



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:39 PM UTC

PDB ID : 6BYT / pdb_00006byt
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

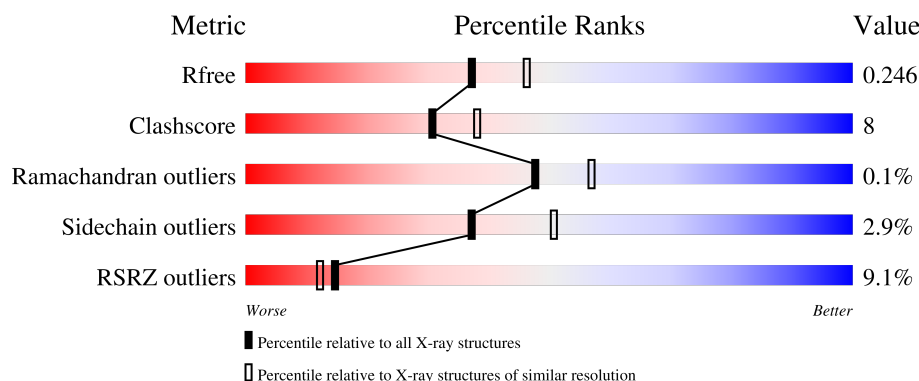
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	506	83% 12% 5%
1	B	506	16% 73% 21% 5%
2	C	4	50% 50%
2	D	4	75% 25%

2 Entry composition

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.

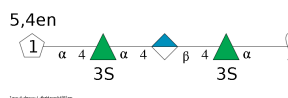
- Molecule 1 is a protein called Short ulvan lyase.

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.

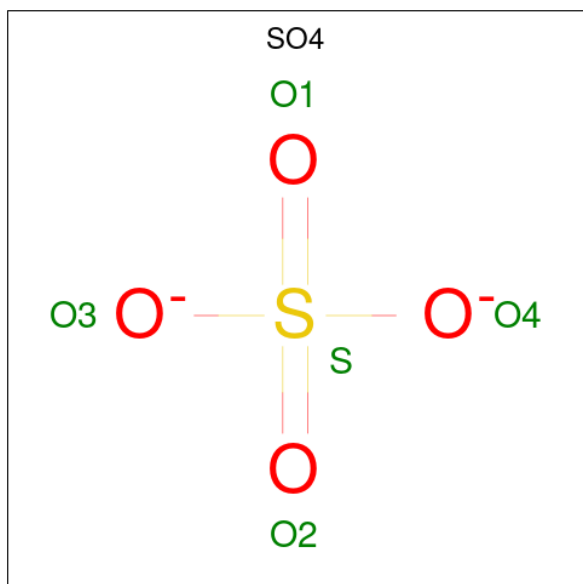


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	4	Total	C	H	O	S	0	0	0
			82	24	30	26	2			
2	D	4	Total	C	H	O	S	0	0	0
			82	24	30	26	2			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



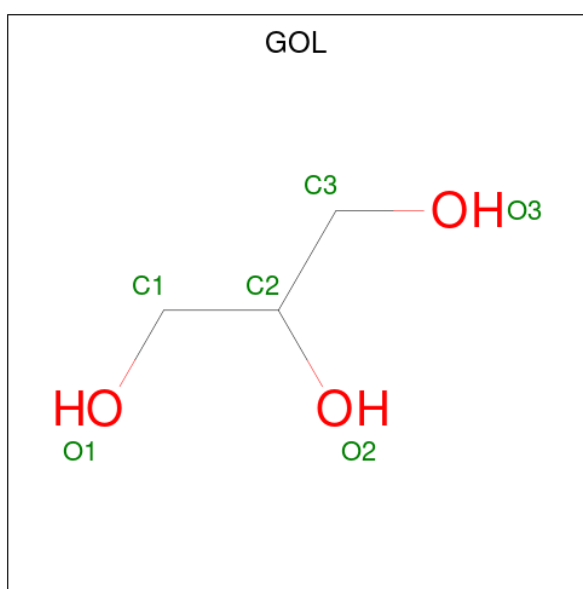
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

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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 (CCD ID: 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

