Full wwPDB X-ray Structure Validation Report ⓘ

Mar 3, 2024 – 07:44 AM EST

PDB ID	:	6BYT
Title	:	Complex structure of LOR107 mutant (R320) with tetrasaccharide substrate
Authors	:	Ulaganathan, T.S.; Cygler, M.
Deposited on	:	2017-12-21
Resolution	:	2.20 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:

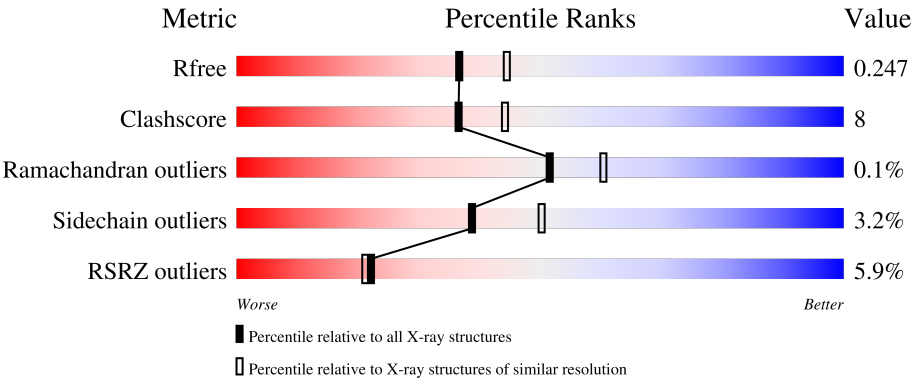
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	506	3% 83% 12% 5%
1	B	506	9% 74% 20% • 5%
2	C	4	50% 50%
2	D	4	75% 25%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8204 atoms, of which 84 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.

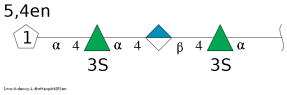
- Molecule 1 is a protein called Short ulvan lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	1	0
			3843	2446	652	736	9			
1	B	482	Total	C	N	O	S	0	0	0
			3791	2411	641	730	9			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	-	initiating methionine	UNP A0A109PTH9
A	320	ASN	ARG	engineered mutation	UNP A0A109PTH9
A	523	LEU	-	expression tag	UNP A0A109PTH9
A	524	GLU	-	expression tag	UNP A0A109PTH9
A	525	HIS	-	expression tag	UNP A0A109PTH9
A	526	HIS	-	expression tag	UNP A0A109PTH9
A	527	HIS	-	expression tag	UNP A0A109PTH9
A	528	HIS	-	expression tag	UNP A0A109PTH9
A	529	HIS	-	expression tag	UNP A0A109PTH9
A	530	HIS	-	expression tag	UNP A0A109PTH9
B	25	MET	-	initiating methionine	UNP A0A109PTH9
B	320	ASN	ARG	engineered mutation	UNP A0A109PTH9
B	523	LEU	-	expression tag	UNP A0A109PTH9
B	524	GLU	-	expression tag	UNP A0A109PTH9
B	525	HIS	-	expression tag	UNP A0A109PTH9
B	526	HIS	-	expression tag	UNP A0A109PTH9
B	527	HIS	-	expression tag	UNP A0A109PTH9
B	528	HIS	-	expression tag	UNP A0A109PTH9
B	529	HIS	-	expression tag	UNP A0A109PTH9
B	530	HIS	-	expression tag	UNP A0A109PTH9

- Molecule 2 is an oligosaccharide called 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-4)-3-O-sulfo-alpha-L-rhamnopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-4)-3-O-sulfo-alpha-L-rhamnopyranose.

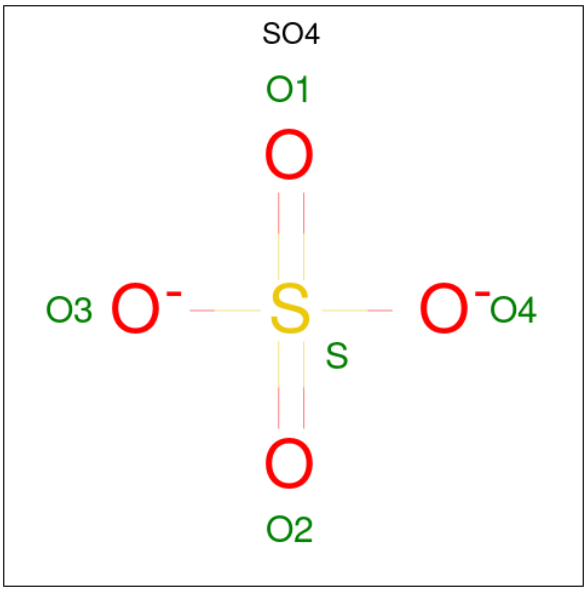


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	C	4	Total C H O S 82 24 30 26 2	0	0	0
2	D	4	Total C H O S 82 24 30 26 2	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Ca 2 2	0	0
3	B	2	Total Ca 2 2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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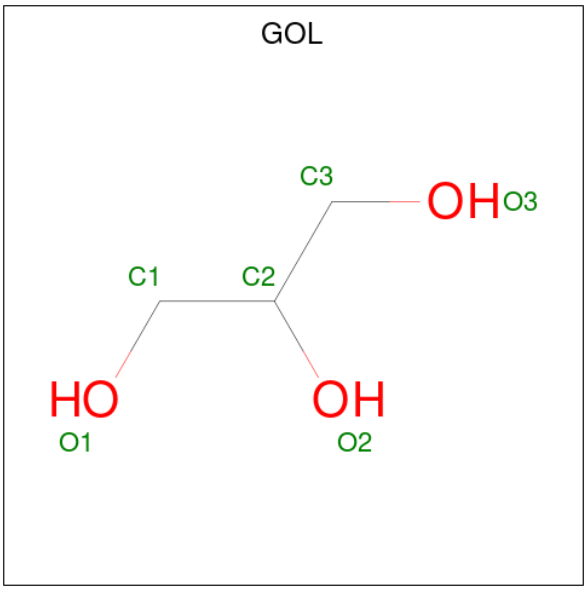
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H O 14 3 8 3	0	0
5	B	1	Total C H O 14 3 8 3	0	0
5	B	1	Total C H O 14 3 8 3	0	0

- Molecule 6 is water.

