



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:38 PM UTC

PDB ID : 6E0W / pdb_00006e0w
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

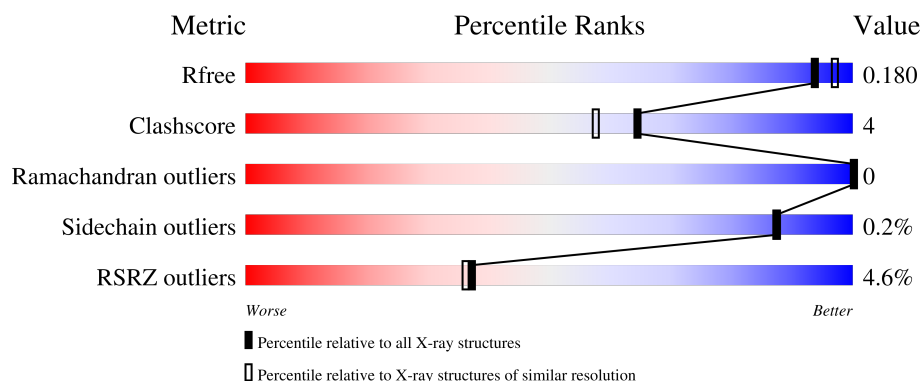
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

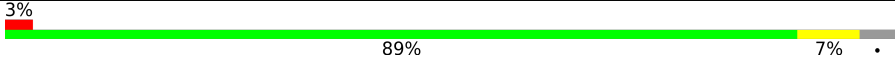
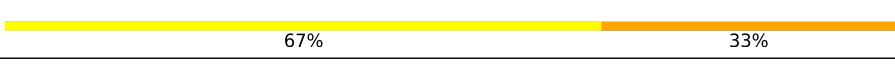
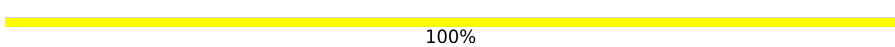
The reported resolution of this entry is 1.80 Å.

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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 $\leq 5\%$. 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	
1	B	626	
2	C	6	
2	D	6	

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	-

2 Entry composition

There are 7 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:

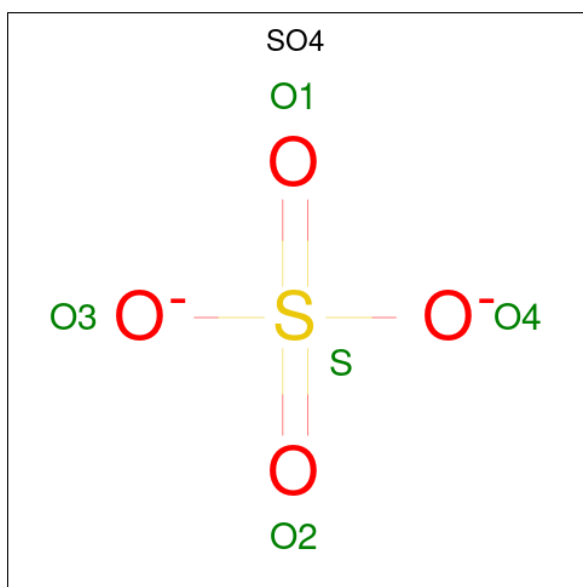
Chain	Residue	Modelled	Actual	Comment	Reference
A	179	SER	-	expression tag	UNP I7I026
B	179	SER	-	expression tag	UNP I7I026

- Molecule 2 is an oligosaccharide called 4,6-O-[(1R)-1-carboxyethylidene]-D-galactopyranose-(1-4)-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	6	Total	C	O	0	0	0
			71	39	32			
2	D	6	Total	C	O	0	0	0
			71	39	32			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