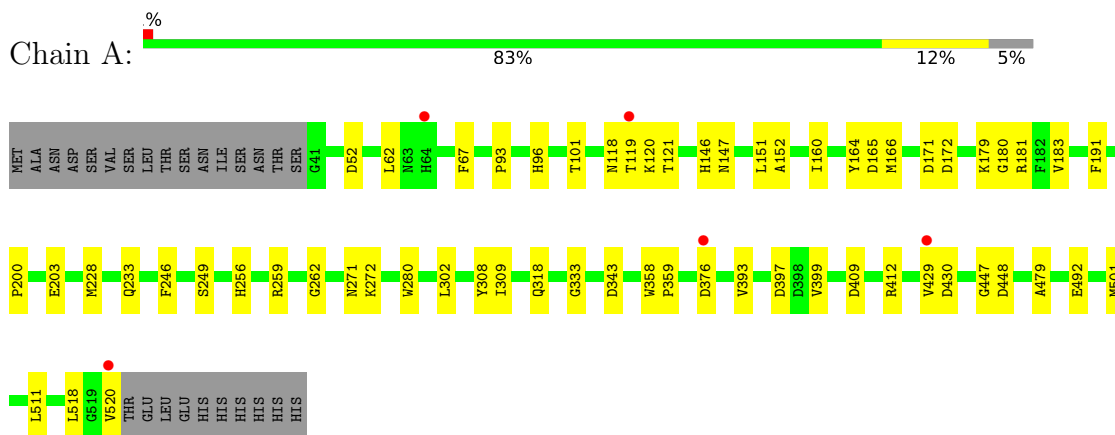
- Molecule 6 is water.

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

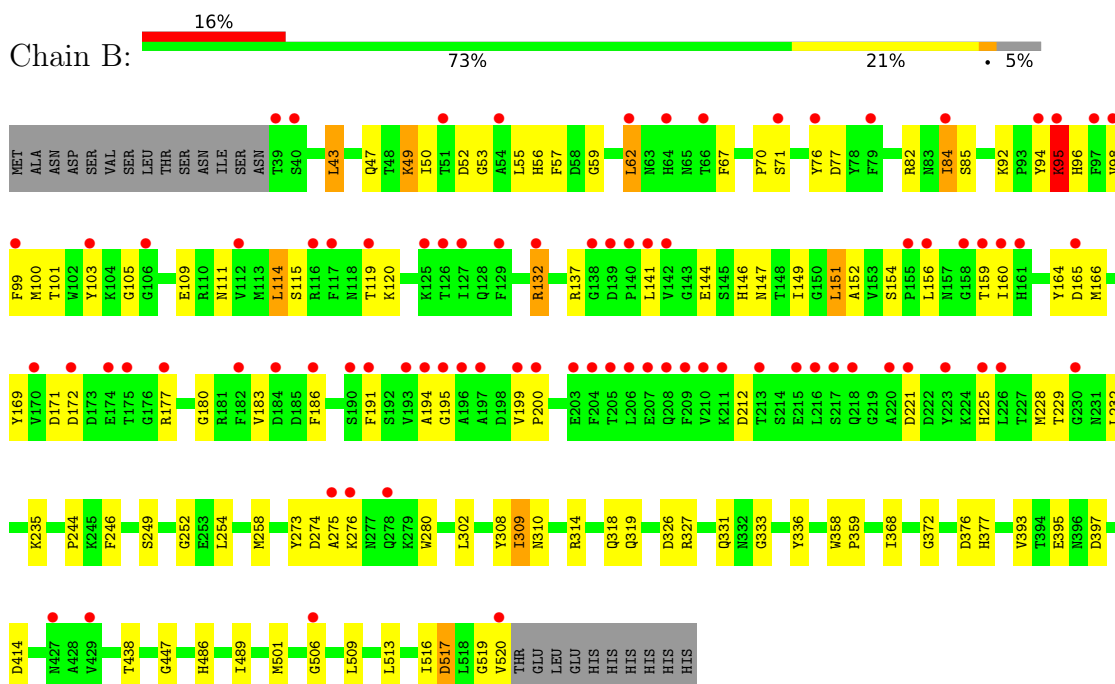
3 Residue-property plots [i](#)

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



- Molecule 1: Short ulvan lyase



- 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:  50% 50%

83Y1
BDP2
83Y3
GCD4

- 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:  75% 25%

83Y1
BDP2
83Y3
GCD4

4 Data and refinement statistics

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 49.05 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.05-2.20) 99.9 (49.05-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.200 , 0.247 0.201 , 0.246	Depositor DCC
R_{free} test set	5067 reflections (4.99%)	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 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.008 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BDP, GOL, CA, 83Y, GCD, SO4

