



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 05:09 AM BST

PDB ID : 3CK9
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 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 : 2.13.1
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) : 2.13.1

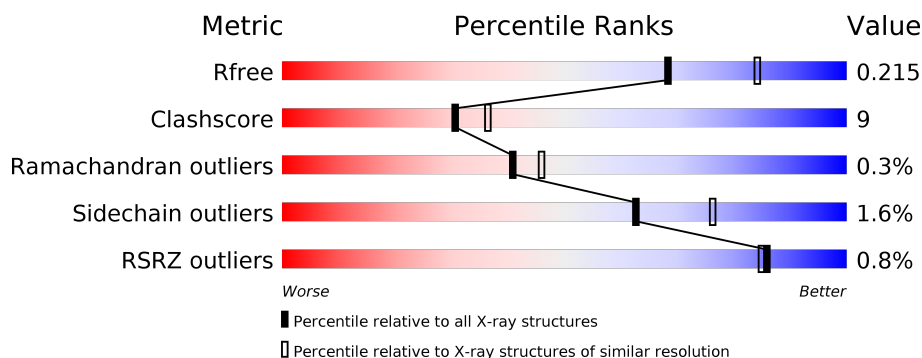
1 Overall quality at a glance

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}	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 on 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	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 80% 16% • • </div> </div>
1	B	527	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green, yellow, orange, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 76% 20% • • </div> </div>
2	C	7	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green, yellow);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 29% 71% </div> </div>
3	D	6	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green, yellow);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 67% 33% </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	C	1	X	-	-	-
3	GLC	D	6	-	-	-	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.

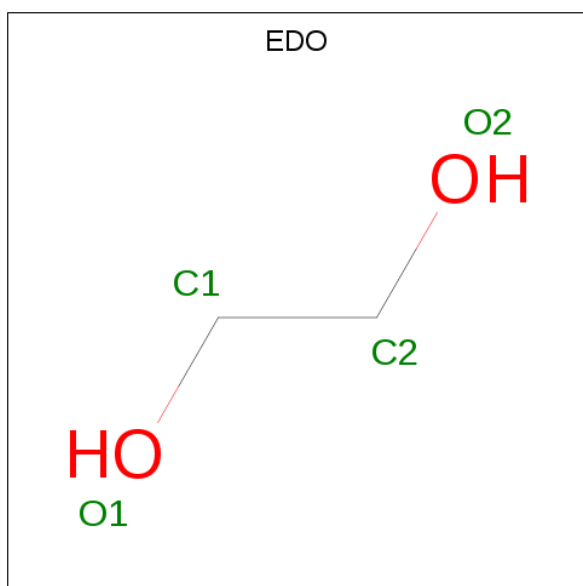


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	6	Total	C	O	0	0	0
			67	36	31			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: 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		

Continued on next page...

Continued from previous page...

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

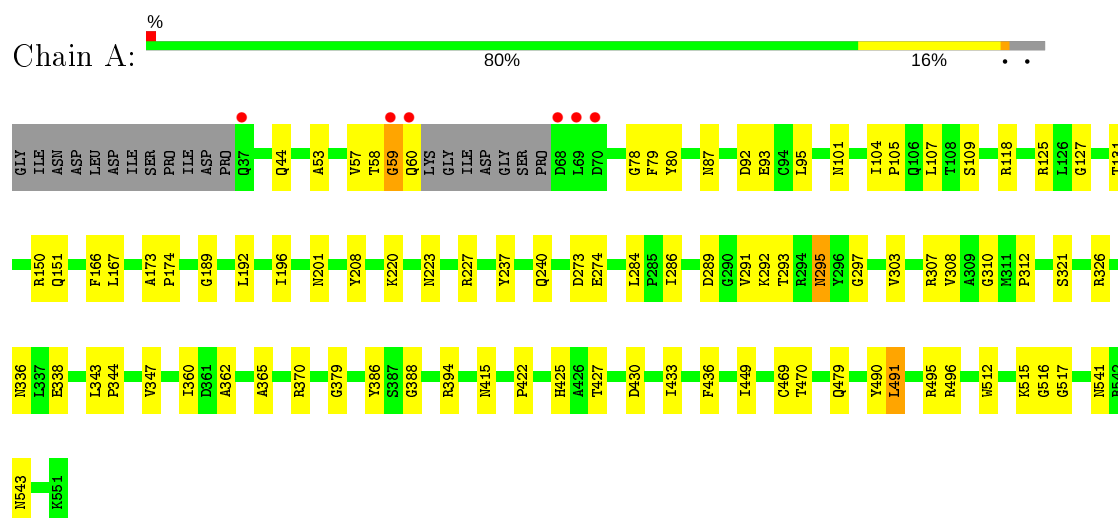
- Molecule 6 is water.

