



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 07:54 AM BST

PDB ID : 4RG5
Title : Crystal Structure of S. Pombe SMN YG-Dimer
Authors : Gupta, K.; Martin, R.S.; Sarachan, K.L.; Sharp, B.; Van Duyne, G.D.
Deposited on : 2014-09-29
Resolution : 1.70 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

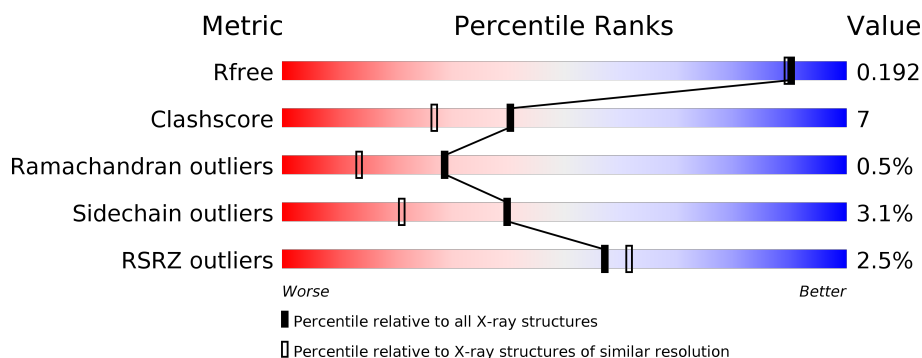
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	401	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>..</div> </div> </div>
1	B	401	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>.</div> </div> </div>
2	C	2	<div> <div></div> <div>100%</div> </div>
2	D	2	<div> <div></div> <div>100%</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
4	MLI	B	504	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7253 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 Maltose-binding periplasmic protein, Survival Motor Neuron protein chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3136	2022	507	600	7			
1	B	400	Total	C	N	O	S	0	1	0
			3133	2021	506	599	7			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	0	0
			23	12	11			
2	D	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is MALONATE ION (three-letter code: MLI) (formula: C₃H₂O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			7	3	4		
4	B	1	Total	C	O	0	0
			7	3	4		

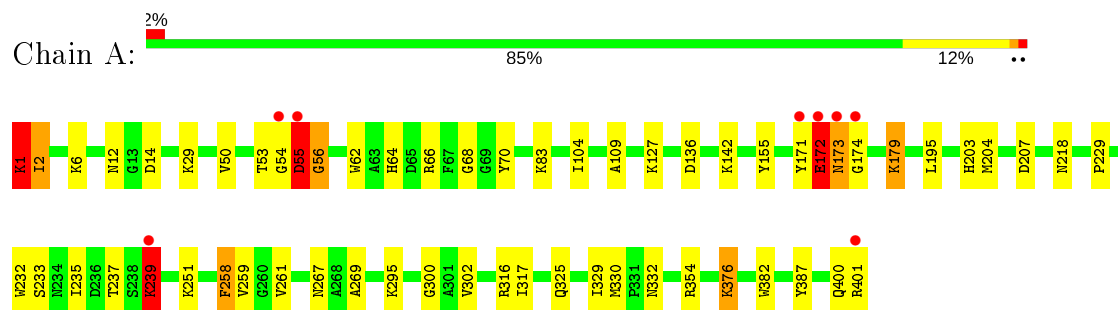
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	615	Total	O	0	0
			615	615		
5	B	274	Total	O	0	0
			274	274		

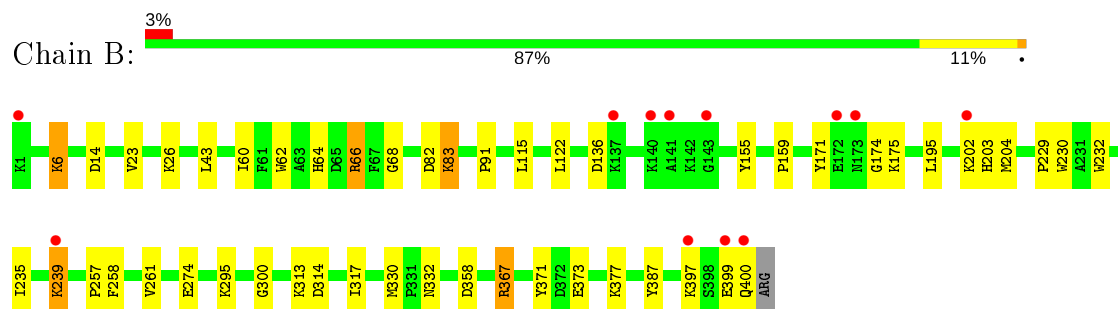
3 Residue-property plots

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.

