24 (4%)	0	100	100
All	All	1210/1252 (97%)	1162 (96%)	48 (4%)	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	494/509 (97%)	493 (100%)	1 (0%)	93	92
1	B	496/509 (97%)	493 (99%)	3 (1%)	86	84
All	All	990/1018 (97%)	986 (100%)	4 (0%)	91	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	ILE
1	B	439	ASP
1	B	629	ASP
1	B	722	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

10 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	BGC	C	1	2	12,12,12	1.11	1 (8%)	17,17,17	0.94	1 (5%)
2	FUC	C	2	2	10,10,11	1.37	2 (20%)	14,14,16	1.06	1 (7%)
2	FUC	C	3	2	10,10,11	0.97	0	14,14,16	0.91	1 (7%)
2	GLA	C	4	2	11,11,12	1.81	3 (27%)	15,15,17	1.32	3 (20%)
2	BDP	C	5	5,2	12,12,13	1.89	3 (25%)	14,17,19	1.35	1 (7%)
2	BGC	D	1	2	12,12,12	1.22	1 (8%)	17,17,17	0.93	0
2	FUC	D	2	2	10,10,11	1.52	2 (20%)	14,14,16	0.76	0
2	FUC	D	3	2	10,10,11	0.69	0	14,14,16	1.16	1 (7%)
2	GLA	D	4	2	11,11,12	1.60	3 (27%)	15,15,17	1.57	2 (13%)
2	BDP	D	5	5,2	12,12,13	1.63	2 (16%)	14,17,19	1.55	2 (14%)

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	BGC	C	1	2	-	2/2/22/22	0/1/1/1
2	FUC	C	2	2	-	-	0/1/1/1
2	FUC	C	3	2	-	-	0/1/1/1
2	GLA	C	4	2	-	1/2/19/22	0/1/1/1
2	BDP	C	5	5,2	-	2/4/21/24	0/1/1/1
2	BGC	D	1	2	-	0/2/22/22	0/1/1/1
2	FUC	D	2	2	-	-	0/1/1/1
2	FUC	D	3	2	-	-	0/1/1/1
2	GLA	D	4	2	-	0/2/19/22	0/1/1/1
2	BDP	D	5	5,2	-	1/4/21/24	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4	GLA	O5-C1	4.80	1.51	1.43
2	C	5	BDP	O5-C1	4.70	1.51	1.43
2	D	5	BDP	O5-C1	3.72	1.49	1.43
2	D	4	GLA	O5-C1	3.53	1.49	1.43
2	D	1	BGC	O5-C1	3.50	1.51	1.42
2	D	2	FUC	O5-C1	-3.09	1.38	1.43
2	C	2	FUC	C4-C5	2.87	1.59	1.52
2	C	1	BGC	O5-C1	2.75	1.49	1.42
2	C	5	BDP	C2-C3	-2.69	1.48	1.52
2	C	5	BDP	O5-C5	2.66	1.48	1.43
2	D	4	GLA	O5-C5	2.54	1.48	1.43
2	C	4	GLA	O5-C5	2.37	1.48	1.43
2	D	5	BDP	O6A-C6	2.31	1.29	1.22
2	D	4	GLA	O3-C3	2.18	1.48	1.43
2	C	4	GLA	C2-C3	-2.13	1.49	1.52
2	D	2	FUC	C1-C2	2.08	1.56	1.52
2	C	2	FUC	C1-C2	2.04	1.56	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	5	BDP	C1-C2-C3	4.53	115.24	109.67
2	D	4	GLA	C1-O5-C5	-4.10	106.63	112.19
2	D	4	GLA	C3-C4-C5	3.50	116.48	110.24
2	C	5	BDP	C1-C2-C3	3.40	113.85	109.67
2	C	4	GLA	C3-C4-C5	2.75	115.15	110.24
2	C	1	BGC	C1-O5-C5	-2.62	108.71	113.66
2	D	3	FUC	O3-C3-C2	-2.33	105.54	109.99
2	C	4	GLA	C1-C2-C3	2.30	112.49	109.67
2	C	2	FUC	O2-C2-C3	-2.28	105.56	110.14
2	C	3	FUC	C3-C4-C5	-2.11	106.49	109.77
2	C	4	GLA	C6-C5-C4	-2.09	108.11	113.00
2	D	5	BDP	O6B-C6-O6A	-2.00	119.54	124.09