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	0/3957	0.54	0/5365
1	B	0.41	2/3901 (0.1%)	0.56	2/5298 (0.0%)
All	All	0.38	2/7858 (0.0%)	0.55	2/10663 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	517	ASP	C-O	-5.95	1.16	1.24
1	B	516	ILE	C-O	-5.61	1.18	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	LYS	CA-C-N	5.97	132.94	121.54
1	B	95	LYS	C-N-CA	5.97	132.94	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3843	0	3563	34	0
1	B	3791	0	3447	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	0
6	B	140	0	0	8	0
All	All	8120	84	7055	123	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 (123) 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:147:ASN:HB3	1:B:165:ASP:HA	1.66	0.78
1:B:56:HIS:CG	1:B:501:MET:HE1	2.21	0.75
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:B:501:MET:HE3	1:B:509:LEU:HD12	1.73	0.69
1:A:200:PRO:HD2	1:A:203:GLU:OE1	1.93	0.68
1:B:56:HIS:ND1	1:B:501:MET:HE1	2.09	0.67
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:98:VAL:HG12	1:B:100:MET:HE2	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:273:TYR:CE2	1:B:275:ALA:HB2	2.39	0.56
1:B:228:MET:HE2	1:B:280:TRP:CD2	2.42	0.55
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:501:MET:HE3	1:B:509:LEU:CD1	2.38	0.54
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:B:212:ASP:CG	6:B:701:HOH:O	2.50	0.53
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:43:LEU:C	1:B:43:LEU:HD12	2.36	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:LEU:HD23	1:B:151:LEU:C	2.38	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:98:VAL:CG1	1:B:100:MET:HE2	2.43	0.47
1:B:318:GLN:HG2	1:B:333:GLY:O	2.15	0.47
1:B:114:LEU:HD23	1:B:115:SER:N	2.29	0.46
1:A:358:TRP:HA	1:A:359:PRO:C	2.40	0.46
1:B:96:HIS:O	1:B:119:THR:HB	2.16	0.46
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:228:MET:HE2	1:A:280:TRP:CD2	2.51	0.45
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:358:TRP:HA	1:B:359:PRO:C	2.41	0.45
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: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:B:114:LEU:C	1:B:114:LEU:CD2	2.91	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:B:49:LYS:C	1:B:50:ILE:HD13	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:A:501:MET:HE3	1:A:511:LEU:HD21	2.04	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	43	51
All	All	959/1012 (95%)	915 (95%)	43 (4%)	1 (0%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	95	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	402/434 (93%)	395 (98%)	7 (2%)	53	69
1	B	386/434 (89%)	370 (96%)	16 (4%)	27	37
All	All	788/868 (91%)	765 (97%)	23 (3%)	37	51

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ASP
1	A	120	LYS
1	A	233	GLN
1	A	309	ILE
1	A	376	ASP
1	A	397	ASP
1	A	518	LEU
1	B	43	LEU
1	B	49	LYS
1	B	52	ASP
1	B	62	LEU
1	B	84	ILE
1	B	114	LEU
1	B	132	ARG
1	B	144	GLU
1	B	151	LEU
1	B	221	ASP
1	B	276	LYS
1	B	309	ILE
1	B	376	ASP
1	B	397	ASP
1	B	438	THR
1	B	489	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	305	GLN
1	A	347	ASN
1	B	128	GLN
1	B	305	GLN

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 ⓘ

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	1.64	2 (13%)	21,23,23	2.05	7 (33%)
2	BDP	C	2	2	12,12,13	1.33	2 (16%)	14,17,19	1.65	3 (21%)
2	83Y	C	3	2	14,14,15	1.12	2 (14%)	18,21,23	1.56	3 (16%)
2	GCD	C	4	2	10,11,12	2.26	2 (20%)	12,15,17	2.76	7 (58%)
2	83Y	D	1	2	15,15,15	1.02	1 (6%)	21,23,23	1.46	5 (23%)
2	BDP	D	2	2	12,12,13	1.22	2 (16%)	14,17,19	1.53	2 (14%)
2	83Y	D	3	2	14,14,15	1.03	1 (7%)	18,21,23	1.20	1 (5%)
2	GCD	D	4	2	10,11,12	2.23	4 (40%)	12,15,17	1.63	3 (25%)

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	-	1/5/22/25	0/1/1/1
2	GCD	C	4	2	-	0/4/17/20	0/1/1/1
2	83Y	D	1	2	-	1/5/25/25	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	6.03	1.45	1.37
2	D	4	GCD	O5-C5	5.26	1.44	1.37
2	C	1	83Y	O3-S	-4.40	1.44	1.57
2	C	1	83Y	O3-C3	-3.32	1.38	1.46
2	C	2	BDP	O6B-C6	-2.73	1.21	1.30
2	D	4	GCD	O6B-C6	-2.72	1.23	1.30
2	D	1	83Y	O3-S	-2.66	1.49	1.57
2	D	2	BDP	O5-C1	-2.58	1.39	1.43
2	D	4	GCD	C5-C6	-2.54	1.43	1.48
2	C	2	BDP	C5-C6	-2.54	1.47	1.53
2	C	3	83Y	O3-S	-2.53	1.49	1.57
2	C	4	GCD	O6B-C6	-2.53	1.23	1.30
2	D	2	BDP	O6B-C6	-2.49	1.22	1.30
2	D	3	83Y	O3-S	-2.41	1.50	1.57
2	D	4	GCD	O5-C1	-2.27	1.41	1.45
2	C	3	83Y	O3-C3	-2.16	1.41	1.46