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

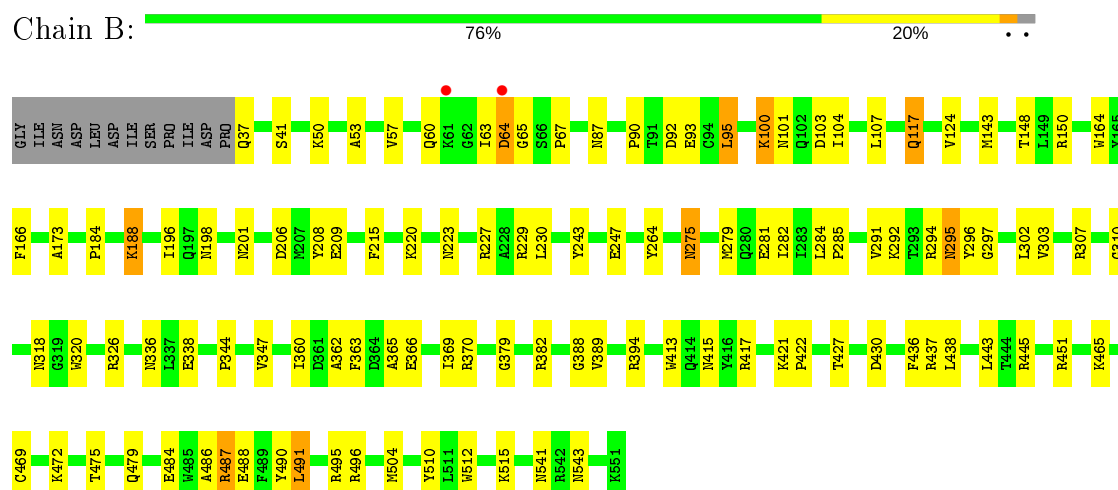
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: SusD



• Molecule 1: SusD



• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose





- 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 60.26 – 2.18	Depositor EDS
% Data completeness (in resolution range)	94.6 (60.20-2.20) 92.0 (60.26-2.18)	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 0.178 , 0.215	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)	0.35 , 46.3	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, GLC, EDO

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	0.34	0/4167	0.56	0/5638
1	B	0.34	0/4215	0.59	1/5704 (0.0%)
All	All	0.34	0/8382	0.58	1/11342 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	GLY	N-CA-C	-6.74	96.25	113.10

