



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:16 PM UTC

PDB ID : 3CK9 / pdb_00003ck9
Title : B. thetaiotaomicron SusD with maltoheptaose
Authors : Koropatkin, N.M.; Martens, E.C.; Gordon, J.I.; Smith, T.J.
Deposited on : 2008-03-14
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

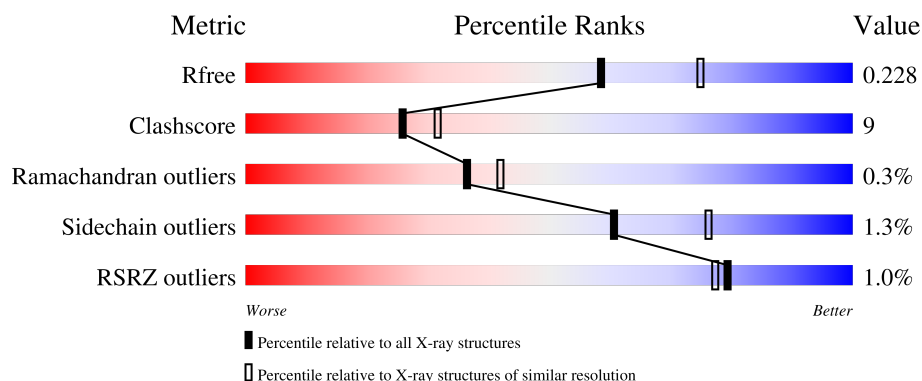
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

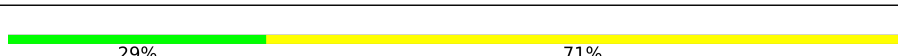
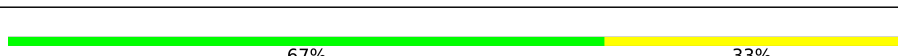
The reported resolution of this entry is 2.20 Å.

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	527	
1	B	527	
2	C	7	
3	D	6	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	C	1	X	-	-	-
5	EDO	B	741	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9125 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called SusD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	508	Total	C	N	O	S	0	0	0
			4075	2562	701	793	19			
1	B	515	Total	C	N	O	S	0	0	0
			4121	2590	709	803	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	GLY	-	expression tag	UNP Q8A1G2
A	100	LYS	GLU	SEE REMARK 999	UNP Q8A1G2
B	25	GLY	-	expression tag	UNP Q8A1G2
B	100	LYS	GLU	SEE REMARK 999	UNP Q8A1G2

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	7	Total	C	O	0	0	0
			78	42	36			

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

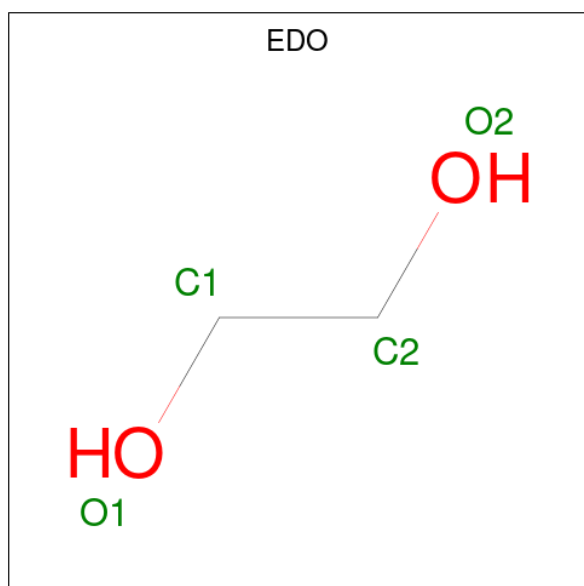


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	6	Total	C	O	0	0	0
			67	36	31			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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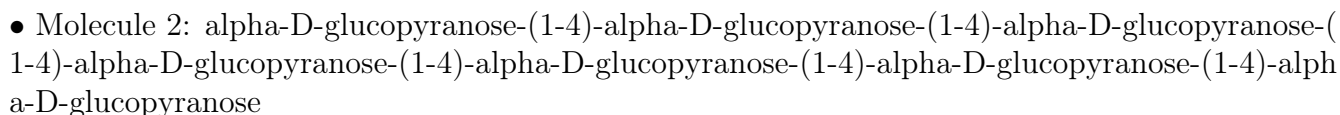
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	407	Total O 407 407	0	0
6	B	321	Total O 321 321	0	0

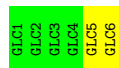
- Molecule 1: SusD





- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain D:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.61Å 73.22Å 83.38Å 65.06° 72.19° 69.73°	Depositor
Resolution (Å)	60.20 – 2.20 60.20 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.6 (60.20-2.20) 93.4 (60.20-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 2.18Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.185 , 0.222 0.192 , 0.228	Depositor DCC
R_{free} test set	5665 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å ²)	13.0	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9125	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, GLC, 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	0.38	0/4167	0.88	14/5638 (0.2%)
1	B	0.39	1/4215 (0.0%)	0.88	11/5704 (0.2%)
All	All	0.38	1/8382 (0.0%)	0.88	25/11342 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	279	MET	SD-CE	-6.18	1.64	1.79