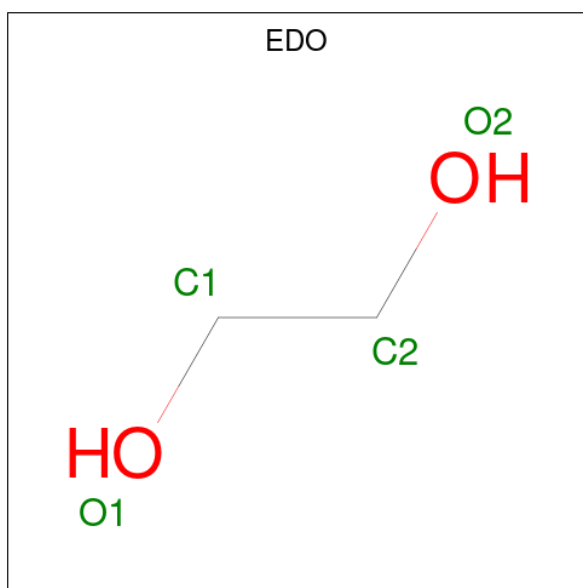


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

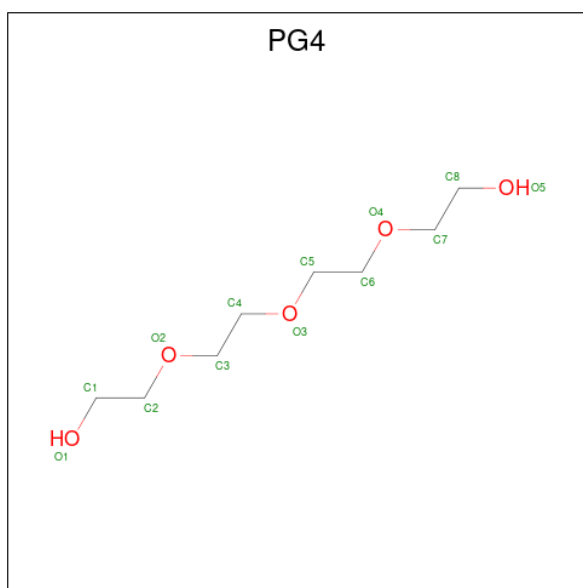
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	2	Total	Mg	0	0
			2	2		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).

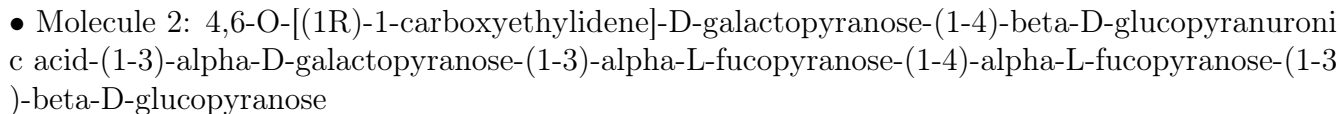


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is water.

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

- Molecule 1: Bacteriophage Phi92 gp150



- Molecule 2: 4,6-O-[(1R)-1-carboxyethylidene]-D-galactopyranose-(1-4)-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:

100%

BGC1
FUC2
FUC3
GLA4
BDP5
HLA6

4 Data and refinement statistics

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 61.46 – 1.80	Depositor EDS
% Data completeness (in resolution range)	95.6 (61.46-1.80) 99.5 (61.46-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 1.81Å)	Xtriage
Refinement program	PHENIX (dev_3092: ???)	Depositor
R, R_{free}	0.153 , 0.176 0.159 , 0.180	Depositor DCC
R_{free} test set	2852 reflections (1.94%)	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)	0.34 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, GLA, MG, SO4, FUC, BDP, BGC, HLA, EDO

