Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 01:50 PM EDT

PDB ID	:	2OK2
Title	:	MutS C-terminal domain fused to Maltose Binding Protein
Authors	:	Putnam, C.D.; Mendillo, M.L.; Kolodner, R.D.
Deposited on	:	2007-01-15
Resolution	:	2.00 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 (i) 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 (i)) were used in the production of this report:

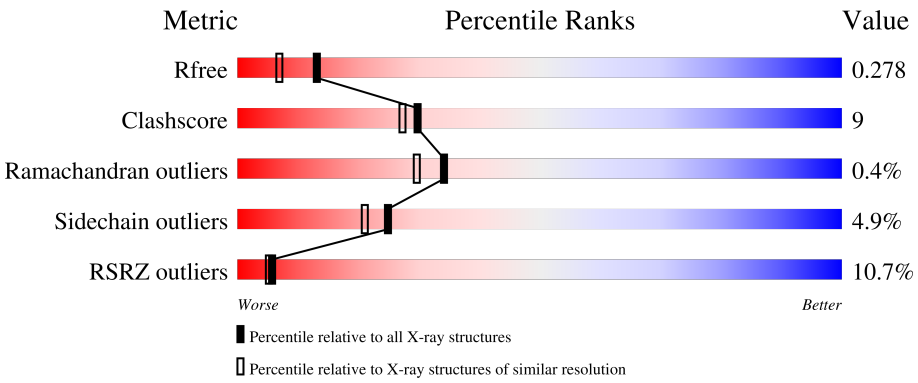
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	402	12% 79% 18% •
1	B	402	9% 84% 14% •
2	C	2	50% 50%
2	D	2	50% 50%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6889 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, DNA mismatch repair protein mutS fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	402	3160	2032	512	608	8	0	3	0
1	B	402	3167	2033	516	610	8	0	4	0

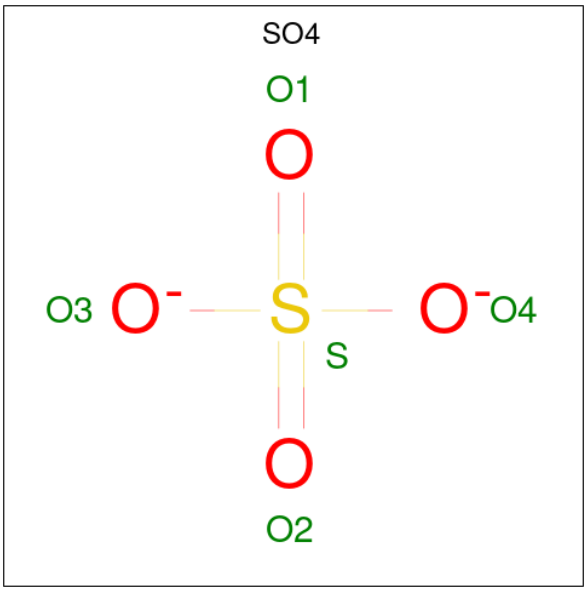
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	cloning artifact	UNP P0AEX9
A	367	HIS	-	cloning artifact	UNP P0AEX9
A	368	MET	-	cloning artifact	UNP P0AEX9
B	1	MET	-	cloning artifact	UNP P0AEX9
B	367	HIS	-	cloning artifact	UNP P0AEX9
B	368	MET	-	cloning artifact	UNP P0AEX9

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

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

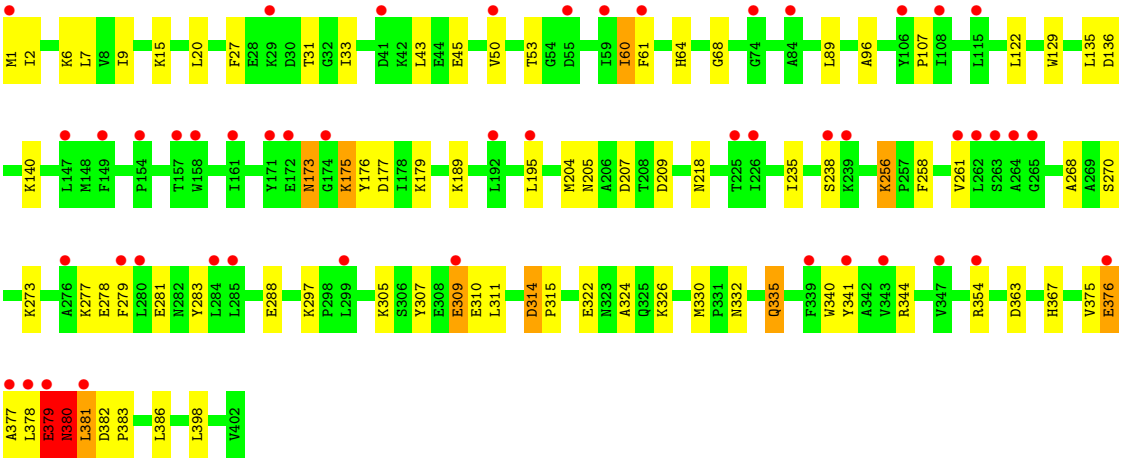
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	287	Total O 287 287	0	0
4	B	224	Total O 224 224	0	0

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.