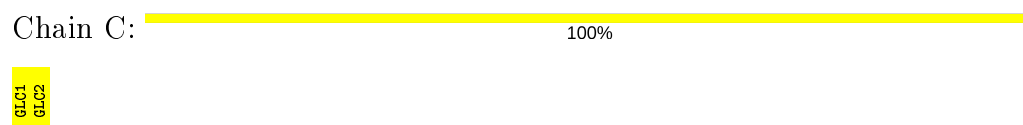
- Molecule 1: Maltose-binding periplasmic protein, Survival Motor Neuron protein chimera



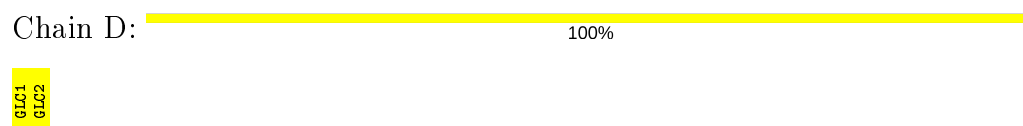
- Molecule 1: Maltose-binding periplasmic protein, Survival Motor Neuron protein chimera



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.43 Å 105.02 Å 107.69 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.01 – 1.70 47.01 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.01-1.70) 99.2 (47.01-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.41 (at 1.70 Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.165 , 0.192 0.165 , 0.192	Depositor DCC
R_{free} test set	5988 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.010 for -h,l,k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7253	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: GLC, MLI, 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	1.19	3/3213 (0.1%)	1.12	15/4360 (0.3%)
1	B	1.18	3/3213 (0.1%)	1.12	14/4360 (0.3%)
All	All	1.18	6/6426 (0.1%)	1.12	29/8720 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	274	GLU	CD-OE1	7.35	1.33	1.25
1	A	233	SER	CB-OG	-6.79	1.33	1.42
1	B	274	GLU	CG-CD	6.54	1.61	1.51
1	A	62	TRP	CE3-CZ3	6.06	1.48	1.38
1	A	56	GLY	N-CA	5.80	1.54	1.46
1	B	230	TRP	CE3-CZ3	5.23	1.47	1.38

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	B	367	ARG	NE-CZ-NH1	-6.84	116.88	120.30
1	A	70	TYR	CB-CG-CD2	-6.67	117.00	121.00
1	B	155	TYR	CB-CG-CD2	-6.55	117.07	121.00
1	B	66	ARG	CG-CD-NE	-6.54	98.06	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	B	155	TYR	CD1-CE1-CZ	-6.34	114.09	119.80
1	B	82	ASP	CB-CG-OD1	6.31	123.98	118.30
1	A	2	ILE	CG1-CB-CG2	-6.24	97.68	111.40
1	A	55	ASP	CB-CG-OD1	6.17	123.86	118.30
1	A	155	TYR	CB-CG-CD2	-6.08	117.35	121.00
1	B	387	TYR	CB-CG-CD2	-5.90	117.46	121.00
1	B	313	LYS	CD-CE-NZ	-5.88	98.17	111.70
1	A	316	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	B	155	TYR	CG-CD2-CE2	-5.64	116.79	121.30
1	A	104	ILE	CG1-CB-CG2	-5.60	99.09	111.40
1	B	358	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	66	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	A	174	GLY	N-CA-C	-5.39	99.62	113.10
1	A	251	LYS	CD-CE-NZ	-5.35	99.41	111.70
1	B	14	ASP	CB-CA-C	-5.25	99.90	110.40
1	A	70	TYR	CB-CG-CD1	5.24	124.14	121.00
1	B	115	LEU	CB-CG-CD2	-5.23	102.11	111.00
1	A	354	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	314	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	400	GLN	CA-CB-CG	5.17	124.77	113.40
1	A	142	LYS	CD-CE-NZ	-5.14	99.87	111.70
1	A	387	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	B	314	ASP	CB-CG-OD2	-5.03	113.77	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	LYS	Peptide
1	A	172	GLU	Peptide
1	A	239	LYS	Peptide

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	3136	0	3100	53	0
1	B	3133	0	3100	42	0
2	C	23	0	21	0	0
2	D	23	0	21	0	0
3	A	30	0	0	0	0
3	B	5	0	0	0	0
4	B	14	0	4	6	0
5	A	615	0	0	13	1
5	B	274	0	0	10	1
All	All	7253	0	6246	91	2

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 7.