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	GLY	N-CA-C	-9.13	96.25	110.77
1	B	533	ILE	N-CA-C	-7.46	101.64	108.95
1	B	370	ARG	N-CA-C	-6.81	101.36	110.55
1	A	507	THR	N-CA-C	6.80	118.63	110.19
1	A	533	ILE	N-CA-C	-6.79	102.79	108.63
1	A	489	PHE	N-CA-C	6.74	121.58	112.88
1	A	396	ILE	N-CA-C	-6.48	105.42	111.45
1	A	175	PHE	N-CA-C	6.25	120.47	109.96
1	A	78	GLY	N-CA-C	6.22	119.08	111.93
1	B	175	PHE	N-CA-C	6.04	120.11	109.96
1	B	489	PHE	N-CA-C	5.66	120.19	112.88
1	A	91	THR	N-CA-C	5.63	119.09	110.36
1	B	323	ILE	N-CA-C	5.59	116.36	108.36
1	B	507	THR	N-CA-C	5.55	118.01	110.35
1	A	188	LYS	N-CA-C	5.53	117.03	109.18
1	B	93	GLU	N-CA-C	5.49	118.44	111.69
1	B	318	ASN	N-CA-C	5.47	117.76	108.02
1	A	222	ALA	N-CA-C	-5.43	105.44	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	ILE	CA-C-N	5.35	125.35	119.90
1	A	349	ILE	C-N-CA	5.35	125.35	119.90
1	B	188	LYS	N-CA-C	5.19	116.55	109.18
1	A	282	ILE	N-CA-C	5.14	114.67	107.37
1	A	370	ARG	N-CA-C	-5.11	102.92	110.48
1	A	97	ALA	N-CA-C	5.03	116.77	111.28
1	B	174	PRO	N-CA-C	-5.02	102.13	112.47

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	4075	0	3879	64	0
1	B	4121	0	3926	90	0
2	C	78	0	66	2	0
3	D	67	0	57	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	20	0	29	2	0
5	B	32	0	48	7	0
6	A	407	0	0	7	0
6	B	321	0	0	8	0
All	All	9125	0	8005	155	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 9.