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	4075	0	3879	62	0
1	B	4121	0	3926	87	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	407	0	0	7	0
6	B	321	0	0	7	0
All	All	9125	0	8005	150	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 (150) 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
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	1.96	0.80
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:HA	1:B:100:LYS:HE3	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:H	1:B:188:LYS:HD3	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:A:87:ASN:ND2	1:A:496:ARG:HB3	2.17	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:PRO:HB2	6:B:1245:HOH:O	2.02	0.59
1:B:275:ASN:H	1:B:279:MET:HE2	1.68	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: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
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:101:ASN:HB2	1:B:104:ILE:HG13	1.89	0.54
1:B:53:ALA:O	1:B:57:VAL:HG22	2.07	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:59:GLY:C	1:A:60:GLN:HG3	2.28	0.53
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:B:484:GLU:CD	1:B:487:ARG:HH12	2.12	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:37:GLN:N	1:B:41:SER:HG	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HG3	1:B:394:ARG:HH11	1.79	0.46
1:B:143:MET:HB2	1:B:148:THR:HG21	1.97	0.46
1:B:87:ASN:HD22	1:B:496:ARG:HD3	1.80	0.46
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: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:150:ARG:HD2	6:B:1034:HOH:O	2.16	0.45
1:B:92:ASP:HB3	1:B:512:TRP:CD2	2.52	0.45
2:C:1:GLC:H1	2:C:7:GLC:C3	2.43	0.45
1:B:417:ARG:HD3	1:B:421:LYS: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:484:GLU:CD	1:B:487:ARG:NH1	2.72	0.42
1:B:295:ASN:HD22	1:B:295:ASN:C	2.23	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:362:ALA:HB1	1:B:422:PRO:HG3	2.01	0.42
1:A:87:ASN:HD22	1:A:496:ARG:HD3	1.84	0.42
1:B:437:ARG:NH2	1:B:488:GLU:OE2	2.42	0.42
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: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:490:TYR:O	1:B:491:LEU:HB2	2.19	0.41
1:B:87:ASN:HA	1:B:87:ASN:HD22	1.69	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: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:295:ASN:HD22	1:A:295:ASN:C	2.23	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:386:TYR:CZ	1:A:388:GLY:HA3	2.56	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:449:ILE:HG23	6:A:1044:HOH:O	2.20	0.40
1:A:59:GLY:N	6:A:879:HOH:O	2.16	0.40
1:B:486:ALA:HB2	1:B:495:ARG:CZ	2.51	0.40
1:A:289:ASP:HB3	1:A:293:THR:H	1.85	0.40
1:A:58:THR:O	1:A:59:GLY:O	2.39	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%)	34	37
1	B	513/527 (97%)	489 (95%)	23 (4%)	1 (0%)	47	55
All	All	1017/1054 (96%)	971 (96%)	43 (4%)	3 (0%)	41	46

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%)	84	91
1	B	430/441 (98%)	419 (97%)	11 (3%)	46	58
All	All	855/882 (97%)	841 (98%)	14 (2%)	62	76

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	240	GLN
1	A	295	ASN
1	A	491	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	64	ASP
1	B	95	LEU
1	B	100	LYS
1	B	117	GLN
1	B	188	LYS
1	B	198	ASN
1	B	275	ASN
1	B	295	ASN
1	B	443	LEU
1	B	487	ARG
1	B	491	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) 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	452	GLN
1	A	479	GLN
1	A	540	ASN
1	A	543	ASN
1	B	44	GLN
1	B	87	ASN
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	479	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	0.76	0
2	GLC	C	2	2	11,11,12	0.96	0	15,15,17	1.02	0
2	GLC	C	3	2	11,11,12	1.13	0	15,15,17	0.81	0
2	GLC	C	4	2	11,11,12	1.31	1 (9%)	15,15,17	1.08	1 (6%)
2	GLC	C	5	2	11,11,12	1.37	1 (9%)	15,15,17	1.27	2 (13%)
2	GLC	C	6	2	11,11,12	1.31	1 (9%)	15,15,17	1.14	1 (6%)
2	GLC	C	7	2	11,11,12	0.69	0	15,15,17	0.73	0
3	GLC	D	1	3	12,12,12	1.02	0	17,17,17	0.74	0
3	GLC	D	2	3	11,11,12	1.19	0	15,15,17	0.84	0
3	GLC	D	3	3	11,11,12	1.11	0	15,15,17	0.69	0
3	GLC	D	4	3	11,11,12	1.16	0	15,15,17	0.80	0
3	GLC	D	5	3	11,11,12	1.31	1 (9%)	15,15,17	0.97	1 (6%)
3	GLC	D	6	3	11,11,12	1.28	2 (18%)	15,15,17	0.77	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	2.85	1.48	1.43
2	C	4	GLC	C4-C5	2.60	1.58	1.53
3	D	5	GLC	O5-C1	2.38	1.47	1.43
3	D	6	GLC	O5-C1	2.33	1.47	1.43
3	D	6	GLC	C2-C3	2.16	1.55	1.52
2	C	6	GLC	O5-C1	2.14	1.47	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	5	GLC	C1-C2-C3	-2.55	106.53	109.67
2	C	6	GLC	O5-C5-C6	2.43	111.01	107.20
2	C	4	GLC	O4-C4-C3	-2.32	105.00	110.35
2	C	5	GLC	O5-C5-C6	2.16	110.59	107.20
3	D	5	GLC	O5-C5-C6	2.05	110.42	107.20

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

Continued on next page...

