Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 11:37 PM EST

PDB ID	:	8E07
Title	:	Crystal structure of HPSE P6 in complex with triose pentosan inhibitor
Authors	:	Whitefield, C.; Jackson, C.J.
Deposited on	:	2022-08-08
Resolution	:	1.80 Å(reported)

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	:	2.36
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)	:	2.36
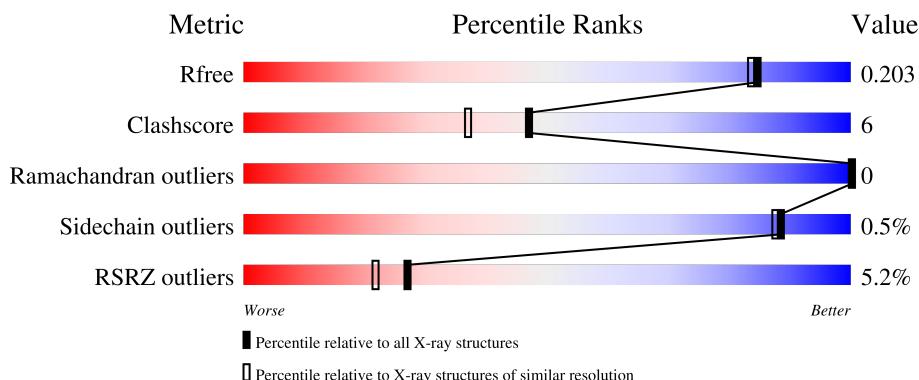
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
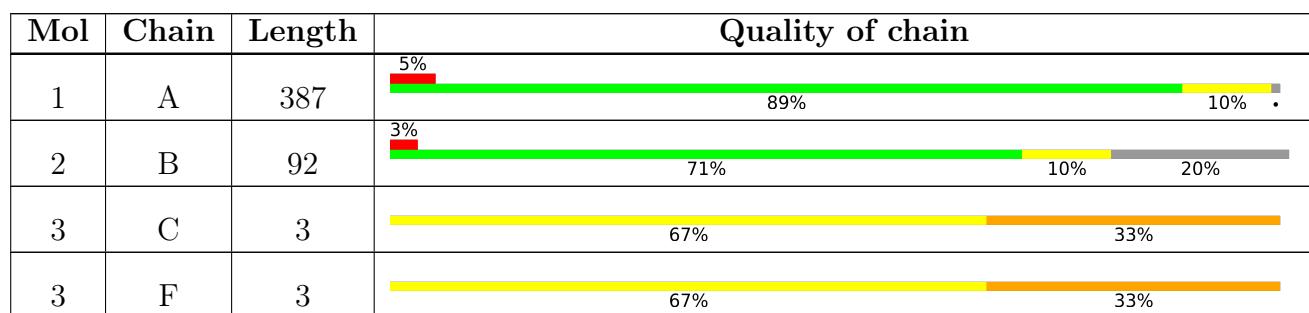
The reported resolution of this entry is 1.80 Å.

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	Percentile Ranks	Value
Rfree		0.203
Clashscore		6
Ramachandran outliers		0
Sidechain outliers		0.5%
RSRZ outliers		5.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

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	387	5% / 89% ... 10% ·
2	B	92	3% / 71% ... 10% ... 20%
3	C	3	67% ... 33%
3	F	3	67% ... 33%

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 4191 atoms, of which 3 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 Heparanase 50 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	385	3076	1981	530	553	12	0	4	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	157	MET	-	initiating methionine	UNP Q9Y251
A	178	LYS	ASN	engineered mutation	UNP Q9Y251
A	195	SER	ALA	engineered mutation	UNP Q9Y251
A	197	GLY	LEU	engineered mutation	UNP Q9Y251
A	212	ALA	SER	engineered mutation	UNP Q9Y251
A	219	ASP	SER	engineered mutation	UNP Q9Y251
A	230	ARG	LEU	engineered mutation	UNP Q9Y251
A	234	GLY	ASP	engineered mutation	UNP Q9Y251
A	244	LYS	GLU	engineered mutation	UNP Q9Y251
A	248	HIS	GLN	engineered mutation	UNP Q9Y251
A	273	GLY	ARG	engineered mutation	UNP Q9Y251
A	292	ALA	SER	engineered mutation	UNP Q9Y251
A	307	LEU	LYS	engineered mutation	UNP Q9Y251
A	318	THR	ILE	engineered mutation	UNP Q9Y251
A	322	GLN	SER	engineered mutation	UNP Q9Y251
A	327	LEU	PHE	engineered mutation	UNP Q9Y251
A	354	GLY	LEU	engineered mutation	UNP Q9Y251
A	426	GLN	SER	engineered mutation	UNP Q9Y251
A	427	ASP	LYS	engineered mutation	UNP Q9Y251
A	477	GLN	LYS	engineered mutation	UNP Q9Y251
A	483	HIS	LEU	engineered mutation	UNP Q9Y251
A	486	ASP	HIS	engineered mutation	UNP Q9Y251
A	498	GLN	LEU	engineered mutation	UNP Q9Y251
A	512	LYS	MET	engineered mutation	UNP Q9Y251
A	513	PRO	GLU	engineered mutation	UNP Q9Y251
A	530	ALA	SER	engineered mutation	UNP Q9Y251
A	540	PRO	ALA	engineered mutation	UNP Q9Y251

