Full wwPDB X-ray Structure Validation Report (i)

Oct 14, 2023 – 08:18 PM EDT

PDB ID	:	8E08
Title	:	Crystal structure of HPSE P6 in complex with tetraose pentosan inhibitor
Authors	:	Whitefield, C.; Jackson, C.J.
Deposited on	:	2022-08-08
Resolution	:	1.93 Å(reported)

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

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

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

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

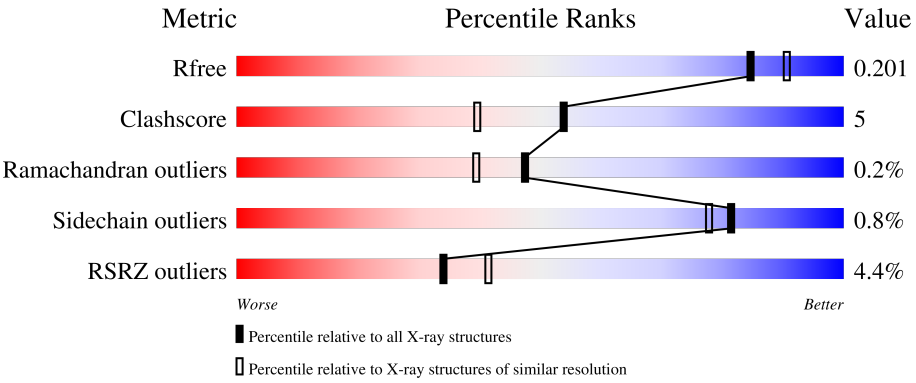
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.93 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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% 88% 11%
2	B	92	2% 71% 10% 20%
3	C	4	50% 50%
3	D	4	25% 75%
3	H	4	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	XY6	H	1	-	-	-	X
3	XY6	H	2	-	-	-	X
3	XY6	H	3	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4264 atoms, of which 81 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	3050	1965	525	549	11	0	1	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	C	N	O	0	0	0
			586	383	95	108			

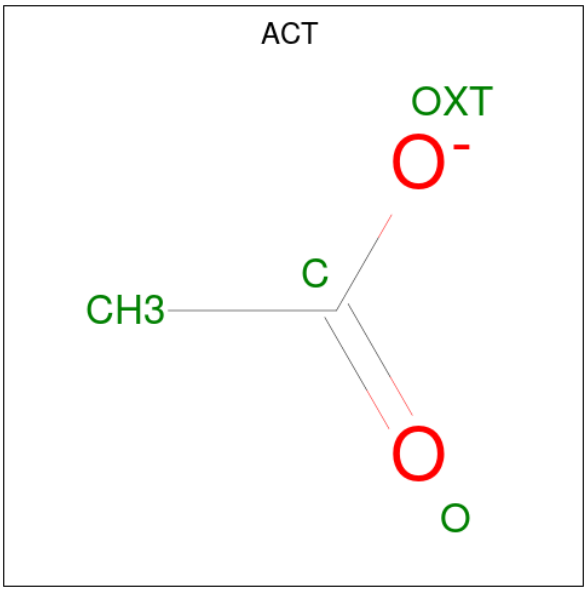
There are 18 discrepancies between the modelled and reference sequences:

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-(1-4)-2,3-di-O-sulfo-beta-D-xylopyranose.

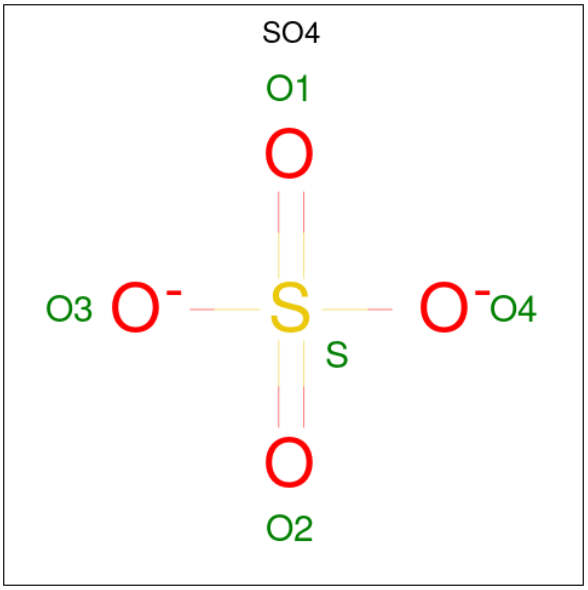
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	4	Total	C	H	O	S	0	0	0
			98	20	25	44	9			
3	D	4	Total	C	H	O	S	0	0	0
			98	20	25	44	9			
3	H	4	Total	C	H	O	S	0	0	0
			98	20	25	44	9			

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



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

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



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

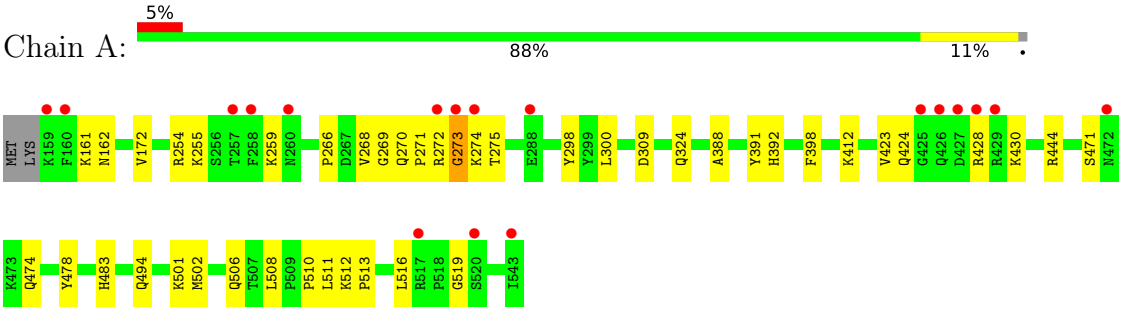
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	253	Total O 253 253	0	0
6	B	57	Total O 57 57	0	0