All (155) 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:C:1:GLC:H1	2:C:7:GLC:O3	1.57	1.05
1:A:44:GLN:HE21	1:A:151:GLN:HE22	1.18	0.90
1:B:484:GLU:HA	1:B:487:ARG:HH12	1.39	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:ASN:HD22	1:B:227:ARG:HH12	1.22	0.85
1:B:484:GLU:HA	1:B:487:ARG:NH1	1.93	0.84
1:B:275:ASN:N	1:B:279:MET:HE2	1.94	0.82
1:A:174:PRO:O	5:A:737:EDO:H22	1.84	0.78
1:A:93:GLU:HG3	1:A:495:ARG:HG2	1.66	0.77
1:A:166:PHE:HB3	1:A:173:ALA:HB2	1.66	0.77
1:A:44:GLN:HE21	1:A:151:GLN:NE2	1.83	0.77
1:B:100:LYS:HE3	1:B:100:LYS:HA	1.68	0.76
1:A:201:ASN:HD22	1:A:227:ARG:HH12	1.37	0.71
1:B:90:PRO:HB3	1:B:107:LEU:O	1.90	0.71
1:B:284:LEU:HB3	1:B:436:PHE:HB2	1.71	0.71
1:B:487:ARG:HH11	1:B:487:ARG:HB2	1.56	0.71
1:B:166:PHE:HB3	1:B:173:ALA:HB2	1.73	0.69
1:A:291:VAL:HG23	1:A:292:LYS:HG3	1.75	0.69
1:A:101:ASN:HB2	1:A:104:ILE:HG13	1.73	0.68
1:B:201:ASN:HD22	1:B:227:ARG:NH1	1.91	0.68
1:B:295:ASN:ND2	1:B:297:GLY:H	1.92	0.67
1:A:470:THR:HG21	6:A:1151:HOH:O	1.94	0.66
1:A:284:LEU:HB3	1:A:436:PHE:HB2	1.76	0.66
1:B:93:GLU:HG3	1:B:495:ARG:HG2	1.78	0.66
1:A:87:ASN:HD22	1:A:496:ARG:HB3	1.62	0.64
1:A:295:ASN:ND2	1:A:297:GLY:H	1.96	0.63
1:B:504:MET:HB3	1:B:510:TYR:HB3	1.79	0.63
1:B:291:VAL:HG23	1:B:292:LYS:HG3	1.81	0.62
1:B:188:LYS:HD3	1:B:188:LYS:H	1.65	0.61
1:B:150:ARG:HD3	1:B:208:TYR:CE1	2.37	0.60
1:B:303:VAL:O	1:B:307:ARG:HG2	2.02	0.60
1:B:275:ASN:H	1:B:279:MET:HE2	1.67	0.59
1:A:87:ASN:ND2	1:A:496:ARG:HB3	2.17	0.59
1:B:184:PRO:HB2	6:B:1245:HOH:O	2.02	0.59
1:A:59:GLY:C	1:A:60:GLN:HG3	2.28	0.58
1:A:344:PRO:HB2	1:A:347:VAL:HG23	1.86	0.58
1:B:150:ARG:HG3	1:B:150:ARG:HH11	1.69	0.58
1:B:484:GLU:CD	1:B:487:ARG:HH12	2.12	0.57
1:A:479:GLN:NE2	6:A:1211:HOH:O	2.36	0.57
1:B:67:PRO:HG2	1:B:124:VAL:CG1	2.34	0.57
1:A:422:PRO:HG3	1:B:362:ALA:HB1	1.87	0.57
1:B:365:ALA:HB2	1:B:370:ARG:HD3	1.86	0.56
1:B:320:TRP:HE1	5:B:741:EDO:H11	1.70	0.56
1:B:363:PHE:CE1	1:B:389:VAL:HG11	2.41	0.55
1:B:344:PRO:HB2	1:B:347:VAL:HG23	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:THR:HG21	5:B:741:EDO:H21	1.87	0.55
1:B:95:LEU:HD13	1:B:326:ARG:NE	2.22	0.54
1:B:53:ALA:O	1:B:57:VAL:HG22	2.07	0.54
1:B:101:ASN:HB2	1:B:104:ILE:HG13	1.89	0.54
1:B:209:GLU:OE2	1:B:220:LYS:HE3	2.08	0.54
1:B:201:ASN:ND2	1:B:227:ARG:HH12	2.00	0.54
1:A:273:ASP:OD1	1:A:274:GLU:HG3	2.09	0.53
1:A:150:ARG:HD3	1:A:208:TYR:CE1	2.44	0.53
1:B:164:TRP:CZ2	1:B:229:ARG:HD3	2.44	0.53
1:A:365:ALA:HB2	1:A:370:ARG:HD3	1.92	0.52
1:A:289:ASP:OD1	1:A:291:VAL:HG22	2.08	0.52
1:B:487:ARG:HH11	1:B:487:ARG:CB	2.23	0.52
1:B:541:ASN:ND2	6:B:1245:HOH:O	2.43	0.52
1:B:60:GLN:HB2	1:B:63:ILE:HB	1.92	0.51
1:B:541:ASN:OD1	1:B:543:ASN:HB2	2.11	0.51
1:A:53:ALA:O	1:A:57:VAL:HG22	2.11	0.51
1:A:394:ARG:HG2	1:A:394:ARG:HH11	1.76	0.50
1:B:243:TYR:CZ	1:B:451:ARG:HD2	2.46	0.50
1:A:344:PRO:HB3	6:A:1193:HOH:O	2.11	0.50
1:B:366:GLU:HG3	6:B:1191:HOH:O	2.12	0.50
1:B:318:ASN:HD22	5:B:741:EDO:C1	2.25	0.50
1:A:78:GLY:HA3	6:A:808:HOH:O	2.11	0.50
1:B:296:TYR:CE1	5:B:742:EDO:H21	2.48	0.49
1:A:104:ILE:HB	1:A:105:PRO:HD3	1.94	0.49
1:A:95:LEU:HG	1:A:326:ARG:HG2	1.95	0.49
1:B:310:GLY:O	1:B:360:ILE:HD13	2.12	0.49
1:A:127:GLY:O	1:A:131:THR:HG23	2.12	0.49
1:B:150:ARG:HG3	1:B:150:ARG:NH1	2.27	0.49
1:B:50:LYS:HG3	6:B:1062:HOH:O	2.12	0.49
1:B:281:GLU:HG3	1:B:438:LEU:HB3	1.96	0.48
1:A:166:PHE:CB	1:A:173:ALA:HB2	2.41	0.47
1:B:484:GLU:CD	1:B:487:ARG:NH1	2.72	0.47
1:B:208:TYR:O	1:B:220:LYS:HG3	2.15	0.47
1:A:201:ASN:HD22	1:A:227:ARG:NH1	2.09	0.47
1:B:486:ALA:O	1:B:490:TYR:HB3	2.15	0.47
1:A:80:TYR:CE2	1:A:433:ILE:HG21	2.50	0.47