- Molecule 2 is a protein called Heparanase 8 kDa subunit.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	74	Total 602	C 394	N 99	O 109	0	2	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	18	MET	-	initiating methionine	UNP Q9Y251
B	19	GLY	-	expression tag	UNP Q9Y251
B	20	SER	-	expression tag	UNP Q9Y251
B	21	SER	-	expression tag	UNP Q9Y251
B	22	HIS	-	expression tag	UNP Q9Y251
B	23	HIS	-	expression tag	UNP Q9Y251
B	24	HIS	-	expression tag	UNP Q9Y251
B	25	HIS	-	expression tag	UNP Q9Y251
B	26	HIS	-	expression tag	UNP Q9Y251
B	27	HIS	-	expression tag	UNP Q9Y251
B	28	SER	-	expression tag	UNP Q9Y251
B	29	GLN	-	expression tag	UNP Q9Y251
B	30	ASP	-	expression tag	UNP Q9Y251
B	31	PRO	-	expression tag	UNP Q9Y251
B	32	ASN	-	expression tag	UNP Q9Y251
B	33	SER	-	expression tag	UNP Q9Y251
B	34	SER	-	expression tag	UNP Q9Y251
B	35	SER	-	expression tag	UNP Q9Y251

- Molecule 3 is an oligosaccharide called 2,3,4-tri-O-sulfo-beta-D-xylopyranose-(1-4)-2,3-di-O-sulfo-beta-D-xylopyranose-(1-4)-2,3-di-O-sulfo-beta-D-xylopyranose.
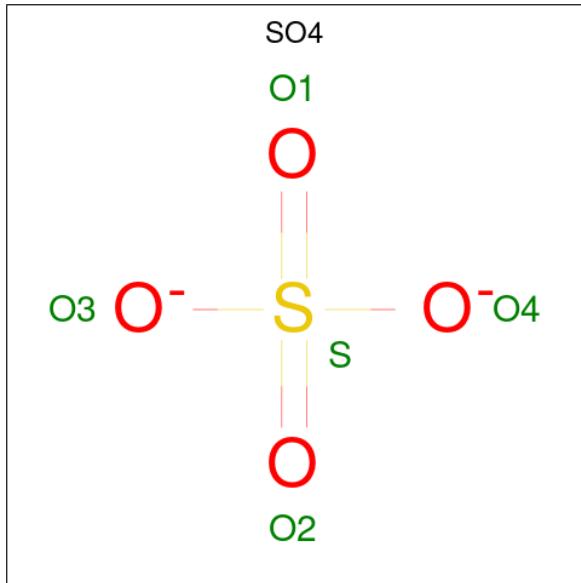
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total 56	C 15	O 34	S 7	0	0	0
3	F	3	Total 56	C 15	O 34	S 7	0	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

ACT

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	7	2	3	2	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4
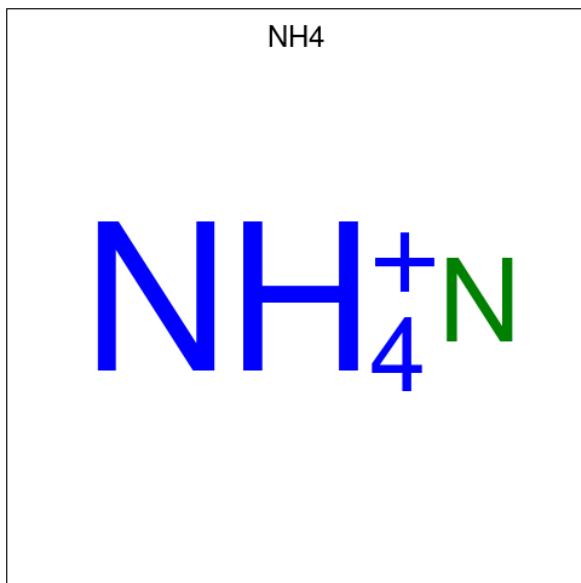
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	A	1	5	4	1	0	0
5	A	1	Total 5	O 4	S 1	0	0
5	A	1	Total 5	O 4	S 1	0	0

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W O R L D W I D E

PDB

PROTEIN DATA BANK

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

- Molecule 6 is AMMONIUM ION (three-letter code: NH4) (formula: H_4N).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total N 1 1		0	0
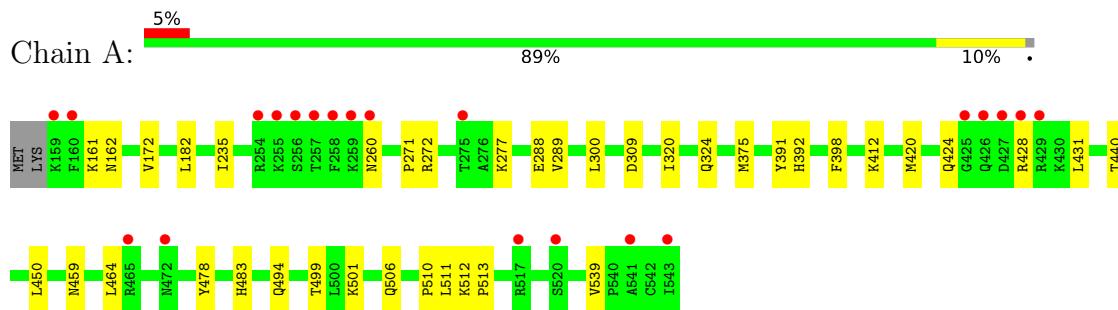
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	303	Total O 303 303		0	0
7	B	65	Total O 65 65		0	0
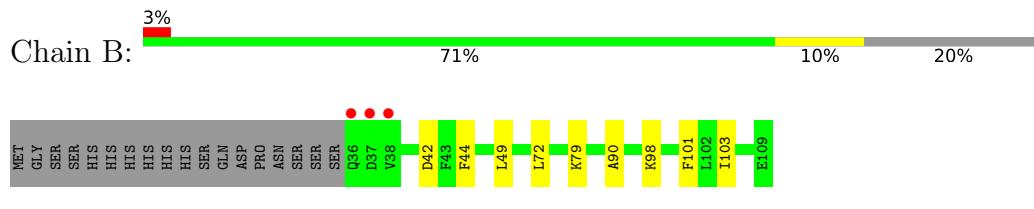
3 Residue-property plots ⓘ