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	BGC	C4-C5-C6-O6
2	C	1	BGC	O5-C5-C6-O6
2	C	4	GLA	C4-C5-C6-O6
2	C	5	BDP	O5-C5-C6-O6A

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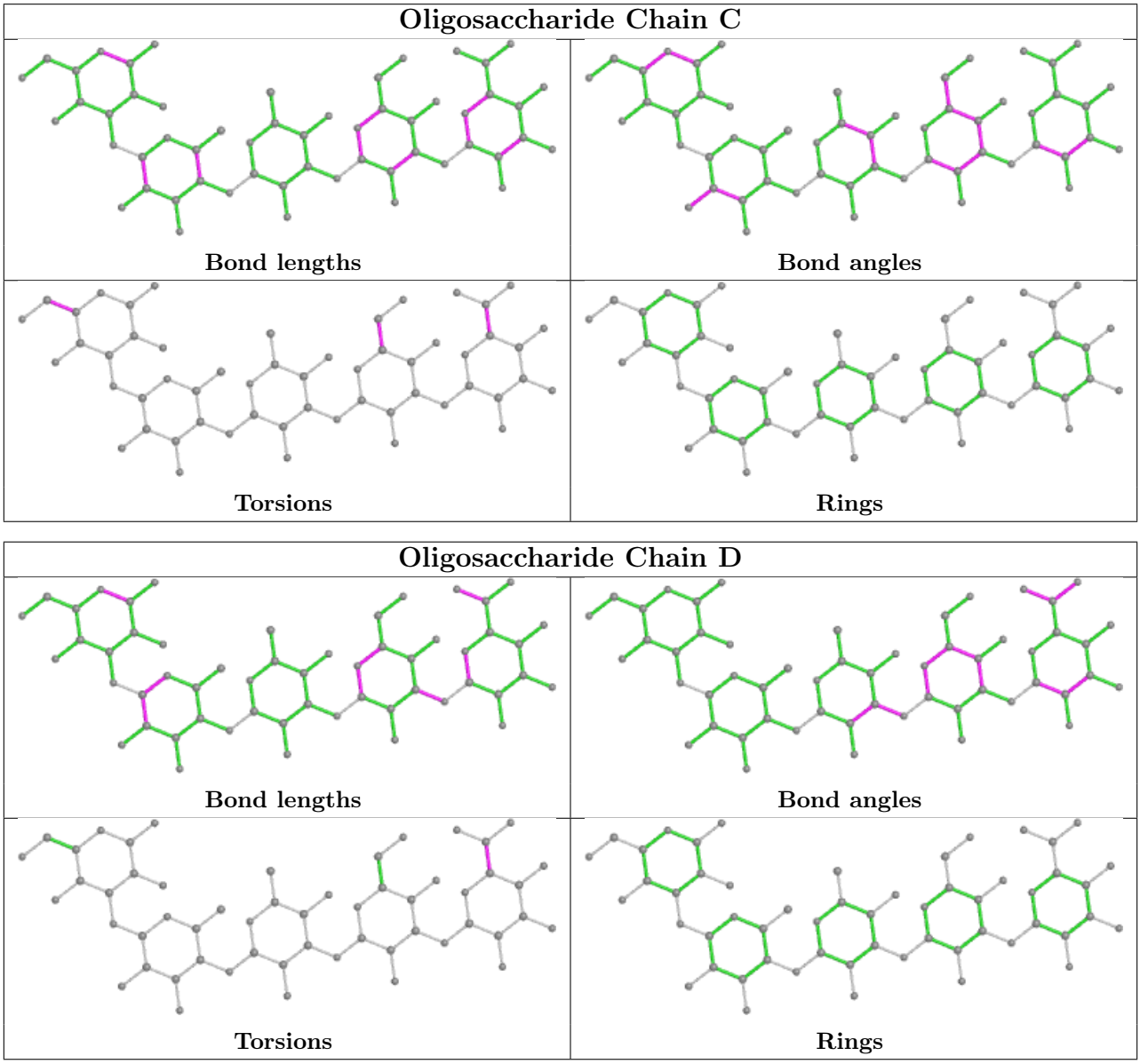
Mol	Chain	Res	Type	Atoms
2	C	5	BDP	O5-C5-C6-O6B
2	D	5	BDP	O5-C5-C6-O6A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	4	GLA	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 (i)