1:B:188:LYS:HD3	1:B:188:LYS:N	2.29	0.47
1:A:310:GLY:O	1:A:360:ILE:HD13	2.15	0.46
1:B:394:ARG:HH11	1:B:394:ARG:HG3	1.79	0.46
1:B:87:ASN:HD22	1:B:496:ARG:HD3	1.80	0.46
1:B:143:MET:HB2	1:B:148:THR:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ASN:ND2	1:A:227:ARG:HH12	2.11	0.46
1:B:379:GLY:O	1:B:469:CYS:HA	2.15	0.46
1:A:92:ASP:HB3	1:A:512:TRP:CD2	2.51	0.46
1:B:282:ILE:HG21	1:B:285:PRO:HB3	1.98	0.46
1:B:294:ARG:HB2	5:B:742:EDO:H12	1.97	0.46
1:B:427:THR:CG2	5:B:741:EDO:H21	2.45	0.46
1:A:308:VAL:HB	1:A:321:SER:HB3	1.97	0.46
1:B:295:ASN:C	1:B:295:ASN:HD22	2.23	0.46
1:B:487:ARG:NH1	1:B:487:ARG:HB2	2.29	0.46
1:A:336:ASN:OD1	1:A:338:GLU:HB2	2.16	0.46
1:A:312:PRO:HD3	1:A:360:ILE:HG21	1.98	0.46
1:B:223:ASN:O	1:B:227:ARG:HG3	2.16	0.45
1:B:302:LEU:HD13	1:B:413:TRP:CE2	2.51	0.45
1:A:220:LYS:O	1:A:223:ASN:HB3	2.16	0.45
1:B:92:ASP:HB3	1:B:512:TRP:CD2	2.52	0.45
1:B:150:ARG:HD2	6:B:1034:HOH:O	2.16	0.45
2:C:1:GLC:H1	2:C:7:GLC:C3	2.43	0.45
1:A:295:ASN:HD22	1:A:295:ASN:C	2.23	0.45
1:B:417:ARG:HD3	1:B:421:LYS:O	2.16	0.44
1:B:143:MET:HE3	6:B:1225:HOH:O	2.16	0.44
1:A:512:TRP:CE2	1:A:515:LYS:HB2	2.52	0.44
1:A:107:LEU:HD22	1:A:118:ARG:HD2	2.00	0.44
1:B:264:TYR:CE1	1:B:382:ARG:HG2	2.53	0.44
1:A:286:ILE:HB	1:A:433:ILE:HB	2.00	0.44
1:B:87:ASN:HA	1:B:496:ARG:HB3	2.00	0.43
1:B:247:GLU:HG3	1:B:445:ARG:HG3	1.99	0.43
1:B:103:ASP:HB2	1:B:117:GLN:HG2	1.99	0.43
1:A:415:ASN:HD21	1:A:430:ASP:H	1.64	0.43
1:B:295:ASN:ND2	1:B:295:ASN:C	2.76	0.43
1:A:303:VAL:O	1:A:307:ARG:HG2	2.19	0.43
1:A:425:HIS:CE1	1:A:427:THR:HB	2.54	0.43
1:B:92:ASP:HB3	1:B:512:TRP:CG	2.53	0.43
1:A:192:LEU:O	1:A:196:ILE:HG13	2.19	0.43
1:A:490:TYR:O	1:A:491:LEU:HB2	2.19	0.43
1:B:150:ARG:NH1	1:B:206:ASP:O	2.51	0.43
1:A:466:ARG:HD2	1:A:466:ARG:C	2.44	0.42
1:A:379:GLY:O	1:A:469:CYS:HA	2.19	0.42
1:B:415:ASN:HD21	1:B:430:ASP:H	1.68	0.42
1:A:87:ASN:HD22	1:A:496:ARG:HD3	1.84	0.42
1:A:362:ALA:HB1	1:B:422:PRO:HG3	2.01	0.42
1:B:437:ARG:NH2	1:B:488:GLU:OE2	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:SER:HB2	1:A:517:GLY:N	2.34	0.42
1:B:369:ILE:HD12	1:B:388:GLY:HA2	2.02	0.42
5:A:731:EDO:H21	6:A:1135:HOH:O	2.19	0.42
1:B:109:SER:HB2	1:B:516:GLY:C	2.45	0.41
1:B:336:ASN:OD1	1:B:338:GLU:HB2	2.20	0.41
1:B:284:LEU:CB	1:B:436:PHE:HB2	2.46	0.41
1:A:109:SER:O	1:A:516:GLY:HA2	2.20	0.41
1:B:87:ASN:HD22	1:B:87:ASN:HA	1.69	0.41
1:B:490:TYR:O	1:B:491:LEU:HB2	2.19	0.41
1:B:196:ILE:HG22	1:B:230:LEU:HD11	2.03	0.41
1:B:515:LYS:HA	6:B:1097:HOH:O	2.21	0.41
1:A:295:ASN:ND2	1:A:295:ASN:C	2.78	0.41
1:B:215:PHE:CZ	1:B:285:PRO:HG3	2.56	0.41
1:B:479:GLN:HB2	6:B:1071:HOH:O	2.19	0.41
1:A:386:TYR:CZ	1:A:388:GLY:HA3	2.56	0.41
1:A:541:ASN:OD1	1:A:543:ASN:HB2	2.21	0.41
1:B:475:THR:HG23	1:B:475:THR:O	2.20	0.41
1:A:167:LEU:HD11	1:A:237:TYR:HB3	2.02	0.40
1:A:79:PHE:HA	1:A:125:ARG:HG2	2.03	0.40
1:A:92:ASP:HB3	1:A:512:TRP:CG	2.56	0.40
1:A:59:GLY:N	6:A:879:HOH:O	2.16	0.40
1:A:449:ILE:HG23	6:A:1044:HOH:O	2.20	0.40
1:B:486:ALA:HB2	1:B:495:ARG:CZ	2.51	0.40
1:B:527:TYR:C	1:B:527:TYR:CD1	2.99	0.40
1:A:58:THR:O	1:A:59:GLY:O	2.39	0.40
1:A:289:ASP:HB3	1:A:293:THR:H	1.85	0.40
1:B:294:ARG:CB	5:B:742:EDO:H12	2.51	0.40
1:B:465:LYS:HG3	1:B:472:LYS:HE3	2.03	0.40
1:A:343:LEU:HD12	1:A:344:PRO:HD2	2.02	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	504/527 (96%)	482 (96%)	20 (4%)	2 (0%)	30	34
1	B	513/527 (97%)	489 (95%)	23 (4%)	1 (0%)	43	51
All	All	1017/1054 (96%)	971 (96%)	43 (4%)	3 (0%)	36	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	GLY
1	B	64	ASP
1	A	189	GLY