All (91) 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:91:PRO:HB2	5:B:764:HOH:O	1.43	1.16
1:B:204:MET:SD	5:B:795:HOH:O	2.07	1.12
1:A:179:LYS:HE3	1:A:179:LYS:HA	1.43	0.99
1:A:55:ASP:OD2	1:A:269:ALA:HB3	1.62	0.99
1:B:64:HIS:HD2	1:B:261:VAL:H	1.14	0.94
1:B:83:LYS:HE2	5:B:641:HOH:O	1.72	0.88
1:B:43:LEU:CD1	1:B:60:ILE:HD11	2.04	0.87
1:A:64:HIS:HD2	1:A:261:VAL:H	1.20	0.85
1:B:43:LEU:HD13	1:B:60:ILE:HD11	1.59	0.82
1:A:239:LYS:HA	5:A:1001:HOH:O	1.80	0.81
1:B:64:HIS:CD2	1:B:261:VAL:H	1.97	0.80
1:A:173:ASN:HB3	5:A:1087:HOH:O	1.81	0.79
1:A:195:LEU:CD1	1:A:204:MET:HE1	2.15	0.77
1:B:235:ILE:HG13	5:B:851:HOH:O	1.88	0.73
1:A:64:HIS:CD2	1:A:261:VAL:H	2.05	0.73
1:B:26:LYS:CB	4:B:504:MLI:H11	2.19	0.73
1:A:12:ASN:ND2	1:A:14:ASP:OD1	2.19	0.70
1:A:55:ASP:HB2	1:A:56:GLY:CA	2.24	0.68
1:A:55:ASP:CB	1:A:56:GLY:HA3	2.23	0.68
1:A:207:ASP:OD2	1:B:399:GLU:HB3	1.94	0.67
1:A:55:ASP:HB2	1:A:56:GLY:HA3	1.77	0.67
1:B:43:LEU:HD13	1:B:60:ILE:CD1	2.26	0.66
1:A:195:LEU:HD11	1:A:204:MET:HE1	1.77	0.65
1:B:195:LEU:CD1	1:B:204:MET:HE1	2.27	0.65
1:B:6:LYS:HD3	5:B:644:HOH:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:HIS:HE1	1:A:330:MET:O	1.82	0.63
1:B:136:ASP:OD2	1:B:203:HIS:HD2	1.81	0.63
1:A:237:THR:O	1:A:239:LYS:HE2	1.99	0.62
1:A:203:HIS:HE1	5:A:763:HOH:O	1.82	0.62
1:B:235:ILE:N	5:B:851:HOH:O	2.32	0.62
1:A:171:TYR:O	1:A:172:GLU:HB3	2.00	0.61
1:A:50:VAL:O	1:A:55:ASP:HA	2.00	0.61
1:B:26:LYS:HB3	4:B:504:MLI:H11	1.81	0.61
1:A:136:ASP:OD2	1:A:203:HIS:HD2	1.86	0.59
1:A:300:GLY:HA3	5:A:1175:HOH:O	2.02	0.59
1:A:2:ILE:HB	5:A:1189:HOH:O	2.01	0.59
1:B:64:HIS:HE1	1:B:330:MET:O	1.86	0.59
1:A:55:ASP:OD2	1:A:269:ALA:CB	2.43	0.59
5:A:871:HOH:O	1:B:203:HIS:HE1	1.86	0.58
1:B:23:VAL:HA	4:B:504:MLI:H12	1.86	0.58
1:A:376:LYS:HB2	1:A:376:LYS:NZ	2.19	0.57
1:B:235:ILE:CG1	5:B:851:HOH:O	2.51	0.57
1:A:317:ILE:HD11	5:A:933:HOH:O	2.07	0.55
1:B:371:TYR:HE2	1:B:373:GLU:OE2	1.90	0.55
1:A:195:LEU:HD11	1:A:204:MET:CE	2.37	0.54
1:A:55:ASP:HB3	1:A:267:ASN:HD21	1.73	0.54
1:B:171:TYR:OH	1:B:174:GLY:HA2	2.08	0.54
1:B:295:LYS:HE2	5:B:630:HOH:O	2.08	0.53
1:A:54:GLY:O	1:A:55:ASP:O	2.26	0.53
1:A:376:LYS:CB	1:A:376:LYS:NZ	2.72	0.52
1:A:195:LEU:HD12	1:A:204:MET:HE1	1.88	0.52
1:B:195:LEU:HD12	1:B:204:MET:HE1	1.92	0.51
1:B:43:LEU:C	1:B:43:LEU:HD12	2.31	0.51
1:A:376:LYS:CB	1:A:376:LYS:HZ3	2.24	0.51
1:B:171:TYR:CZ	1:B:174:GLY:HA2	2.46	0.50
5:A:944:HOH:O	1:B:300:GLY:HA3	2.11	0.50
1:B:62:TRP:CD1	1:B:66:ARG:HG3	2.47	0.50
1:B:26:LYS:CG	4:B:504:MLI:H11	2.42	0.49
1:B:26:LYS:HG2	4:B:504:MLI:H11	1.94	0.49
1:A:237:THR:O	1:A:239:LYS:CE	2.60	0.49
1:A:382:TRP:CZ2	1:B:367:ARG:CG	2.95	0.49
1:A:179:LYS:CA	1:A:179:LYS:HE3	2.26	0.48
1:A:68:GLY:HA3	1:A:332:ASN:O	2.14	0.47
1:A:2:ILE:HD12	1:A:55:ASP:CG	2.36	0.47
5:A:955:HOH:O	1:B:239:LYS:HA	2.14	0.47
1:A:317:ILE:CG1	5:A:933:HOH:O	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LYS:NZ	5:A:1077:HOH:O	2.48	0.46
1:A:325:GLN:NE2	5:A:1069:HOH:O	2.47	0.46
1:B:136:ASP:OD2	1:B:203:HIS:CD2	2.66	0.46
1:A:55:ASP:CB	1:A:56:GLY:CA	2.89	0.46
1:B:68:GLY:HA3	1:B:332:ASN:O	2.15	0.46
1:A:218:ASN:HD21	1:A:235:ILE:HG12	1.81	0.45
1:A:53:THR:OG1	1:A:54:GLY:N	2.48	0.45
1:B:159:PRO:HG3	1:B:257:PRO:HA	1.99	0.44
1:A:382:TRP:CH2	1:B:367:ARG:HD3	2.52	0.44
1:A:376:LYS:HZ2	1:A:376:LYS:HB2	1.83	0.44
1:A:12:ASN:ND2	1:A:14:ASP:CG	2.71	0.44
1:A:179:LYS:HD3	5:A:1150:HOH:O	2.17	0.44
1:A:195:LEU:CD1	1:A:204:MET:CE	2.90	0.43
1:B:122:LEU:HD11	5:B:682:HOH:O	2.18	0.43
1:B:229:PRO:HA	1:B:232:TRP:CE2	2.52	0.43
1:B:295:LYS:CE	5:B:630:HOH:O	2.66	0.43
1:A:2:ILE:HG13	1:A:56:GLY:O	2.19	0.42
1:A:229:PRO:HA	1:A:232:TRP:CE2	2.55	0.42
1:A:109:ALA:HA	1:A:302:VAL:HA	2.02	0.42
1:B:300:GLY:O	1:B:317:ILE:HD12	2.20	0.41
1:A:258:PHE:HA	1:A:258:PHE:HD1	1.78	0.41
1:A:1:LYS:HE2	1:A:1:LYS:HB3	1.92	0.41
1:A:259:VAL:HB	1:A:329:ILE:HD13	2.03	0.41
1:B:26:LYS:HG2	4:B:504:MLI:O9	2.21	0.40
1:A:382:TRP:CZ2	1:B:367:ARG:HD3	2.57	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:830:HOH:O	5:A:1202:HOH:O[4_555]	1.80	0.40
5:B:625:HOH:O	5:B:821:HOH:O[4_445]	2.14	0.06