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.
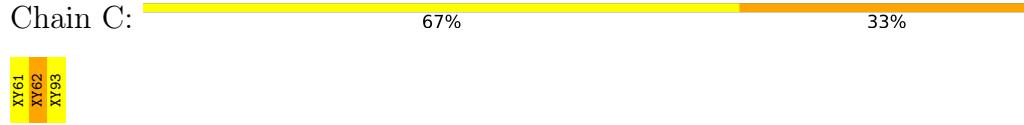
- Molecule 1: Heparanase 50 kDa subunit

Chain A:
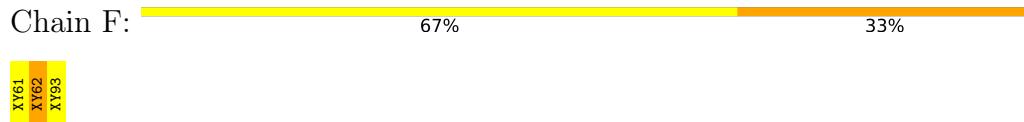
- Molecule 2: Heparanase 8 kDa subunit

Chain B:

- Molecule 3: 2,3,4-tri-O-sulfo-beta-D-xylopyranose-(1-4)-2,3-di-O-sulfo-beta-D-xylopyranose-(1-4)-2,3-di-O-sulfo-beta-D-xylopyranose

Chain C:

- Molecule 3: 2,3,4-tri-O-sulfo-beta-D-xylopyranose-(1-4)-2,3-di-O-sulfo-beta-D-xylopyranose-(1-4)-2,3-di-O-sulfo-beta-D-xylopyranose

Chain F:

4 Data and refinement statistics (i)

| Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	59.54Å 76.19Å 124.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.91 – 1.80 46.91 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.91-1.80) 99.4 (46.91-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.23 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.172 , 0.203 0.171 , 0.203	Depositor DCC
R_{free} test set	2712 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	25.3	Xtriage
Anisotropy	0.627	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.0	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4191	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: XY6, ACT, SO4, NH4, XY9

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	0.35	0/3155	0.57	0/4267
2	B	0.34	0/619	0.56	0/839
All	All	0.35	0/3774	0.57	0/5106

There are no bond length outliers.

There are no bond angle outliers.

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	3076	0	3100	40	0
2	B	602	0	620	18	0
3	C	56	0	0	1	0
3	F	56	0	0	1	0
4	A	4	3	3	0	0
5	A	25	0	0	0	0
6	A	1	0	0	0	0
7	A	303	0	0	14	0
7	B	65	0	0	1	0
All	All	4188	3	3723	47	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 6.