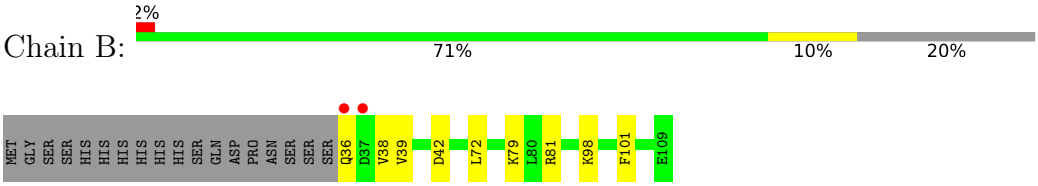
3 Residue-property plots

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



• Molecule 2: Heparanase 8 kDa subunit



• 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-(1-4)-2,3-di-O-sulfo-beta-D-xylopyranose

• 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-(1-4)-2,3-di-O-sulfo-beta-D-xylopyranose

• 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-(1-4)-2,3-di-O-sulfo-beta-D-xylopyranose


XY61
XY62
XY63
XY64

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	59.27Å 75.63Å 125.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.28 – 1.93 48.28 – 1.93	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.28-1.93) 100.0 (48.28-1.93)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 1.92Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.173 , 0.202 0.171 , 0.201	Depositor DCC
R_{free} test set	2114 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	30.2	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4264	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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: SO4, XY6, ACT, 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	0.40	0/3125	0.60	0/4228
2	B	0.40	0/600	0.58	0/814
All	All	0.40	0/3725	0.60	0/5042

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	3050	0	3067	34	1
2	B	586	0	597	12	0
3	C	73	25	0	1	1
3	D	73	25	0	3	0
3	H	73	25	0	0	0
4	A	8	6	6	1	0
5	A	10	0	0	0	0
6	A	253	0	0	6	0
6	B	57	0	0	2	0
All	All	4183	81	3670	40	1

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

hydrogen atoms). The all-atom clashscore for this structure is 5.

All (40) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:GLN:HG3	2:B:38:VAL:H	1.50	0.75
1:A:483:HIS:HB2	1:A:494:GLN:HG3	1.72	0.72
1:A:423:VAL:HG13	2:B:39:VAL:CG1	2.22	0.70
1:A:423:VAL:HG13	2:B:39:VAL:HG13	1.75	0.69
1:A:324:GLN:HG2	6:A:925:HOH:O	1.95	0.67
1:A:266:PRO:HG2	1:A:268:VAL:HG13	1.86	0.57
1:A:274:LYS:HE3	3:C:2:XY6:O24	2.06	0.56
2:B:81:ARG:NH2	6:B:201:HOH:O	2.38	0.55
1:A:254:ARG:HA	1:A:254:ARG:NE	2.22	0.55
1:A:162:ASN:HA	2:B:101:PHE:O	2.08	0.53
1:A:172:VAL:HG21	2:B:72:LEU:HG	1.90	0.53
1:A:501:LYS:NZ	6:A:704:HOH:O	2.42	0.53
1:A:398:PHE:O	2:B:79:LYS:HE2	2.09	0.51
1:A:412:LYS:HD3	1:A:511:LEU:HD12	1.94	0.49
2:B:98:LYS:HE3	3:D:2:XY6:O30	2.13	0.48
2:B:72:LEU:C	2:B:72:LEU:HD23	2.33	0.48
1:A:424:GLN:HG2	2:B:42:ASP:OD2	2.14	0.48
1:A:161:LYS:HG3	6:A:702:HOH:O	2.13	0.47
1:A:471:SER:O	1:A:519:GLY:HA2	2.15	0.46
1:A:506:GLN:NE2	6:A:706:HOH:O	2.43	0.46
2:B:81:ARG:HB2	6:B:233:HOH:O	2.15	0.45
1:A:300:LEU:HD11	1:A:309:ASP:HB3	1.98	0.45
1:A:412:LYS:CD	1:A:511:LEU:HD12	2.47	0.45
3:D:3:XY6:O2	3:D:3:XY6:O4	2.35	0.44
1:A:483:HIS:HD2	6:A:899:HOH:O	1.99	0.44
1:A:298:TYR:OH	4:A:601:ACT:H2	2.18	0.44
1:A:388:ALA:HB3	3:D:1:XY6:O31	2.18	0.44
1:A:272:ARG:O	1:A:273:GLY:C	2.57	0.44
1:A:269:GLY:O	1:A:275:THR:HG21	2.18	0.43
1:A:259:LYS:HD3	1:A:259:LYS:HA	1.59	0.43
1:A:474:GLN:NE2	1:A:516:LEU:O	2.47	0.43
1:A:254:ARG:HA	1:A:254:ARG:HE	1.83	0.41
1:A:270:GLN:HB2	1:A:271:PRO:HD2	2.02	0.41
1:A:511:LEU:O	6:A:701:HOH:O	2.22	0.41
1:A:502[B]:MET:SD	1:A:508:LEU:HD23	2.60	0.41
1:A:478:TYR:CZ	1:A:513:PRO:HB3	2.56	0.41
1:A:428:ARG:HD2	1:A:430:LYS:HD2	2.02	0.41
1:A:502[A]:MET:SD	2:B:79:LYS:HE3	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:PRO:HB2	1:A:512:LYS:HD3	2.02	0.40
1:A:271:PRO:O	1:A:272:ARG:HG3	2.21	0.40