Of 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 for Mogul analysis.

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	SO4	B	903	-	4,4,4	0.41	0	6,6,6	0.32	0
7	PG4	B	910	-	12,12,12	0.53	0	11,11,11	0.65	0
3	SO4	B	902	-	4,4,4	0.12	0	6,6,6	0.19	0
3	SO4	B	906	-	4,4,4	0.14	0	6,6,6	0.21	0
3	SO4	A	904	-	4,4,4	0.53	0	6,6,6	0.55	0
5	HLA	A	906	2	16,17,17	1.70	2 (12%)	23,26,26	1.76	4 (17%)
3	SO4	A	901	-	4,4,4	0.12	0	6,6,6	0.45	0
6	EDO	B	909	-	3,3,3	0.45	0	2,2,2	0.45	0
5	HLA	B	911	2	16,17,17	1.81	2 (12%)	23,26,26	1.59	5 (21%)
3	SO4	B	904	-	4,4,4	0.30	0	6,6,6	0.95	0
3	SO4	B	905	-	4,4,4	0.14	0	6,6,6	0.31	0
3	SO4	A	903	-	4,4,4	0.49	0	6,6,6	0.53	0
3	SO4	A	902	-	4,4,4	0.12	0	6,6,6	0.28	0
3	SO4	B	901	-	4,4,4	0.16	0	6,6,6	0.55	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
5	HLA	B	911	2	-	1/5/34/34	0/2/2/2
7	PG4	B	910	-	-	3/10/10/10	-
5	HLA	A	906	2	-	1/5/34/34	0/2/2/2
6	EDO	B	909	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	911	HLA	O6-CAM	5.66	1.48	1.42
5	A	906	HLA	O6-CAM	4.80	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	911	HLA	O4-CAM	3.42	1.47	1.42
5	A	906	HLA	O4-CAM	3.24	1.47	1.42

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	906	HLA	C6-O6-CAM	-4.46	110.04	113.94
5	A	906	HLA	O4-C4-C3	4.39	113.86	109.27
5	B	911	HLA	O6-CAM-CAN	3.30	110.21	106.27
5	B	911	HLA	O5-C5-C6	-2.98	105.28	108.27
5	B	911	HLA	C1-O5-C5	2.91	116.14	112.19
5	A	906	HLA	CAM-O4-C4	-2.48	108.06	114.18
5	A	906	HLA	O6-CAM-CAN	2.27	108.98	106.27
5	B	911	HLA	C1-C2-C3	-2.17	107.00	109.67
5	B	911	HLA	O4-C4-C3	2.14	111.51	109.27

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	910	PG4	O4-C7-C8-O5
7	B	910	PG4	O3-C5-C6-O4
6	B	909	EDO	O1-C1-C2-O2
5	A	906	HLA	O6-CAM-CAO-OAQ
5	B	911	HLA	O6-CAM-CAO-OAQ
7	B	910	PG4	O2-C3-C4-O3

