Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2025 – 05:02 PM EDT

PDB ID	:	9CPN / pdb_00009cpn
Title	:	Structural basis of BAK sequestration by MCL-1 and consequences for apoptosis initiation
Authors	:	Aggarwal, A.; Jayaraman, S.; Dey, R.; Moldoveanu, T.
Deposited on	:	2024-07-18
Resolution	:	1.89 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:

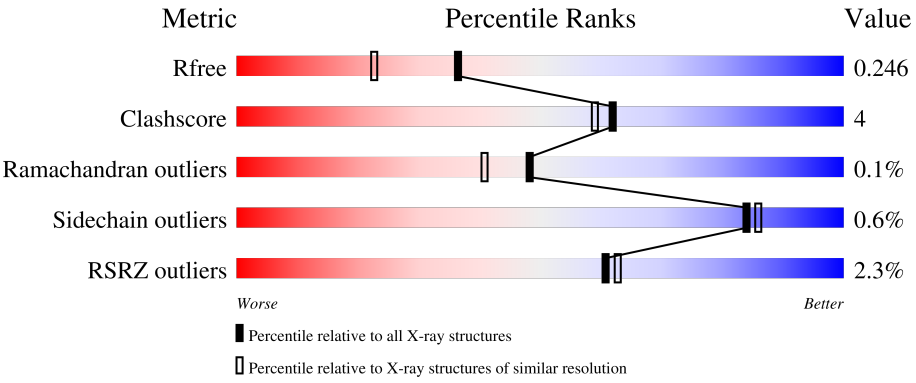
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 1.89 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}	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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	517	91% 8%
1	B	517	3% 89% 9%
1	C	517	3% 93% 6%
1	D	517	2% 90% 9%
2	E	22	5% 95% 5%

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Mol	Chain	Length	Quality of chain
2	F	22	5% 73% 18% 9%
2	G	22	68% 23% 5% 5%
2	H	22	82% 14% 5%
3	I	2	50% 50%
3	J	2	100%
3	K	2	100%
3	L	2	100%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 33942 atoms, of which 16182 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 Induced myeloid leukemia cell differentiation protein Mcl-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	514	Total	C	H	N	O	S	0	4	0
			8012	2575	3985	674	768	10			
1	B	505	Total	C	H	N	O	S	0	4	0
			7740	2506	3821	655	749	9			
1	C	511	Total	C	H	N	O	S	0	3	0
			7741	2515	3804	655	758	9			
1	D	510	Total	C	H	N	O	S	0	3	0
			7746	2514	3818	653	751	10			

- Molecule 2 is a protein called Bcl-2 homologous antagonist/killer.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	22	Total	C	H	N	O	S	0	2	0
			358	107	179	36	35	1			
2	F	22	Total	C	H	N	O	S	0	0	0
			340	102	170	34	33	1			
2	G	21	Total	C	H	N	O	S	0	0	0
			329	99	165	33	31	1			
2	H	21	Total	C	H	N	O	S	0	0	0
			311	97	152	30	31	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	2	Total	C	H	O	0	0	0
			45	12	22	11			
3	J	2	Total	C	H	O	0	0	0
			45	12	22	11			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	K	2	Total C H O 45 12 22 11	0	0	0
3	L	2	Total C H O 45 12 22 11	0	0	0

- Molecule 4 is water.

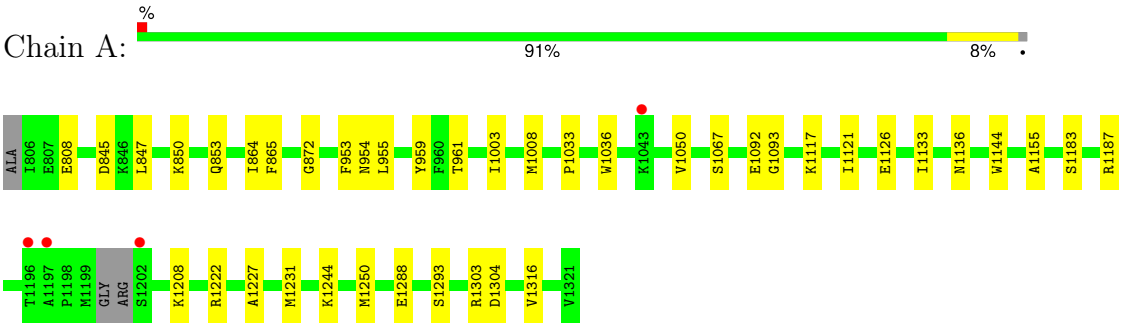
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	357	Total O 357 357	0	0
4	B	255	Total O 255 255	0	0
4	C	265	Total O 265 265	0	0
4	D	242	Total O 242 242	0	0
4	E	18	Total O 18 18	0	0
4	F	16	Total O 16 16	0	0
4	G	16	Total O 16 16	0	0
4	H	16	Total O 16 16	0	0

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.

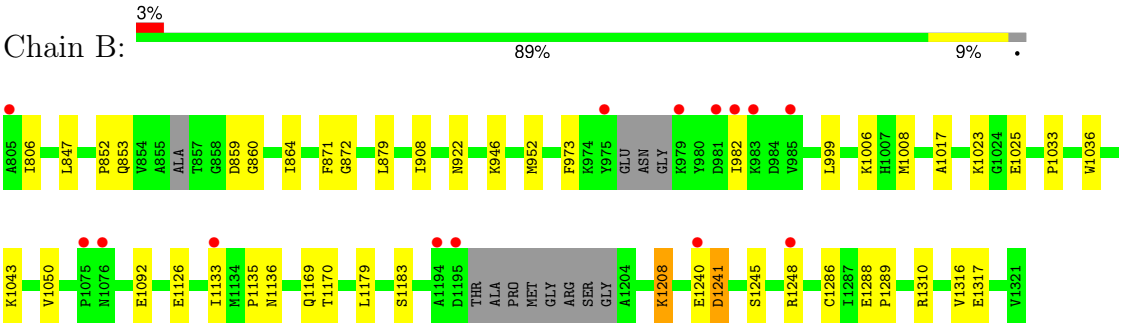
• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain A:



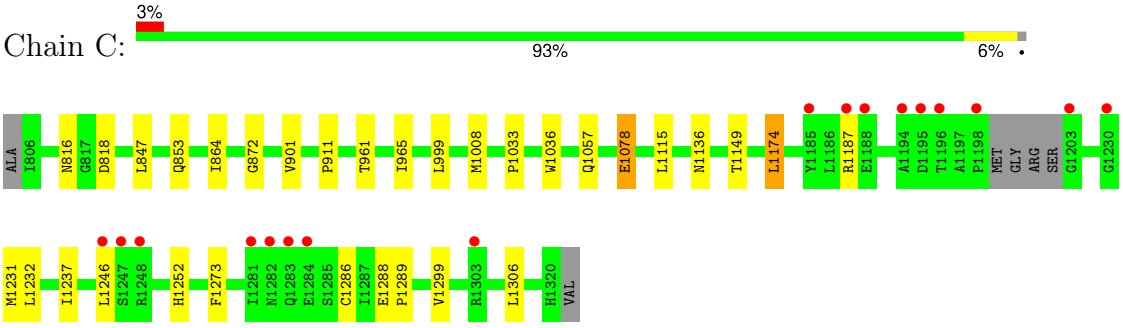
• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain B:



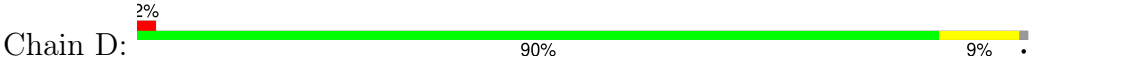
• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

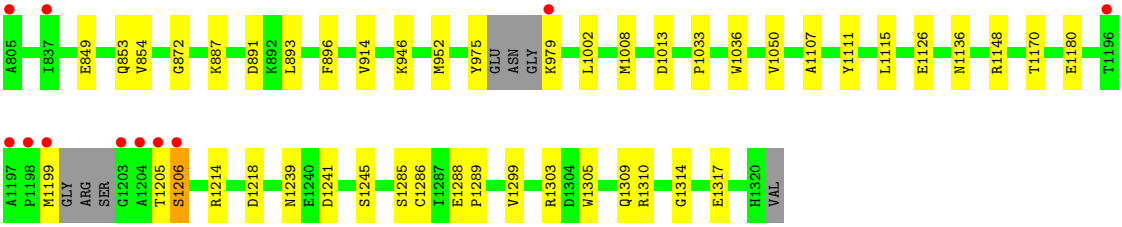
Chain C:



• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain D:





• Molecule 2: Bcl-2 homologous antagonist/killer

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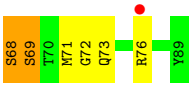

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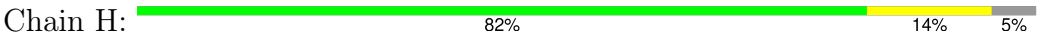
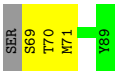
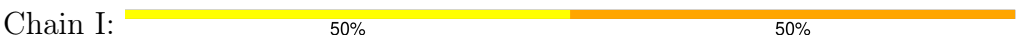




• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



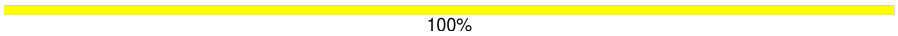
• Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

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

Chain K:

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

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	88.61Å 109.33Å 125.13Å 90.00° 100.68° 90.00°	Depositor
Resolution (Å)	34.69 – 1.89 34.69 – 1.89	Depositor EDS
% Data completeness (in resolution range)	98.3 (34.69-1.89) 98.4 (34.69-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 1.89Å)	Xtriage
Refinement program	PHENIX (1.21_5207: ???)	Depositor
R, R_{free}	0.191 , 0.243 0.196 , 0.246	Depositor DCC
R_{free} test set	9310 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	23.3	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 42.2	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	0.96	EDS
Total number of atoms	33942	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 66.73 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.7646e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

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

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	0.60	0/4128	0.73	0/5596
1	B	0.60	0/4023	0.74	1/5462 (0.0%)
1	C	0.58	0/4035	0.76	0/5488
1	D	0.57	0/4025	0.74	1/5471 (0.0%)
2	E	0.67	0/187	0.75	0/249
2	F	0.70	0/170	1.06	0/226
2	G	1.08	2/164 (1.2%)	0.73	0/218
2	H	0.62	0/159	0.72	0/212
All	All	0.60	2/16891 (0.0%)	0.75	2/22922 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	75	GLY	C-N	-8.87	1.21	1.34
2	G	76	ARG	C-N	-6.54	1.25	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1205	THR	N-CA-C	-5.36	106.24	112.89
1	B	1135	PRO	CA-C-O	-5.18	115.54	121.86

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	4027	3985	3990	39	0
1	B	3919	3821	3818	31	0
1	C	3937	3804	3808	25	0
1	D	3928	3818	3820	31	0
2	E	179	179	167	7	0
2	F	170	170	170	5	0
2	G	164	165	165	4	0
2	H	159	152	156	2	0
3	I	23	22	21	3	0
3	J	23	22	21	0	0
3	K	23	22	21	0	0
3	L	23	22	21	0	0
4	A	357	0	0	6	0
4	B	255	0	0	3	0
4	C	265	0	0	2	0
4	D	242	0	0	5	0
4	E	18	0	0	0	0
4	F	16	0	0	0	0
4	G	16	0	0	0	0
4	H	16	0	0	0	0
All	All	17760	16182	16178	131	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 4.