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	0.62	0/4688	0.69	0/6376
1	B	0.66	0/4703	0.71	1/6397 (0.0%)
All	All	0.64	0/9391	0.70	1/12773 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	283	ARG	NE-CZ-NH1	-5.62	115.88	121.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4590	0	4396	32	0
1	B	4605	0	4405	36	0
2	C	71	0	44	2	0
2	D	71	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	4	0	6	1	0
6	B	13	0	18	1	0
7	A	604	0	0	13	6
7	B	575	0	0	15	1
All	All	10586	0	8913	71	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 (71) 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	7:A:1001:HOH:O	1.98	0.81
1:A:203:VAL:O	7:A:1002:HOH:O	2.00	0.80
1:B:561:GLU:OE1	7:B:1001:HOH:O	2.03	0.75
1:A:439:ASP:HB3	7:A:1018:HOH:O	1.88	0.73
1:B:262:ASN:OD1	7:B:1002:HOH:O	2.08	0.72
1:A:315:LYS:NZ	2:C:6:HLA:O2	2.24	0.71
1:A:201:SER:N	7:A:1007:HOH:O	2.25	0.69
1:B:748:PRO:O	7:B:1003:HOH:O	2.10	0.69
1:A:268:ASP:O	7: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	7:B:1004:HOH:O	2.15	0.64
1:B:714:LYS:HD2	1:B:787:ASN:HB3	1.80	0.64
1:B:315:LYS:NZ	7:B:1010:HOH:O	2.30	0.63
1:B:439:ASP:OD2	1:B:466:LYS:NZ	2.32	0.63
1:B:551:GLU:OE2	7:B:1005:HOH:O	2.16	0.59
6:B:910:PG4:H22	7:B:1425:HOH:O	2.03	0.57
1:A:296:MET:HE2	1:A:298:SER:HB3	1.85	0.57
1:A:296:MET:CE	1:A:298:SER:HB3	2.36	0.56
1:A:218:GLY:O	7:A:1004:HOH:O	2.18	0.55
1:B:749:GLY:HA2	1:B:754:GLY:O	2.09	0.53
5:B:909:EDO:O2	7:B:1006:HOH:O	2.18	0.53
1:B:466:LYS:NZ	7:B:1021:HOH:O	2.43	0.51
1:B:718:THR:CG2	1:B:784:THR:H	2.24	0.51
1:B:249:GLN:NE2	7:B:1023:HOH:O	2.44	0.50
1:A:296:MET:HE3	1:A:315:LYS:HB3	1.92	0.50
1:B:283:ARG:HD2	7: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	7:A:1019:HOH:O	2.46	0.49
1:A:727:SER:HB2	1:A:732:TRP:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:CYS:O	1:A:477:PRO:HA	2.15	0.47
1:B:586:ASN:ND2	7: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	7:A:1014:HOH:O	2.43	0.46
7:A:1376: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:A:711:ASP:OD1	7:A:1005:HOH:O	2.21	0.45
1:B:203:VAL:HG13	1:B:216:MET:HE1	1.98	0.45
1:B:456:CYS:O	1:B:477:PRO:HA	2.17	0.45
1:A:614:GLN:NE2	7:A:1023:HOH:O	2.49	0.45
1:B:471:ARG:HD2	7:B:1078:HOH:O	2.17	0.45
1:A:802:ASN:ND2	7:A:1022:HOH:O	2.47	0.44
1:B:444:ARG:HA	1:B:466:LYS:O	2.17	0.44
1:B:629:ASP:OD1	1:B:629:ASP:N	2.50	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	7: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	7:A:1142: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:305:GLU:HA	1:A:324:TYR:O	2.21	0.41
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	7: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:A:1045:HOH:O	7:A:1069:HOH:O[3_565]	1.96	0.24
7:A:1452:HOH:O	7:B:1085:HOH:O[8_554]	2.00	0.20
7:A:1295:HOH:O	7:A:1356:HOH:O[2_665]	2.05	0.15
7:A:1523:HOH:O	7:A:1544:HOH:O[3_565]	2.05	0.15
7:A:1332:HOH:O	7:A:1436:HOH:O[2_665]	2.12	0.08
7:A:1412:HOH:O	7:A:1417: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
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 ⓘ

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%)	87	87
1	B	496/509 (97%)	495 (100%)	1 (0%)	87	87
All	All	990/1018 (97%)	988 (100%)	2 (0%)	87	87

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	ILE
1	B	629	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	GLN
1	A	261	ASN
1	A	392	ASN
1	A	568	ASN
1	A	587	ASN
1	B	392	ASN
1	B	420	ASN
1	B	542	ASN
1	B	568	ASN
1	B	587	ASN
1	B	693	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 ⓘ