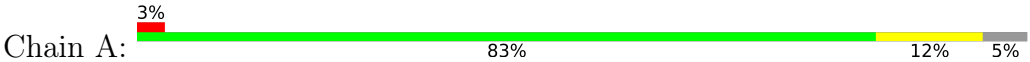
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	185	Total O 185 185	0	0
6	B	140	Total O 140 140	0	0

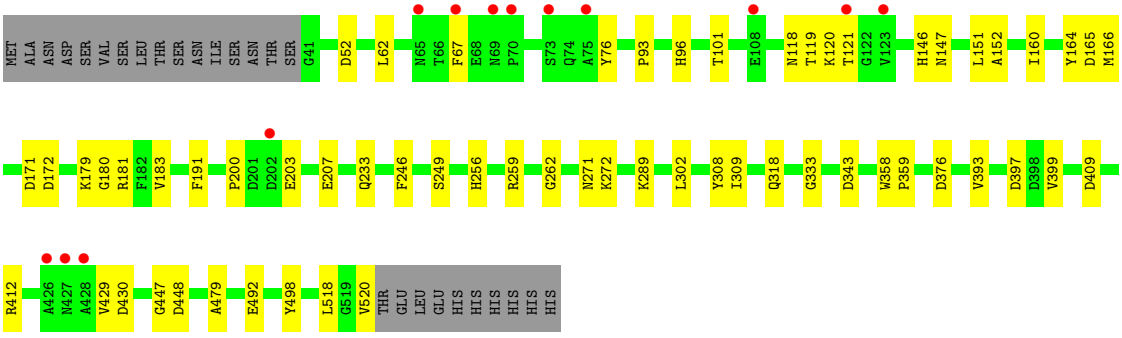
3 Residue-property plots (i)

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: Short ulvan lyase

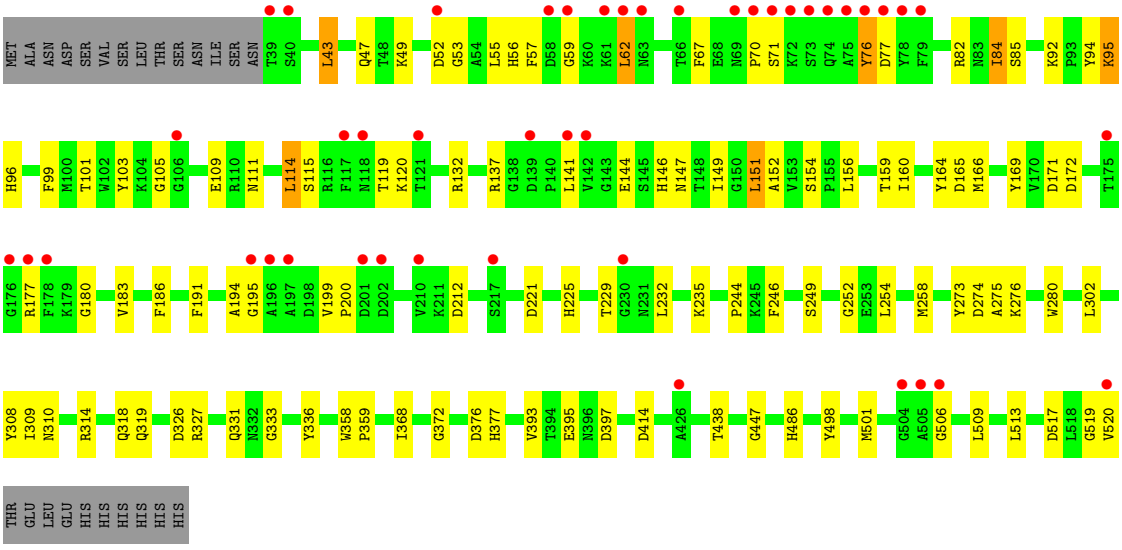
Chain A:





• Molecule 1: Short ulvan lyase

Chain B:



• Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-4)-3-O-sulfo-alpha-L-rhamnopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-4)-3-O-sulfo-alpha-L-rhamnopyranose

Chain C:

• Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-4)-3-O-sulfo-alpha-L-rhamnopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-4)-3-O-sulfo-alpha-L-rhamnopyranose

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.22Å 120.66Å 127.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.05 – 2.20 49.04 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.05-2.20) 99.0 (49.04-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.200 , 0.247 0.200 , 0.247	Depositor DCC
R_{free} test set	5067 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	37.1	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.008 for -h,l,k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8204	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.93 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.8204e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: GCD, SO4, BDP, 83Y, GOL, CA

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	0.43	0/3957	0.59	0/5365
1	B	0.44	0/3901	0.61	0/5298
All	All	0.44	0/7858	0.60	0/10663

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	3843	0	3563	33	0
1	B	3791	0	3447	84	0
2	C	52	30	11	2	0
2	D	52	30	11	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	15	0	0	0	0
4	B	20	0	0	1	0
5	A	6	8	7	1	0
5	B	12	16	16	0	0
6	A	185	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	140	0	0	8	0
All	All	8120	84	7055	117	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 8.