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	GCD	O5-C5-C6	5.63	122.19	111.85
2	C	4	GCD	O5-C5-C4	-5.36	120.02	124.94
2	C	1	83Y	O5-C1-C2	-4.09	103.10	110.30
2	C	1	83Y	C4-C3-C2	4.05	116.48	110.86
2	D	4	GCD	O5-C5-C4	-3.64	121.59	124.94
2	C	1	83Y	C6-C5-C4	-3.47	106.73	113.08
2	C	2	BDP	O4-C4-C5	-3.27	102.30	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	83Y	C3-O3-S	3.25	126.83	119.04
2	C	1	83Y	O4-C4-C5	-3.21	102.65	109.74
2	C	3	83Y	O4-C4-C5	-3.16	102.76	109.74
2	D	1	83Y	O5-C1-C2	-2.97	105.08	110.30
2	D	2	BDP	O4-C4-C5	-2.88	103.17	109.76
2	C	1	83Y	O3S-S-O2S	2.81	118.37	108.56
2	D	4	GCD	O5-C5-C6	2.73	116.87	111.85
2	C	4	GCD	O6B-C6-C5	2.67	120.12	114.06
2	C	4	GCD	C4-C5-C6	-2.66	117.79	123.56
2	C	3	83Y	O3S-S-O3	2.63	112.41	106.37
2	C	2	BDP	O6B-C6-C5	2.60	123.03	113.64
2	C	4	GCD	O3-C3-C4	-2.49	103.65	109.27
2	D	1	83Y	O3S-S-O3	2.48	112.07	106.37
2	D	4	GCD	C1-C2-C3	2.44	113.20	109.64
2	C	1	83Y	O5-C5-C4	2.32	113.73	109.55
2	D	1	83Y	O5-C5-C4	2.30	113.70	109.55
2	D	3	83Y	O4-C4-C3	-2.25	104.17	109.94
2	C	2	BDP	O6A-C6-C5	-2.15	113.03	120.81
2	D	1	83Y	O4-C4-C5	-2.13	105.04	109.74
2	D	2	BDP	O3-C3-C2	-2.13	105.71	110.05
2	C	1	83Y	C1-C2-C3	-2.07	106.17	110.37
2	C	4	GCD	O6B-C6-O6A	-2.04	119.05	123.90
2	C	4	GCD	C1-O5-C5	2.00	119.67	115.42
2	D	1	83Y	O2S-S-O1S	-2.00	104.51	112.24

There are no chirality outliers.

All (14) 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
2	C	3	83Y	C2-C3-O3-S

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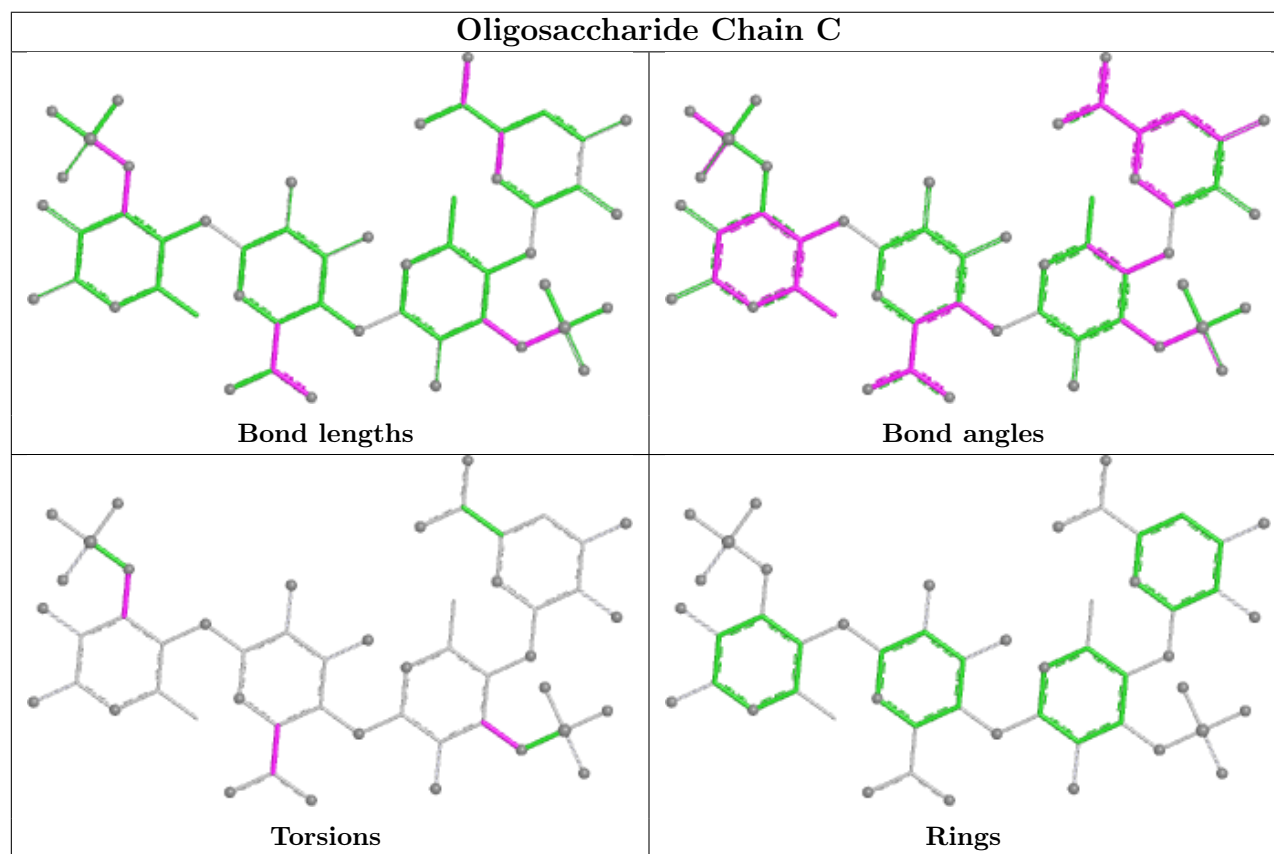
Mol	Chain	Res	Type	Atoms
2	D	1	83Y	C4-C3-O3-S