All (1) 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)
1:A:444:ARG:NH2	3:C:1:XY6:O31[1_655]	1.30	0.90

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	384/387 (99%)	377 (98%)	6 (2%)	1 (0%)	41 32
2	B	72/92 (78%)	71 (99%)	1 (1%)	0	100 100
All	All	456/479 (95%)	448 (98%)	7 (2%)	1 (0%)	47 39

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	273	GLY

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	330/332 (99%)	327 (99%)	3 (1%)	78 75
2	B	66/83 (80%)	66 (100%)	0	100 100
All	All	396/415 (95%)	393 (99%)	3 (1%)	81 78

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	LYS
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 (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	$\#\|Z\| > 2$
3	XY6	C	1	3	18,18,18	1.72	6 (33%)	20,28,28	1.54	4 (20%)
3	XY6	C	2	3	17,17,18	1.90	4 (23%)	15,26,28	1.58	4 (26%)
3	XY6	C	3	3	17,17,18	1.99	5 (29%)	15,26,28	1.47	2 (13%)
3	XY9	C	4	3	21,21,22	2.10	7 (33%)	20,33,35	1.80	5 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	XY6	D	1	3	18,18,18	1.70	5 (27%)	20,28,28	1.48	7 (35%)
3	XY6	D	2	3	17,17,18	1.83	4 (23%)	15,26,28	2.48	6 (40%)
3	XY6	D	3	3	17,17,18	2.05	5 (29%)	15,26,28	2.52	6 (40%)
3	XY9	D	4	3	21,21,22	2.02	7 (33%)	20,33,35	1.88	5 (25%)
3	XY6	H	1	3	18,18,18	1.72	5 (27%)	20,28,28	1.39	3 (15%)
3	XY6	H	2	3	17,17,18	1.92	5 (29%)	15,26,28	2.42	6 (40%)
3	XY6	H	3	3	17,17,18	1.87	4 (23%)	15,26,28	1.58	3 (20%)
3	XY9	H	4	3	21,21,22	2.23	6 (28%)	20,33,35	2.48	7 (35%)

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	-	8/10/27/27	0/1/1/1
3	XY6	C	2	3	-	0/10/24/27	0/1/1/1
3	XY6	C	3	3	-	0/10/24/27	0/1/1/1
3	XY9	C	4	3	-	0/15/29/32	0/1/1/1
3	XY6	D	1	3	-	0/10/27/27	0/1/1/1
3	XY6	D	2	3	-	3/10/24/27	0/1/1/1
3	XY6	D	3	3	-	1/10/24/27	0/1/1/1
3	XY9	D	4	3	-	5/15/29/32	0/1/1/1
3	XY6	H	1	3	-	5/10/27/27	0/1/1/1
3	XY6	H	2	3	-	4/10/24/27	0/1/1/1
3	XY6	H	3	3	-	0/10/24/27	0/1/1/1
3	XY9	H	4	3	-	0/15/29/32	0/1/1/1

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	4	XY9	O4-C4	-5.25	1.39	1.47
3	C	2	XY6	O2-C2	-4.61	1.40	1.47
3	C	3	XY6	O2-C2	-4.48	1.40	1.47
3	D	3	XY6	O2-C2	-4.40	1.40	1.47
3	D	4	XY9	O4-C4	-4.39	1.40	1.47
3	C	4	XY9	O2-C2	-4.36	1.40	1.47
3	H	4	XY9	O2-C2	-4.33	1.40	1.47
3	C	4	XY9	O4-C4	-4.21	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2	XY6	O2-C2	-4.19	1.40	1.47
3	H	3	XY6	O2-C2	-4.19	1.40	1.47
3	H	2	XY6	O3-C3	-3.79	1.38	1.46
3	H	2	XY6	O2-S23	3.57	1.67	1.57
3	D	3	XY6	C1-C2	3.44	1.57	1.51
3	C	1	XY6	O3-S28	3.41	1.67	1.57
3	H	4	XY9	O3-C3	-3.40	1.39	1.46
3	D	1	XY6	O3-S28	3.29	1.67	1.57
3	H	2	XY6	O2-C2	-3.27	1.42	1.47
3	D	4	XY9	O2-C2	-3.21	1.42	1.47
3	H	4	XY9	O2-S33	3.19	1.66	1.57
3	D	4	XY9	O3-S38	3.17	1.66	1.57
3	C	3	XY6	O3-C3	-3.15	1.39	1.46
3	D	2	XY6	O3-C3	-3.10	1.40	1.46
3	H	3	XY6	O2-S23	3.02	1.66	1.57
3	D	4	XY9	O2-S33	3.01	1.66	1.57
3	D	4	XY9	O4-S43	2.98	1.66	1.57
3	D	3	XY6	O2-S23	2.94	1.66	1.57
3	D	3	XY6	O3-S28	2.92	1.65	1.57
3	C	4	XY9	O3-S38	2.92	1.65	1.57
3	H	1	XY6	O2-S23	2.91	1.65	1.57
3	H	3	XY6	O3-S28	2.90	1.65	1.57
3	C	2	XY6	O2-S23	2.90	1.65	1.57
3	H	4	XY9	O4-S43	2.89	1.65	1.57
3	H	4	XY9	O3-S38	2.88	1.65	1.57
3	D	2	XY6	O2-S23	2.88	1.65	1.57
3	C	4	XY9	O4-S43	2.88	1.65	1.57
3	C	2	XY6	O3-S28	2.87	1.65	1.57
3	D	1	XY6	O2-C2	-2.87	1.40	1.46
3	D	1	XY6	O3-C3	-2.85	1.40	1.46
3	H	1	XY6	O3-C3	-2.82	1.40	1.46
3	C	3	XY6	O3-S28	2.82	1.65	1.57
3	D	3	XY6	O3-C3	-2.81	1.40	1.46
3	C	1	XY6	O2-S23	2.78	1.65	1.57
3	H	3	XY6	O3-C3	-2.76	1.40	1.46
3	C	3	XY6	O2-S23	2.75	1.65	1.57
3	H	1	XY6	O3-S28	2.75	1.65	1.57
3	C	4	XY9	O3-C3	-2.74	1.40	1.46
3	D	1	XY6	O2-S23	2.72	1.65	1.57
3	C	4	XY9	O2-S33	2.71	1.65	1.57
3	C	1	XY6	O2-C2	-2.63	1.40	1.46
3	H	1	XY6	O2-C2	-2.62	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	2	XY6	O3-S28	2.60	1.65	1.57
3	C	4	XY9	O5-C5	-2.59	1.37	1.42
3	C	2	XY6	O3-C3	-2.51	1.41	1.46
3	H	2	XY6	O4-C4	-2.49	1.38	1.43
3	C	1	XY6	O5-C5	-2.45	1.39	1.43
3	D	2	XY6	O3-S28	2.40	1.64	1.57
3	D	4	XY9	O3-C3	-2.40	1.41	1.46
3	C	1	XY6	O5-C1	-2.28	1.39	1.43
3	C	1	XY6	O3-C3	-2.27	1.41	1.46
3	D	1	XY6	C1-C2	2.25	1.54	1.52
3	C	3	XY6	O5-C5	-2.09	1.38	1.42
3	H	1	XY6	O4-C4	-2.02	1.39	1.43
3	D	4	XY9	O5-C5	-2.00	1.39	1.42