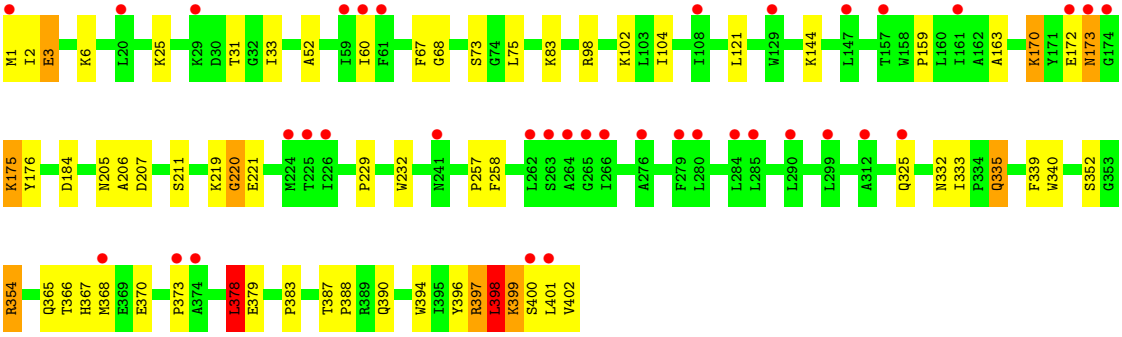
• Molecule 1: Maltose-binding periplasmic protein, DNA mismatch repair protein mutS fusion protein

Chain A:



• Molecule 1: Maltose-binding periplasmic protein, DNA mismatch repair protein mutS fusion protein

Chain B:



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

Chain C:

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

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	174.29Å 88.36Å 61.35Å 90.00° 106.80° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 24.92 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.00) 97.8 (24.92-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.201 , 0.277 0.201 , 0.278	Depositor DCC
R_{free} test set	2998 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	34.4	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6889	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, 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	1.36	9/3237 (0.3%)	0.94	8/4398 (0.2%)
1	B	0.94	4/3243 (0.1%)	0.88	2/4404 (0.0%)
All	All	1.17	13/6480 (0.2%)	0.91	10/8802 (0.1%)

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	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	376	GLU	CD-OE1	46.33	1.76	1.25
1	A	379	GLU	C-N	13.04	1.64	1.34
1	A	376	GLU	CD-OE2	12.84	1.39	1.25
1	A	379	GLU	CD-OE1	10.13	1.36	1.25
1	B	221	GLU	CB-CG	7.38	1.66	1.52
1	A	324	ALA	CA-CB	6.64	1.66	1.52
1	A	380	ASN	CG-ND2	5.88	1.47	1.32
1	A	129	TRP	CE3-CZ3	5.57	1.48	1.38
1	A	376	GLU	CG-CD	5.43	1.60	1.51
1	B	219	LYS	CE-NZ	5.38	1.62	1.49
1	B	163	ALA	CA-CB	5.04	1.63	1.52
1	B	220	GLY	C-O	5.04	1.31	1.23
1	A	379	GLU	CD-OE2	5.03	1.31	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	GLU	OE1-CD-OE2	10.99	136.49	123.30
1	A	379	GLU	OE1-CD-OE2	-8.20	113.46	123.30
1	A	376	GLU	CG-CD-OE1	-7.70	102.89	118.30
1	B	398	LEU	CA-CB-CG	6.87	131.11	115.30
1	A	386	LEU	CA-CB-CG	6.12	129.37	115.30
1	A	314	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	379	GLU	CG-CD-OE1	-5.55	107.19	118.30
1	A	386	LEU	CB-CG-CD1	-5.37	101.87	111.00
1	A	209	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	378	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	379	GLU	Sidechain