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	BGC	C	1	2	12,12,12	1.11	1 (8%)	17,17,17	0.93	1 (5%)
2	FUC	C	2	2	10,10,11	1.34	1 (10%)	14,14,16	0.97	1 (7%)
2	FUC	C	3	2	10,10,11	0.97	0	14,14,16	0.88	1 (7%)
2	GLA	C	4	2	11,11,12	1.76	3 (27%)	15,15,17	1.23	1 (6%)
2	BDP	C	5	2	12,12,13	1.82	3 (25%)	14,17,19	1.21	1 (7%)
2	HLA	C	6	2	16,17,18	2.10	2 (12%)	19,26,28	1.56	2 (10%)
2	BGC	D	1	2	12,12,12	1.24	1 (8%)	17,17,17	0.93	0
2	FUC	D	2	2	10,10,11	1.46	1 (10%)	14,14,16	0.74	0
2	FUC	D	3	2	10,10,11	0.70	0	14,14,16	1.11	1 (7%)
2	GLA	D	4	2	11,11,12	1.57	3 (27%)	15,15,17	1.55	2 (13%)
2	BDP	D	5	2	12,12,13	1.59	2 (16%)	14,17,19	1.39	1 (7%)
2	HLA	D	6	2	16,17,18	2.30	2 (12%)	19,26,28	1.85	4 (21%)

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	2	-	0/4/21/24	0/1/1/1
2	HLA	C	6	2	-	0/6/34/37	0/2/2/2
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLA	D	4	2	-	0/2/19/22	0/1/1/1
2	BDP	D	5	2	-	1/4/21/24	0/1/1/1
2	HLA	D	6	2	-	0/6/34/37	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	6	HLA	O6-CAM	7.87	1.48	1.41
2	C	6	HLA	O6-CAM	6.80	1.47	1.41
2	C	4	GLA	O5-C1	4.58	1.51	1.43
2	C	5	BDP	O5-C1	4.48	1.51	1.43
2	D	6	HLA	O4-CAM	3.64	1.47	1.42
2	D	1	BGC	O5-C1	3.59	1.51	1.42
2	D	5	BDP	O5-C1	3.55	1.49	1.43
2	C	6	HLA	O4-CAM	3.44	1.47	1.42
2	D	4	GLA	O5-C1	3.37	1.49	1.43
2	D	2	FUC	O5-C1	-2.92	1.38	1.43
2	C	2	FUC	C4-C5	2.89	1.59	1.52
2	C	1	BGC	O5-C1	2.82	1.49	1.42
2	D	4	GLA	O5-C5	2.65	1.48	1.43
2	C	5	BDP	C2-C3	-2.57	1.48	1.52
2	C	5	BDP	O5-C5	2.54	1.48	1.43
2	C	4	GLA	O5-C5	2.47	1.48	1.43
2	D	5	BDP	O6A-C6	2.39	1.29	1.22
2	D	4	GLA	O3-C3	2.08	1.48	1.43
2	C	4	GLA	C2-C3	-2.03	1.49	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	6	HLA	O6-CAM-CAN	5.04	110.21	106.89
2	C	6	HLA	O4-C4-C3	4.43	113.86	109.28
2	D	4	GLA	C1-O5-C5	-4.14	106.63	112.19
2	D	5	BDP	C1-C2-C3	3.84	115.24	109.64
2	D	4	GLA	C3-C4-C5	3.44	116.48	110.23
2	C	6	HLA	O6-CAM-CAN	3.17	108.98	106.89
2	D	6	HLA	O5-C5-C6	-3.04	105.28	108.30
2	D	6	HLA	C1-O5-C5	2.95	116.14	112.19
2	C	5	BDP	C1-C2-C3	2.89	113.85	109.64
2	C	4	GLA	C3-C4-C5	2.71	115.15	110.23
2	C	1	BGC	C1-O5-C5	-2.55	108.71	113.65
2	C	2	FUC	O2-C2-C3	-2.21	105.56	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	FUC	O3-C3-C2	-2.21	105.54	110.05
2	C	3	FUC	C3-C4-C5	-2.19	106.49	109.81
2	D	6	HLA	O4-C4-C3	2.16	111.51	109.28

There are no chirality outliers.