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	399/401 (100%)	386 (97%)	10 (2%)	3 (1%)	19	6
1	B	399/401 (100%)	390 (98%)	8 (2%)	1 (0%)	41	24
All	All	798/802 (100%)	776 (97%)	18 (2%)	4 (0%)	29	13

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ASP
1	A	239	LYS
1	A	172	GLU
1	B	239	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	322/322 (100%)	310 (96%)	12 (4%)	34	15
1	B	322/322 (100%)	314 (98%)	8 (2%)	47	29
All	All	644/644 (100%)	624 (97%)	20 (3%)	40	21

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LYS
1	A	6	LYS
1	A	29	LYS
1	A	55	ASP
1	A	83	LYS
1	A	173	ASN
1	A	179	LYS
1	A	239	LYS
1	A	258	PHE

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Mol	Chain	Res	Type
1	A	295	LYS
1	A	376	LYS
1	A	401	ARG
1	B	6	LYS
1	B	83	LYS
1	B	175	LYS
1	B	202	LYS
1	B	258	PHE
1	B	377	LYS
1	B	397	LYS
1	B	400	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	201	ASN
1	A	203	HIS
1	A	218	ASN
1	A	253	GLN
1	B	12	ASN
1	B	64	HIS
1	B	203	HIS
1	B	218	ASN
1	B	400	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 ⓘ

4 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	1.51	2 (16%)	17,17,17	1.61	2 (11%)
2	GLC	C	2	2	11,11,12	1.50	2 (18%)	15,15,17	1.62	4 (26%)
2	GLC	D	1	2	12,12,12	1.93	3 (25%)	17,17,17	3.00	8 (47%)
2	GLC	D	2	2	11,11,12	1.07	0	15,15,17	1.92	6 (40%)