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	3	XY6	O2-C2-C3	5.84	113.12	106.65
3	H	4	XY9	C4-O4-S43	-5.84	110.30	117.91
3	D	2	XY6	C5-C4-C3	5.11	115.34	109.17
3	D	4	XY9	C1-C2-C3	4.93	116.76	109.40
3	D	3	XY6	C5-C4-C3	-4.87	103.29	109.17
3	D	2	XY6	O5-C1-C2	-4.79	101.38	110.18
3	H	4	XY9	O4-C4-C3	4.60	111.75	106.65
3	H	2	XY6	O2-C2-C3	4.56	111.70	106.65
3	H	4	XY9	O2-C2-C3	4.56	111.70	106.65
3	H	4	XY9	C3-O3-S38	-4.44	110.29	118.88
3	H	2	XY6	O5-C1-C2	4.25	117.98	110.18
3	C	1	XY6	C5-O5-C1	-4.21	105.63	112.71
3	D	2	XY6	O2-C2-C3	-4.18	102.02	106.65
3	D	3	XY6	C5-O5-C1	3.85	117.45	111.52
3	C	2	XY6	C2-O2-S23	-3.73	113.04	117.91
3	C	4	XY9	C1-C2-C3	3.73	114.97	109.40
3	H	2	XY6	C5-O5-C1	3.62	117.08	111.52
3	H	2	XY6	C2-O2-S23	3.53	122.51	117.91
3	H	3	XY6	O2-C2-C3	3.37	110.38	106.65
3	C	4	XY9	O35-S33-O34	-3.14	99.60	112.22
3	H	1	XY6	O5-C1-C2	3.09	113.99	109.51
3	H	1	XY6	C5-C4-C3	-3.04	105.50	109.17
3	D	4	XY9	O35-S33-O34	-2.93	100.44	112.22
3	D	4	XY9	C2-O2-S33	2.89	121.68	117.91
3	D	3	XY6	O30-S28-O29	-2.82	100.92	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	2	XY6	C3-O3-S28	-2.79	113.48	118.88
3	H	1	XY6	O26-S23-O24	-2.75	101.17	112.22
3	C	4	XY9	O46-S43-O45	-2.73	101.25	112.22
3	H	4	XY9	C2-O2-S33	-2.71	114.37	117.91
3	H	3	XY6	O30-S28-O29	-2.68	101.47	112.22
3	C	4	XY9	C4-O4-S43	-2.67	114.42	117.91
3	D	2	XY6	C5-O5-C1	-2.65	107.44	111.52
3	C	4	XY9	O41-S38-O39	-2.65	101.57	112.22
3	D	4	XY9	O46-S43-O45	-2.65	101.58	112.22
3	C	1	XY6	O31-S28-O29	-2.60	99.47	108.49
3	C	1	XY6	O26-S23-O24	-2.55	101.99	112.22
3	H	2	XY6	O25-S23-O24	-2.54	99.67	108.49
3	C	3	XY6	O2-C2-C3	2.54	109.46	106.65
3	D	1	XY6	O5-C1-C2	2.52	113.17	109.51
3	C	3	XY6	C3-O3-S28	-2.47	114.10	118.88
3	C	2	XY6	O25-S23-O24	-2.47	99.91	108.49
3	H	4	XY9	O46-S43-O45	-2.38	102.67	112.22
3	D	1	XY6	C5-C4-C3	-2.32	106.37	109.17
3	D	1	XY6	O5-C5-C4	-2.30	107.22	110.77
3	C	1	XY6	C5-C4-C3	2.29	111.94	109.17
3	D	2	XY6	C1-C2-C3	-2.28	105.99	109.40
3	D	3	XY6	O5-C1-C2	2.25	114.32	110.18
3	H	3	XY6	O25-S23-O24	-2.19	100.89	108.49
3	D	1	XY6	C4-C3-C2	-2.15	107.75	111.37
3	C	2	XY6	O31-S28-O30	-2.15	101.02	108.49
3	D	1	XY6	O2-C2-C1	-2.13	104.72	107.58
3	D	4	XY9	C4-O4-S43	-2.11	115.16	117.91
3	H	4	XY9	O36-S33-O34	-2.10	101.18	108.49
3	D	3	XY6	O25-S23-O24	-2.09	101.22	108.49
3	D	1	XY6	O31-S28-O29	-2.07	101.28	108.49
3	D	2	XY6	O25-S23-O24	-2.02	101.45	108.49
3	C	2	XY6	C5-C4-C3	2.02	111.62	109.17
3	D	1	XY6	O25-S23-O26	-2.02	101.47	108.49