All (4) torsion outliers are listed below:

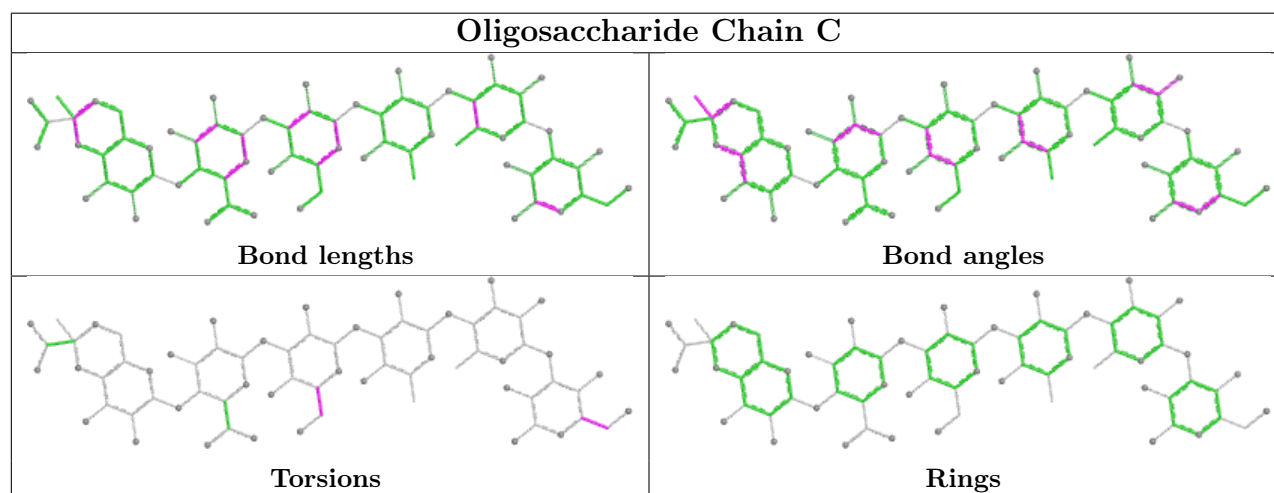
Mol	Chain	Res	Type	Atoms
2	C	1	BGC	C4-C5-C6-O6
2	C	1	BGC	O5-C5-C6-O6
2	C	4	GLA	C4-C5-C6-O6
2	D	5	BDP	O5-C5-C6-O6A