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	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	D	1	2	-	2/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	GLC	O2-C2	3.92	1.52	1.43
2	C	2	GLC	C4-C5	3.30	1.60	1.53
2	D	1	GLC	C1-C2	3.18	1.59	1.52
2	D	1	GLC	O1-C1	3.06	1.49	1.39
2	C	1	GLC	C1-C2	3.00	1.59	1.52
2	C	1	GLC	O2-C2	2.56	1.49	1.43
2	C	2	GLC	O3-C3	2.14	1.48	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	GLC	O2-C2-C1	5.99	123.05	109.16
2	D	1	GLC	C6-C5-C4	-5.89	99.20	113.00
2	D	1	GLC	C4-C3-C2	4.82	119.24	110.82
2	C	1	GLC	O4-C4-C3	-4.43	100.10	110.35
2	D	1	GLC	O1-C1-C2	4.11	120.61	109.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	GLC	C2-C3-C4	-3.49	104.86	110.89
2	D	2	GLC	C1-O5-C5	3.45	116.86	112.19
2	D	1	GLC	O4-C4-C3	-3.34	102.64	110.35
2	C	2	GLC	C1-O5-C5	3.33	116.71	112.19
2	D	1	GLC	C1-O5-C5	3.23	119.75	113.66
2	C	2	GLC	O5-C5-C6	-3.08	102.37	107.20
2	C	1	GLC	C3-C4-C5	2.74	115.13	110.24
2	C	2	GLC	O5-C1-C2	-2.62	106.73	110.77
2	D	2	GLC	O5-C1-C2	-2.46	106.97	110.77
2	D	1	GLC	O1-C1-O5	2.41	117.63	110.38
2	D	2	GLC	C1-C2-C3	2.21	112.38	109.67
2	C	2	GLC	O4-C4-C3	2.20	115.44	110.35
2	D	2	GLC	O3-C3-C2	2.18	114.17	109.99
2	D	1	GLC	C3-C4-C5	-2.11	106.47	110.24
2	D	2	GLC	O2-C2-C3	-2.08	105.97	110.14

There are no chirality outliers.

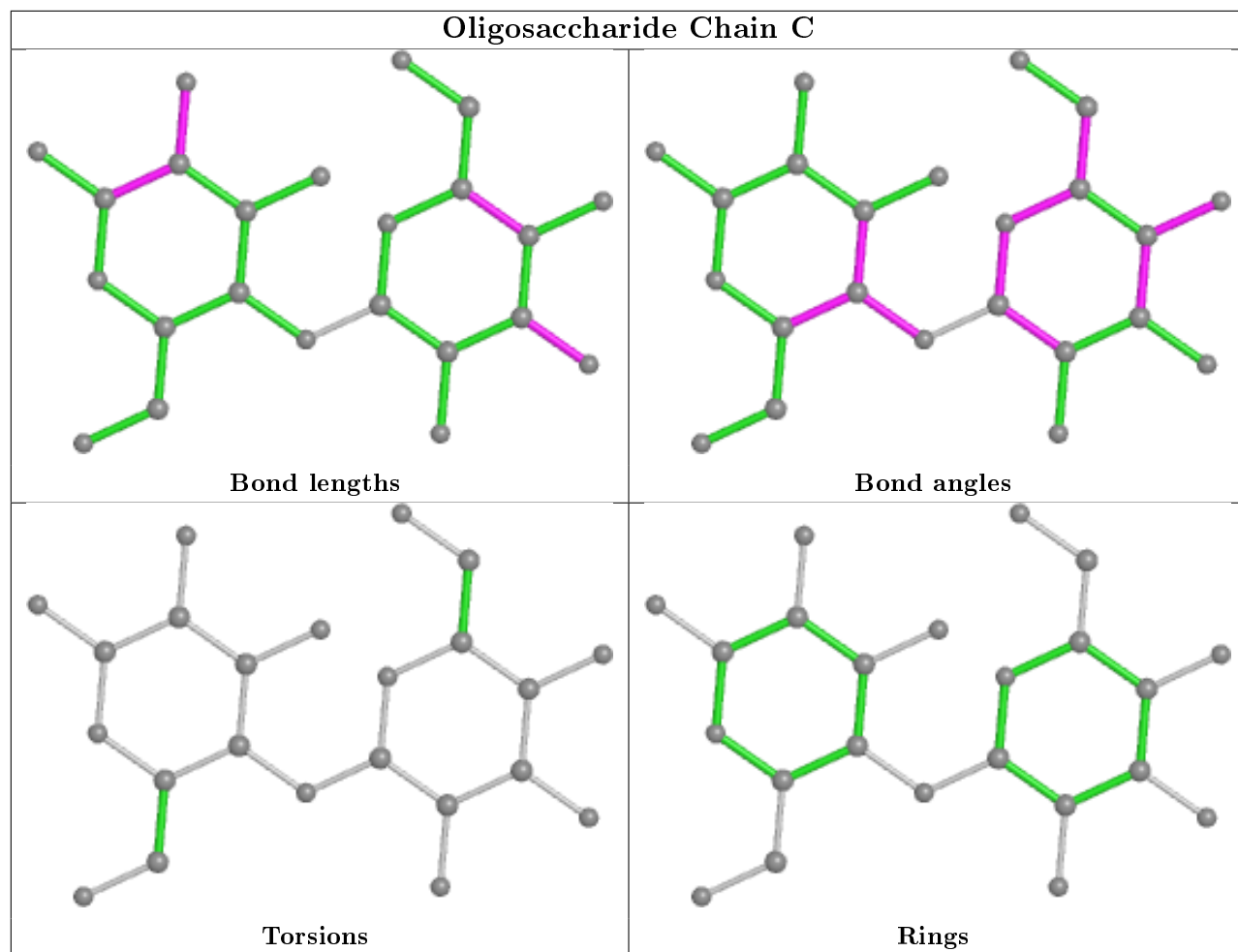
All (2) torsion outliers are listed below:

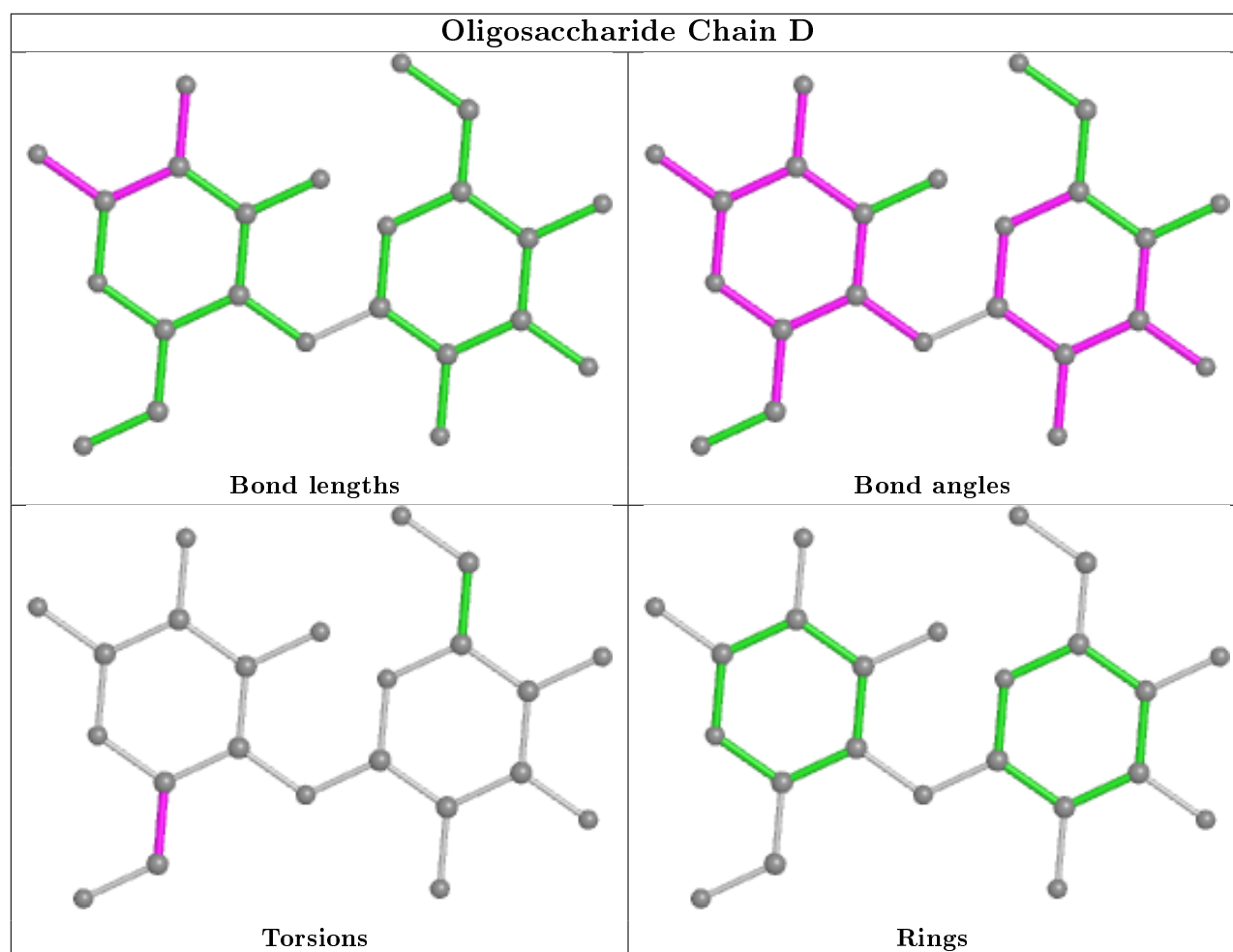
Mol	Chain	Res	Type	Atoms
2	D	1	GLC	O5-C5-C6-O6
2	D	1	GLC	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	504	-	4,4,4	0.74	0	6,6,6	0.31	0
3	SO4	B	502	-	4,4,4	0.53	0	6,6,6	0.77	0
4	MLI	B	503	-	0,6,6	0.00	-	0,7,7	0.00	-
3	SO4	A	507	-	4,4,4	0.44	0	6,6,6	0.33	0
3	SO4	A	503	-	4,4,4	1.18	1 (25%)	6,6,6	1.18	1 (16%)
3	SO4	A	502	-	4,4,4	0.44	0	6,6,6	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	505	-	4,4,4	0.53	0	6,6,6	0.30	0
4	MLI	B	504	-	0,6,6	0.00	-	0,7,7	0.00	-
3	SO4	A	506	-	4,4,4	0.37	0	6,6,6	0.57	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
4	MLI	B	504	-	-	0/0/4/4	-
4	MLI	B	503	-	-	0/0/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	SO4	O1-S	2.02	1.57	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	SO4	O4-S-O1	2.24	120.98	109.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	504	MLI	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	401/401 (100%)	-0.33	8 (1%) 65 69	17, 24, 44, 83	0
1	B	400/401 (99%)	-0.01	12 (3%) 50 54	18, 26, 47, 78	0
All	All	801/802 (99%)	-0.17	20 (2%) 57 61	17, 25, 45, 83	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	173	ASN	6.5
1	A	172	GLU	5.2
1	A	401	ARG	4.9
1	B	143	GLY	4.1
1	B	397	LYS	4.1
1	A	239	LYS	4.0
1	B	400	GLN	3.8
1	A	55	ASP	3.6
1	B	141	ALA	3.6
1	A	174	GLY	3.4
1	A	171	TYR	3.1
1	B	173	ASN	2.8
1	B	172	GLU	2.7
1	B	399	GLU	2.7
1	B	239	LYS	2.7
1	B	202	LYS	2.6
1	B	137	LYS	2.5
1	A	54	GLY	2.5
1	B	1	LYS	2.4
1	B	140	LYS	2.4