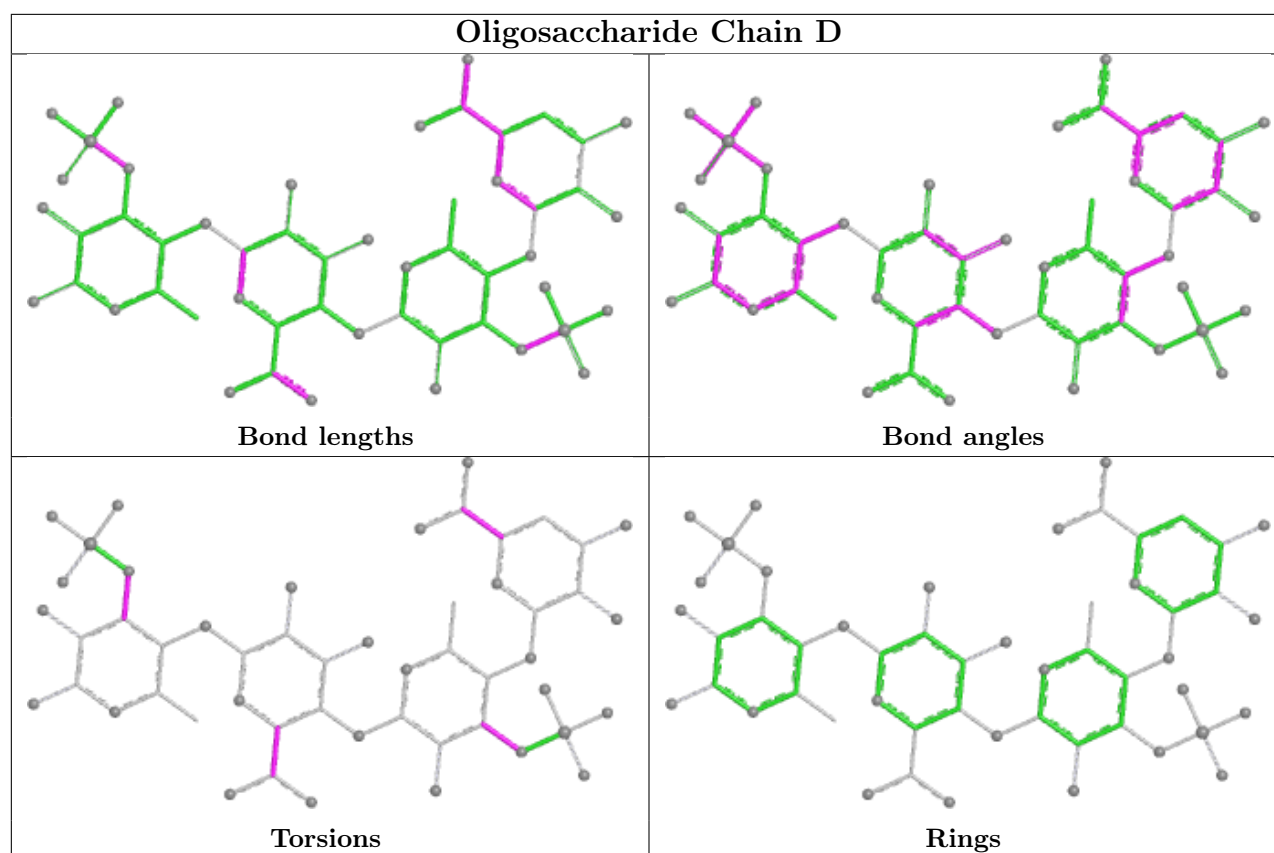
There are no ring outliers.