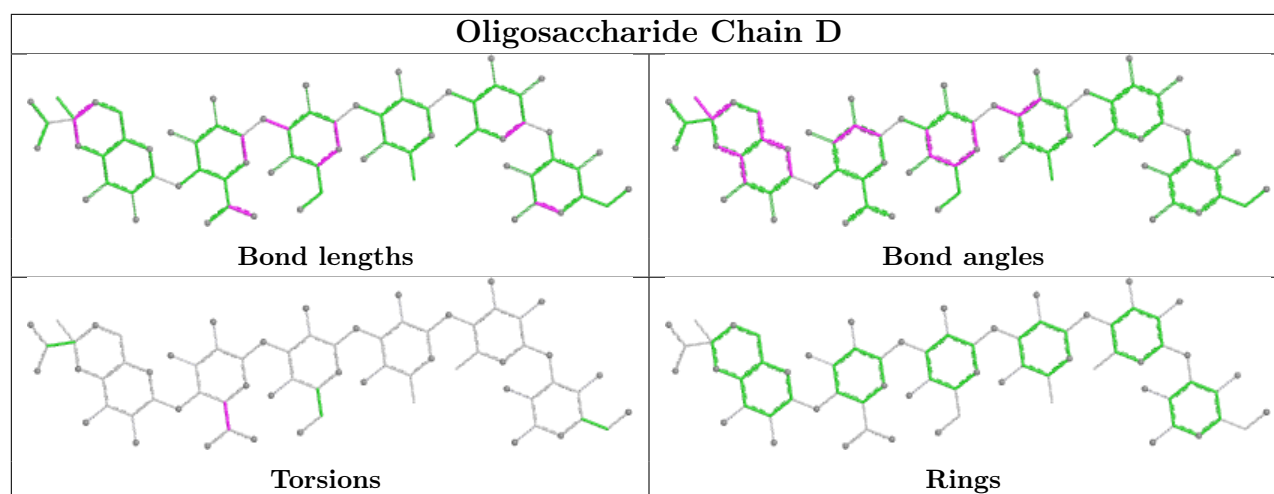
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	6	HLA	1	0
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 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 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	A	903	-	4,4,4	0.58	0	6,6,6	0.52	0
3	SO4	B	902	-	4,4,4	0.24	0	6,6,6	0.17	0
3	SO4	B	901	-	4,4,4	0.24	0	6,6,6	0.50	0
3	SO4	B	904	-	4,4,4	0.39	0	6,6,6	0.85	0
3	SO4	A	902	-	4,4,4	0.21	0	6,6,6	0.25	0
3	SO4	B	905	-	4,4,4	0.23	0	6,6,6	0.29	0
5	EDO	B	909	-	3,3,3	0.43	0	2,2,2	0.47	0
3	SO4	A	901	-	4,4,4	0.14	0	6,6,6	0.42	0
3	SO4	B	906	-	4,4,4	0.23	0	6,6,6	0.21	0
3	SO4	B	903	-	4,4,4	0.48	0	6,6,6	0.34	0
3	SO4	A	904	-	4,4,4	0.61	0	6,6,6	0.56	0
6	PG4	B	910	-	12,12,12	0.54	0	11,11,11	0.64	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	EDO	B	909	-	-	1/1/1/1	-
6	PG4	B	910	-	-	2/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	910	PG4	O4-C7-C8-O5
6	B	910	PG4	O3-C5-C6-O4
5	B	909	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	909	EDO	1	0
3	B	906	SO4	0	7
6	B	910	PG4	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, 95th 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%)	-0.12	16 (2%) 56 56	12, 34, 88, 130	4 (0%)
1	B	602/626 (96%)	-0.09	39 (6%) 25 23	14, 33, 97, 130	6 (0%)
All	All	1204/1252 (96%)	-0.10	55 (4%) 37 36	12, 33, 91, 130	10 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	790	ILE	4.4
1	B	757	LEU	3.7
1	B	752	ALA	3.3
1	B	781	VAL	3.2
1	B	715	ILE	3.2
1	B	746	VAL	3.2
1	B	758	VAL	3.1
1	B	750	ALA	3.0
1	B	719	VAL	3.0
1	A	218	GLY	2.9
1	B	748	PRO	2.9
1	B	747	ILE	2.9
1	B	780	ILE	2.9
1	A	212	THR	2.9
1	B	725	LEU	2.9
1	B	745	ILE	2.9
1	B	771	LEU	2.8
1	B	717	ALA	2.7
1	A	202	TYR	2.6
1	B	793	LEU	2.6
1	B	707	ALA	2.6
1	B	785	ALA	2.6
1	B	730	LEU	2.6
1	B	761	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	203	VAL	2.6
1	B	762	ALA	2.6
1	B	760	THR	2.5
1	A	226	LEU	2.4
1	B	759	THR	2.4
1	A	217	VAL	2.4
1	B	767	VAL	2.4
1	B	782	THR	2.3
1	A	201	SER	2.3
1	A	230	TYR	2.3
1	A	802	ASN	2.3
1	B	802	ASN	2.3
1	B	751	GLY	2.3
1	B	718	THR	2.3
1	B	720	THR	2.3
1	A	207	LEU	2.3
1	B	724	TYR	2.2
1	B	629	ASP	2.2
1	B	755	GLY	2.2
1	B	792	ALA	2.2
1	A	228	ALA	2.2
1	A	255	ILE	2.1
1	A	219	LEU	2.1
1	B	753	ASN	2.1
1	B	756	ASP	2.1
1	A	325	ARG	2.1
1	B	754	GLY	2.0
1	B	709	PHE	2.0
1	B	788	THR	2.0
1	A	220	PRO	2.0
1	A	282	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