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

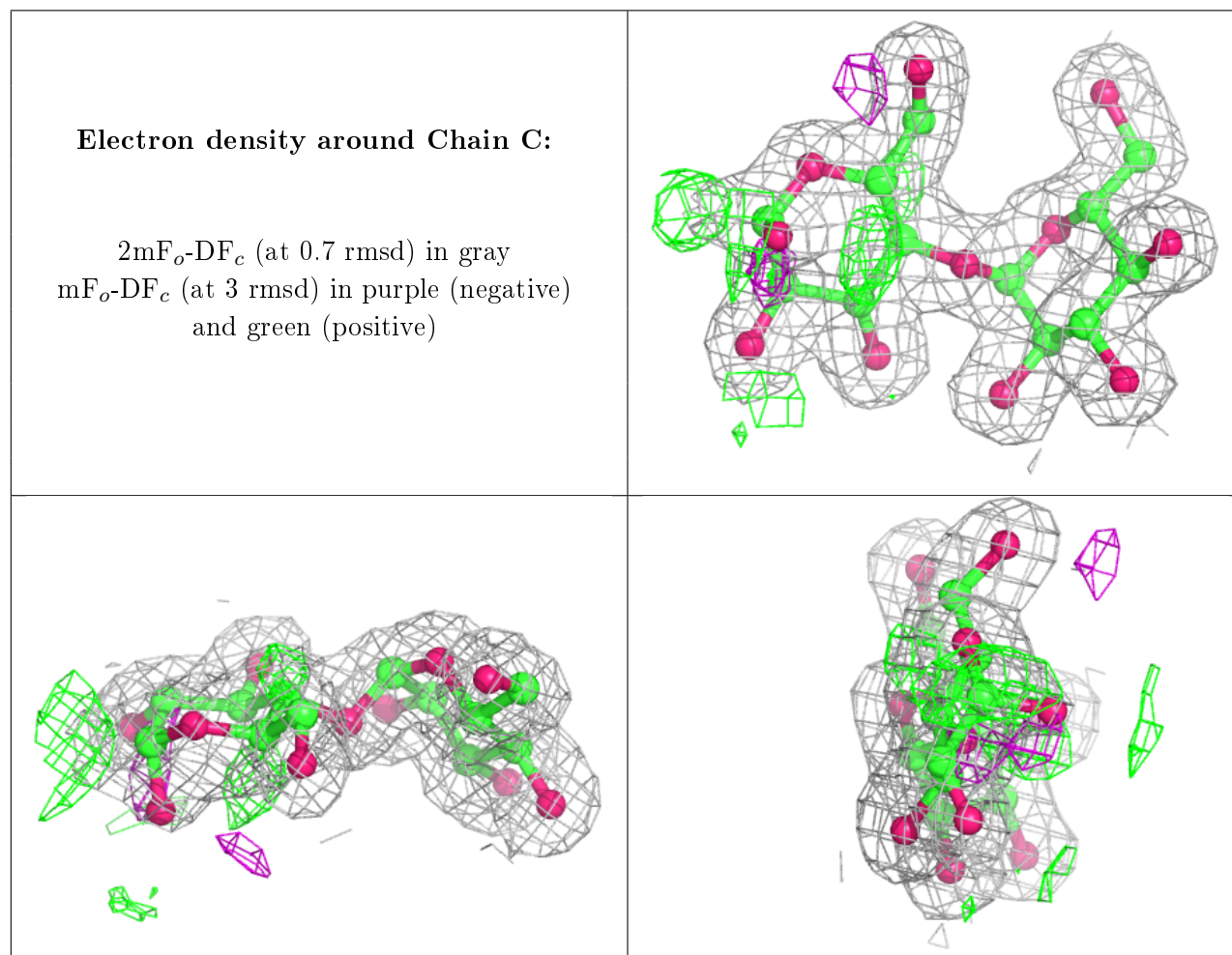
There are no non-standard protein/DNA/RNA residues in this entry.