All (117) 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:B:101:THR:HG23	1:B:151:LEU:HD12	1.52	0.90
1:A:147:ASN:HB3	1:A:165:ASP:HA	1.53	0.90
1:B:119:THR:HG23	1:B:120:LYS:HD2	1.58	0.85
1:B:501:MET:HE3	1:B:509:LEU:HD12	1.63	0.79
1:B:147:ASN:HB3	1:B:165:ASP:HA	1.66	0.78
1:B:156:LEU:HD21	1:B:252:GLY:O	1.88	0.74
1:B:327:ARG:NH2	1:B:377:HIS:O	2.20	0.74
1:A:171:ASP:OD1	1:A:183:VAL:HA	1.89	0.72
1:B:70:PRO:HG2	1:B:141:LEU:HD13	1.72	0.71
1:B:212:ASP:HB2	6:B:701:HOH:O	1.90	0.71
1:A:200:PRO:HD2	1:A:203:GLU:OE1	1.93	0.68
1:B:152:ALA:HB2	1:B:246:PHE:CG	2.29	0.67
1:B:171:ASP:OD1	1:B:183:VAL:HA	1.94	0.67
1:B:84:ILE:HG23	1:B:103:TYR:HD2	1.61	0.66
1:B:146:HIS:NE2	2:D:2:BDP:H5	2.10	0.66
1:A:146:HIS:NE2	2:C:2:BDP:H5	2.10	0.65
1:B:212:ASP:CB	6:B:701:HOH:O	2.46	0.63
1:B:506:GLY:HA3	6:B:721:HOH:O	1.98	0.62
1:B:309:ILE:HG21	1:B:393:VAL:HB	1.82	0.61
1:A:318:GLN:HG2	1:A:333:GLY:O	2.01	0.61
1:B:274:ASP:HA	6:B:755:HOH:O	1.99	0.61
1:B:225:HIS:HA	6:B:701:HOH:O	2.01	0.60
1:B:119:THR:HG23	1:B:120:LYS:CD	2.29	0.59
1:A:93:PRO:HG2	1:A:492:GLU:OE1	2.03	0.59
1:B:517:ASP:OD1	1:B:519:GLY:N	2.31	0.59
1:A:289:LYS:NZ	6:A:703:HOH:O	2.36	0.58
1:A:172:ASP:O	1:A:180:GLY:HA2	2.03	0.58
1:B:164:TYR:O	1:B:166:MET:HG3	2.04	0.58
1:A:262:GLY:HA2	2:C:1:83Y:C6	2.34	0.57
1:B:326:ASP:HA	4:B:604:SO4:O1	2.04	0.57
1:B:172:ASP:O	1:B:180:GLY:HA2	2.04	0.57
1:A:259[A]:ARG:HH11	1:A:302:LEU:H	1.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:TYR:CE2	1:B:275:ALA:HB2	2.39	0.56
1:B:151:LEU:HD23	1:B:152:ALA:N	2.21	0.55
1:B:62:LEU:HG	1:B:67:PHE:HA	1.88	0.55
1:B:59:GLY:N	1:B:76:TYR:O	2.38	0.54
1:B:137:ARG:HD3	1:B:177:ARG:HG2	1.88	0.54
1:B:84:ILE:HG23	1:B:103:TYR:CD2	2.40	0.54
1:A:256:HIS:HB3	1:A:271:ASN:OD1	2.08	0.53
1:B:95:LYS:O	1:B:96:HIS:ND1	2.41	0.53
1:B:84:ILE:HD12	1:B:103:TYR:CE2	2.43	0.53
1:B:169:TYR:O	1:B:186:PHE:HB2	2.08	0.53
1:B:395:GLU:OE1	1:B:447:GLY:HA2	2.09	0.52
1:B:159:THR:CG2	1:B:194:ALA:HA	2.40	0.52
1:A:62:LEU:HD13	1:A:67:PHE:HA	1.90	0.52
1:B:152:ALA:HB2	1:B:246:PHE:CB	2.41	0.51
1:B:71:SER:HB3	1:B:77:ASP:OD2	2.11	0.51
1:A:479:ALA:HB3	6:B:813:HOH:O	2.10	0.51
1:B:336:TYR:HB3	1:B:368:ILE:HD11	1.93	0.51
1:B:94:TYR:HB3	1:B:99:PHE:HE1	1.76	0.50
1:B:137:ARG:CZ	1:B:177:ARG:HH11	2.24	0.50
1:B:232:LEU:O	1:B:235:LYS:HB3	2.11	0.50
1:A:448:ASP:OD1	1:A:520:VAL:CG1	2.60	0.50
1:B:199:VAL:HB	1:B:200:PRO:HD2	1.94	0.49
1:B:212:ASP:CG	6:B:701:HOH:O	2.50	0.49
1:B:195:GLY:HA2	6:B:800:HOH:O	2.13	0.49
1:B:273:TYR:HB2	1:B:280:TRP:CH2	2.48	0.49
1:B:96:HIS:HB2	1:B:119:THR:HG22	1.95	0.49
1:B:109:GLU:HA	1:B:109:GLU:OE1	2.13	0.48
1:B:101:THR:HB	1:B:149:ILE:HG21	1.95	0.48
1:B:111:ASN:HA	1:B:132:ARG:HG2	1.95	0.48