Continued from previous page...

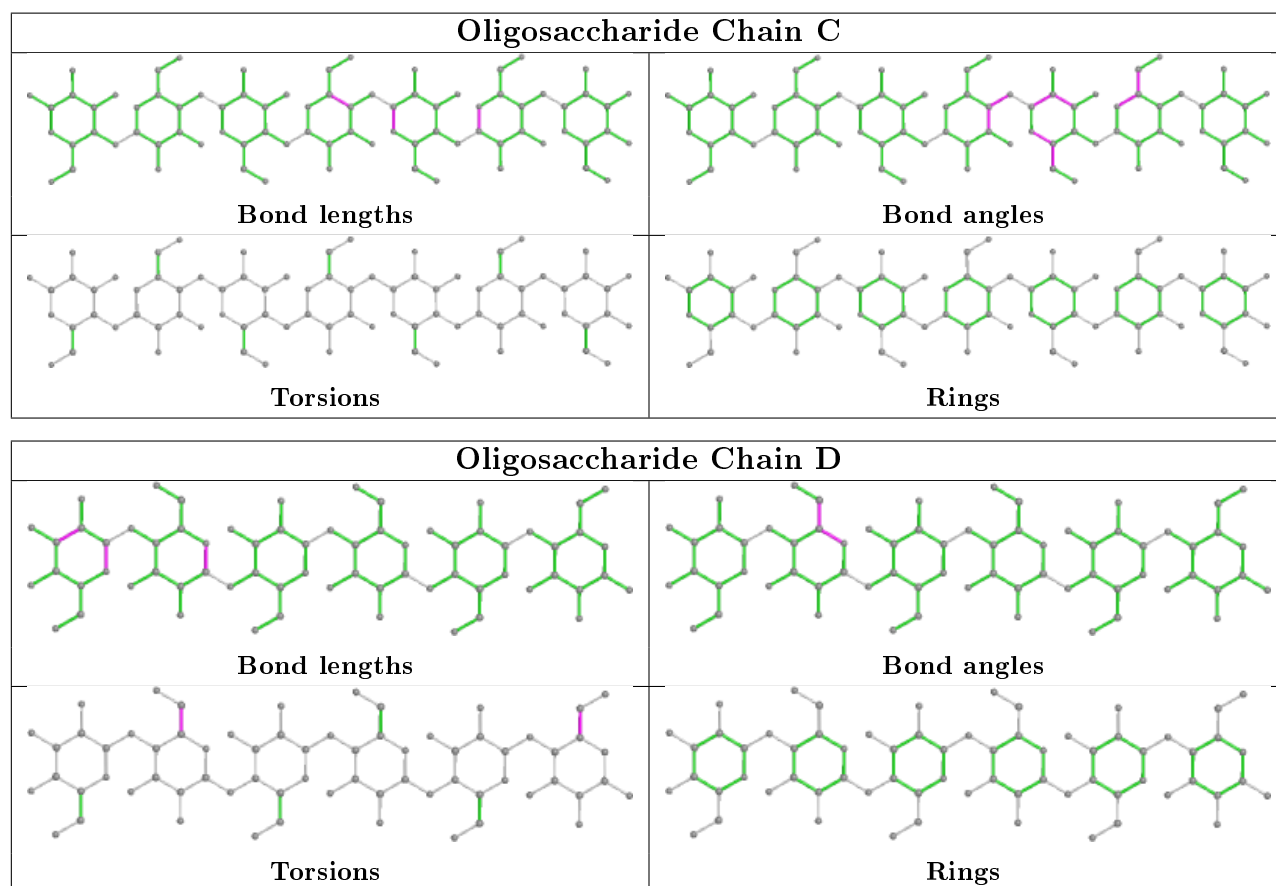
Mol	Chain	Res	Type	Atoms
3	D	5	GLC	C4-C5-C6-O6
3	D	1	GLC	C4-C5-C6-O6
3	D	1	GLC	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	7	GLC	2	0
2	C	1	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	737	-	3,3,3	0.55	0	2,2,2	0.42	0
5	EDO	B	742	-	3,3,3	0.66	0	2,2,2	0.29	0
5	EDO	B	749	-	3,3,3	0.62	0	2,2,2	0.38	0
5	EDO	A	747	-	3,3,3	0.69	0	2,2,2	0.31	0
5	EDO	B	734	-	3,3,3	0.68	0	2,2,2	0.30	0
5	EDO	A	730	-	3,3,3	0.65	0	2,2,2	0.26	0
5	EDO	B	744	-	3,3,3	0.64	0	2,2,2	0.33	0
5	EDO	A	731	4	3,3,3	0.63	0	2,2,2	0.25	0
5	EDO	B	733	-	3,3,3	0.70	0	2,2,2	0.31	0
5	EDO	A	736	-	3,3,3	0.63	0	2,2,2	0.31	0
5	EDO	B	732	-	3,3,3	0.66	0	2,2,2	0.30	0
5	EDO	B	748	-	3,3,3	0.67	0	2,2,2	0.32	0
5	EDO	B	741	-	3,3,3	0.61	0	2,2,2	0.32	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	737	-	-	1/1/1/1	-
5	EDO	B	742	-	-	0/1/1/1	-
5	EDO	B	749	-	-	0/1/1/1	-
5	EDO	A	747	-	-	0/1/1/1	-
5	EDO	B	734	-	-	0/1/1/1	-
5	EDO	A	730	-	-	1/1/1/1	-
5	EDO	B	744	-	-	0/1/1/1	-
5	EDO	A	731	4	-	1/1/1/1	-
5	EDO	B	733	-	-	1/1/1/1	-
5	EDO	A	736	-	-	0/1/1/1	-
5	EDO	B	732	-	-	0/1/1/1	-
5	EDO	B	748	-	-	0/1/1/1	-
5	EDO	B	741	-	-	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	737	EDO	1	0
5	B	742	EDO	3	0
5	A	731	EDO	1	0
5	B	741	EDO	4	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%)	-0.40	6 (1%) 79 77	5, 14, 29, 49	0
1	B	515/527 (97%)	-0.35	2 (0%) 92 91	7, 15, 30, 45	0
All	All	1023/1054 (97%)	-0.38	8 (0%) 86 85	5, 15, 29, 49	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	60	GLN	4.9
1	A	59	GLY	4.3
1	A	70	ASP	3.5
1	B	61	LYS	3.1
1	B	64	ASP	3.0
1	A	68	ASP	2.4
1	A	69	LEU	2.4
1	A	37	GLN	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.