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	425/441 (96%)	422 (99%)	3 (1%)	76	87
1	B	430/441 (98%)	422 (98%)	8 (2%)	50	66
All	All	855/882 (97%)	844 (99%)	11 (1%)	61	76

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	240	GLN
1	A	318	ASN
1	A	491	LEU
1	B	64	ASP
1	B	95	LEU
1	B	100	LYS
1	B	117	GLN
1	B	188	LYS
1	B	443	LEU
1	B	487	ARG
1	B	491	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	87	ASN
1	A	151	GLN
1	A	201	ASN
1	A	240	GLN
1	A	295	ASN
1	A	331	GLN
1	A	415	ASN
1	A	479	GLN
1	A	508	ASN
1	A	540	ASN
1	A	543	ASN
1	B	44	GLN
1	B	72	GLN
1	B	87	ASN
1	B	99	GLN
1	B	151	GLN
1	B	201	ASN
1	B	275	ASN
1	B	295	ASN
1	B	318	ASN
1	B	331	GLN
1	B	415	ASN
1	B	452	GLN
1	B	540	ASN
1	B	543	ASN

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 ⓘ

13 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	GLC	C	1	2	12,12,12	0.85	0	17,17,17	0.75	0
2	GLC	C	2	2	11,11,12	0.94	0	15,15,17	0.93	0
2	GLC	C	3	2	11,11,12	1.12	0	15,15,17	0.76	0
2	GLC	C	4	2	11,11,12	1.29	1 (9%)	15,15,17	1.04	1 (6%)
2	GLC	C	5	2	11,11,12	1.34	1 (9%)	15,15,17	1.10	1 (6%)
2	GLC	C	6	2	11,11,12	1.28	1 (9%)	15,15,17	0.99	0
2	GLC	C	7	2	11,11,12	0.68	0	15,15,17	0.65	0
3	GLC	D	1	3	12,12,12	1.03	0	17,17,17	0.73	0
3	GLC	D	2	3	11,11,12	1.16	0	15,15,17	0.75	0
3	GLC	D	3	3	11,11,12	1.10	0	15,15,17	0.62	0
3	GLC	D	4	3	11,11,12	1.14	0	15,15,17	0.71	0
3	GLC	D	5	3	11,11,12	1.29	1 (9%)	15,15,17	0.84	0
3	GLC	D	6	3	11,11,12	1.25	2 (18%)	15,15,17	0.68	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
2	GLC	C	1	2	1/1/5/5	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1
2	GLC	C	4	2	-	0/2/19/22	0/1/1/1
2	GLC	C	5	2	-	0/2/19/22	0/1/1/1
2	GLC	C	6	2	-	0/2/19/22	0/1/1/1
2	GLC	C	7	2	-	0/2/19/22	0/1/1/1
3	GLC	D	1	3	-	2/2/22/22	0/1/1/1
3	GLC	D	2	3	-	0/2/19/22	0/1/1/1
3	GLC	D	3	3	-	0/2/19/22	0/1/1/1
3	GLC	D	4	3	-	0/2/19/22	0/1/1/1
3	GLC	D	5	3	-	2/2/19/22	0/1/1/1
3	GLC	D	6	3	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	5	GLC	O5-C1	2.72	1.48	1.43
2	C	4	GLC	C4-C5	2.58	1.58	1.53
3	D	5	GLC	O5-C1	2.27	1.47	1.43
3	D	6	GLC	O5-C1	2.23	1.47	1.43
3	D	6	GLC	C2-C3	2.09	1.55	1.52
2	C	6	GLC	O5-C1	2.04	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	GLC	O4-C4-C3	-2.28	105.00	110.38
2	C	5	GLC	C1-C2-C3	-2.14	106.53	109.64

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1	GLC	C1

All (4) torsion outliers are listed below:

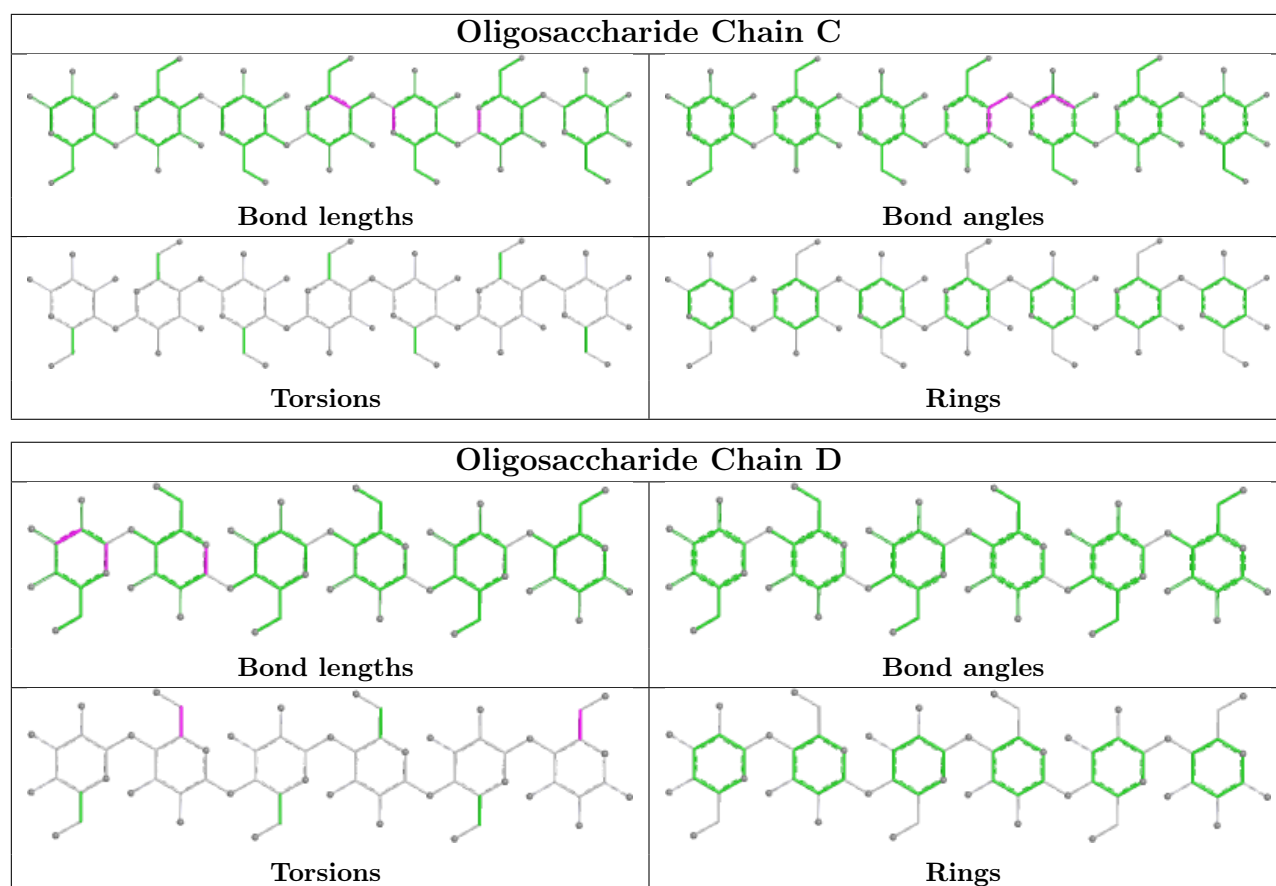
Mol	Chain	Res	Type	Atoms
3	D	5	GLC	O5-C5-C6-O6
3	D	5	GLC	C4-C5-C6-O6
3	D	1	GLC	C4-C5-C6-O6
3	D	1	GLC	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	GLC	2	0
2	C	7	GLC	2	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 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	EDO	A	736	-	3,3,3	0.59	0	2,2,2	0.35	0
5	EDO	A	731	4	3,3,3	0.59	0	2,2,2	0.30	0
5	EDO	B	742	-	3,3,3	0.61	0	2,2,2	0.34	0
5	EDO	B	749	-	3,3,3	0.58	0	2,2,2	0.42	0
5	EDO	B	741	-	3,3,3	0.57	0	2,2,2	0.37	0
5	EDO	A	747	-	3,3,3	0.64	0	2,2,2	0.35	0
5	EDO	B	733	-	3,3,3	0.66	0	2,2,2	0.35	0
5	EDO	B	734	-	3,3,3	0.64	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	B	744	-	3,3,3	0.60	0	2,2,2	0.37	0
5	EDO	B	748	-	3,3,3	0.62	0	2,2,2	0.36	0
5	EDO	A	737	-	3,3,3	0.51	0	2,2,2	0.46	0
5	EDO	A	730	-	3,3,3	0.61	0	2,2,2	0.31	0
5	EDO	B	732	-	3,3,3	0.62	0	2,2,2	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	736	-	-	0/1/1/1	-
5	EDO	A	731	4	-	1/1/1/1	-
5	EDO	B	742	-	-	0/1/1/1	-
5	EDO	B	749	-	-	0/1/1/1	-
5	EDO	B	741	-	-	0/1/1/1	-
5	EDO	A	747	-	-	0/1/1/1	-
5	EDO	B	733	-	-	1/1/1/1	-
5	EDO	B	734	-	-	0/1/1/1	-
5	EDO	B	744	-	-	0/1/1/1	-
5	EDO	B	748	-	-	0/1/1/1	-
5	EDO	A	737	-	-	1/1/1/1	-
5	EDO	A	730	-	-	1/1/1/1	-
5	EDO	B	732	-	-	0/1/1/1	-

There are no bond length outliers.