1:A:259[A]:ARG:NH1	1:A:302:LEU:H	2.10	0.48
1:A:152:ALA:HB2	1:A:246:PHE:CG	2.48	0.48
1:B:53:GLY:O	1:B:105:GLY:HA3	2.14	0.48
1:B:55:LEU:HD11	1:B:76:TYR:HE2	1.78	0.48
1:B:156:LEU:HD22	1:B:156:LEU:N	2.29	0.47
1:B:156:LEU:CD2	1:B:252:GLY:O	2.57	0.47
1:B:519:GLY:O	1:B:520:VAL:HG13	2.14	0.47
1:B:154:SER:HA	1:B:254:LEU:HD11	1.96	0.47
1:B:318:GLN:HG2	1:B:333:GLY:O	2.15	0.47
1:B:43:LEU:C	1:B:43:LEU:HD12	2.36	0.46
1:B:114:LEU:HD23	1:B:115:SER:N	2.29	0.46
1:B:96:HIS:O	1:B:119:THR:HB	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:GLN:HA	1:B:513:LEU:O	2.16	0.46
1:B:327:ARG:NH1	1:B:372:GLY:O	2.49	0.46
1:A:429:VAL:HG23	1:A:430:ASP:H	1.81	0.45
1:B:159:THR:HG23	1:B:194:ALA:HA	1.97	0.45
1:B:96:HIS:HB2	1:B:119:THR:CG2	2.46	0.45
1:B:151:LEU:HD23	1:B:151:LEU:C	2.38	0.44
1:A:409:ASP:O	1:A:412:ARG:HG2	2.18	0.44
1:B:414:ASP:OD1	1:B:414:ASP:N	2.45	0.44
1:B:57:PHE:HB2	1:B:82:ARG:HA	2.00	0.44
1:A:358:TRP:CD1	1:A:359:PRO:HA	2.52	0.44
1:B:229:THR:HG22	1:B:280:TRP:O	2.17	0.43
1:B:56:HIS:ND1	1:B:501:MET:HE1	2.34	0.43
1:A:447:GLY:HA2	5:A:606:GOL:H12	2.01	0.43
1:B:94:TYR:HB3	1:B:99:PHE:CE1	2.54	0.43
1:A:160:ILE:O	1:A:191:PHE:HA	2.19	0.43
1:A:101:THR:HG23	1:A:151:LEU:HD22	2.00	0.43
1:A:272:LYS:HD2	1:A:343:ASP:OD1	2.19	0.42
1:A:429:VAL:HG23	1:A:430:ASP:N	2.34	0.42
1:A:393:VAL:HG22	1:A:399:VAL:HG22	2.00	0.42
1:A:164:TYR:O	1:A:166:MET:HG3	2.19	0.42
1:B:273:TYR:CZ	1:B:275:ALA:HA	2.54	0.42
1:A:259[A]:ARG:NH2	1:A:262:GLY:O	2.42	0.42
1:B:156:LEU:HD22	1:B:156:LEU:H	1.84	0.42
1:B:310:ASN:HB2	1:B:314:ARG:NH2	2.34	0.42
1:A:249:SER:HA	1:A:308:TYR:CE2	2.55	0.42
1:B:137:ARG:NH1	1:B:177:ARG:HH11	2.18	0.42
1:B:249:SER:HA	1:B:308:TYR:CE2	2.55	0.42
1:B:302:LEU:HD12	1:B:302:LEU:N	2.34	0.42
1:B:154:SER:CA	1:B:254:LEU:HD11	2.50	0.42
1:B:92:LYS:HB2	1:B:151:LEU:HD22	2.02	0.41
1:B:486:HIS:HE1	1:B:501:MET:HE1	1.84	0.41
1:A:358:TRP:HA	1:A:359:PRO:C	2.40	0.41
1:B:319:GLN:O	1:B:331:GLN:HA	2.20	0.41
1:A:96:HIS:O	1:A:119:THR:HG22	2.20	0.41
1:A:259[A]:ARG:HH11	1:A:302:LEU:N	2.18	0.41
1:B:55:LEU:HD11	1:B:76:TYR:CE2	2.55	0.41
1:B:56:HIS:CG	1:B:501:MET:HE3	2.56	0.41
1:A:179:LYS:HD2	1:A:181:ARG:NH2	2.35	0.41
1:B:519:GLY:O	1:B:520:VAL:CG1	2.69	0.41
1:B:160:ILE:O	1:B:191:PHE:HA	2.20	0.40
1:A:118:ASN:HB3	1:A:121:THR:OG1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:TRP:HA	1:B:359:PRO:C	2.41	0.40
1:B:85:SER:O	1:B:486:HIS:NE2	2.55	0.40
1:B:244:PRO:HA	1:B:258:MET:HG2	2.03	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	479/506 (95%)	459 (96%)	20 (4%)	0	100 100
1	B	480/506 (95%)	456 (95%)	23 (5%)	1 (0%)	47 55
All	All	959/1012 (95%)	915 (95%)	43 (4%)	1 (0%)	51 60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	95	LYS