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.





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	0.24	0	6,6,6	0.24	0
4	SO4	B	603	-	4,4,4	0.27	0	6,6,6	0.31	0
5	GOL	A	606	-	5,5,5	1.26	1 (20%)	5,5,5	0.99	0
4	SO4	B	606	-	4,4,4	0.24	0	6,6,6	0.12	0
4	SO4	A	603	-	4,4,4	0.29	0	6,6,6	0.27	0
5	GOL	B	607	-	5,5,5	1.13	0	5,5,5	0.86	0
5	GOL	B	608	-	5,5,5	1.22	0	5,5,5	0.97	0
4	SO4	B	604	-	4,4,4	0.25	0	6,6,6	0.24	0
4	SO4	A	604	-	4,4,4	0.26	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	605	-	4,4,4	0.25	0	6,6,6	0.06	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	A	606	-	-	1/4/4/4	-
5	GOL	B	608	-	-	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	-2.30	1.36	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (4) 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-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	606	GOL	1	0
4	B	604	SO4	1	0

5.7 Other polymers [i](#)

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(Å ²)	Q<0.9
1	A	480/506 (94%)	-0.21	5 (1%) 79 77	23, 42, 70, 88	1 (0%)
1	B	482/506 (95%)	0.74	83 (17%) 4 3	25, 57, 90, 114	0
All	All	962/1012 (95%)	0.26	88 (9%) 15 12	23, 47, 86, 114	1 (0%)

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	160	ILE	6.2
1	B	196	ALA	6.2
1	B	210	VAL	5.1
1	B	200	PRO	4.8
1	B	197	ALA	4.3
1	B	230	GLY	4.1
1	B	39	THR	3.8
1	A	520	VAL	3.8
1	B	520	VAL	3.8
1	B	117	PHE	3.7
1	B	429	VAL	3.5
1	B	209	PHE	3.5
1	B	220	ALA	3.5
1	B	40	SER	3.5
1	B	158	GLY	3.5
1	B	211	LYS	3.4
1	B	216	LEU	3.4
1	B	94	TYR	3.4
1	B	156	LEU	3.3
1	B	275	ALA	3.2
1	B	126	THR	3.2
1	B	193	VAL	3.1
1	B	194	ALA	3.0
1	B	177	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	138	GLY	2.9
1	B	97	PHE	2.9
1	B	184	ASP	2.9
1	B	186	PHE	2.8
1	B	207	GLU	2.8
1	B	213	THR	2.8
1	B	206	LEU	2.7
1	B	223	TYR	2.7
1	B	129	PHE	2.7
1	B	98	VAL	2.7
1	B	95	LYS	2.7
1	A	376	ASP	2.6
1	B	141	LEU	2.6
1	B	195	GLY	2.6
1	B	506	GLY	2.6
1	B	62	LEU	2.6
1	B	119	THR	2.6
1	B	125	LYS	2.6
1	B	203	GLU	2.5
1	B	140	PRO	2.5
1	B	199	VAL	2.5
1	B	276	LYS	2.5
1	A	64	HIS	2.5
1	A	119	THR	2.5
1	B	79	PHE	2.4
1	B	226	LEU	2.4
1	B	278	GLN	2.4
1	B	155	PRO	2.4
1	B	217	SER	2.4
1	B	172	ASP	2.4
1	B	106	GLY	2.4
1	B	182	PHE	2.4
1	B	218	GLN	2.4
1	B	132	ARG	2.3
1	B	175	THR	2.3
1	B	221	ASP	2.3
1	B	64	HIS	2.3
1	A	429	VAL	2.3
1	B	170	VAL	2.3
1	B	103	TYR	2.3
1	B	205	THR	2.3
1	B	190	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	127	ILE	2.3
1	B	204	PHE	2.2
1	B	191	PHE	2.2
1	B	174	GLU	2.2
1	B	142	VAL	2.2
1	B	54	ALA	2.2
1	B	66	THR	2.2
1	B	76	TYR	2.2
1	B	139	ASP	2.2
1	B	225	HIS	2.2
1	B	84	ILE	2.1
1	B	112	VAL	2.1
1	B	215	GLU	2.1
1	B	208	GLN	2.1
1	B	51	THR	2.1
1	B	71	SER	2.1
1	B	161	HIS	2.1
1	B	165	ASP	2.1
1	B	99	PHE	2.1
1	B	159	THR	2.0
1	B	116	ARG	2.0
1	B	427	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