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	910	PG4	1	0
3	B	906	SO4	0	7
5	A	906	HLA	1	0
6	B	909	EDO	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	602/626 (96%)	0.09	33 (5%)	25	20	22, 34, 88, 130	0
1	B	602/626 (96%)	0.09	39 (6%)	18	15	20, 33, 97, 130	0
All	All	1204/1252 (96%)	0.09	72 (5%)	21	17	20, 34, 91, 130	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	202	TYR	11.7
1	A	207	LEU	6.6
1	A	222	GLY	6.3
1	A	203	VAL	5.9
1	B	746	VAL	5.9
1	B	790	ILE	5.9
1	B	750	ALA	5.3
1	B	747	ILE	5.0
1	B	758	VAL	5.0
1	B	785	ALA	4.6
1	A	244	VAL	4.5
1	A	206	ASN	4.4
1	A	211	THR	4.3
1	B	789	GLN	4.2
1	B	771	LEU	4.2
1	B	781	VAL	4.2
1	B	714	LYS	4.1
1	B	755	GLY	4.1
1	B	788	THR	4.0
1	B	757	LEU	3.9
1	B	708	PHE	3.8
1	A	230	TYR	3.8
1	A	226	LEU	3.8
1	A	208	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	256	THR	3.7
1	B	759	THR	3.7
1	A	239	ALA	3.7
1	B	780	ILE	3.7
1	B	710	SER	3.7
1	A	257	PHE	3.7
1	B	782	THR	3.6
1	B	715	ILE	3.6
1	A	251	ILE	3.6
1	A	218	GLY	3.5
1	A	221	SER	3.4
1	A	241	GLY	3.3
1	A	273	PHE	3.3
1	A	214	ALA	3.3
1	B	760	THR	3.2
1	B	777	ALA	3.2
1	B	709	PHE	3.1
1	A	201	SER	3.1
1	B	793	LEU	3.0
1	B	753	ASN	3.0
1	A	252	LEU	2.9
1	B	718	THR	2.8
1	A	234	PRO	2.8
1	A	237	PHE	2.8
1	A	271	TYR	2.6
1	A	227	GLN	2.6
1	A	219	LEU	2.6
1	B	798	PHE	2.5
1	A	210	SER	2.5
1	B	754	GLY	2.4
1	B	711	ASP	2.4
1	B	751	GLY	2.4
1	A	243	GLY	2.4
1	B	707	ALA	2.3
1	B	768	THR	2.3
1	A	238	GLY	2.3
1	B	791	LYS	2.3
1	A	262	ASN	2.3
1	A	249	GLN	2.2
1	B	756	ASP	2.2
1	B	762	ALA	2.2
1	B	745	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	723	THR	2.1
1	B	728	ASN	2.1
1	B	202	TYR	2.1
1	A	250	ALA	2.0
1	B	802	ASN	2.0
1	A	223	GLY	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)