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	402/434 (93%)	392 (98%)	10 (2%)	47 60
1	B	386/434 (89%)	371 (96%)	15 (4%)	32 41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	788/868 (91%)	763 (97%)	25 (3%)	39 50

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ASP
1	A	76	TYR
1	A	120	LYS
1	A	207	GLU
1	A	233	GLN
1	A	309	ILE
1	A	376	ASP
1	A	397	ASP
1	A	498	TYR
1	A	518	LEU
1	B	43	LEU
1	B	49	LYS
1	B	52	ASP
1	B	62	LEU
1	B	76	TYR
1	B	84	ILE
1	B	114	LEU
1	B	144	GLU
1	B	151	LEU
1	B	221	ASP
1	B	276	LYS
1	B	376	ASP
1	B	397	ASP
1	B	438	THR
1	B	498	TYR

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 (i)

8 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	83Y	C	1	2	15,15,15	1.69	2 (13%)	17,23,23	2.21	7 (41%)
2	BDP	C	2	2	12,12,13	1.31	2 (16%)	14,17,19	1.80	5 (35%)
2	83Y	C	3	2	14,14,15	1.16	2 (14%)	16,21,23	1.67	2 (12%)
2	GCD	C	4	2	10,11,12	2.15	2 (20%)	13,15,17	3.00	6 (46%)
2	83Y	D	1	2	15,15,15	1.04	1 (6%)	17,23,23	1.45	3 (17%)
2	BDP	D	2	2	12,12,13	1.23	2 (16%)	14,17,19	1.65	3 (21%)
2	83Y	D	3	2	14,14,15	1.06	1 (7%)	16,21,23	1.36	3 (18%)
2	GCD	D	4	2	10,11,12	2.13	4 (40%)	13,15,17	1.82	3 (23%)

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	83Y	C	1	2	-	2/5/25/25	0/1/1/1
2	BDP	C	2	2	-	2/4/21/24	0/1/1/1
2	83Y	C	3	2	-	0/5/22/25	0/1/1/1
2	GCD	C	4	2	-	0/4/17/20	0/1/1/1
2	83Y	D	1	2	-	0/5/25/25	0/1/1/1
2	BDP	D	2	2	-	2/4/21/24	0/1/1/1
2	83Y	D	3	2	-	2/5/22/25	0/1/1/1
2	GCD	D	4	2	-	4/4/17/20	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4	GCD	O5-C5	5.72	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	GCD	O5-C5	4.99	1.44	1.37
2	C	1	83Y	O3-S	-4.46	1.44	1.57
2	C	1	83Y	O3-C3	-3.61	1.38	1.46
2	D	2	BDP	O5-C1	-2.73	1.39	1.43
2	D	1	83Y	O3-S	-2.69	1.49	1.57
2	C	2	BDP	O6B-C6	-2.63	1.21	1.30
2	C	3	83Y	O3-S	-2.56	1.49	1.57
2	D	4	GCD	O6B-C6	-2.54	1.23	1.30
2	C	2	BDP	C5-C6	-2.47	1.47	1.53
2	D	4	GCD	O5-C1	-2.43	1.41	1.45
2	D	3	83Y	O3-S	-2.43	1.50	1.57
2	D	2	BDP	O6B-C6	-2.39	1.22	1.30
2	C	4	GCD	O6B-C6	-2.37	1.23	1.30
2	C	3	83Y	O3-C3	-2.33	1.41	1.46
2	D	4	GCD	C5-C6	-2.29	1.43	1.48

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	4	GCD	O5-C5-C6	7.11	122.19	111.52
2	C	4	GCD	O5-C5-C4	-5.68	120.02	124.81
2	C	3	83Y	C3-O3-S	4.12	126.83	118.88
2	C	1	83Y	O5-C1-C2	-4.02	103.10	110.28
2	C	1	83Y	C4-C3-C2	3.90	116.48	110.85
2	D	4	GCD	O5-C5-C4	-3.81	121.59	124.81
2	D	4	GCD	O5-C5-C6	3.57	116.87	111.52
2	C	1	83Y	C6-C5-C4	-3.43	106.73	113.07
2	C	2	BDP	O4-C4-C5	-3.32	102.30	109.74
2	C	1	83Y	O4-C4-C5	-3.16	102.65	109.67
2	C	3	83Y	O4-C4-C5	-3.12	102.76	109.67
2	D	2	BDP	O4-C4-C5	-2.93	103.17	109.74
2	D	1	83Y	O5-C1-C2	-2.92	105.08	110.28
2	D	4	GCD	C1-C2-C3	2.88	113.20	109.67
2	C	2	BDP	O5-C1-C2	-2.87	106.34	110.77
2	C	1	83Y	O3S-S-O2S	2.84	118.37	108.49
2	C	4	GCD	C4-C5-C6	-2.72	117.79	123.65
2	C	2	BDP	O6B-C6-C5	2.56	123.03	113.65
2	C	4	GCD	O3-C3-C4	-2.52	103.65	109.31
2	D	3	83Y	C3-O3-S	2.43	123.56	118.88
2	D	2	BDP	O5-C1-C2	-2.39	107.08	110.77
2	C	4	GCD	O6B-C6-C5	2.37	120.12	114.20
2	C	1	83Y	O5-C5-C4	2.34	113.73	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	83Y	O5-C5-C4	2.33	113.70	109.52
2	C	2	BDP	O2-C2-C1	2.25	113.76	109.15
2	D	2	BDP	O3-C3-C2	-2.24	105.71	109.99
2	D	3	83Y	O4-C4-C3	-2.18	104.17	109.94
2	D	3	83Y	O5-C1-C2	-2.17	107.42	110.77
2	C	2	BDP	O6A-C6-C5	-2.12	113.03	120.81
2	D	1	83Y	O4-C4-C5	-2.09	105.04	109.67
2	C	1	83Y	C1-C2-C3	-2.01	106.17	110.33
2	C	4	GCD	C2-C3-C4	2.01	115.07	112.32

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	83Y	C2-C3-O3-S
2	C	2	BDP	C4-C5-C6-O6A
2	C	2	BDP	C4-C5-C6-O6B
2	D	2	BDP	C4-C5-C6-O6A
2	D	2	BDP	C4-C5-C6-O6B
2	D	3	83Y	C2-C3-O3-S
2	D	4	GCD	C4-C5-C6-O6A
2	D	4	GCD	C4-C5-C6-O6B
2	D	4	GCD	O5-C5-C6-O6A
2	D	4	GCD	O5-C5-C6-O6B
2	C	1	83Y	C4-C3-O3-S
2	D	3	83Y	C4-C3-O3-S

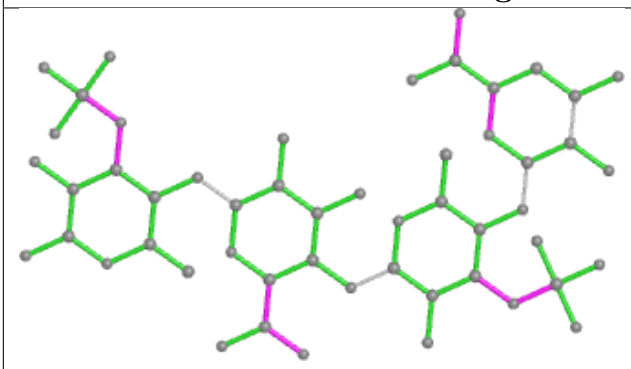
There are no ring outliers.