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

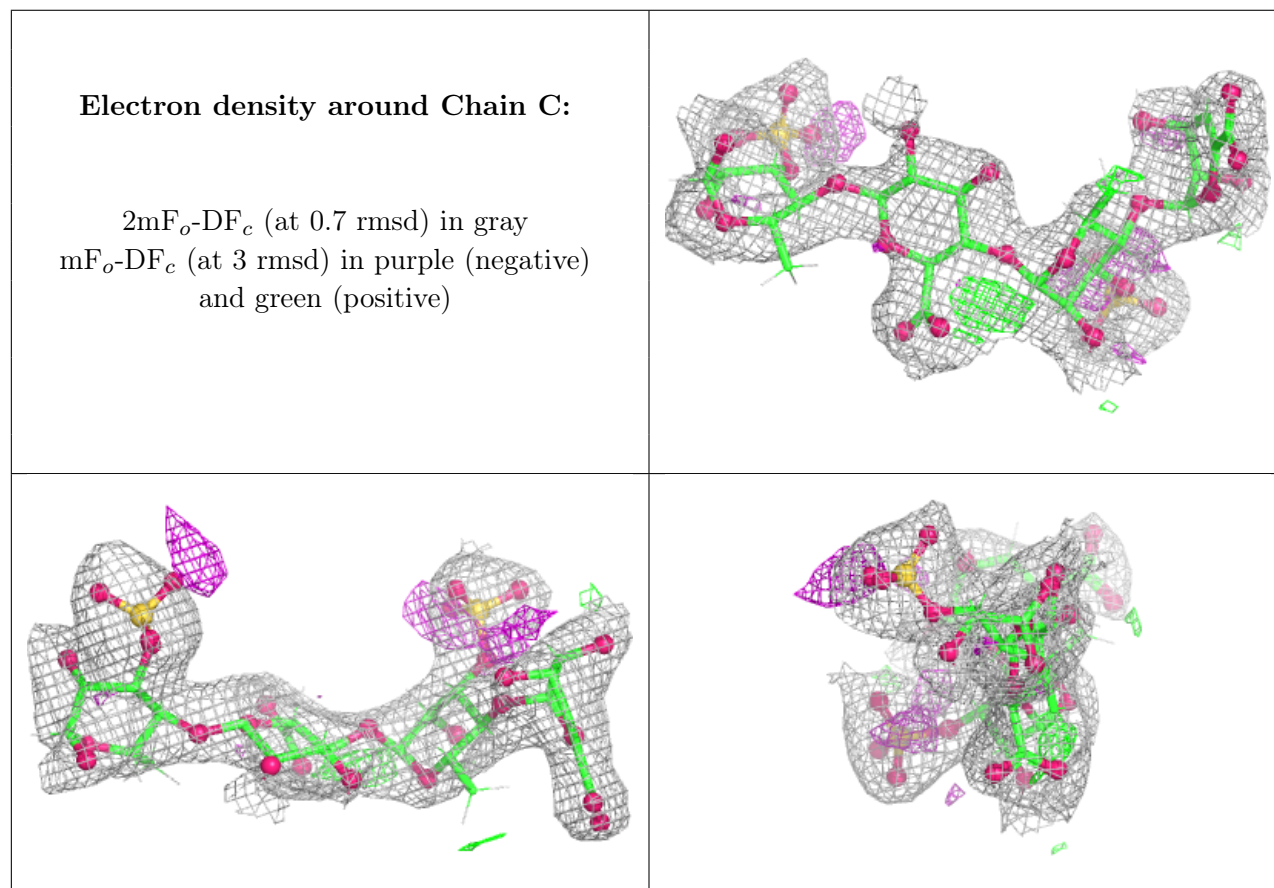
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	83Y	D	1	15/15	0.68	0.18	96,114,135,140	0
2	GCD	D	4	11/12	0.75	0.14	88,100,121,123	0
2	BDP	C	2	12/13	0.76	0.16	68,101,121,125	0
2	BDP	D	2	12/13	0.79	0.14	76,94,113,114	0
2	83Y	D	3	14/15	0.80	0.16	78,99,119,123	0
2	GCD	C	4	11/12	0.80	0.13	82,88,102,104	0