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	3160	0	3118	74	0
1	B	3167	0	3126	54	0
2	C	23	0	21	1	0
2	D	23	0	21	1	0
3	A	5	0	0	0	0
4	A	287	0	0	7	0
4	B	224	0	0	6	0
All	All	6889	0	6286	119	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 (119) 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:A:376:GLU:OE1	1:A:376:GLU:CD	1.76	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:SER:O	1:A:273:LYS:HE2	1.65	0.97
1:A:175:LYS:HD3	1:A:176:TYR:H	1.29	0.96
1:A:31:THR:HG22	1:A:33:ILE:HD13	1.47	0.95
1:A:367:HIS:ND1	4:A:8336:HOH:O	2.04	0.91
1:B:31:THR:HG22	1:B:33:ILE:HG12	1.55	0.88
1:A:175:LYS:HA	1:A:175:LYS:HE2	1.56	0.86
1:A:378:LEU:HD11	1:B:398:LEU:HD21	1.57	0.86
1:B:399:LYS:O	1:B:402:VAL:HG23	1.76	0.86
1:B:172:GLU:HG3	1:B:173:ASN:H	1.43	0.84
1:A:268:ALA:O	1:A:273:LYS:NZ	2.15	0.79
1:A:288:GLU:HB2	4:A:8380:HOH:O	1.82	0.78
1:A:378:LEU:HD11	1:B:398:LEU:CD2	2.14	0.78
1:A:175:LYS:HD3	1:A:176:TYR:N	2.02	0.74
1:A:68:GLY:HA3	1:A:332:ASN:O	1.86	0.74
1:A:175:LYS:CD	1:A:176:TYR:H	2.02	0.72
1:B:387:THR:OG1	1:B:390:GLN:HG3	1.89	0.72
1:A:305:LYS:O	1:A:309:GLU:HG2	1.90	0.71
1:B:172:GLU:HG3	1:B:173:ASN:N	2.04	0.71
1:B:175:LYS:HE3	1:B:176:TYR:H	1.56	0.71
1:B:31:THR:CG2	1:B:33:ILE:HG12	2.21	0.70
1:B:205[B]:ASN:HD22	1:B:207:ASP:H	1.38	0.69
1:A:89:LEU:HD23	1:A:107:PRO:HG2	1.76	0.68
1:A:64:HIS:HB3	1:A:261[A]:VAL:HG13	1.74	0.68
1:A:31:THR:CG2	1:A:33:ILE:HD13	2.21	0.68
1:A:363:ASP:OD2	4:A:8361:HOH:O	2.13	0.67
1:B:172:GLU:HG2	1:B:175:LYS:O	1.95	0.67
1:A:64:HIS:HB3	1:A:261[A]:VAL:CG1	2.26	0.65
1:B:366:THR:O	1:B:370:GLU:HG2	1.97	0.64
1:A:60:ILE:C	1:A:60:ILE:HD13	2.18	0.63
1:A:378:LEU:CD1	1:B:398:LEU:HD21	2.28	0.63
1:A:398:LEU:HB3	1:B:378:LEU:HD21	1.82	0.62
1:A:341[A]:TYR:CD1	1:A:367:HIS:NE2	2.68	0.62
1:B:354:ARG:HD2	4:B:8396:HOH:O	2.01	0.61
1:A:307:TYR:CZ	1:A:311:LEU:HD21	2.36	0.61
1:A:64:HIS:ND1	1:A:261[A]:VAL:HG12	2.15	0.60
1:A:341[B]:TYR:CD1	1:A:344:ARG:NH1	2.70	0.60
1:A:31:THR:HG22	1:A:33:ILE:CD1	2.29	0.58
1:B:333:ILE:HD12	1:B:335:GLN:HE21	1.69	0.57
1:B:67:PHE:HB3	1:B:104:ILE:HD12	1.87	0.57
1:A:9:ILE:HG21	1:A:20:LEU:HD21	1.85	0.57
1:A:27:PHE:O	1:A:31:THR:HB	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:LEU:HD12	1:A:381:LEU:H	1.69	0.56
1:B:383:PRO:HD2	4:B:8409:HOH:O	2.05	0.56
1:A:218:ASN:O	1:A:238:SER:OG	2.22	0.56
1:A:60:ILE:HD13	1:A:61:PHE:N	2.21	0.55
1:A:205:ASN:OD1	1:A:207:ASP:HB2	2.07	0.54
1:B:159:PRO:HG3	1:B:257:PRO:HA	1.90	0.54
1:B:25:LYS:HD3	1:B:25:LYS:C	2.27	0.54
1:B:205[B]:ASN:ND2	1:B:207:ASP:H	2.03	0.54
1:B:333:ILE:HD12	1:B:335:GLN:NE2	2.24	0.53
1:B:172:GLU:CG	1:B:173:ASN:H	2.09	0.53
1:B:335:GLN:NE2	1:B:335:GLN:H	2.07	0.53
1:B:1:MET:C	1:B:3:GLU:H	2.12	0.53
1:A:381:LEU:O	1:B:399:LYS:HE2	2.09	0.52
1:A:136:ASP:OD2	1:A:140:LYS:HE3	2.09	0.52
1:A:398:LEU:CB	1:B:378:LEU:HD11	2.40	0.52