All (47) 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:483:HIS:HB2	1:A:494:GLN:HG3	1.71	0.72
7:A:856:HOH:O	2:B:79:LYS:HE3	1.90	0.70
1:A:420[B]:MET:HB3	2:B:44:PHE:HB3	1.75	0.69
2:B:79:LYS:HG3	7:B:247:HOH:O	1.93	0.67
1:A:320:ILE:HG12	1:A:375[B]:MET:HE1	1.76	0.65
1:A:511:LEU:O	7:A:701:HOH:O	2.14	0.65
1:A:459:ASN:HB2	7:A:866:HOH:O	1.96	0.64
1:A:235:ILE:HD11	7:A:988:HOH:O	1.96	0.64
1:A:161:LYS:HG3	7:A:927:HOH:O	1.98	0.63
1:A:277:LYS:NZ	3:F:2:XY6:O5	2.33	0.62
1:A:420[B]:MET:HE2	2:B:49:LEU:HD11	1.82	0.61
1:A:512:LYS:NZ	7:A:703:HOH:O	2.34	0.59
1:A:420[B]:MET:CE	2:B:49:LEU:HD11	2.32	0.59
1:A:324:GLN:HG2	7:A:980:HOH:O	2.04	0.58
1:A:483:HIS:HB2	1:A:494:GLN:CG	2.35	0.55
1:A:300:LEU:HD11	1:A:309:ASP:HB3	1.90	0.54
1:A:424:GLN:HG2	2:B:42:ASP:OD2	2.10	0.52
1:A:440:THR:HA	7:A:718:HOH:O	2.09	0.51
1:A:510:PRO:HB2	1:A:512:LYS:HE2	1.93	0.50
1:A:172:VAL:HG11	2:B:72[A]:LEU:HG	1.93	0.50
1:A:431:LEU:HD21	1:A:464:LEU:HD21	1.94	0.49
7:A:971:HOH:O	2:B:103:ILE:HD11	2.11	0.49
2:B:98:LYS:HE3	3:C:2:XY6:O25	2.11	0.49
1:A:288[B]:GLU:HG2	1:A:289:VAL:HG13	1.94	0.49
1:A:412:LYS:HE2	1:A:511:LEU:HD12	1.96	0.48
1:A:162:ASN:HA	2:B:101:PHE:O	2.14	0.48
1:A:478:TYR:CZ	1:A:513:PRO:HB3	2.49	0.48
1:A:172:VAL:HG21	2:B:72[B]:LEU:HD22	1.97	0.46
1:A:431:LEU:HD21	1:A:464:LEU:CD2	2.45	0.45
1:A:412:LYS:CD	1:A:511:LEU:HD12	2.47	0.45
1:A:428:ARG:HB2	7:A:906:HOH:O	2.16	0.45
1:A:412:LYS:HD3	1:A:511:LEU:HD12	1.99	0.44
1:A:260:ASN:HB2	7:A:925:HOH:O	2.17	0.44
7:A:883:HOH:O	2:B:79:LYS:HD3	2.18	0.44
1:A:499:THR:HG21	1:A:501:LYS:HE2	1.99	0.43
7:A:875:HOH:O	2:B:79:LYS:HD2	2.18	0.43
1:A:420[A]:MET:HB2	2:B:49:LEU:HD11	2.01	0.43
1:A:450:LEU:HD21	1:A:539:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:PHE:HB2	2:B:79:LYS:HE2	2.01	0.42
1:A:182:LEU:HD22	2:B:90:ALA:HB3	2.01	0.41
1:A:271:PRO:O	1:A:272:ARG:HB2	2.21	0.41
1:A:172:VAL:HG21	2:B:72[B]:LEU:CD2	2.51	0.41
1:A:320:ILE:HG23	1:A:375[B]:MET:HE2	2.02	0.41
1:A:506:GLN:NE2	7:A:707:HOH:O	2.46	0.41
1:A:431:LEU:HD12	1:A:431:LEU:HA	1.90	0.40
1:A:320:ILE:HG12	1:A:375[B]:MET:CE	2.48	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	387/387 (100%)	379 (98%)	8 (2%)	0	100	100
2	B	74/92 (80%)	73 (99%)	1 (1%)	0	100	100
All	All	461/479 (96%)	452 (98%)	9 (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	334/332 (101%)	332 (99%)	2 (1%)	86	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	68/83 (82%)	68 (100%)	0	100	100
All	All	402/415 (97%)	400 (100%)	2 (0%)	88	87

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

Mol	Chain	Res	Type
1	A	391	TYR
1	A	392	HIS

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

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

6 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	XY6	C	1	3	18,18,18	2.66	7 (38%)	20,28,28	1.62	5 (25%)
3	XY6	C	2	3	17,17,18	2.17	5 (29%)	15,26,28	3.12	3 (20%)
3	XY9	C	3	3	21,21,22	2.29	8 (38%)	20,33,35	3.58	5 (25%)
3	XY6	F	1	3	18,18,18	2.97	9 (50%)	20,28,28	2.08	5 (25%)
3	XY6	F	2	3	17,17,18	2.33	5 (29%)	15,26,28	3.48	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	XY9	F	3	3	21,21,22	2.43	5 (23%)	20,33,35	3.27	8 (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
3	XY6	C	1	3	-	0/10/27/27	0/1/1/1
3	XY6	C	2	3	-	3/10/24/27	0/1/1/1
3	XY9	C	3	3	-	10/15/29/32	0/1/1/1
3	XY6	F	1	3	-	4/10/27/27	0/1/1/1
3	XY6	F	2	3	-	2/10/24/27	0/1/1/1
3	XY9	F	3	3	-	3/15/29/32	0/1/1/1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	XY6	C1-C2	6.49	1.58	1.52
3	C	1	XY6	C1-C2	6.08	1.58	1.52
3	F	3	XY9	O2-C2	-5.91	1.38	1.47
3	F	3	XY9	O4-C4	-5.47	1.38	1.47
3	F	2	XY6	C1-C2	5.46	1.60	1.51
3	C	2	XY6	O2-C2	-5.44	1.38	1.47
3	F	1	XY6	C3-C2	5.32	1.63	1.52
3	C	3	XY9	O4-C4	-5.24	1.39	1.47
3	F	2	XY6	O2-C2	-5.21	1.39	1.47
3	C	1	XY6	C3-C2	4.72	1.62	1.52
3	C	1	XY6	O2-C2	-4.46	1.37	1.46
3	F	1	XY6	O3-S28	4.28	1.69	1.57
3	F	3	XY9	C1-C2	4.07	1.58	1.51
3	F	1	XY6	O2-S23	4.06	1.69	1.57
3	C	2	XY6	C1-C2	4.01	1.58	1.51
3	C	3	XY9	O2-C2	-4.01	1.41	1.47
3	F	1	XY6	O3-C3	-3.65	1.38	1.46
3	F	3	XY9	O3-C3	-3.62	1.38	1.46
3	C	1	XY6	C4-C3	3.60	1.60	1.52
3	C	3	XY9	O3-S38	3.58	1.67	1.57
3	F	1	XY6	C4-C3	3.45	1.59	1.52
3	C	1	XY6	O3-S28	3.42	1.67	1.57
3	F	2	XY6	O3-C3	-3.39	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	XY6	O5-C5	-3.33	1.38	1.43
3	C	3	XY9	O3-C3	-3.32	1.39	1.46
3	C	1	XY6	O3-C3	-3.28	1.39	1.46
3	C	2	XY6	O3-S28	3.18	1.66	1.57
3	F	3	XY9	O3-S38	3.13	1.66	1.57
3	C	3	XY9	C1-C2	3.09	1.56	1.51
3	F	1	XY6	O2-C2	-2.94	1.40	1.46
3	F	2	XY6	O2-S23	2.89	1.65	1.57
3	C	2	XY6	O2-S23	2.88	1.65	1.57
3	C	3	XY9	O2-S33	2.86	1.65	1.57
3	C	2	XY6	O3-C3	-2.63	1.41	1.46
3	F	2	XY6	O3-S28	2.41	1.64	1.57
3	C	1	XY6	O2-S23	2.38	1.64	1.57
3	F	1	XY6	O5-C1	-2.17	1.40	1.43
3	C	3	XY9	O5-C1	-2.16	1.38	1.42
3	C	3	XY9	O4-S43	2.07	1.63	1.57