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	XY6	C2-O2-S23-O24
3	C	1	XY6	C3-O3-S28-O29
3	C	1	XY6	C3-O3-S28-O30
3	D	2	XY6	C3-O3-S28-O29

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Mol	Chain	Res	Type	Atoms
3	D	4	XY9	C2-C3-O3-S38
3	D	4	XY9	C3-O3-S38-O39
3	D	4	XY9	C3-O3-S38-O40
3	D	4	XY9	C3-O3-S38-O41
3	H	1	XY6	C3-C2-O2-S23
3	H	1	XY6	C2-O2-S23-O24
3	H	1	XY6	C2-O2-S23-O25
3	H	1	XY6	C2-O2-S23-O26
3	H	2	XY6	C3-C2-O2-S23
3	H	2	XY6	C3-O3-S28-O31
3	C	1	XY6	C2-O2-S23-O26
3	D	2	XY6	C3-O3-S28-O30
3	H	2	XY6	C3-O3-S28-O29
3	H	2	XY6	C3-O3-S28-O30
3	C	1	XY6	C2-O2-S23-O25
3	C	1	XY6	C3-O3-S28-O31
3	D	2	XY6	C3-O3-S28-O31
3	C	1	XY6	C1-C2-O2-S23
3	H	1	XY6	C1-C2-O2-S23
3	C	1	XY6	C3-C2-O2-S23
3	D	3	XY6	C2-C3-O3-S28
3	D	4	XY9	C4-C3-O3-S38

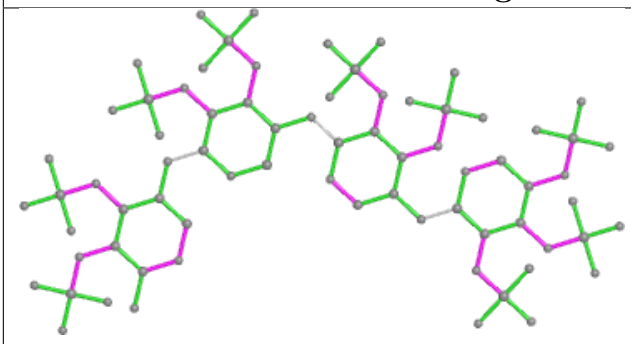
There are no ring outliers.

5 monomers are involved in 5 short contacts:

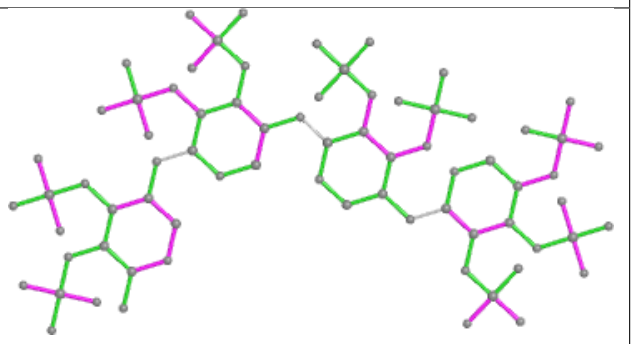
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1	XY6	1	0
3	C	1	XY6	0	1
3	D	2	XY6	1	0
3	D	3	XY6	1	0
3	C	2	XY6	1	0