1:B:98:ARG:NH1	4:B:8366:HOH:O	2.42	0.52
1:B:398:LEU:C	1:B:398:LEU:HD23	2.31	0.51
1:A:341[B]:TYR:HD1	1:A:344:ARG:NH1	2.08	0.51
1:A:50:VAL:O	1:A:53:THR:HG22	2.10	0.50
1:B:52:ALA:HB1	1:B:397:ARG:NE	2.27	0.50
1:A:173[A]:ASN:ND2	1:A:173[A]:ASN:H	2.08	0.50
1:B:205[B]:ASN:ND2	1:B:207:ASP:OD1	2.43	0.50
1:A:398:LEU:HB2	1:B:378:LEU:HD11	1.94	0.49
1:B:25:LYS:HD3	1:B:25:LYS:O	2.11	0.49
1:A:195:LEU:HD12	1:A:204:MET:HE1	1.93	0.49
1:A:341[A]:TYR:CE1	1:A:367:HIS:CE1	3.01	0.48
1:B:339:PHE:HA	1:B:368:MET:HE2	1.96	0.48
1:B:229:PRO:HA	1:B:232:TRP:CE2	2.49	0.48
1:B:352:SER:OG	1:B:354:ARG:HG2	2.13	0.48
1:A:6:LYS:HG2	1:A:7:LEU:N	2.29	0.47
1:A:136:ASP:O	1:A:140:LYS:HG3	2.14	0.47
1:A:45:GLU:HG2	1:A:380:ASN:HD22	1.80	0.46
1:A:175:LYS:HA	1:A:175:LYS:CE	2.36	0.46
1:B:365[B]:GLN:NE2	4:B:8210:HOH:O	2.48	0.46
1:A:64:HIS:CE1	1:A:330:MET:HB2	2.51	0.46
1:A:378:LEU:HA	1:A:381:LEU:CD1	2.46	0.46
1:B:367:HIS:CE1	1:B:379:GLU:OE1	2.68	0.46
1:A:64:HIS:CG	1:A:261[A]:VAL:HG12	2.51	0.46
1:A:189:LYS:NZ	4:A:8385:HOH:O	2.49	0.46
1:A:376:GLU:OE1	1:A:376:GLU:CG	2.63	0.45
1:B:340:TRP:CE3	2:D:2:GLC:H61	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LYS:HE2	4:A:8063:HOH:O	2.17	0.45
1:B:170:LYS:NZ	4:B:8393:HOH:O	2.48	0.45
1:B:205[B]:ASN:HD22	1:B:206:ALA:N	2.14	0.45
1:A:177:ASP:OD1	1:A:179:LYS:HB3	2.17	0.45
1:A:335:GLN:NE2	1:A:335:GLN:H	2.15	0.45
1:B:175:LYS:CE	1:B:176:TYR:H	2.26	0.45
1:A:314:ASP:HA	1:A:315:PRO:HD2	1.79	0.44
1:A:340:TRP:CD1	2:C:2:GLC:H4	2.53	0.44
1:B:68:GLY:HA3	1:B:332:ASN:O	2.17	0.44
1:B:144:LYS:HE2	1:B:220:GLY:O	2.16	0.44
1:A:354:ARG:HA	1:A:354:ARG:HD2	1.73	0.43
1:A:122:LEU:HD11	1:A:135:LEU:HD11	2.00	0.43
1:A:382:ASP:HB3	4:A:8492:HOH:O	2.17	0.43
1:B:399:LYS:O	1:B:402:VAL:CG2	2.60	0.43
1:A:235:ILE:O	1:A:238:SER:HB3	2.18	0.43
1:A:341[B]:TYR:HD1	1:A:344:ARG:HH11	1.67	0.43
1:B:401:LEU:N	1:B:402:VAL:HA	2.33	0.43
1:A:43:LEU:C	1:A:43:LEU:HD12	2.39	0.42
1:B:339:PHE:HD1	1:B:368:MET:HE1	1.82	0.42
1:B:394:TRP:O	1:B:398:LEU:HB3	2.19	0.42
1:B:102:LYS:NZ	4:B:8286:HOH:O	2.47	0.42
1:A:96:ALA:HB3	1:A:261[A]:VAL:HG11	2.01	0.41
1:A:322:GLU:HG2	1:A:326:LYS:HE3	2.02	0.41
1:A:375:VAL:O	1:A:379:GLU:HG3	2.20	0.41
1:A:45:GLU:HG2	1:A:380:ASN:ND2	2.36	0.41
1:A:383:PRO:HB2	1:B:396:TYR:CE2	2.56	0.41
1:B:184:ASP:HB2	1:B:365[B]:GLN:HB2	2.02	0.41
1:A:173[A]:ASN:H	1:A:173[A]:ASN:HD22	1.67	0.41
1:A:277:LYS:O	1:A:281:GLU:HB2	2.19	0.41
1:B:184:ASP:HB2	1:B:365[A]:GLN:HB2	2.02	0.41
1:A:279:PHE:O	1:A:283:TYR:HB2	2.21	0.41
1:B:73:SER:HB2	1:B:75:LEU:HG	2.02	0.41
1:A:377:ALA:O	1:A:380:ASN:HB2	2.21	0.40
1:A:398:LEU:HB3	1:B:378:LEU:HD11	2.03	0.40
1:A:256:LYS:HD3	4:A:8045:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	403/402 (100%)	391 (97%)	11 (3%)	1 (0%)	47	44
1	B	404/402 (100%)	393 (97%)	9 (2%)	2 (0%)	29	23
All	All	807/804 (100%)	784 (97%)	20 (2%)	3 (0%)	34	30