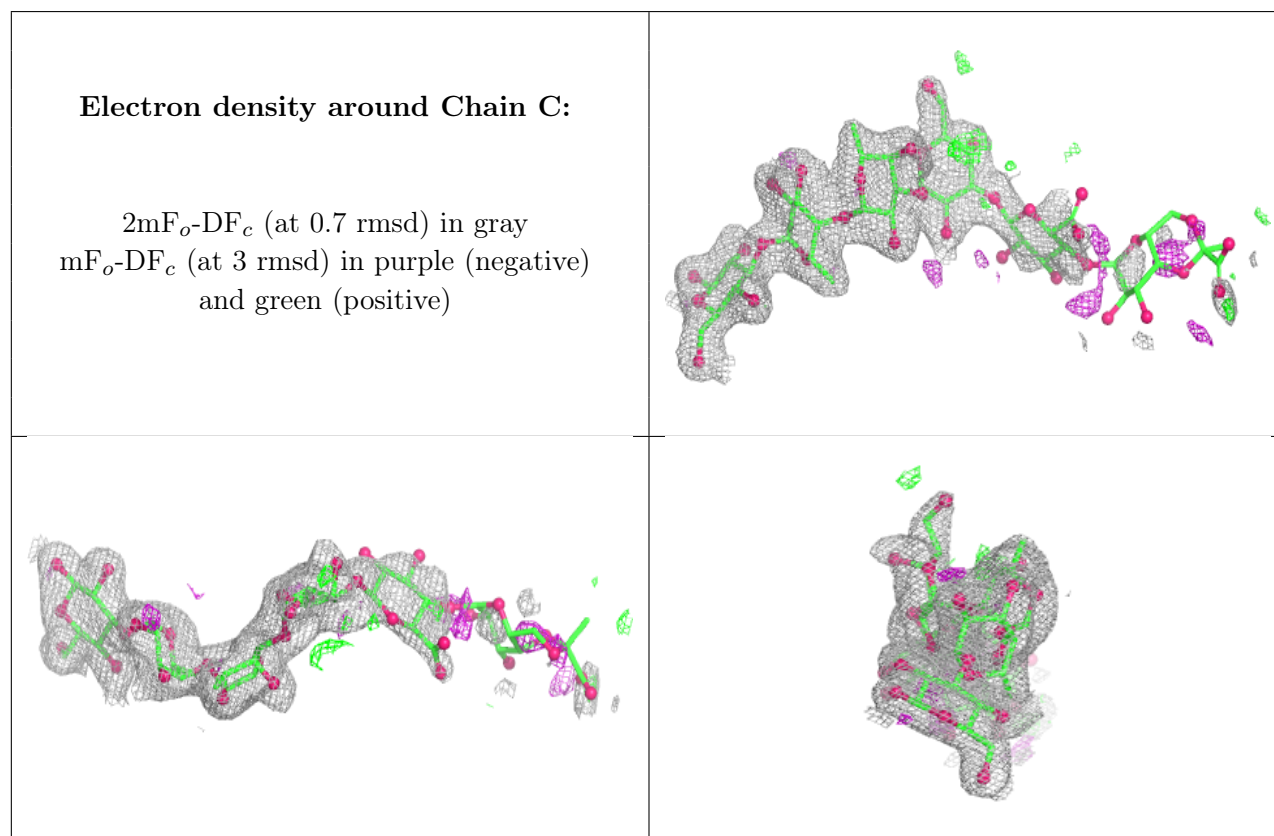
There are no non-standard protein/DNA/RNA residues in this entry.