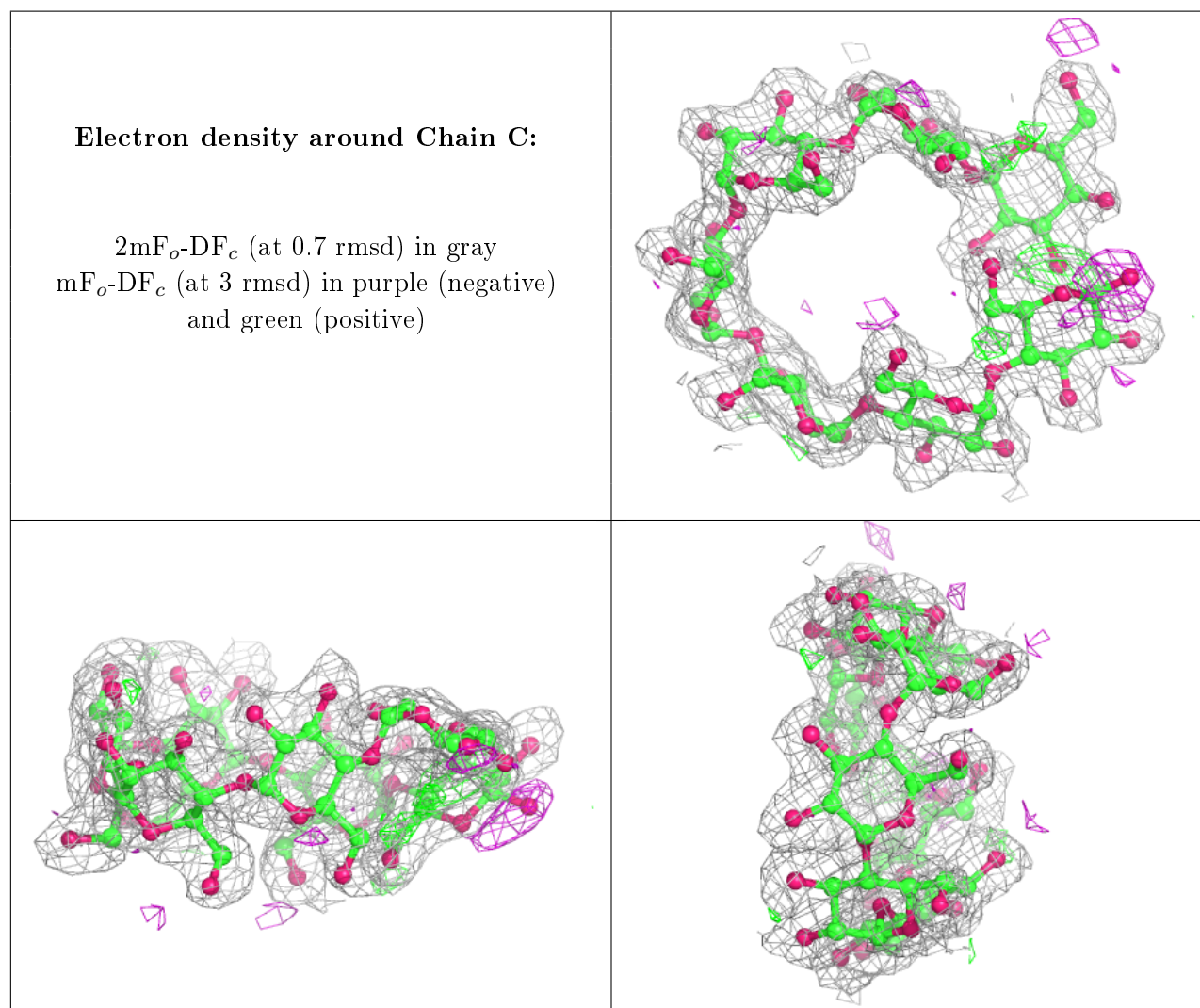
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GLC	D	6	11/12	0.52	0.51	50,51,52,54	0