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	3	XY9	C2-O2-S33	10.85	132.05	117.91
3	F	2	XY6	C2-O2-S23	10.19	131.20	117.91
3	C	2	XY6	C2-O2-S23	9.34	130.09	117.91
3	F	3	XY9	C2-O2-S33	8.92	129.54	117.91
3	C	3	XY9	C4-O4-S43	6.98	127.02	117.91
3	C	3	XY9	C3-O3-S38	6.34	131.12	118.88
3	F	2	XY6	C3-O3-S28	6.22	130.89	118.88
3	F	3	XY9	C4-O4-S43	6.00	125.74	117.91
3	C	2	XY6	C3-O3-S28	5.76	130.01	118.88
3	F	3	XY9	C3-O3-S38	5.41	129.34	118.88
3	F	1	XY6	C2-O2-S23	5.32	129.15	118.88
3	C	3	XY9	O4-C4-C3	4.93	112.11	106.65
3	F	1	XY6	C3-O3-S28	4.74	128.03	118.88
3	F	3	XY9	C1-C2-C3	4.69	116.41	109.40
3	F	3	XY9	O4-C4-C3	4.12	111.22	106.65
3	C	2	XY6	C5-O5-C1	4.11	117.84	111.52
3	F	2	XY6	C1-C2-C3	3.46	114.57	109.40
3	C	1	XY6	C2-O2-S23	3.07	124.81	118.88
3	F	2	XY6	O5-C1-C2	3.04	115.75	110.18
3	F	1	XY6	O1-C1-O5	-2.93	102.07	109.72
3	C	1	XY6	C3-O3-S28	2.83	124.35	118.88
3	F	3	XY9	O40-S38-O41	2.70	117.87	108.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	XY6	O4-C4-C5	-2.68	103.66	109.15
3	F	2	XY6	C5-O5-C1	2.66	115.62	111.52
3	F	1	XY6	O4-C4-C5	-2.66	103.71	109.15
3	C	3	XY9	O40-S38-O41	2.62	117.61	108.49
3	C	1	XY6	O5-C1-C2	2.58	113.25	109.51
3	F	1	XY6	O5-C1-C2	2.57	113.24	109.51
3	C	1	XY6	O31-S28-O30	2.44	116.98	108.49
3	F	3	XY9	C4-C3-C2	2.41	115.96	110.37
3	F	2	XY6	C5-C4-C3	-2.19	106.53	109.17
3	F	3	XY9	C1-O5-C5	2.09	114.73	111.52

There are no chirality outliers.