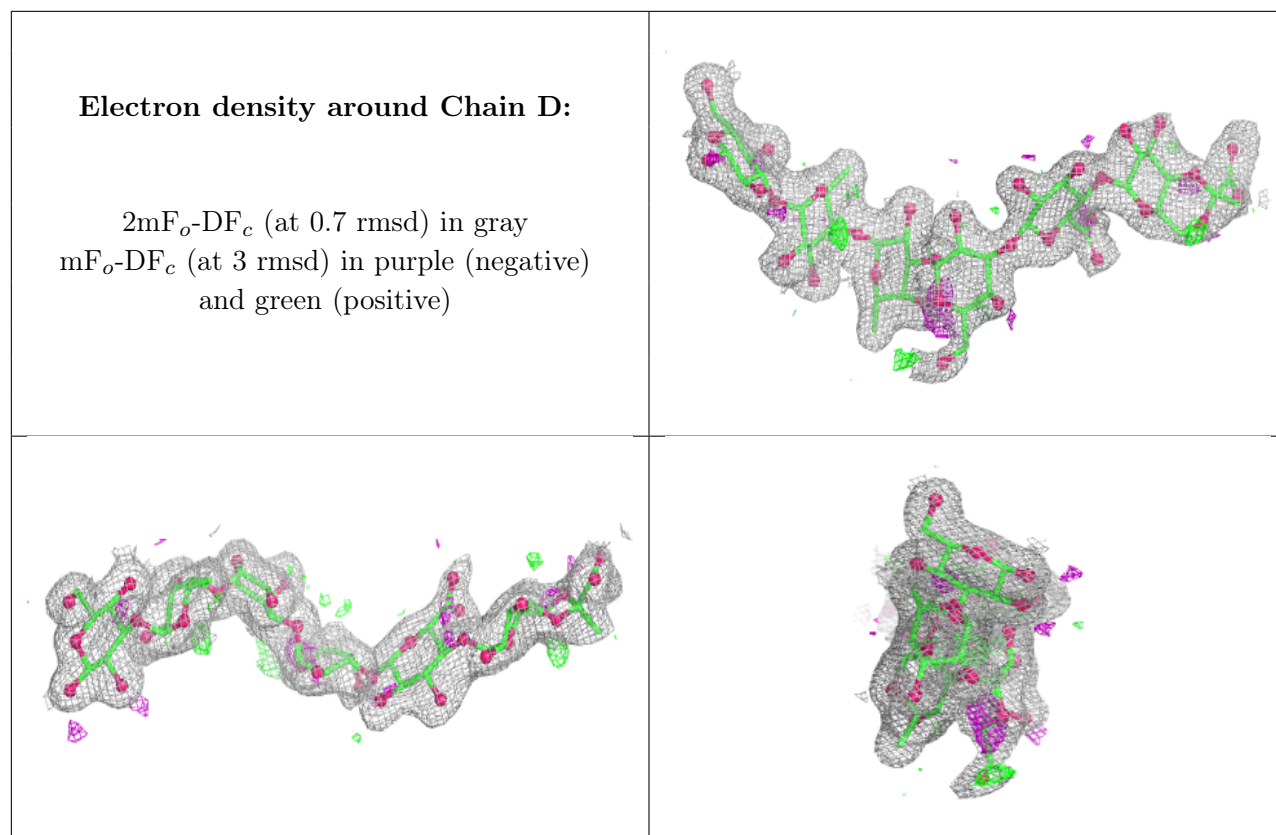
6.3 Carbohydrates [i](#)

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, 95th 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($\text{\AA}^2$)	Q<0.9
2	HLA	C	6	16/17	0.33	0.21	137,144,148,148	0
2	BDP	C	5	12/13	0.58	0.15	107,118,122,130	0
2	GLA	C	4	11/12	0.72	0.14	75,84,88,96	0
2	HLA	D	6	16/17	0.77	0.14	72,81,86,87	0
2	GLA	D	4	11/12	0.86	0.11	47,53,65,67	0
2	BDP	D	5	12/13	0.88	0.10	48,59,71,74	0
2	FUC	C	3	10/11	0.93	0.10	48,56,59,66	0
2	FUC	D	3	10/11	0.94	0.07	31,34,36,37	0
2	BGC	C	1	12/12	0.94	0.08	37,40,43,44	0
2	FUC	D	2	10/11	0.95	0.09	30,34,35,36	0
2	FUC	C	2	10/11	0.96	0.06	36,40,44,50	0
2	BGC	D	1	12/12	0.97	0.06	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.





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, 95th 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($\text{\AA}^2$)	Q<0.9
3	SO4	B	906	5/5	0.80	0.15	175,175,175,175	0
6	PG4	B	910	13/13	0.89	0.14	35,46,60,63	0
3	SO4	B	905	5/5	0.90	0.12	70,73,77,78	0
3	SO4	B	902	5/5	0.92	0.10	65,67,71,73	0
3	SO4	A	901	5/5	0.93	0.09	41,47,58,59	0
3	SO4	A	903	5/5	0.93	0.11	44,47,49,60	0
3	SO4	A	904	5/5	0.94	0.10	37,43,51,61	0
3	SO4	B	901	5/5	0.95	0.07	40,45,47,53	0
3	SO4	A	902	5/5	0.95	0.08	59,60,64,69	0
5	EDO	B	909	4/4	0.95	0.14	37,40,44,45	0
3	SO4	B	903	5/5	0.95	0.09	40,51,53,58	0
3	SO4	B	904	5/5	0.96	0.07	34,37,46,51	0
4	MG	B	908	1/1	0.98	0.08	32,32,32,32	0
4	MG	B	907	1/1	0.99	0.03	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	A	905	1/1	0.99	0.03	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.