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2	ILE
1	A	2	ILE
1	B	373	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	329/326 (101%)	315 (96%)	14 (4%)	29	26
1	B	330/326 (101%)	311 (94%)	19 (6%)	20	15
All	All	659/652 (101%)	626 (95%)	33 (5%)	25	20

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	60	ILE
1	A	173[A]	ASN

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Mol	Chain	Res	Type
1	A	173[B]	ASN
1	A	175	LYS
1	A	256	LYS
1	A	258	PHE
1	A	278	GLU
1	A	297	LYS
1	A	309	GLU
1	A	310	GLU
1	A	335	GLN
1	A	380	ASN
1	A	381	LEU
1	B	3	GLU
1	B	6	LYS
1	B	60	ILE
1	B	83	LYS
1	B	121	LEU
1	B	170	LYS
1	B	173	ASN
1	B	175	LYS
1	B	211	SER
1	B	258	PHE
1	B	325	GLN
1	B	335	GLN
1	B	354	ARG
1	B	378	LEU
1	B	388	PRO
1	B	397	ARG
1	B	398	LEU
1	B	399	LYS
1	B	400	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	100	ASN
1	A	201	ASN
1	A	218	ASN
1	A	335	GLN
1	A	380	ASN
1	B	124	ASN
1	B	218	ASN

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Mol	Chain	Res	Type
1	B	282	ASN
1	B	325	GLN
1	B	335	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

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	0.60	0	17,17,17	1.23	2 (11%)
2	GLC	C	2	2	11,11,12	0.85	0	15,15,17	1.04	1 (6%)
2	GLC	D	1	2	12,12,12	0.85	0	17,17,17	1.12	2 (11%)
2	GLC	D	2	2	11,11,12	0.70	0	15,15,17	2.24	5 (33%)

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	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2	GLC	C1-O5-C5	6.12	120.49	112.19
2	D	2	GLC	C1-C2-C3	-3.96	104.79	109.67
2	C	1	GLC	O5-C1-C2	3.14	115.88	110.28
2	D	1	GLC	O1-C1-O5	-2.73	102.19	110.38
2	D	2	GLC	O5-C5-C6	2.54	111.18	107.20
2	D	2	GLC	O5-C1-C2	2.45	114.56	110.77
2	C	2	GLC	C1-O5-C5	2.21	115.19	112.19
2	D	2	GLC	O2-C2-C3	2.16	114.47	110.14
2	D	1	GLC	C4-C3-C2	-2.04	107.27	110.82
2	C	1	GLC	C1-O5-C5	2.00	117.44	113.66

There are no chirality outliers.

There are no torsion outliers.

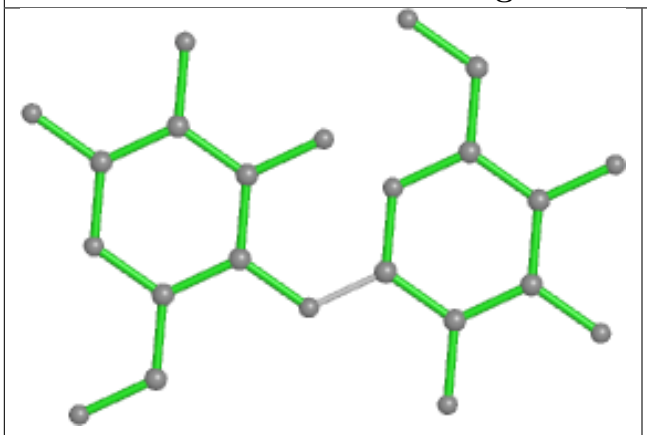
There are no ring outliers.

2 monomers are involved in 2 short contacts:

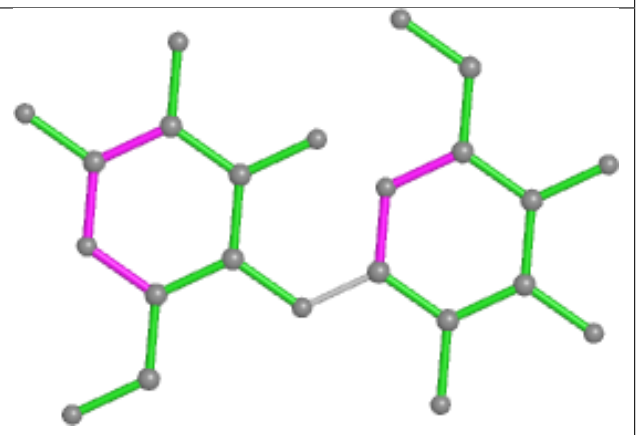
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	GLC	1	0
2	C	2	GLC	1	0