3 monomers are involved in 3 short contacts:

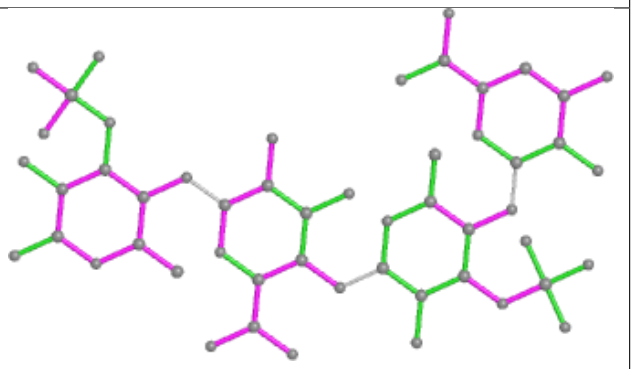
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	BDP	1	0
2	C	1	83Y	1	0
2	D	2	BDP	1	0

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

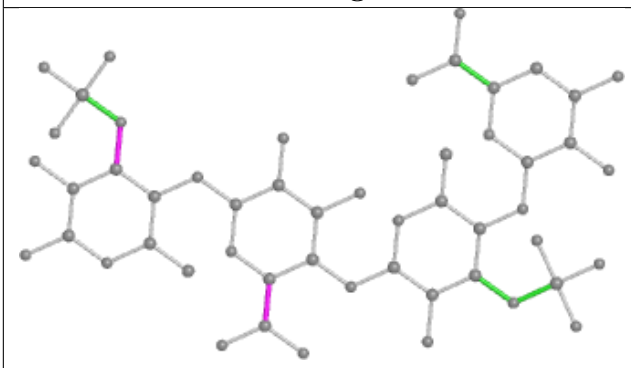
Oligosaccharide Chain C



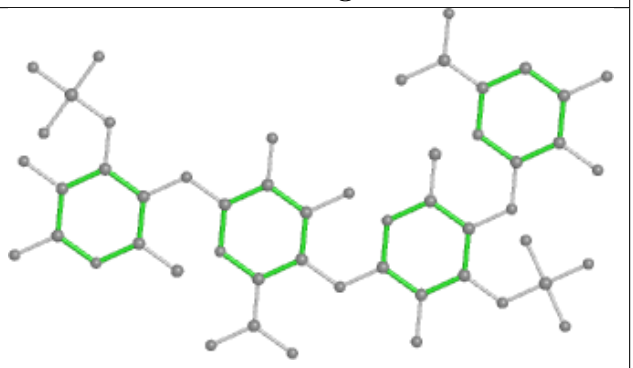
Bond lengths



Bond angles

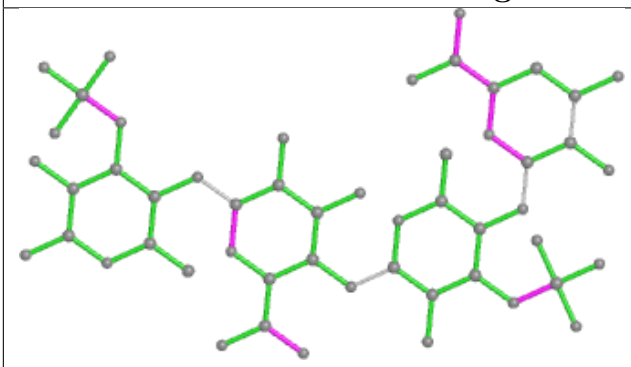


Torsions

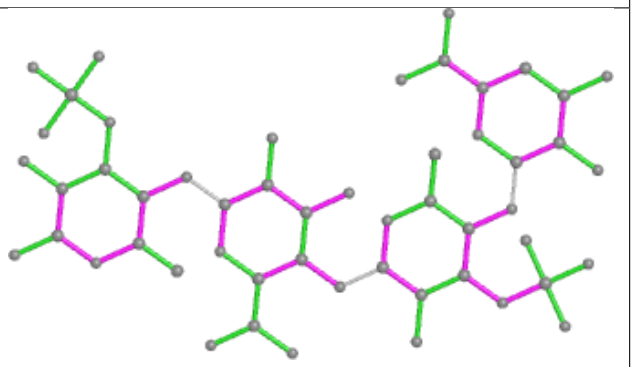


Rings

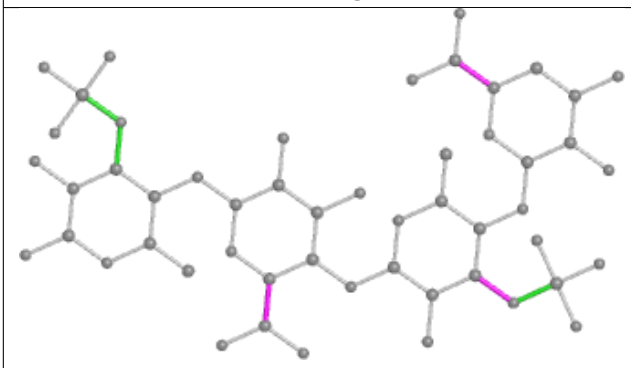
Oligosaccharide Chain D



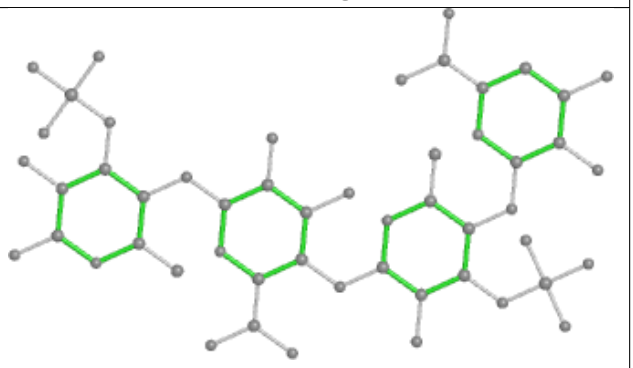
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
4	SO4	B	605	-	4,4,4	0.13	0	6,6,6	0.22	0
4	SO4	A	605	-	4,4,4	0.15	0	6,6,6	0.10	0
4	SO4	B	606	-	4,4,4	0.12	0	6,6,6	0.14	0
4	SO4	B	604	-	4,4,4	0.14	0	6,6,6	0.24	0
4	SO4	B	603	-	4,4,4	0.17	0	6,6,6	0.32	0
4	SO4	A	604	-	4,4,4	0.17	0	6,6,6	0.17	0
5	GOL	B	607	-	5,5,5	1.07	0	5,5,5	0.80	0
5	GOL	B	608	-	5,5,5	1.15	0	5,5,5	0.90	0
4	SO4	A	603	-	4,4,4	0.19	0	6,6,6	0.24	0
5	GOL	A	606	-	5,5,5	1.22	1 (20%)	5,5,5	0.92	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	GOL	B	607	-	-	1/4/4/4	-
5	GOL	B	608	-	-	2/4/4/4	-
5	GOL	A	606	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	606	GOL	O2-C2	-2.24	1.36	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	608	GOL	C1-C2-C3-O3
5	B	608	GOL	O2-C2-C3-O3
5	A	606	GOL	O2-C2-C3-O3
5	B	607	GOL	O1-C1-C2-C3