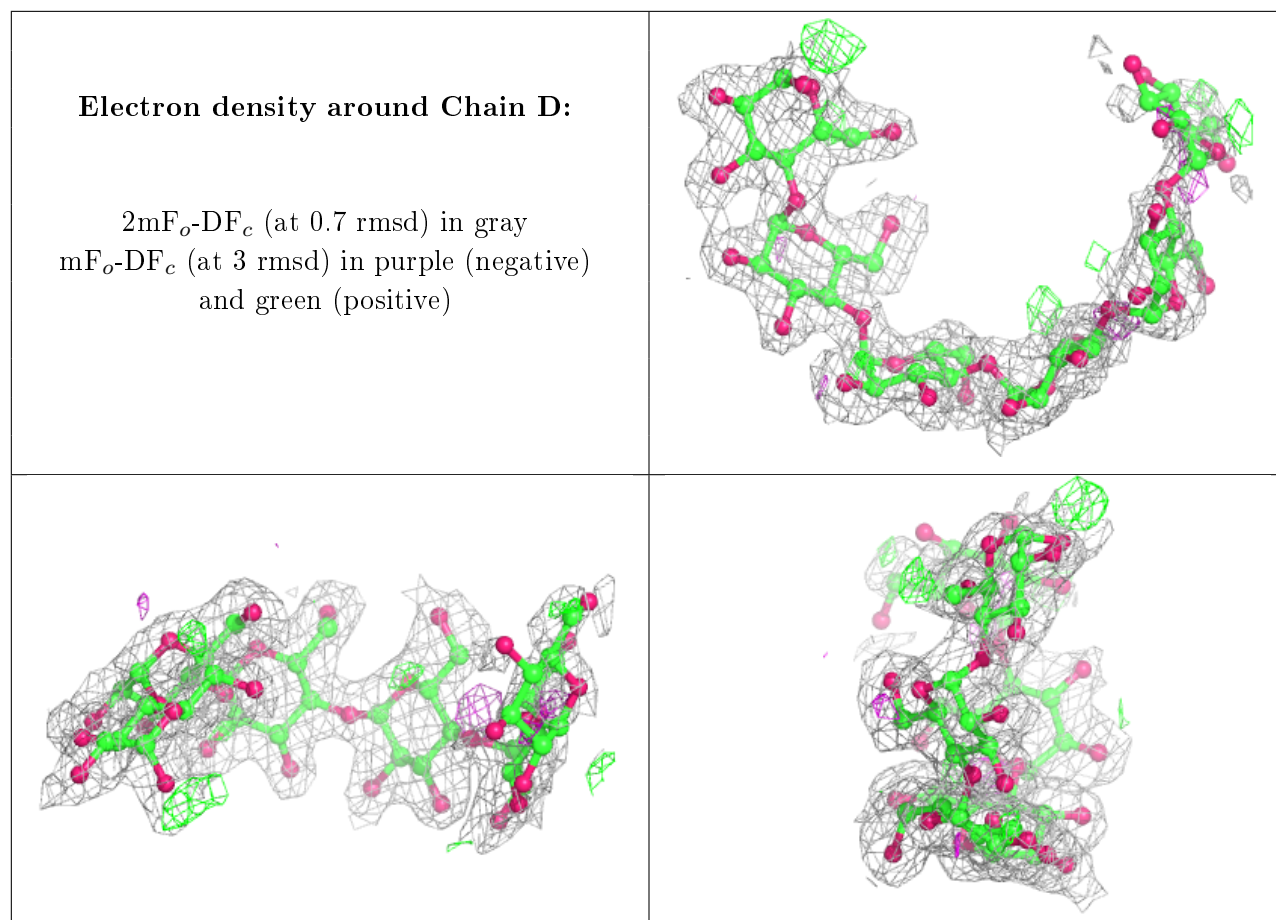
Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GLC	C	1	12/12	0.74	0.26	24,29,30,36	0
2	GLC	C	7	11/12	0.77	0.22	28,34,36,36	0
3	GLC	D	5	11/12	0.81	0.25	36,40,45,46	0
2	GLC	C	6	11/12	0.83	0.15	28,30,31,33	0
3	GLC	D	4	11/12	0.88	0.17	22,25,28,34	0
3	GLC	D	1	12/12	0.88	0.13	22,24,26,30	0
2	GLC	C	4	11/12	0.91	0.12	24,25,27,28	0
3	GLC	D	3	11/12	0.93	0.13	11,15,17,20	0
3	GLC	D	2	11/12	0.94	0.13	16,17,18,18	0
2	GLC	C	2	11/12	0.94	0.11	20,21,22,23	0
2	GLC	C	5	11/12	0.94	0.12	27,28,31,33	0
2	GLC	C	3	11/12	0.95	0.10	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 ⓘ