All (131) 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:C:1174:LEU:HD12	1:C:1299:VAL:HG22	1.55	0.88
1:A:853:GLN:HG2	1:A:1288[B]:GLU:HG2	1.53	0.88
1:B:847:LEU:HD13	1:B:864:ILE:HD11	1.59	0.85
1:D:1050:VAL:HG21	1:D:1126:GLU:OE2	1.77	0.85
1:C:1237:ILE:HD11	1:C:1246:LEU:HD21	1.61	0.82
1:A:808:GLU:OE2	4:A:1401:HOH:O	2.03	0.77
1:A:1231:MET:HE2	2:E:77[B]:GLN:HB3	1.70	0.74
1:A:1208:LYS:HE2	1:A:1316:VAL:HG11	1.72	0.72
1:B:847:LEU:CD1	1:B:864:ILE:HD11	2.20	0.71
2:F:72:GLY:O	2:F:76:ARG:HG3	1.92	0.70
1:C:853:GLN:HG2	1:C:1288:GLU:HG2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1050:VAL:HG22	1:A:1126:GLU:HG2	1.77	0.66
1:C:853:GLN:HG2	1:C:1288:GLU:CG	2.26	0.66
1:B:853:GLN:HG2	1:B:1288:GLU:HG2	1.79	0.65
1:A:1222:ARG:O	1:B:946:LYS:HG3	1.97	0.64
1:A:1187:ARG:HD2	1:A:1288[A]:GLU:OE2	1.98	0.63
1:C:1231:MET:HE2	2:G:77:GLN:HB2	1.81	0.63
1:B:1310:ARG:NH2	1:B:1317:GLU:OE2	2.28	0.63
1:C:847:LEU:C	1:C:847:LEU:HD12	2.24	0.63
1:C:1078:GLU:CD	1:C:1078:GLU:H	2.06	0.62
1:D:872:GLY:HA3	1:D:1136:ASN:O	2.01	0.60
1:D:1310:ARG:NH2	1:D:1317:GLU:OE2	2.34	0.60
1:D:1050:VAL:HG22	1:D:1126:GLU:HG2	1.85	0.59
1:C:1252:HIS:ND1	2:G:72:GLY:HA2	2.18	0.58
1:D:1286:CYS:C	1:D:1289:PRO:HD2	2.29	0.58
1:B:847:LEU:HD13	1:B:864:ILE:CD1	2.31	0.58
1:A:955:LEU:HA	4:A:1402:HOH:O	2.03	0.57
1:B:847:LEU:HD12	1:B:847:LEU:C	2.28	0.57
1:B:1092:GLU:H	1:B:1092:GLU:CD	2.13	0.57
1:A:1303:ARG:NH1	1:A:1304:ASP:OD1	2.38	0.56
1:B:1245:SER:O	1:B:1248:ARG:HD3	2.04	0.56
1:D:1180:GLU:HG2	1:D:1199:MET:HE3	1.87	0.56
1:C:1174:LEU:CD1	1:C:1299:VAL:HG22	2.33	0.56
1:A:872:GLY:HA3	1:A:1136:ASN:O	2.06	0.55
1:A:961:THR:HG23	4:A:1402:HOH:O	2.07	0.55
1:D:1299:VAL:O	1:D:1303:ARG:HG2	2.07	0.54
1:A:845:ASP:O	1:A:850:LYS:HE2	2.08	0.54
1:A:953:PHE:CE1	1:A:1008:MET:HE1	2.43	0.54
1:C:961[A]:THR:CG2	1:C:999:LEU:HD22	2.39	0.53
1:B:859:ASP:OD1	1:B:860:GLY:N	2.35	0.53
1:C:1033:PRO:HA	1:C:1036:TRP:CE2	2.44	0.53
1:B:1245:SER:HB3	2:F:71:MET:HE1	1.90	0.53
1:C:1231:MET:HE2	2:G:77:GLN:CB	2.38	0.53
2:H:69:SER:OG	2:H:70:THR:N	2.40	0.52
1:B:973:PHE:CD2	1:B:982:ILE:HA	2.44	0.52
1:A:1244:LYS:NZ	1:A:1244:LYS:HB2	2.24	0.52
1:B:859:ASP:CG	1:B:860:GLY:H	2.18	0.52
1:A:1033:PRO:HA	1:A:1036:TRP:CE2	2.45	0.52
1:A:1227:ALA:HB1	2:E:77[B]:GLN:OE1	2.09	0.52
1:C:816:ASN:ND2	1:C:818:ASP:OD1	2.44	0.51
1:D:1239:ASN:OD1	1:D:1241:ASP:HB2	2.11	0.50
1:C:1232:LEU:HD12	1:C:1273:PHE:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:849:GLU:OE2	4:D:1401:HOH:O	2.20	0.50
1:C:1115:LEU:HD12	4:C:1515:HOH:O	2.10	0.50
1:A:847:LEU:CD1	1:A:864:ILE:HD11	2.43	0.49
1:C:999:LEU:HD12	1:C:1008:MET:HE1	1.94	0.49
1:B:1179:LEU:O	1:B:1183:SER:HB3	2.12	0.49
1:D:1033:PRO:HA	1:D:1036:TRP:CE2	2.48	0.49
1:D:1013:ASP:OD1	1:D:1013:ASP:C	2.54	0.49
1:C:1286:CYS:C	1:C:1289:PRO:HD2	2.38	0.49
1:B:1050:VAL:HG22	1:B:1126:GLU:HG2	1.93	0.49
1:D:1245:SER:OG	2:H:71:MET:HE1	2.13	0.49
1:A:1231:MET:HE3	2:E:77[A]:GLN:HG3	1.95	0.48
1:A:1231:MET:CE	2:E:77[A]:GLN:HG3	2.44	0.48
1:B:1286:CYS:HA	1:B:1289:PRO:HG2	1.94	0.48
1:B:872:GLY:HA3	1:B:1136:ASN:O	2.12	0.48
1:A:1250:MET:HE1	1:A:1293:SER:OG	2.13	0.48
1:B:1286:CYS:C	1:B:1289:PRO:HD2	2.38	0.48
1:C:961[A]:THR:HG21	1:C:999:LEU:HD22	1.95	0.48
1:C:872:GLY:HA3	1:C:1136:ASN:O	2.14	0.47
2:F:68:SER:O	2:F:69:SER:CB	2.62	0.47
1:C:1288:GLU:O	1:C:1288:GLU:OE1	2.31	0.47
1:B:952:MET:HE2	1:B:1017:ALA:HA	1.97	0.47
1:A:1231:MET:HE3	2:E:77[B]:GLN:CD	2.39	0.47
1:B:999:LEU:CD1	1:B:1008:MET:HE1	2.45	0.46
1:A:1231:MET:CE	2:E:77[B]:GLN:HB3	2.44	0.46
1:C:847:LEU:HD13	1:C:864:ILE:HD11	1.98	0.46
1:A:1050:VAL:CG2	1:A:1126:GLU:HG2	2.43	0.46
1:A:1144:TRP:CD1	3:I:2:GLC:H4	2.50	0.46
2:G:69:SER:OG	2:G:70:THR:N	2.47	0.46
2:F:68:SER:N	2:F:73:GLN:HE21	2.13	0.46
1:A:1183[B]:SER:OG	1:A:1288[B]:GLU:OE1	2.34	0.46
1:C:1149:THR:HG21	4:C:1475:HOH:O	2.16	0.45
1:D:1050:VAL:CG2	1:D:1126:GLU:OE2	2.55	0.45
1:B:1025:GLU:OE1	4:B:1401:HOH:O	2.21	0.45
1:D:1309:GLN:O	1:D:1314:GLY:HA3	2.17	0.45
1:C:901:VAL:HG21	1:C:911:PRO:HD3	1.97	0.45
2:F:68:SER:O	2:F:69:SER:HB3	2.17	0.45
1:A:1121:ILE:HD11	4:A:1440:HOH:O	2.15	0.45
1:D:1170:THR:HG23	4:D:1408:HOH:O	2.16	0.45
1:D:887:LYS:HD2	1:D:891:ASP:CG	2.42	0.45
1:A:847:LEU:HD13	1:A:864:ILE:CD1	2.48	0.44
1:D:952:MET:HG2	4:D:1518:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1305:TRP:CZ2	1:D:1309:GLN:HG3	2.53	0.44
1:A:847:LEU:C	1:A:847:LEU:HD12	2.42	0.44
1:D:1288:GLU:N	1:D:1289:PRO:CD	2.81	0.44
1:A:847:LEU:HD13	1:A:864:ILE:HD11	2.00	0.44
1:A:1231:MET:HE3	2:E:77[A]:GLN:CG	2.48	0.44
1:D:946:LYS:HE2	4:D:1465:HOH:O	2.19	0.43
1:A:1092:GLU:HG2	1:A:1093:GLY:N	2.33	0.43
1:A:1117:LYS:HE2	1:A:1117:LYS:HB3	1.88	0.43
1:D:854:VAL:HG12	1:D:1285:SER:HB2	2.01	0.43
1:B:1033:PRO:HA	1:B:1036:TRP:CE2	2.54	0.42
1:D:1002:LEU:CD1	1:D:1008:MET:HE2	2.50	0.42
1:B:852:PRO:HA	1:B:879:LEU:HD13	2.01	0.42
1:C:961[A]:THR:HG22	1:C:965:ILE:CD1	2.49	0.42
1:C:1174:LEU:HD11	1:C:1306:LEU:HD13	2.02	0.42
1:A:959:TYR:HB2	3:I:2:GLC:O5	2.19	0.42
1:B:1043:LYS:HA	4:B:1449:HOH:O	2.18	0.42
1:B:871:PHE:HB3	1:B:908:ILE:HD12	2.02	0.42
1:A:1133:ILE:HG22	4:A:1689:HOH:O	2.19	0.42
1:D:896:PHE:CZ	1:D:914:VAL:HG21	2.54	0.42
1:D:887:LYS:HD2	1:D:891:ASP:OD1	2.20	0.41
1:A:853:GLN:HG2	1:A:1288[B]:GLU:CG	2.37	0.41
1:B:922:ASN:C	1:B:922:ASN:OD1	2.62	0.41
1:B:1023:LYS:CE	4:B:1418:HOH:O	2.68	0.41
1:B:1310:ARG:HH11	1:B:1310:ARG:HG3	1.86	0.41
1:A:954:ASN:O	4:A:1402:HOH:O	2.22	0.41
1:D:849:GLU:O	1:D:853:GLN:HG3	2.20	0.41
1:A:1003:ILE:HD13	1:A:1155:ALA:HB1	2.03	0.41
1:D:1148:ARG:NH1	4:D:1429:HOH:O	2.54	0.41
1:A:865:PHE:HA	1:A:1067:SER:O	2.21	0.41
1:D:1199:MET:HE2	1:D:1206:SER:HB3	2.03	0.41
1:A:1144:TRP:CE3	3:I:2:GLC:H61	2.56	0.41
1:B:1208:LYS:HG2	1:B:1316:VAL:HG11	2.04	0.40
1:D:975:TYR:CE1	1:D:979:LYS:N	2.90	0.40
1:D:1111:TYR:CE2	1:D:1115:LEU:HD21	2.56	0.40
1:D:1214:ARG:O	1:D:1218:ASP:HB2	2.22	0.40
1:B:1169:GLN:O	1:B:1170:THR:C	2.64	0.40
1:B:1240:GLU:O	1:B:1241:ASP:HB2	2.21	0.40
1:D:893:LEU:HA	1:D:1107:ALA:O	2.22	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	514/517 (99%)	507 (99%)	7 (1%)	0	100 100
1	B	501/517 (97%)	492 (98%)	7 (1%)	2 (0%)	30 22
1	C	510/517 (99%)	500 (98%)	10 (2%)	0	100 100
1	D	507/517 (98%)	498 (98%)	9 (2%)	0	100 100
2	E	22/22 (100%)	21 (96%)	1 (4%)	0	100 100
2	F	20/22 (91%)	19 (95%)	0	1 (5%)	1 0
2	G	19/22 (86%)	19 (100%)	0	0	100 100
2	H	19/22 (86%)	19 (100%)	0	0	100 100
All	All	2112/2156 (98%)	2075 (98%)	34 (2%)	3 (0%)	48 41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1241	ASP
2	F	69	SER
1	B	806	ILE