5	A	606	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	604	SO4	1	0
5	A	606	GOL	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	480/506 (94%)	-0.05	13 (2%) 54 52	23, 42, 70, 88	0
1	B	482/506 (95%)	0.47	44 (9%) 9 8	25, 57, 90, 114	0
All	All	962/1012 (95%)	0.21	57 (5%) 22 21	23, 47, 86, 114	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	40	SER	6.4
1	B	196	ALA	6.3
1	B	70	PRO	5.3
1	B	73	SER	4.9
1	B	69	ASN	4.7
1	B	74	GLN	4.4
1	B	177	ARG	4.3
1	B	77	ASP	4.2
1	B	197	ALA	4.1
1	B	75	ALA	4.1
1	B	506	GLY	4.0
1	B	505	ALA	3.8
1	B	142	VAL	3.7
1	A	427	ASN	3.6
1	B	141	LEU	3.6
1	B	78	TYR	3.5
1	B	66	THR	3.4
1	B	62	LEU	3.4
1	B	59	GLY	3.3
1	B	71	SER	3.1
1	B	117	PHE	3.1
1	A	73	SER	2.8
1	B	178	PHE	2.8
1	A	202	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	175	THR	2.8
1	B	201	ASP	2.8
1	A	70	PRO	2.8
1	B	176	GLY	2.8
1	B	139	ASP	2.7
1	B	230	GLY	2.7
1	A	69	ASN	2.7
1	B	504	GLY	2.7
1	A	121	THR	2.7
1	B	217	SER	2.6
1	B	118	ASN	2.6
1	B	106	GLY	2.6
1	B	121	THR	2.6
1	A	65	ASN	2.6
1	A	75	ALA	2.6
1	B	61	LYS	2.6
1	B	520	VAL	2.5
1	B	63	ASN	2.5
1	A	123	VAL	2.4
1	B	72	LYS	2.4
1	B	426	ALA	2.4
1	B	52	ASP	2.4
1	B	58	ASP	2.4
1	A	67	PHE	2.3
1	B	202	ASP	2.3
1	A	108	GLU	2.2
1	B	195	GLY	2.2
1	B	210	VAL	2.2
1	B	76	TYR	2.1
1	B	39	THR	2.1
1	A	426	ALA	2.0
1	A	428	ALA	2.0
1	B	79	PHE	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)

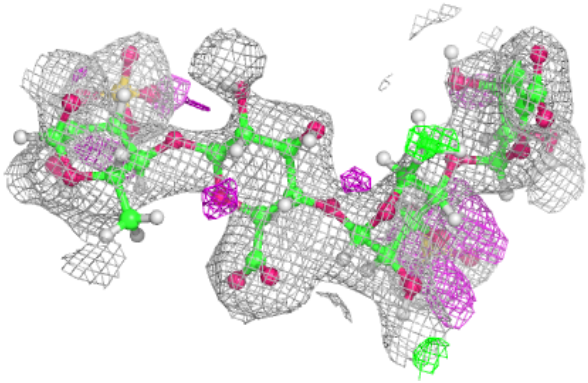
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