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

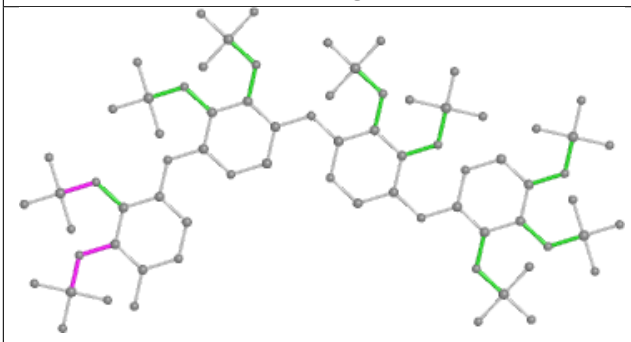
Oligosaccharide Chain C



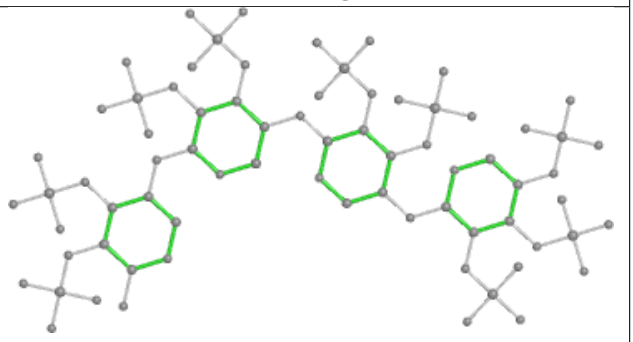
Bond lengths



Bond angles

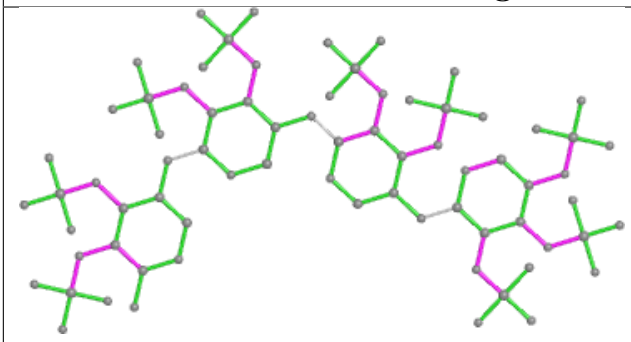


Torsions

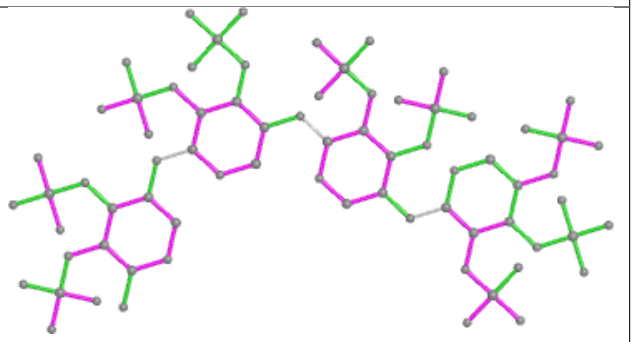


Rings

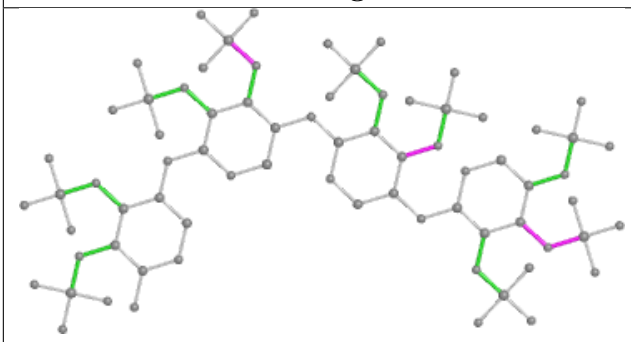
Oligosaccharide Chain D



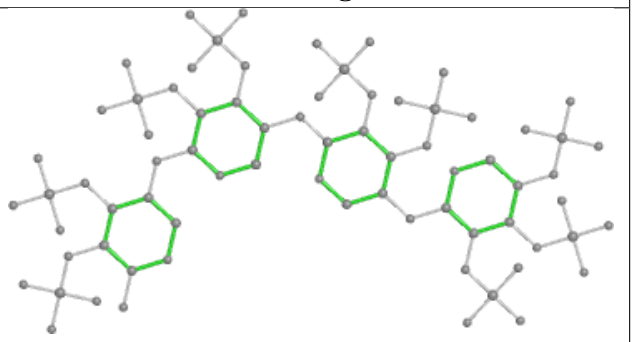
Bond lengths



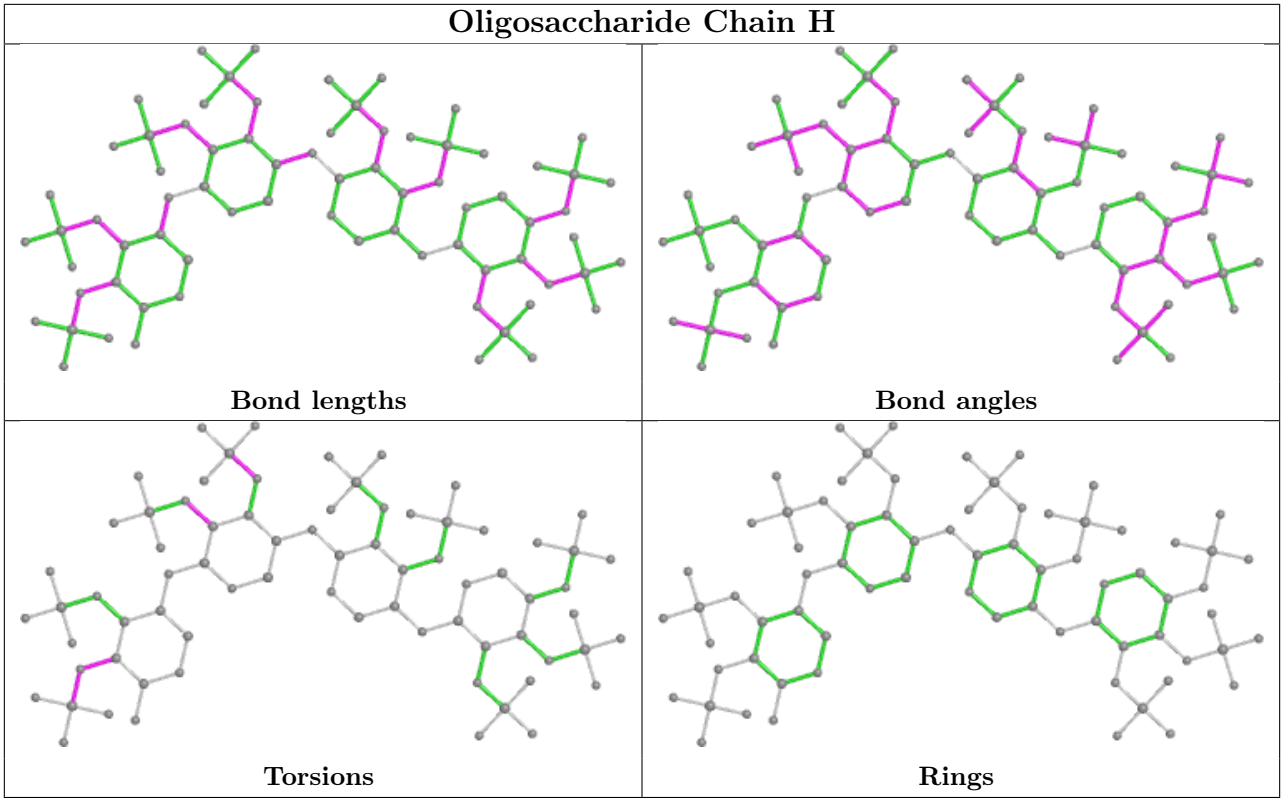
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
4	ACT	A	601	-	3,3,3	1.05	0	3,3,3	1.48	0
5	SO4	A	602	-	4,4,4	0.13	0	6,6,6	0.15	0
5	SO4	A	604	-	4,4,4	0.19	0	6,6,6	0.10	0
4	ACT	A	603	-	3,3,3	0.86	0	3,3,3	1.45	1 (33%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	603	ACT	OXT-C-O	2.03	129.52	122.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	ACT	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	385/387 (99%)	0.18	18 (4%) 31 39	20, 31, 52, 87	0
2	B	74/92 (80%)	0.10	2 (2%) 54 61	21, 29, 53, 75	0
All	All	459/479 (95%)	0.17	20 (4%) 34 41	20, 31, 53, 87	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	160	PHE	5.7
1	A	543	ILE	5.0
1	A	425	GLY	4.6
1	A	520	SER	4.0
1	A	273	GLY	3.7
1	A	159	LYS	3.1
1	A	260	ASN	3.0
1	A	426	GLN	2.9
1	A	428	ARG	2.8
1	A	429	ARG	2.8
1	A	272	ARG	2.6
1	A	258	PHE	2.6
1	A	472	ASN	2.5
1	A	517	ARG	2.4
2	B	37	ASP	2.4
2	B	36	GLN	2.3
1	A	288	GLU	2.3
1	A	427	ASP	2.2
1	A	274	LYS	2.1
1	A	257	THR	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)