All (22) torsion outliers are listed below:
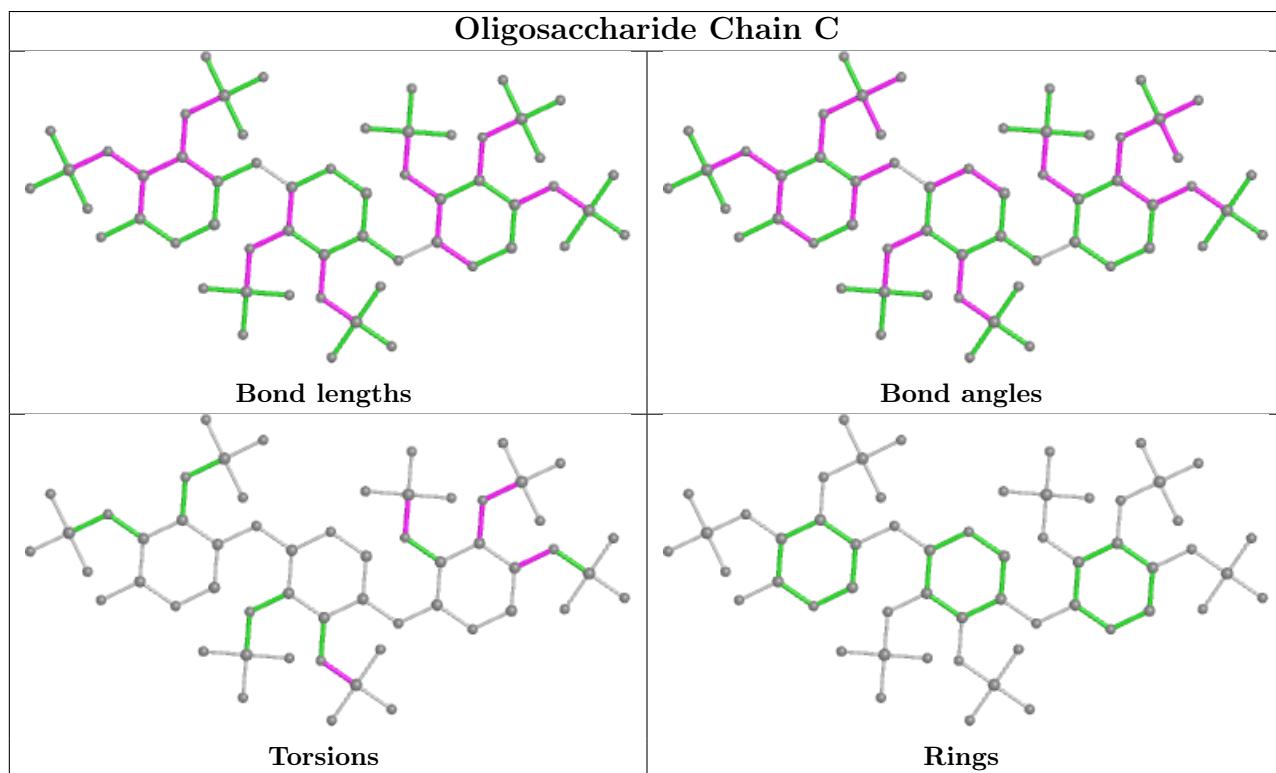
Mol	Chain	Res	Type	Atoms
3	C	2	XY6	C3-O3-S28-O30
3	C	2	XY6	C3-O3-S28-O31
3	C	3	XY9	C2-C3-O3-S38
3	C	3	XY9	C4-C3-O3-S38
3	C	3	XY9	C5-C4-O4-S43
3	C	3	XY9	C3-C4-O4-S43
3	C	3	XY9	C2-O2-S33-O36
3	C	3	XY9	C3-O3-S38-O39
3	C	3	XY9	C3-O3-S38-O40
3	C	3	XY9	C3-O3-S38-O41
3	F	1	XY6	C1-C2-O2-S23
3	F	1	XY6	C3-C2-O2-S23
3	F	1	XY6	C2-C3-O3-S28
3	F	1	XY6	C4-C3-O3-S28
3	F	2	XY6	C1-C2-O2-S23
3	F	3	XY9	C3-O3-S38-O40
3	C	2	XY6	C3-O3-S28-O29
3	C	3	XY9	C2-O2-S33-O35
3	F	3	XY9	C3-O3-S38-O41
3	F	3	XY9	C3-O3-S38-O39
3	C	3	XY9	C2-O2-S33-O34
3	F	2	XY6	C2-O2-S23-O24
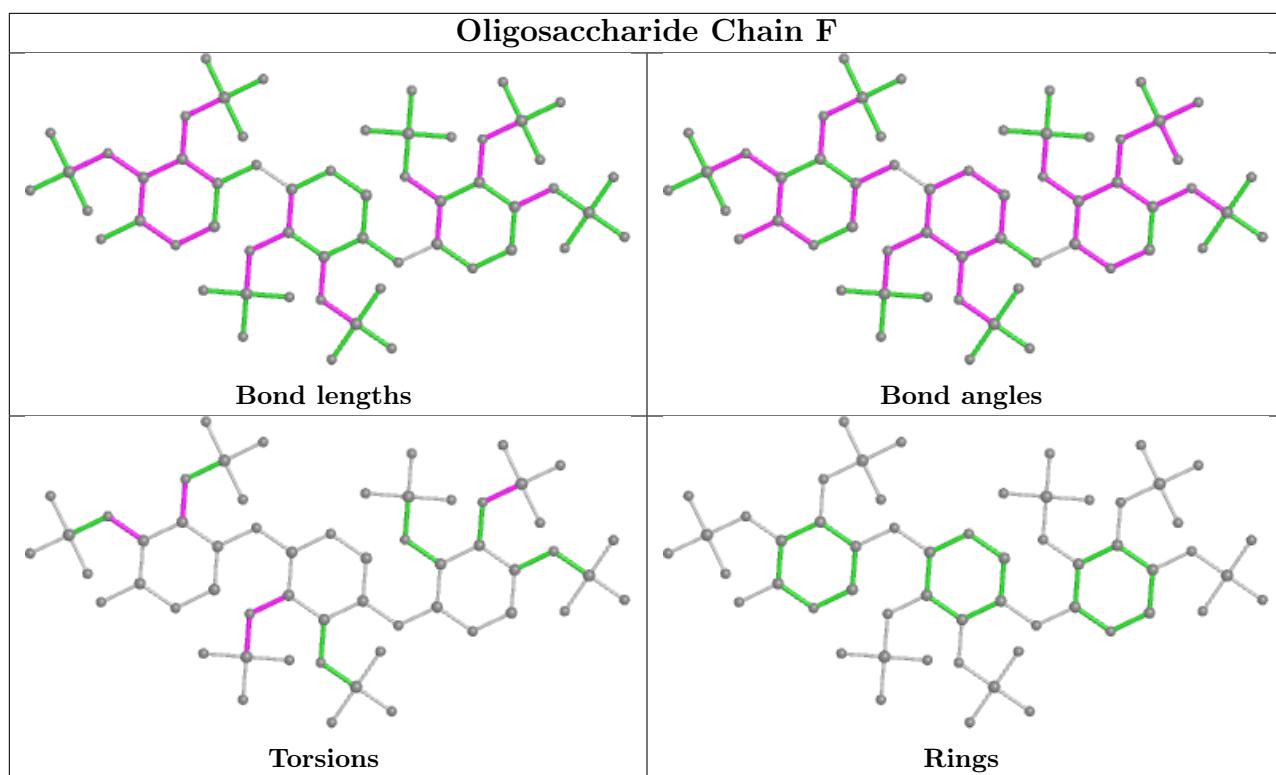
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	XY6	1	0
3	C	2	XY6	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 C