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

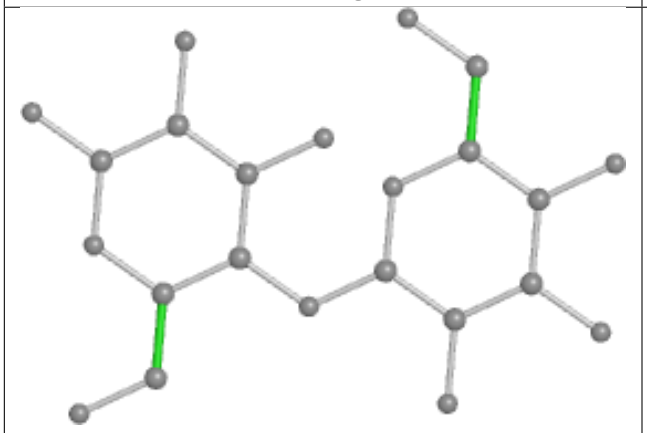
Oligosaccharide Chain C



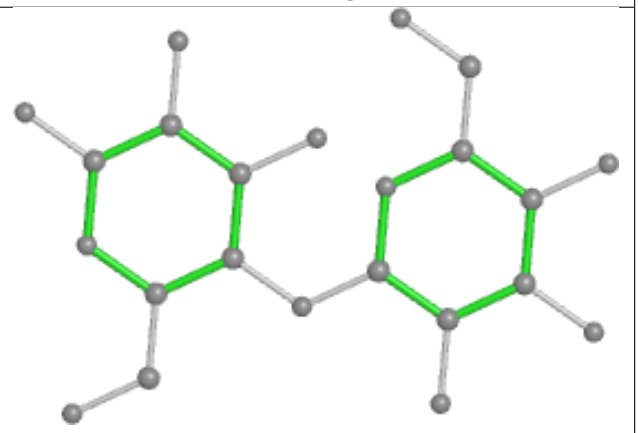
Bond lengths



Bond angles

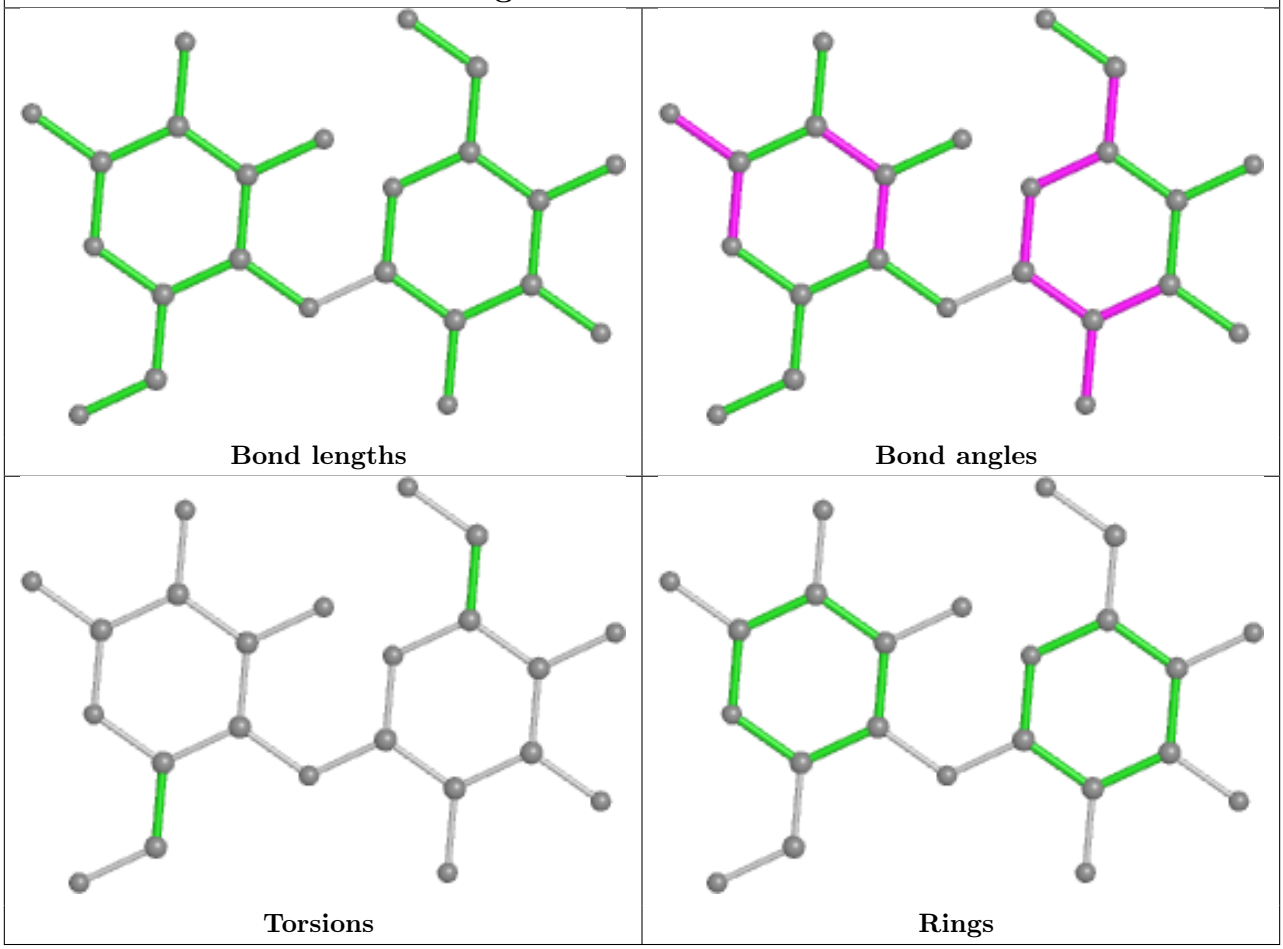


Torsions



Rings

Oligosaccharide Chain D



5.6 Ligand geometry (i)

1 ligand is 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	5000	-	4,4,4	0.18	0	6,6,6	0.43	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	379:GLU	C	380:ASN	N	1.64

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	402/402 (100%)	0.57	49 (12%)	4	3	29, 41, 47, 58	0
1	B	402/402 (100%)	0.59	37 (9%)	9	8	29, 41, 46, 61	0
All	All	804/804 (100%)	0.58	86 (10%)	6	5	29, 41, 46, 61	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	280	LEU	6.1
1	B	1	MET	5.9
1	A	108	ILE	5.3
1	B	173	ASN	5.3
1	A	1	MET	5.2
1	B	108	ILE	5.1
1	B	280	LEU	5.0
1	B	264	ALA	4.8
1	B	374	ALA	4.7
1	B	401	LEU	4.5
1	B	284	LEU	4.5
1	A	284	LEU	4.5
1	A	264	ALA	4.1
1	A	172	GLU	3.9
1	B	285	LEU	3.8
1	A	341[A]	TYR	3.8
1	A	106	TYR	3.6
1	B	59	ILE	3.5
1	B	60	ILE	3.5
1	B	226	ILE	3.5
1	A	261[A]	VAL	3.5
1	A	226	ILE	3.4
1	B	161	ILE	3.4