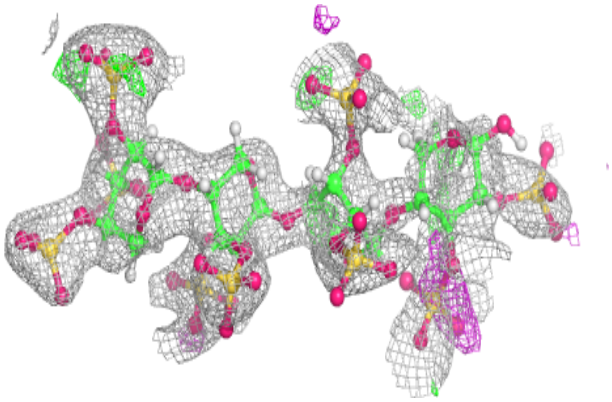
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

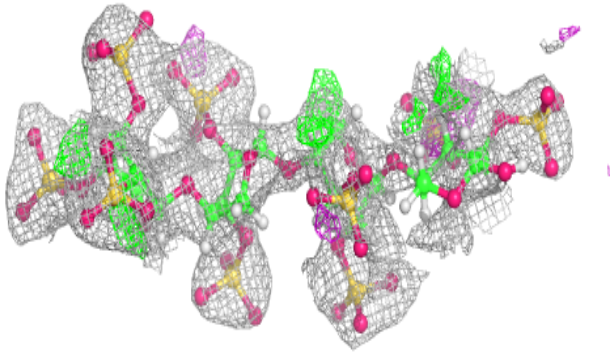
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	XY6	H	1	18/18	0.09	1.01	105,119,140,146	25
3	XY6	H	2	17/18	0.18	0.77	110,121,141,145	23
3	XY6	H	3	17/18	0.37	0.68	80,98,118,126	23
3	XY6	C	1	18/18	0.58	0.39	70,92,112,112	25
3	XY6	D	3	17/18	0.59	0.27	82,98,115,118	23
3	XY9	D	4	21/22	0.70	0.25	79,97,119,119	27
3	XY6	C	2	17/18	0.75	0.28	78,87,104,106	23
3	XY6	D	1	18/18	0.76	0.24	33,54,66,73	25
3	XY6	D	2	17/18	0.81	0.26	51,79,93,101	23
3	XY9	H	4	21/22	0.86	0.23	45,59,78,88	27
3	XY6	C	3	17/18	0.87	0.12	64,76,87,90	23
3	XY9	C	4	21/22	0.92	0.17	38,65,78,85	27

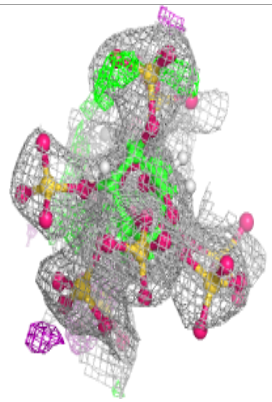
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