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	EDO	B	733	4/4	0.82	0.27	40,40,41,41	0
5	EDO	A	737	4/4	0.84	0.15	28,30,30,34	0
5	EDO	B	734	4/4	0.85	0.22	33,34,34,35	0
5	EDO	A	736	4/4	0.85	0.13	27,28,29,29	0
5	EDO	B	742	4/4	0.86	0.23	39,40,41,41	0
5	EDO	B	741	4/4	0.87	0.17	34,35,35,36	0
5	EDO	B	732	4/4	0.90	0.22	36,37,37,37	0
5	EDO	B	744	4/4	0.92	0.17	30,32,33,34	0
5	EDO	B	749	4/4	0.92	0.14	24,25,25,28	0
5	EDO	A	730	4/4	0.93	0.11	27,27,28,28	0
5	EDO	A	747	4/4	0.95	0.18	20,21,23,24	0
5	EDO	A	731	4/4	0.96	0.15	21,22,23,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	B	748	4/4	0.96	0.17	15,19,20,21	0
4	CA	B	720	1/1	0.98	0.06	20,20,20,20	0
4	CA	B	700	1/1	0.99	0.07	15,15,15,15	0
4	CA	A	600	1/1	0.99	0.09	15,15,15,15	0
4	CA	A	710	1/1	0.99	0.09	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.