1	A	265	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	262	LEU	3.4
1	A	285	LEU	3.4
1	A	279	PHE	3.3
1	A	61	PHE	3.3
1	A	343	VAL	3.3
1	A	378	LEU	3.2
1	B	262	LEU	3.2
1	A	59	ILE	3.1
1	A	339	PHE	3.1
1	A	377	ALA	3.0
1	B	172	GLU	2.9
1	B	147	LEU	2.9
1	B	373	PRO	2.9
1	A	84	ALA	2.9
1	A	149	PHE	2.9
1	A	157	THR	2.8
1	A	299	LEU	2.8
1	A	379	GLU	2.8
1	A	347	VAL	2.8
1	B	312	ALA	2.8
1	A	263	SER	2.8
1	B	299	LEU	2.7
1	B	174	GLY	2.7
1	B	265	GLY	2.7
1	B	279	PHE	2.7
1	A	74	GLY	2.7
1	A	376	GLU	2.6
1	B	20	LEU	2.6
1	B	61	PHE	2.6
1	B	224	MET	2.6
1	A	147	LEU	2.6
1	B	29	LYS	2.6
1	A	158	TRP	2.6
1	B	266	ILE	2.6
1	B	325	GLN	2.6
1	A	192	LEU	2.5
1	A	50	VAL	2.5
1	B	368	MET	2.5
1	B	290	LEU	2.5
1	A	225	THR	2.4
1	A	354	ARG	2.4
1	B	225	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	239	LYS	2.4
1	B	157	THR	2.4
1	A	29	LYS	2.3
1	A	115	LEU	2.3
1	A	171	TYR	2.3
1	A	309	GLU	2.3
1	A	174	GLY	2.2
1	A	276	ALA	2.2
1	B	241[A]	ASN	2.2
1	B	129	TRP	2.2
1	A	381	LEU	2.2
1	B	400	SER	2.2
1	A	195	LEU	2.1
1	A	41	ASP	2.1
1	A	154	PRO	2.1
1	A	238	SER	2.1
1	B	276	ALA	2.1
1	A	55	ASP	2.0
1	A	161	ILE	2.0
1	B	263	SER	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)