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	422/421 (100%)	422 (100%)	0	100 100
1	B	405/421 (96%)	402 (99%)	3 (1%)	81 83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	402/421 (96%)	398 (99%)	4 (1%)	73 74
1	D	402/421 (96%)	401 (100%)	1 (0%)	92 93
2	E	20/18 (111%)	20 (100%)	0	100 100
2	F	18/18 (100%)	17 (94%)	1 (6%)	17 10
2	G	17/18 (94%)	16 (94%)	1 (6%)	16 9
2	H	16/18 (89%)	16 (100%)	0	100 100
All	All	1702/1756 (97%)	1692 (99%)	10 (1%)	84 86

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1006	LYS
1	B	1133	ILE
1	B	1208	LYS
1	C	1057	GLN
1	C	1078	GLU
1	C	1174	LEU
1	C	1187	ARG
1	D	1206	SER
2	F	68	SER
2	G	70	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	876	GLN
1	A	956	GLN
1	A	1045	ASN
1	A	1277	HIS
1	B	904	ASN
1	B	1223	ASN
1	B	1229	GLN
1	C	853	GLN
1	C	1045	ASN
1	C	1086	ASN
1	C	1224	HIS
1	C	1283	GLN
1	D	956	GLN
1	D	1223	ASN

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)

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GLC	I	1	3	12,12,12	0.82	1 (8%)	17,17,17	1.30	2 (11%)
3	GLC	I	2	3	11,11,12	0.73	0	15,15,17	1.29	2 (13%)
3	GLC	J	1	3	12,12,12	0.85	1 (8%)	17,17,17	1.27	3 (17%)
3	GLC	J	2	3	11,11,12	0.88	0	15,15,17	1.24	1 (6%)
3	GLC	K	1	3	12,12,12	0.58	0	17,17,17	1.23	1 (5%)
3	GLC	K	2	3	11,11,12	0.81	0	15,15,17	1.14	2 (13%)
3	GLC	L	1	3	12,12,12	0.68	0	17,17,17	1.04	1 (5%)
3	GLC	L	2	3	11,11,12	0.58	0	15,15,17	1.10	1 (6%)

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
3	GLC	I	1	3	-	0/2/22/22	0/1/1/1
3	GLC	I	2	3	-	0/2/19/22	0/1/1/1
3	GLC	J	1	3	-	0/2/22/22	0/1/1/1
3	GLC	J	2	3	-	0/2/19/22	0/1/1/1
3	GLC	K	1	3	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLC	K	2	3	-	0/2/19/22	0/1/1/1
3	GLC	L	1	3	-	0/2/22/22	0/1/1/1
3	GLC	L	2	3	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1	GLC	O5-C5	-2.18	1.39	1.44
3	J	1	GLC	O5-C5	-2.00	1.39	1.44

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	1	GLC	O5-C1-C2	3.59	116.61	110.30
3	I	1	GLC	O5-C1-C2	3.34	116.18	110.30
3	K	1	GLC	O5-C1-C2	2.96	115.51	110.30
3	J	2	GLC	C1-O5-C5	2.91	116.09	112.19
3	L	1	GLC	O5-C1-C2	2.82	115.25	110.30
3	I	1	GLC	O1-C1-O5	-2.67	102.49	110.41
3	J	1	GLC	C1-O5-C5	2.49	118.47	113.65
3	I	2	GLC	C1-C2-C3	2.49	113.27	109.64
3	L	2	GLC	C2-C3-C4	-2.47	106.53	110.86
3	I	2	GLC	C2-C3-C4	-2.27	106.86	110.86
3	K	2	GLC	C6-C5-C4	-2.24	107.53	113.02
3	J	1	GLC	O1-C1-O5	-2.13	104.09	110.41
3	K	2	GLC	C2-C3-C4	-2.07	107.21	110.86

There are no chirality outliers.

There are no torsion outliers.

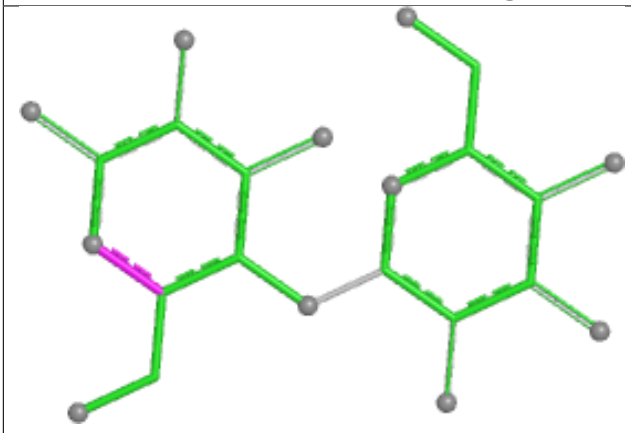
There are no ring outliers.