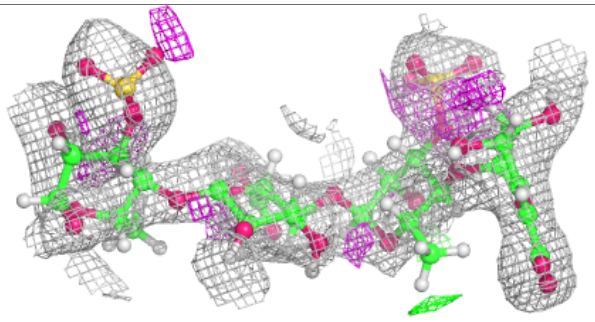
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BDP	D	2	12/13	0.60	0.20	76,94,113,114	0
2	BDP	C	2	12/13	0.63	0.23	68,101,121,125	0
2	83Y	D	3	14/15	0.63	0.27	78,99,119,123	0
2	83Y	D	1	15/15	0.69	0.28	96,114,135,140	0
2	83Y	C	1	15/15	0.75	0.26	84,119,142,144	0
2	GCD	C	4	11/12	0.78	0.19	82,88,102,104	0
2	GCD	D	4	11/12	0.79	0.30	88,100,121,123	0
2	83Y	C	3	14/15	0.86	0.21	58,84,110,110	0

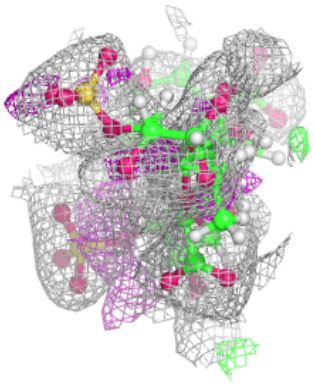
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

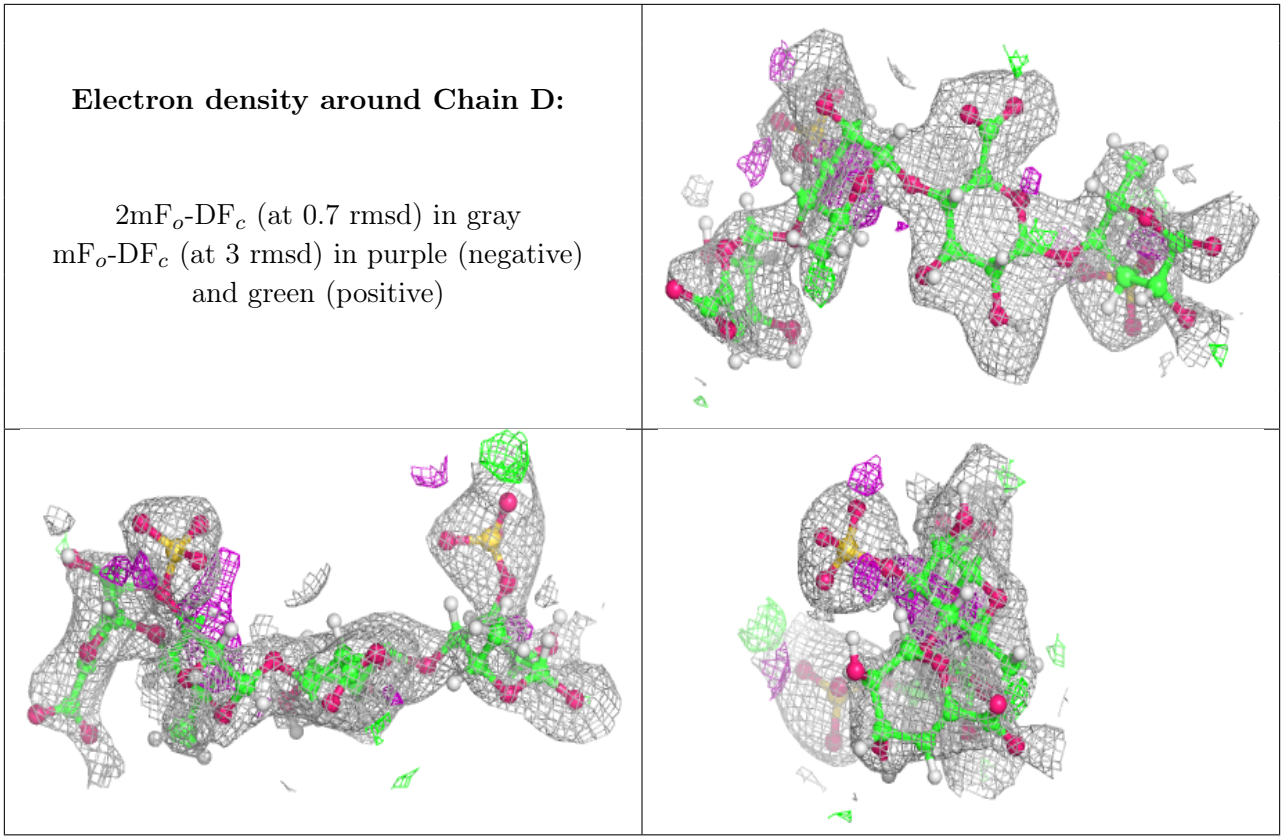






Electron density around Chain D:

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



6.4 Ligands

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	GOL	B	608	6/6	0.65	0.14	49,77,97,98	0
5	GOL	B	607	6/6	0.70	0.29	68,92,108,110	0
5	GOL	A	606	6/6	0.87	0.17	63,78,94,100	0
4	SO4	B	605	5/5	0.88	0.22	92,95,101,107	0
4	SO4	B	606	5/5	0.90	0.15	94,97,101,106	0
4	SO4	B	604	5/5	0.91	0.19	67,84,88,92	0
4	SO4	A	605	5/5	0.93	0.11	93,100,100,103	0
4	SO4	A	604	5/5	0.94	0.24	85,86,88,94	0
3	CA	B	602	1/1	0.97	0.07	55,55,55,55	0
3	CA	A	601	1/1	0.98	0.06	38,38,38,38	0
4	SO4	B	603	5/5	0.98	0.10	57,57,59,63	0
4	SO4	A	603	5/5	0.98	0.10	39,47,56,66	0
3	CA	A	602	1/1	0.98	0.10	42,42,42,42	0
3	CA	B	601	1/1	1.00	0.11	36,36,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.