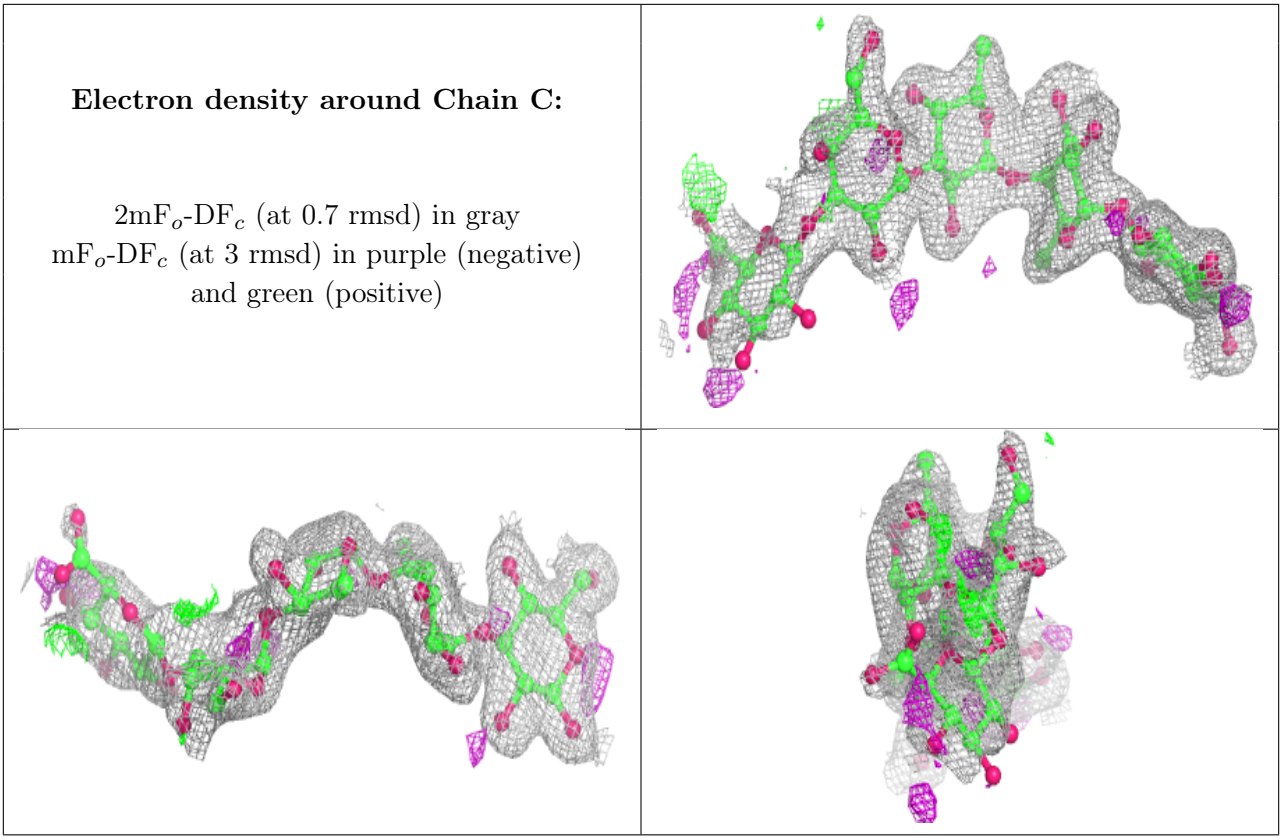
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	BDP	C	5	12/13	0.74	0.33	107,118,122,130	0
2	GLA	C	4	11/12	0.81	0.20	75,84,88,96	0
2	BDP	D	5	12/13	0.81	0.20	48,59,71,74	0
2	GLA	D	4	11/12	0.86	0.25	47,53,65,67	0
2	FUC	C	3	10/11	0.89	0.12	48,56,59,66	0
2	FUC	D	3	10/11	0.91	0.09	31,34,36,37	0
2	FUC	C	2	10/11	0.91	0.10	36,40,44,50	0
2	BGC	C	1	12/12	0.91	0.12	37,40,43,44	0
2	FUC	D	2	10/11	0.92	0.09	30,34,35,36	0
2	BGC	D	1	12/12	0.94	0.09	29,31,38,39	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.