Bond lengths

Bond angles

Torsions

Rings

	Oligosaccharide Chain F	
Bond lengths		Bond angles
Torsions		Rings

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 1 is modelled with single atom - leaving 6 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	#$|Z| > 2$
5	SO4	A	606	-	4,4,4	0.15	0	6,6,6	0.05	0
5	SO4	A	602	-	4,4,4	0.11	0	6,6,6	0.14	0
5	SO4	A	603	-	4,4,4	0.14	0	6,6,6	0.07	0
4	ACT	A	601	-	3,3,3	1.07	0	3,3,3	1.57	0
5	SO4	A	605	-	4,4,4	0.15	0	6,6,6	0.08	0
5	SO4	A	607	-	4,4,4	0.14	0	6,6,6	0.07	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å²)	Q<0.9
1	A	385/387 (99%)	0.09	21 (5%)	25	20	17, 27, 52, 109	0
2	B	74/92 (80%)	-0.02	3 (4%)	37	31	17, 24, 49, 74	0
All	All	459/479 (95%)	0.08	24 (5%)	27	22	17, 27, 52, 109	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	LYS	5.6
1	A	543	ILE	5.5
1	A	257	THR	5.4
1	A	160	PHE	5.1
1	A	259	LYS	4.6
1	A	541	ALA	4.0
1	A	425	GLY	3.6
1	A	426	GLN	3.5
1	A	275	THR	3.3
1	A	260	ASN	3.3
1	A	254	ARG	3.3
2	B	36	GLN	3.2
1	A	472	ASN	3.1
1	A	258	PHE	2.9
1	A	429	ARG	2.8
1	A	255	LYS	2.6
1	A	427	ASP	2.5
1	A	520	SER	2.4
1	A	428	ARG	2.4
2	B	37	ASP	2.2
1	A	517	ARG	2.2
1	A	465	ARG	2.1