1 monomer is involved in 3 short contacts:

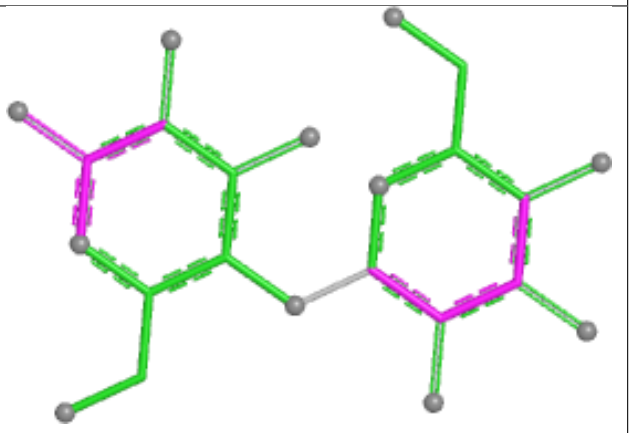
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	2	GLC	3	0

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

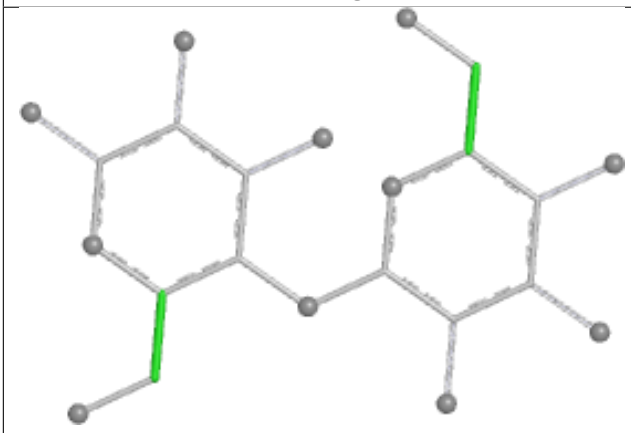
Oligosaccharide Chain I



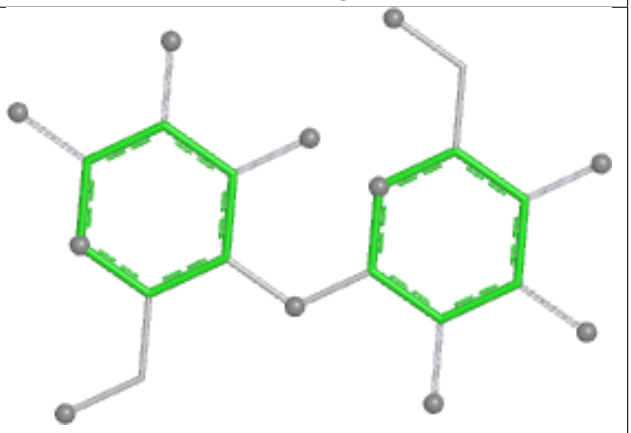
Bond lengths



Bond angles

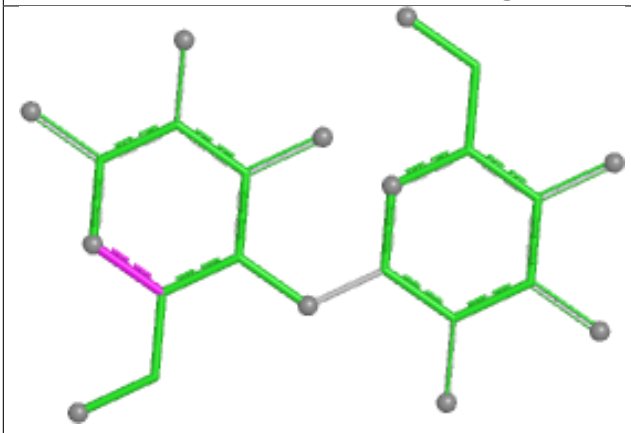


Torsions

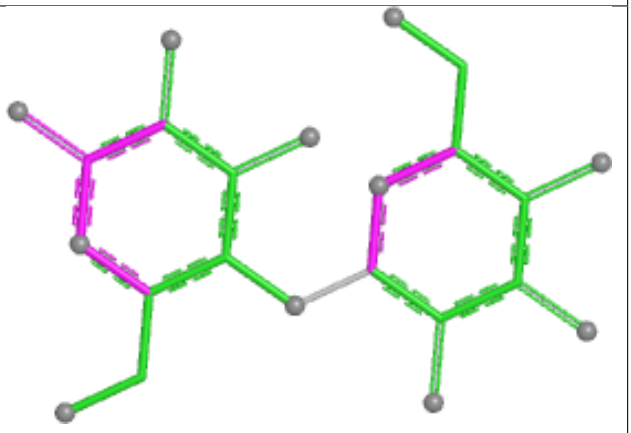


Rings

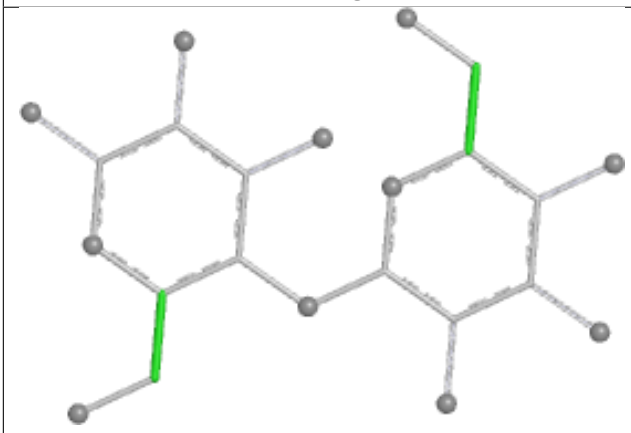