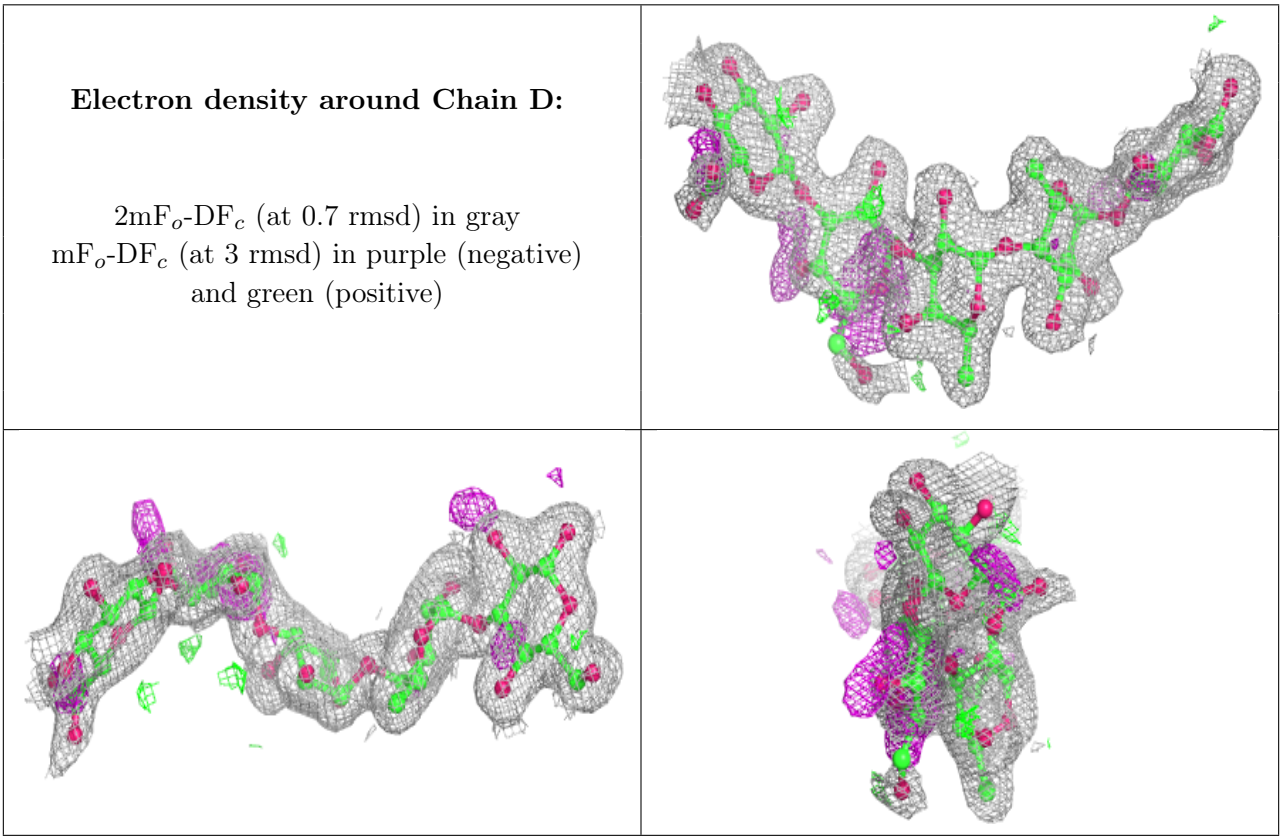
Electron density around Chain C:

$2mF_o$-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 (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
5	HLA	A	906	16/16	0.15	0.58	137,144,148,148	0
3	SO4	B	906	5/5	0.71	0.31	175,175,175,175	0
5	HLA	B	911	16/16	0.73	0.24	72,81,86,87	0
7	PG4	B	910	13/13	0.84	0.15	35,46,60,63	0
3	SO4	A	904	5/5	0.95	0.14	37,43,51,61	0
3	SO4	B	902	5/5	0.95	0.09	65,67,71,73	0
3	SO4	B	903	5/5	0.96	0.15	40,51,53,58	0
3	SO4	B	904	5/5	0.97	0.12	34,37,46,51	0
3	SO4	B	905	5/5	0.97	0.14	70,73,77,78	0
6	EDO	B	909	4/4	0.97	0.11	37,40,44,45	0
3	SO4	A	903	5/5	0.97	0.13	44,47,49,60	0
3	SO4	B	901	5/5	0.98	0.08	40,45,47,53	0
3	SO4	A	901	5/5	0.98	0.09	41,47,58,59	0
3	SO4	A	902	5/5	0.99	0.08	59,60,64,69	0
4	MG	A	905	1/1	0.99	0.06	29,29,29,29	0
4	MG	B	907	1/1	0.99	0.07	27,27,27,27	0
4	MG	B	908	1/1	0.99	0.05	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.