1	A	256	SER	2.1
2	B	38	VAL	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains (i)
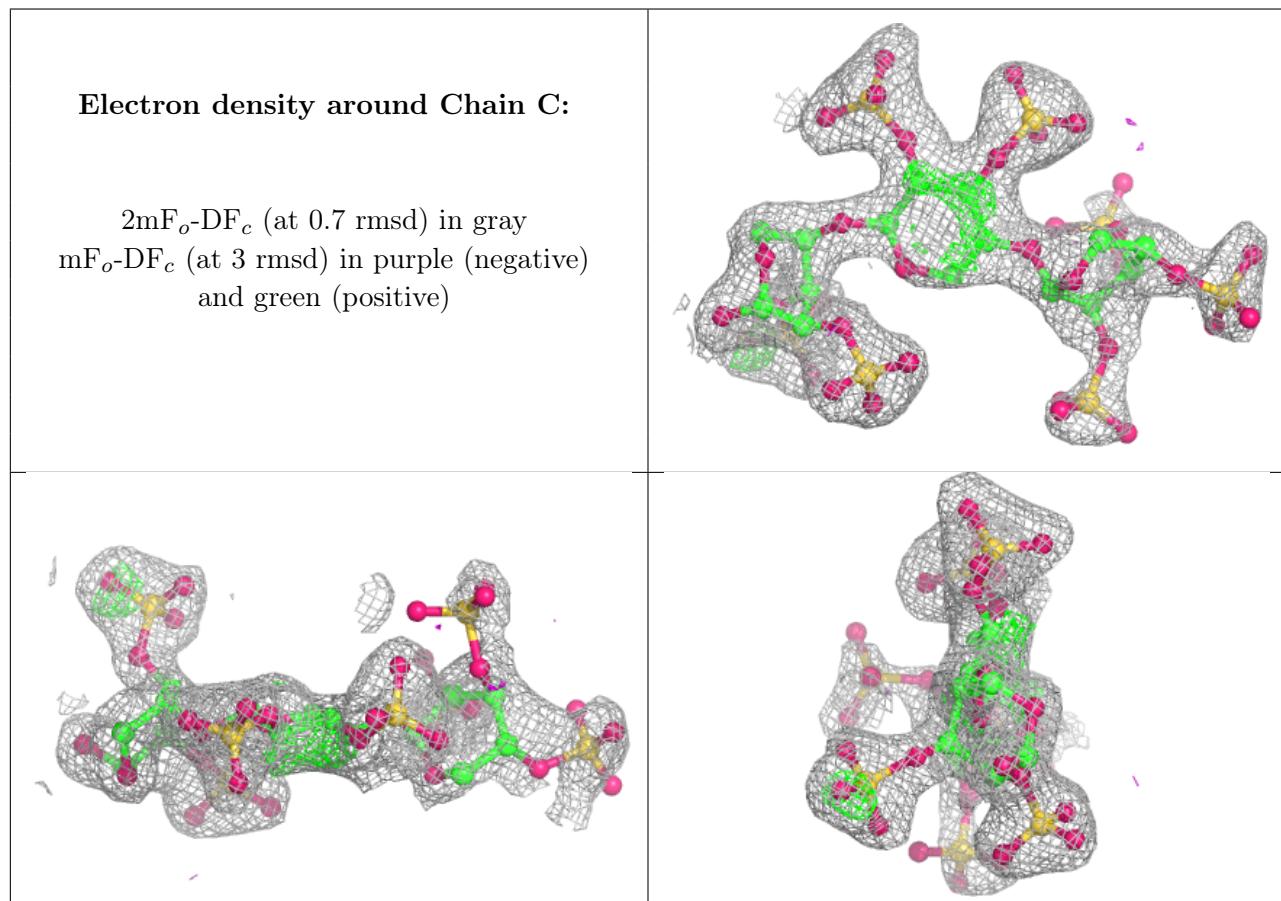
There are no non-standard protein/DNA/RNA residues in this entry.
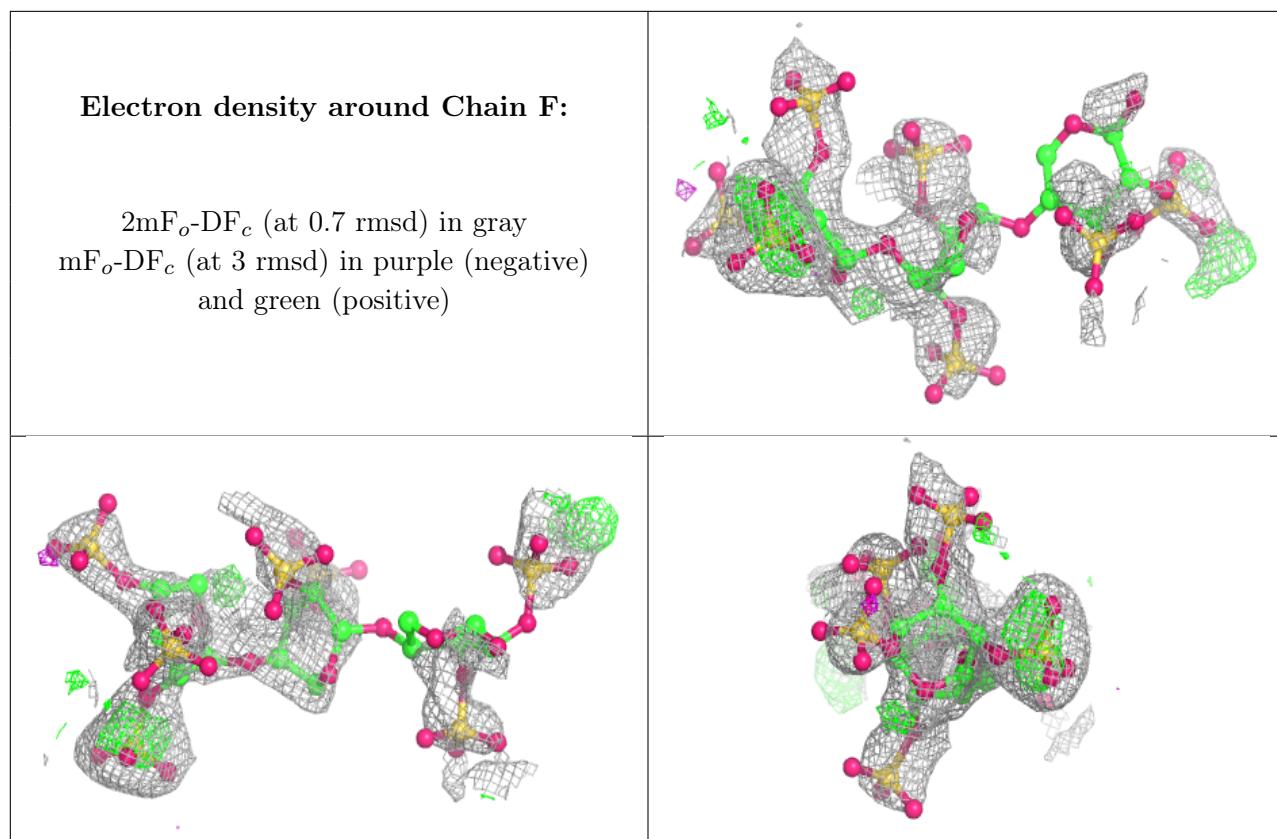
6.3 Carbohydrates (i)

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($\mathring{A}^2$)	Q<0.9
3	XY6	F	1	18/18	0.45	0.39	64,91,102,106	18
3	XY9	C	3	21/22	0.56	0.25	65,74,89,93	21
3	XY6	F	2	17/18	0.74	0.22	77,88,95,95	17
3	XY9	F	3	21/22	0.88	0.23	32,66,80,89	21
3	XY6	C	2	17/18	0.92	0.17	38,47,61,63	17
3	XY6	C	1	18/18	0.95	0.13	22,30,36,38	18

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 F:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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, 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(Å^2)	Q<0.9
5	SO4	A	602	5/5	0.81	0.19	44,61,70,88	0
5	SO4	A	606	5/5	0.87	0.43	67,76,93,96	0
5	SO4	A	607	5/5	0.91	0.37	69,71,81,86	0
5	SO4	A	603	5/5	0.92	0.30	53,57,75,75	0
5	SO4	A	605	5/5	0.93	0.18	73,73,85,95	0
6	NH4	A	604	1/1	0.93	0.24	32,32,32,32	0
4	ACT	A	601	4/4	0.94	0.14	23,28,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.