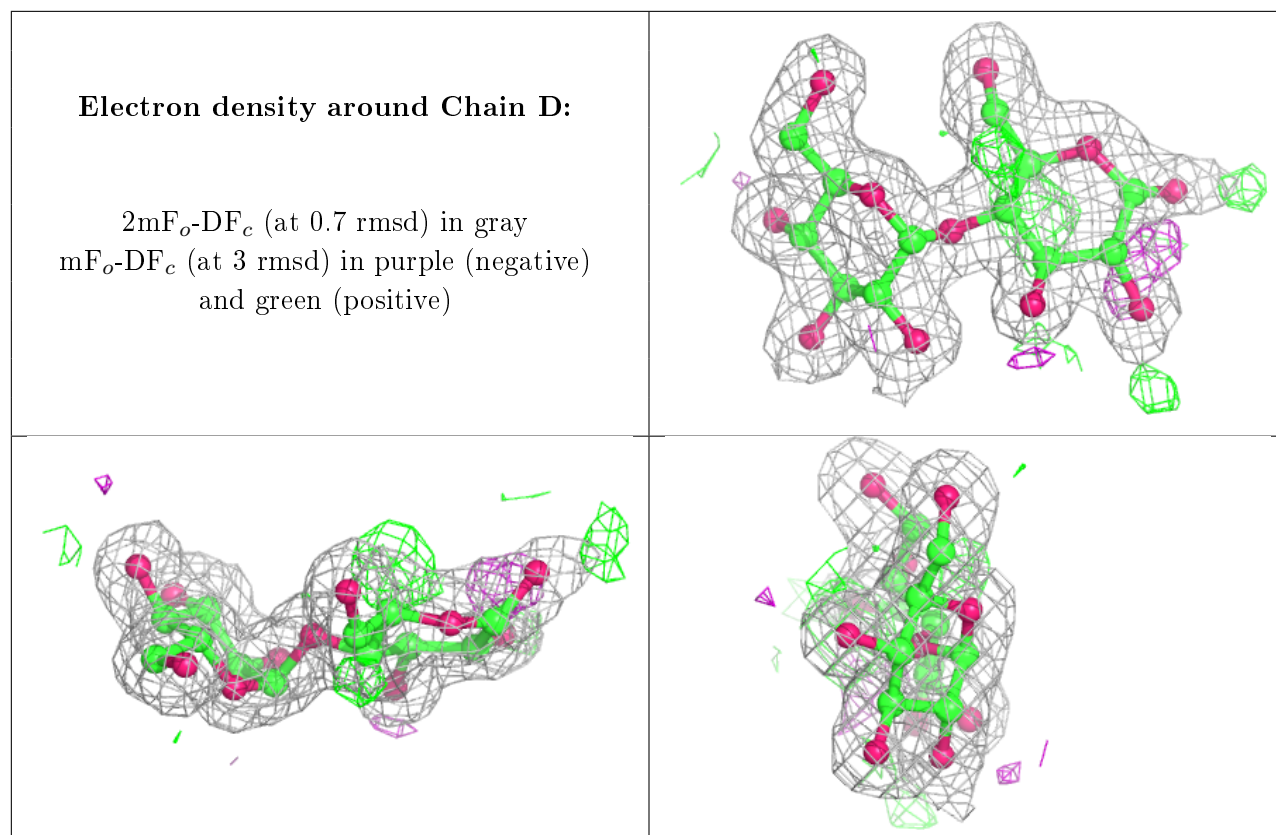
6.3 Carbohydrates [i](#)

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(\AA^2)	Q<0.9
2	GLC	D	1	12/12	0.93	0.12	20,33,41,53	0
2	GLC	C	1	12/12	0.94	0.10	19,26,35,52	0
2	GLC	D	2	11/12	0.98	0.11	19,20,23,23	0
2	GLC	C	2	11/12	0.99	0.07	16,17,18,19	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(\AA^2)	Q<0.9
3	SO4	A	503	5/5	0.81	0.27	36,46,84,92	0
4	MLI	B	504	7/7	0.84	0.22	42,51,64,83	0
3	SO4	B	502	5/5	0.86	0.27	60,83,85,90	0
3	SO4	A	505	5/5	0.89	0.25	72,72,83,95	0
3	SO4	A	506	5/5	0.89	0.24	61,78,87,92	0
4	MLI	B	503	7/7	0.90	0.12	29,31,41,47	0
3	SO4	A	507	5/5	0.92	0.18	70,83,90,94	0
3	SO4	A	504	5/5	0.93	0.25	64,67,69,69	0
3	SO4	A	502	5/5	0.95	0.19	47,62,66,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.