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	733	EDO	O1-C1-C2-O2
5	A	737	EDO	O1-C1-C2-O2
5	A	730	EDO	O1-C1-C2-O2
5	A	731	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	731	EDO	1	0
5	B	742	EDO	3	0
5	B	741	EDO	4	0
5	A	737	EDO	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	508/527 (96%)	-0.23	7 (1%) 73 71	5, 14, 29, 49	0
1	B	515/527 (97%)	-0.15	3 (0%) 85 83	7, 15, 30, 45	0
All	All	1023/1054 (97%)	-0.19	10 (0%) 79 77	5, 15, 29, 49	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	59	GLY	4.5
1	A	70	ASP	3.6
1	A	60	GLN	3.6
1	B	64	ASP	2.9
1	A	69	LEU	2.8
1	A	68	ASP	2.7
1	B	61	LYS	2.5
1	A	71	GLY	2.4
1	A	37	GLN	2.4
1	B	63	ILE	2.3

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

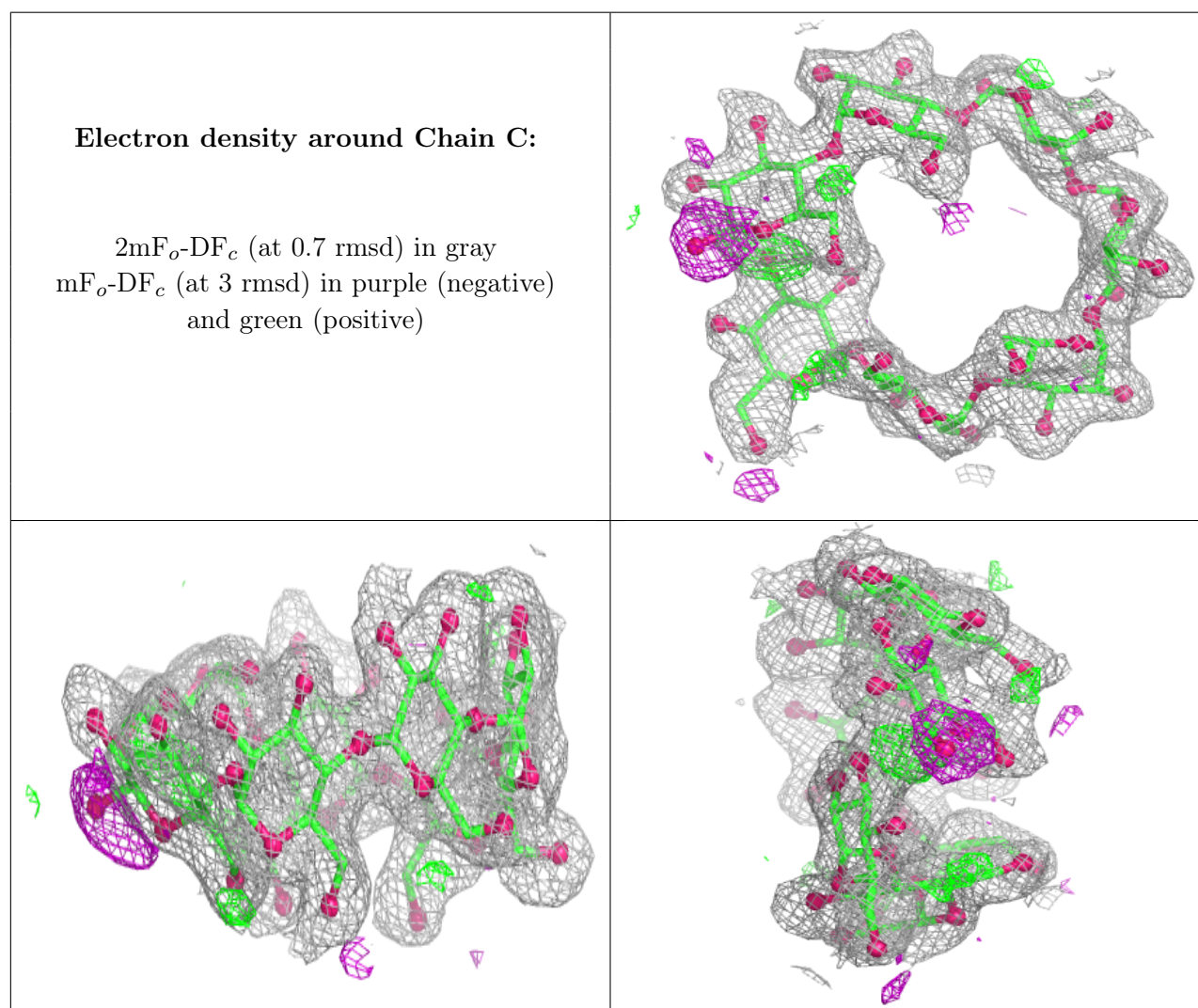
There are no non-standard protein/DNA/RNA residues in this entry.