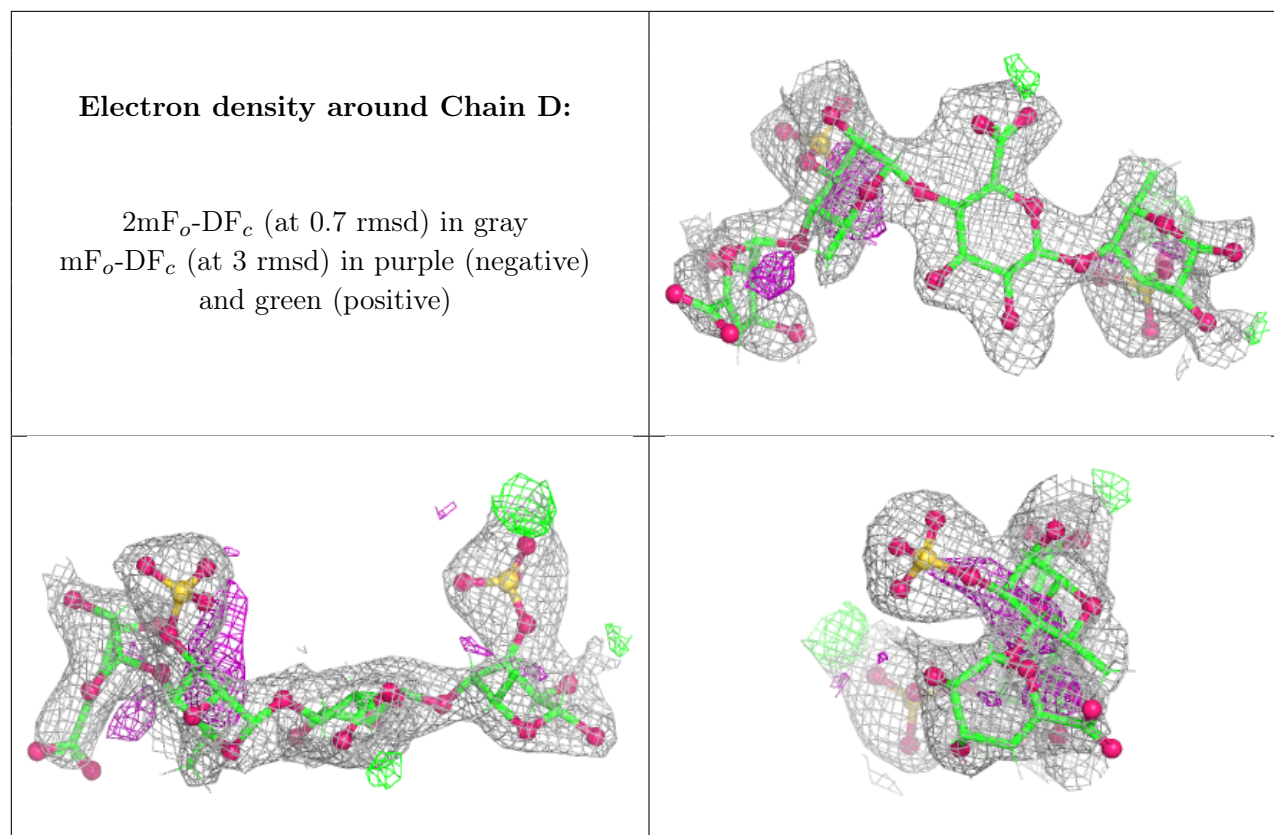
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	83Y	C	1	15/15	0.82	0.16	84,119,142,144	0
2	83Y	C	3	14/15	0.85	0.14	58,84,110,110	0

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.





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, 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	GOL	B	608	6/6	0.70	0.15	49,77,97,98	0
5	GOL	A	606	6/6	0.74	0.17	63,78,94,100	0
5	GOL	B	607	6/6	0.82	0.20	68,92,108,110	0
4	SO4	B	606	5/5	0.84	0.13	94,97,101,106	0
4	SO4	A	605	5/5	0.84	0.14	93,100,100,103	0
4	SO4	B	605	5/5	0.86	0.13	92,95,101,107	0
4	SO4	A	604	5/5	0.90	0.10	85,86,88,94	0
4	SO4	B	604	5/5	0.91	0.10	67,84,88,92	0
3	CA	B	602	1/1	0.95	0.06	55,55,55,55	0
4	SO4	A	603	5/5	0.97	0.07	39,47,56,66	0
4	SO4	B	603	5/5	0.97	0.07	57,57,59,63	0
3	CA	A	601	1/1	0.98	0.05	38,38,38,38	0
3	CA	A	602	1/1	0.99	0.05	42,42,42,42	0
3	CA	B	601	1/1	1.00	0.02	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.