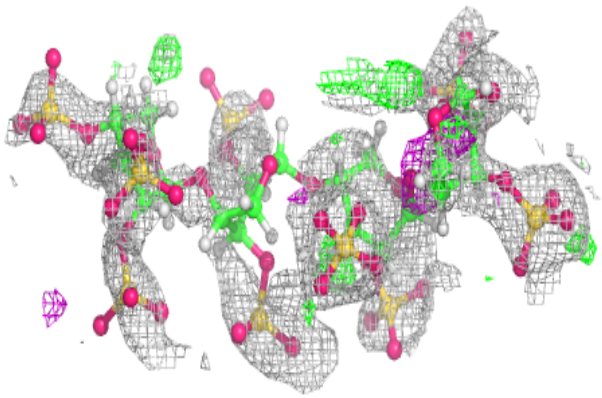


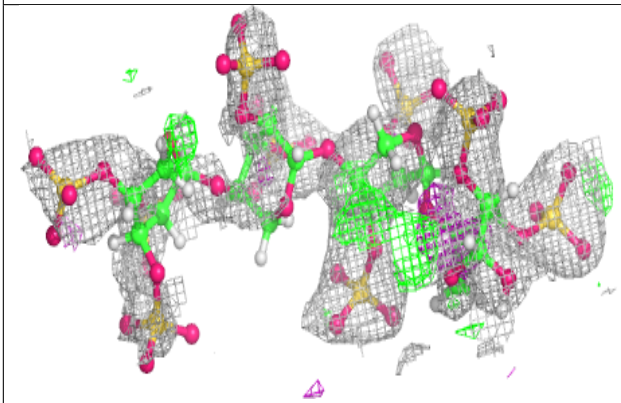


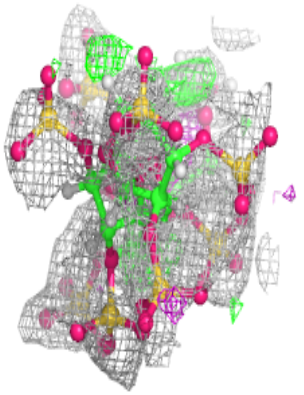


Electron density around Chain D:

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

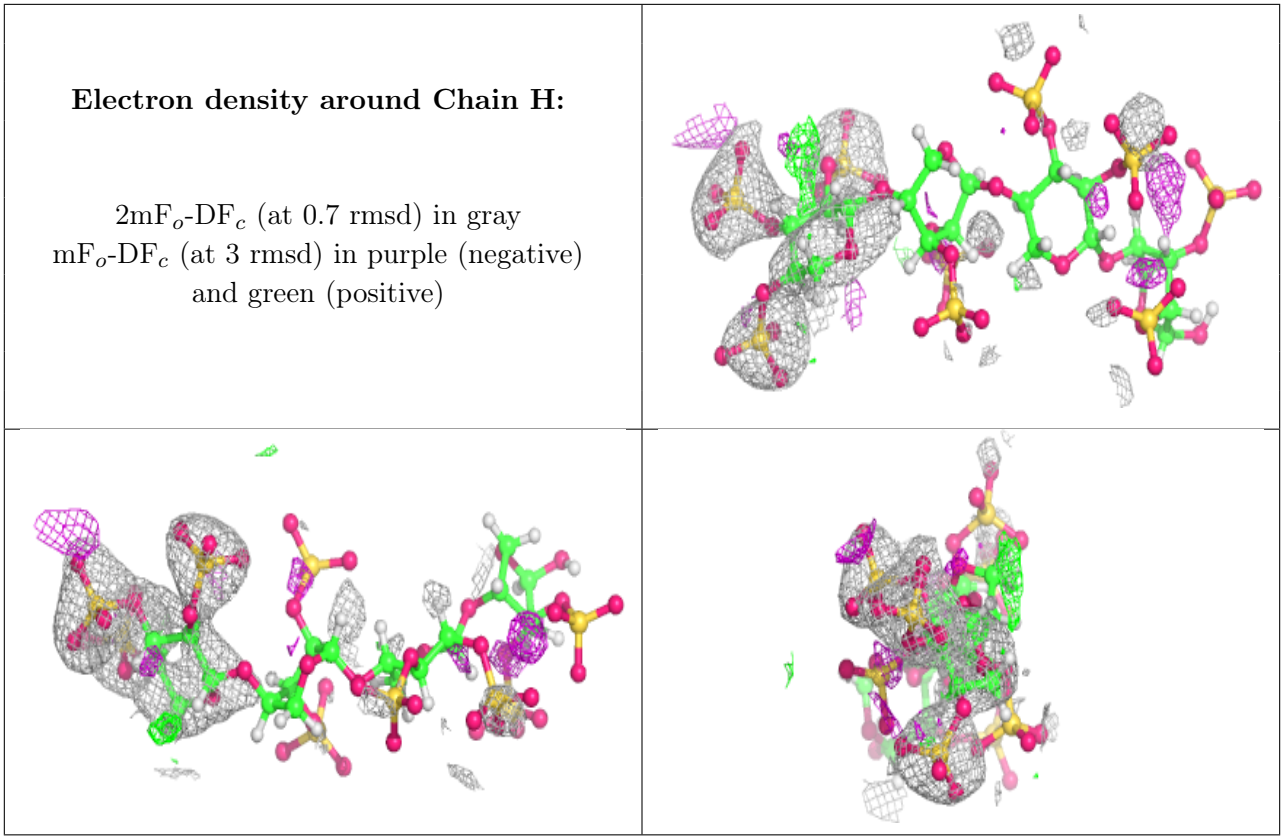






Electron density around Chain H:

$2mF_o$-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
4	ACT	A	603	4/4	0.78	0.15	59,62,72,72	0
5	SO4	A	602	5/5	0.94	0.21	54,62,66,71	0
5	SO4	A	604	5/5	0.94	0.20	49,62,75,75	0
4	ACT	A	601	4/4	0.96	0.13	29,38,52,52	0

6.5 Other polymers

There are no such residues in this entry.