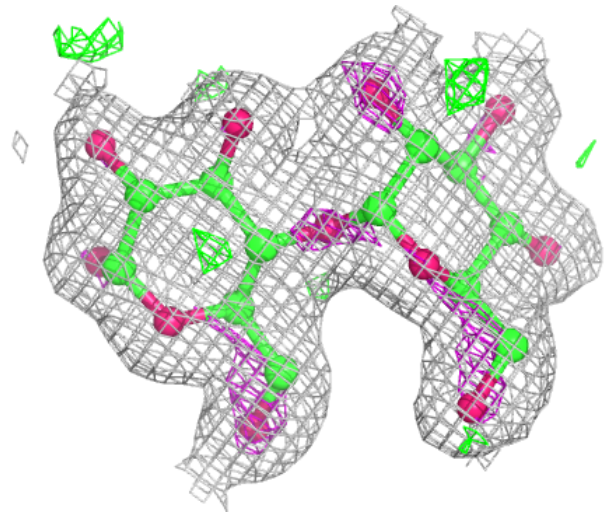
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

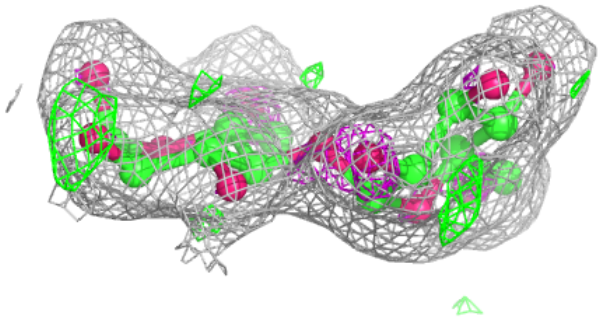
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	D	1	12/12	0.95	0.08	36,40,44,50	0
2	GLC	D	2	11/12	0.96	0.08	35,39,42,43	0
2	GLC	C	1	12/12	0.97	0.06	35,37,43,46	0
2	GLC	C	2	11/12	0.97	0.06	32,35,39,39	0

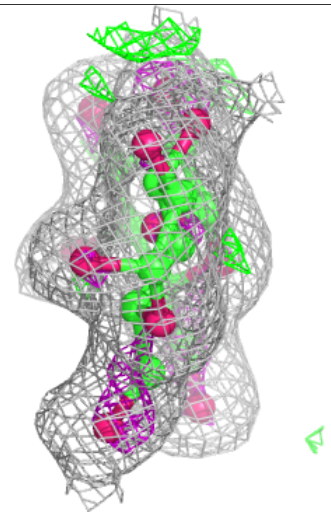
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

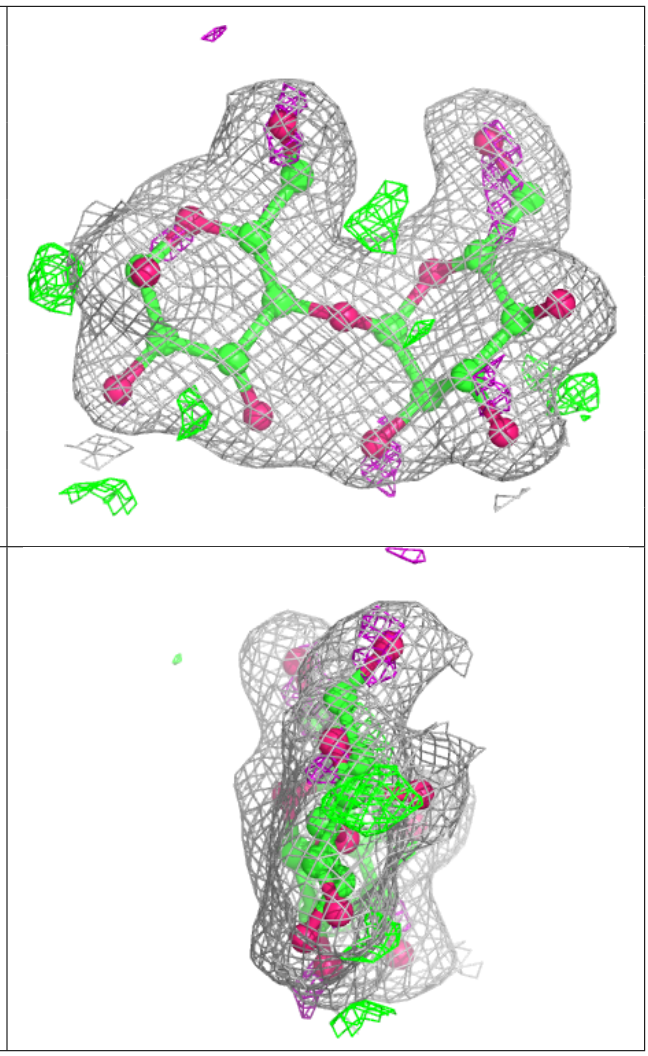






Electron density around Chain D:

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



6.4 Ligands (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	SO4	A	5000	5/5	0.85	0.27	87,88,90,91	0

6.5 Other polymers (i)

There are no such residues in this entry.