Oligosaccharide Chain J



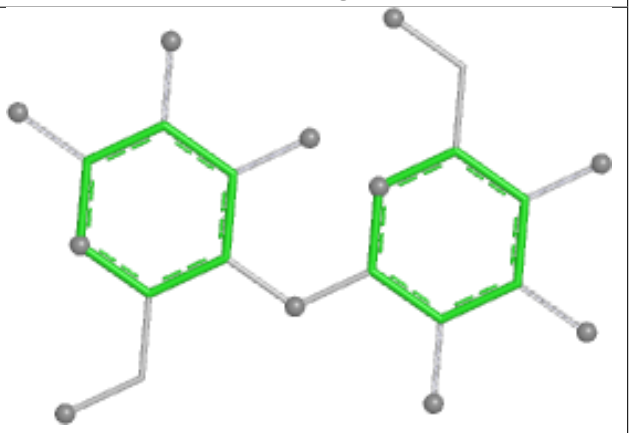
Bond lengths



Bond angles

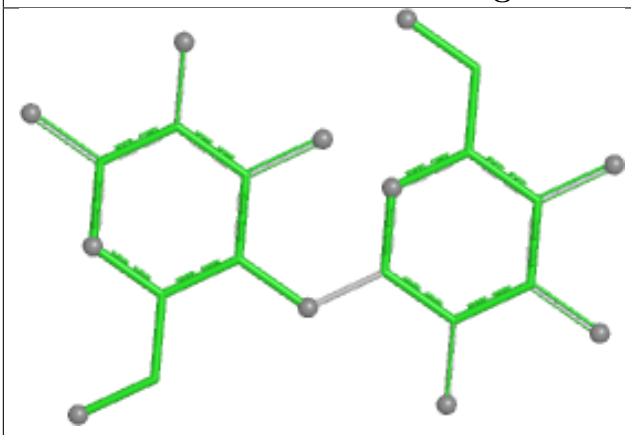


Torsions

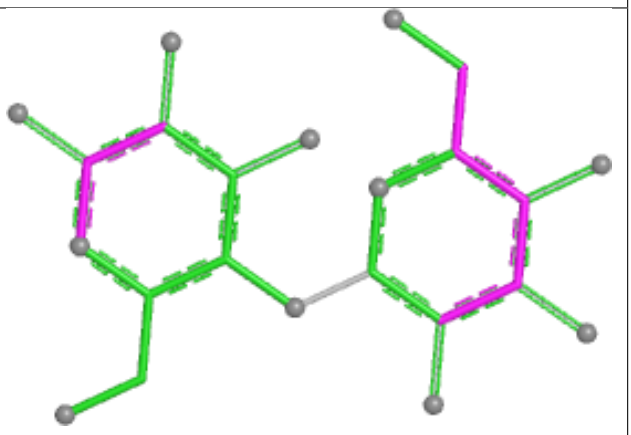


Rings

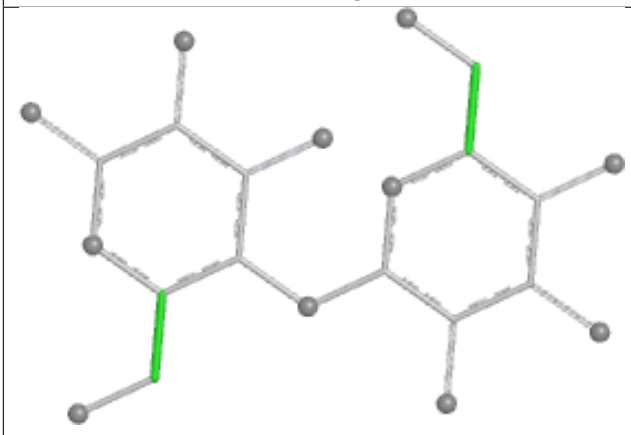
Oligosaccharide Chain K



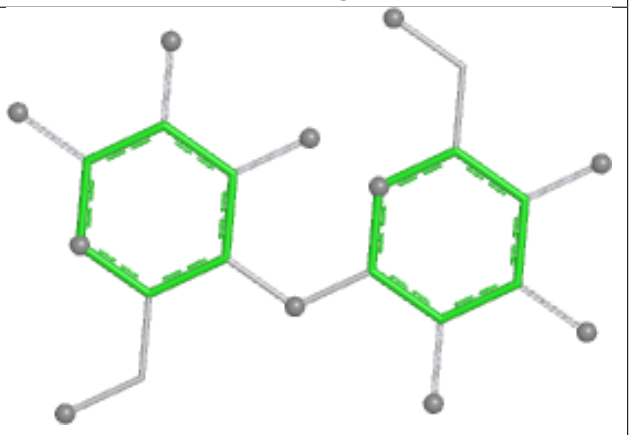
Bond lengths



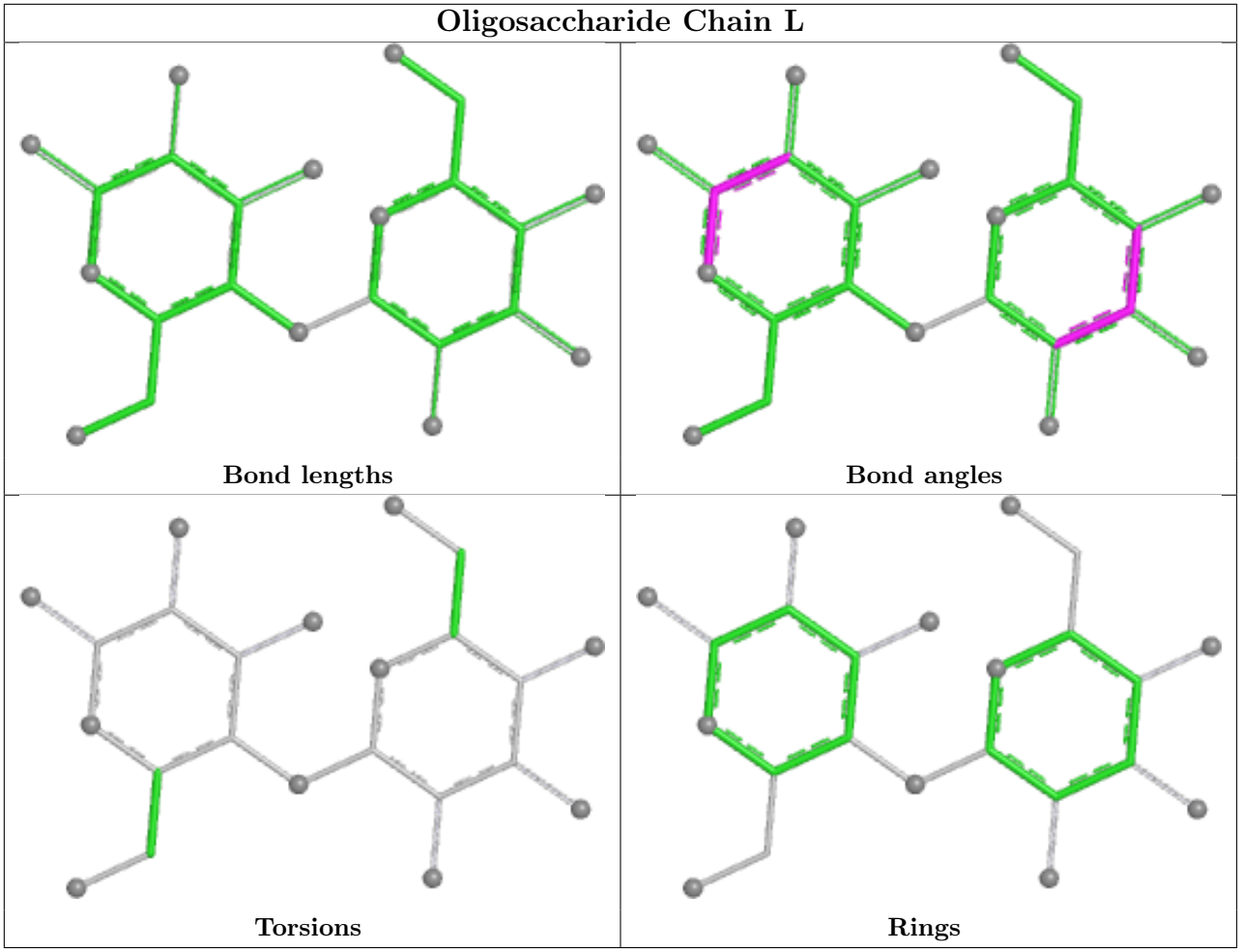
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

There are no ligands in this entry.