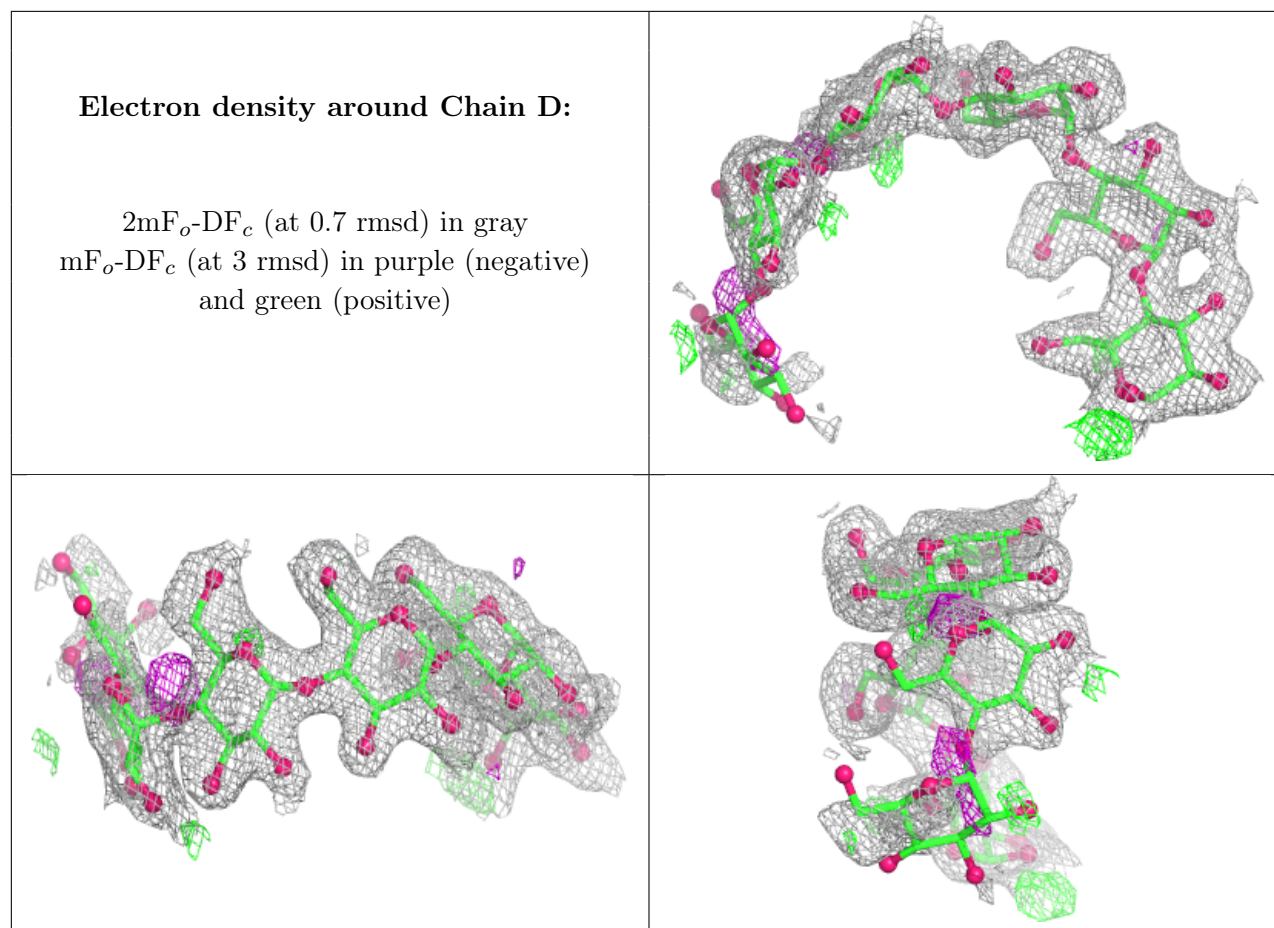
6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GLC	D	6	11/12	0.39	0.22	50,51,52,54	0
2	GLC	C	1	12/12	0.72	0.18	24,29,30,36	0
2	GLC	C	7	11/12	0.75	0.17	28,34,36,36	0
3	GLC	D	5	11/12	0.77	0.14	36,40,45,46	0
2	GLC	C	6	11/12	0.84	0.12	28,30,31,33	0
3	GLC	D	4	11/12	0.84	0.11	22,25,28,34	0
3	GLC	D	1	12/12	0.88	0.09	22,24,26,30	0
2	GLC	C	5	11/12	0.88	0.10	27,28,31,33	0
3	GLC	D	3	11/12	0.91	0.10	11,15,17,20	0
2	GLC	C	4	11/12	0.92	0.08	24,25,27,28	0
3	GLC	D	2	11/12	0.92	0.08	16,17,18,18	0
2	GLC	C	2	11/12	0.92	0.08	20,21,22,23	0
2	GLC	C	3	11/12	0.94	0.07	17,19,20,22	0

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	A	737	4/4	0.72	0.17	28,30,30,34	0
5	EDO	B	734	4/4	0.81	0.17	33,34,34,35	0
5	EDO	B	744	4/4	0.82	0.14	30,32,33,34	0
5	EDO	B	732	4/4	0.85	0.13	36,37,37,37	0
5	EDO	B	742	4/4	0.86	0.13	39,40,41,41	0
5	EDO	B	733	4/4	0.86	0.15	40,40,41,41	0
5	EDO	A	736	4/4	0.88	0.11	27,28,29,29	0
5	EDO	B	741	4/4	0.88	0.14	34,35,35,36	0
5	EDO	A	730	4/4	0.91	0.09	27,27,28,28	0
5	EDO	B	749	4/4	0.92	0.10	24,25,25,28	0
5	EDO	A	747	4/4	0.95	0.10	20,21,23,24	0
5	EDO	A	731	4/4	0.95	0.09	21,22,23,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	B	748	4/4	0.96	0.09	15,19,20,21	0
4	CA	A	710	1/1	0.97	0.03	20,20,20,20	0
4	CA	B	720	1/1	0.98	0.03	20,20,20,20	0
4	CA	A	600	1/1	0.99	0.02	15,15,15,15	0
4	CA	B	700	1/1	0.99	0.02	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.