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, 95^{th} 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	514/517 (99%)	-0.50	4 (0%) 82 84	11, 26, 47, 84	4 (0%)
1	B	505/517 (97%)	-0.22	14 (2%) 55 57	14, 30, 56, 92	3 (0%)
1	C	511/517 (98%)	-0.19	17 (3%) 49 51	14, 31, 56, 89	3 (0%)
1	D	510/517 (98%)	-0.20	11 (2%) 62 64	14, 32, 54, 105	3 (0%)
2	E	22/22 (100%)	-0.52	1 (4%) 39 40	11, 22, 39, 51	1 (4%)
2	F	22/22 (100%)	-0.17	1 (4%) 39 40	14, 23, 43, 55	0
2	G	21/22 (95%)	-0.23	0 100 100	17, 27, 54, 68	0
2	H	21/22 (95%)	-0.24	0 100 100	16, 23, 57, 65	0
All	All	2126/2156 (98%)	-0.28	48 (2%) 61 63	11, 30, 54, 105	14 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1187	ARG	6.4
1	B	975	TYR	6.2
1	D	1203	GLY	5.8
1	C	1198	PRO	5.0
1	B	805	ALA	4.5
1	B	1076	ASN	4.5
1	C	1248	ARG	4.4
2	F	76	ARG	3.8
1	D	1205	THR	3.8
1	D	1204	ALA	3.8
1	C	1203	GLY	3.7
1	B	1195	ASP	3.6
1	C	1283	GLN	3.5
1	B	979	LYS	3.4
1	C	1281	ILE	3.4
1	D	979	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	1197	ALA	3.2
1	C	1246	LEU	3.1
1	D	1198	PRO	3.1
1	C	1303	ARG	3.1
1	D	1199	MET	3.0
1	C	1282	ASN	3.0
1	B	1194	ALA	2.9
1	B	1240	GLU	2.8
1	D	1206	SER	2.8
1	C	1194	ALA	2.7
1	D	1196	THR	2.7
1	B	1248	ARG	2.7
1	C	1284	GLU	2.7
1	B	1133	ILE	2.6
1	A	1196	THR	2.5
1	C	1230	GLY	2.4
1	B	983	LYS	2.3
1	C	1196	THR	2.3
1	B	1075	PRO	2.2
1	A	1197	ALA	2.2
1	B	985	VAL	2.2
2	E	68	SER	2.1
1	A	1202	SER	2.1
1	C	1188	GLU	2.1
1	C	1185	TYR	2.1
1	C	1247	SER	2.1
1	D	837	ILE	2.1
1	B	981	ASP	2.0
1	C	1195	ASP	2.0
1	D	805	ALA	2.0
1	B	982	ILE	2.0
1	A	1043	LYS	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,

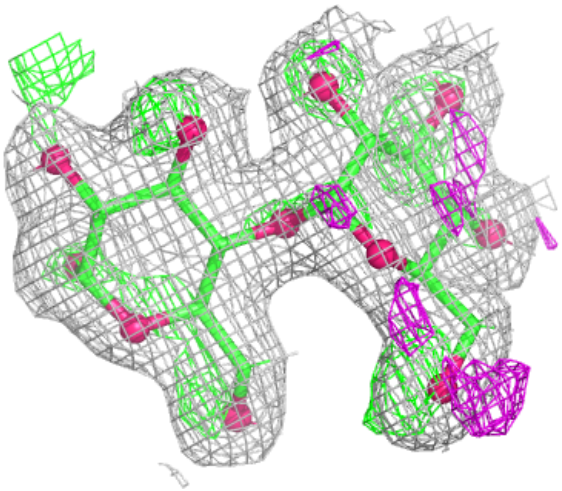
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

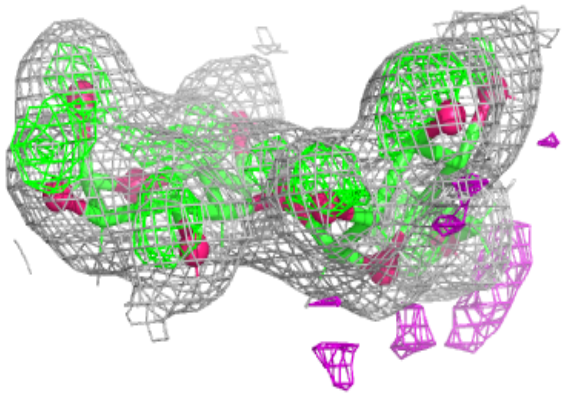
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GLC	I	2	11/12	0.86	0.13	20,25,29,32	0
3	GLC	L	1	12/12	0.88	0.12	24,34,44,48	0
3	GLC	J	1	12/12	0.91	0.09	22,30,40,48	0
3	GLC	I	1	12/12	0.91	0.12	22,29,40,47	0
3	GLC	J	2	11/12	0.92	0.09	21,26,30,32	0
3	GLC	K	2	11/12	0.94	0.07	23,26,32,32	0
3	GLC	K	1	12/12	0.94	0.09	22,33,44,48	0
3	GLC	L	2	11/12	0.95	0.07	21,26,31,34	0

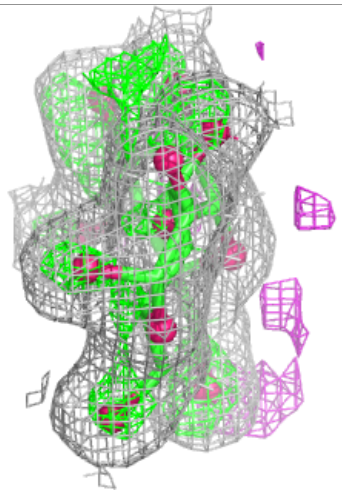
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

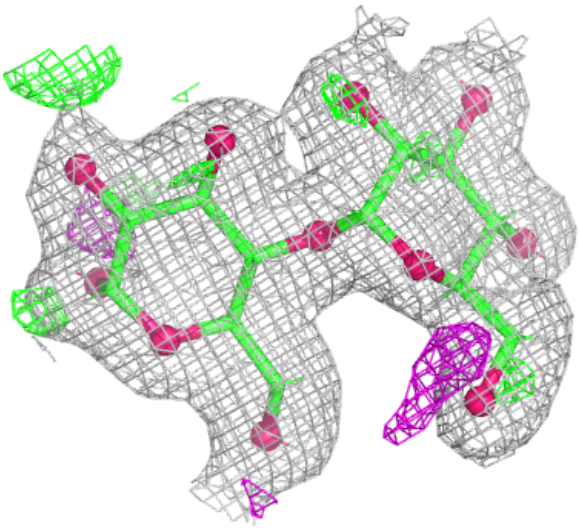


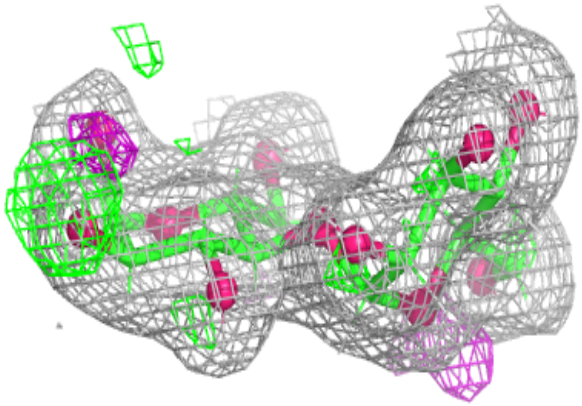


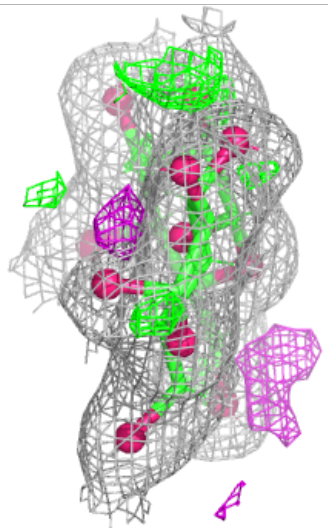


Electron density around Chain J:

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

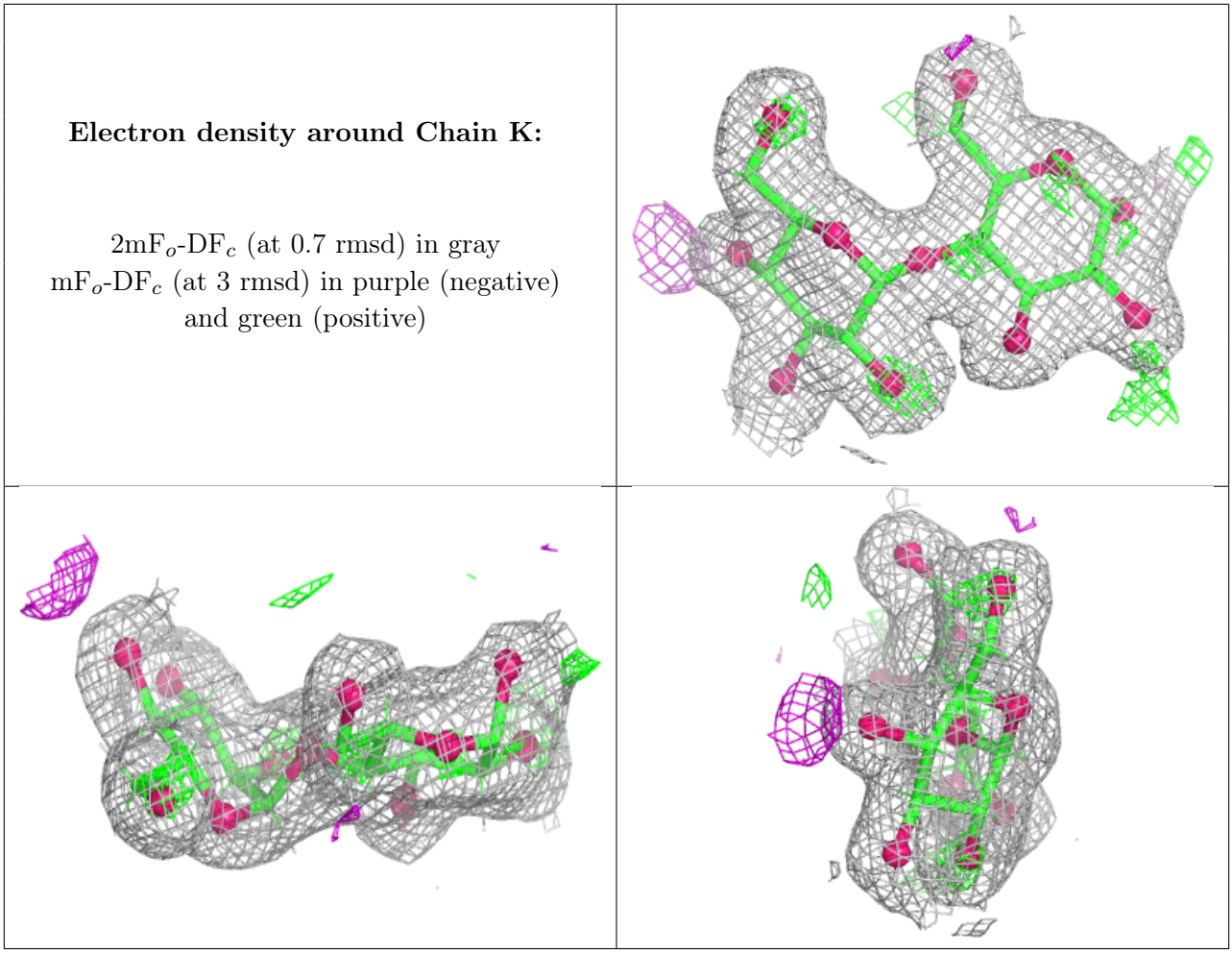






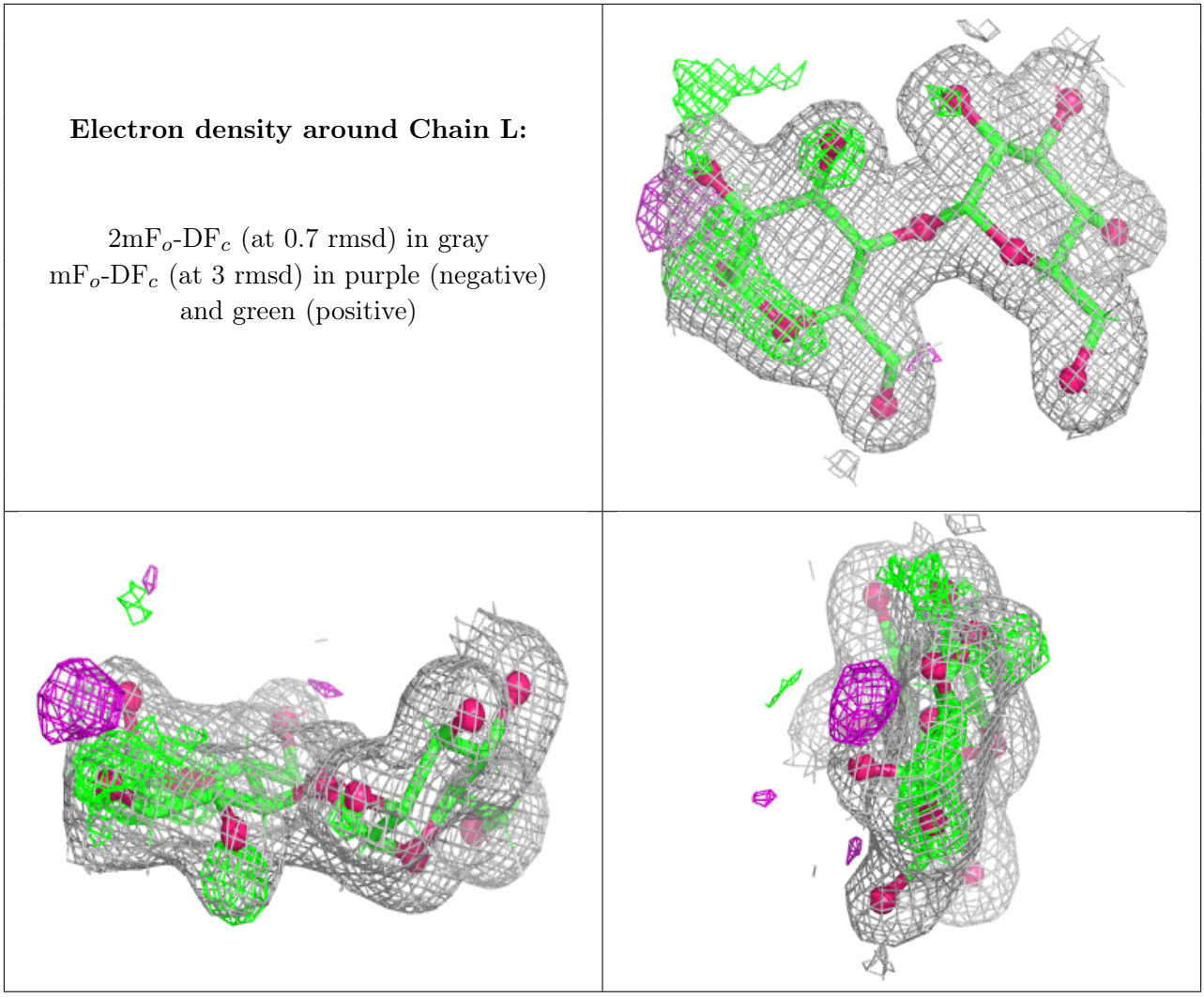
Electron density around Chain K:

$2mF_o$-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 L:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.