Full wwPDB EM Validation Report ⓘ

May 4, 2024 – 11:12 am BST

PDB ID	:	6Z7P
EMDB ID	:	EMD-10388
Title	:	Composite model of the Caulobacter crescentus S-layer bound to the O-antigen of lipopolysaccharide
Authors	:	Bharat, T.A.M.; von Kugelgen, A.
Deposited on	:	2020-06-01
Resolution	:	4.80 Å(reported)
Based on initial models	:	5N8P, 6T72

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

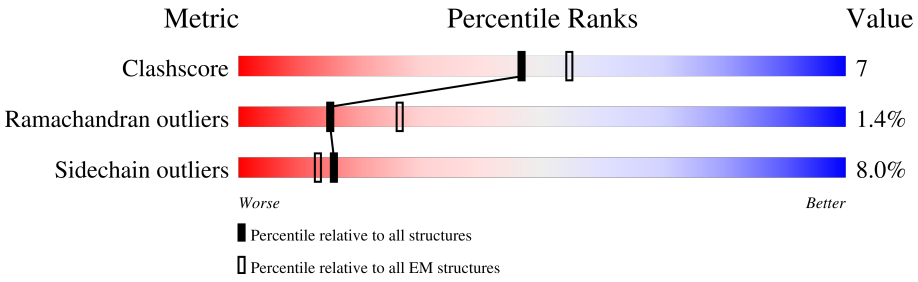
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

Mol	Chain	Length	Quality of chain
1	A	1025	81% 17% .
2	B	9	11% 89%

2 Entry composition

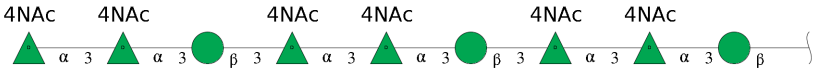
There are 3 unique types of molecules in this entry. The entry contains 7021 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 S-layer protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1025	6888	4228	1148	1509	3	0	0

- Molecule 2 is an oligosaccharide called 4-acetamido-4,6-dideoxy-alpha-D-mannopyranose-(1-3)-4-acetamido-4,6-dideoxy-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-3)-4-acetamido-4,6-dideoxy-alpha-D-mannopyranose-(1-3)-4-acetamido-4,6-dideoxy-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-3)-4-acetamido-4,6-dideoxy-alpha-D-mannopyranose-(1-3)-4-acetamido-4,6-dideoxy-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	9	111	66	6	39	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

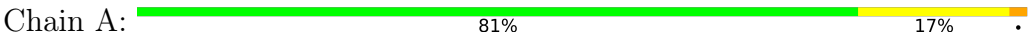
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
3	A	22	22	22	0

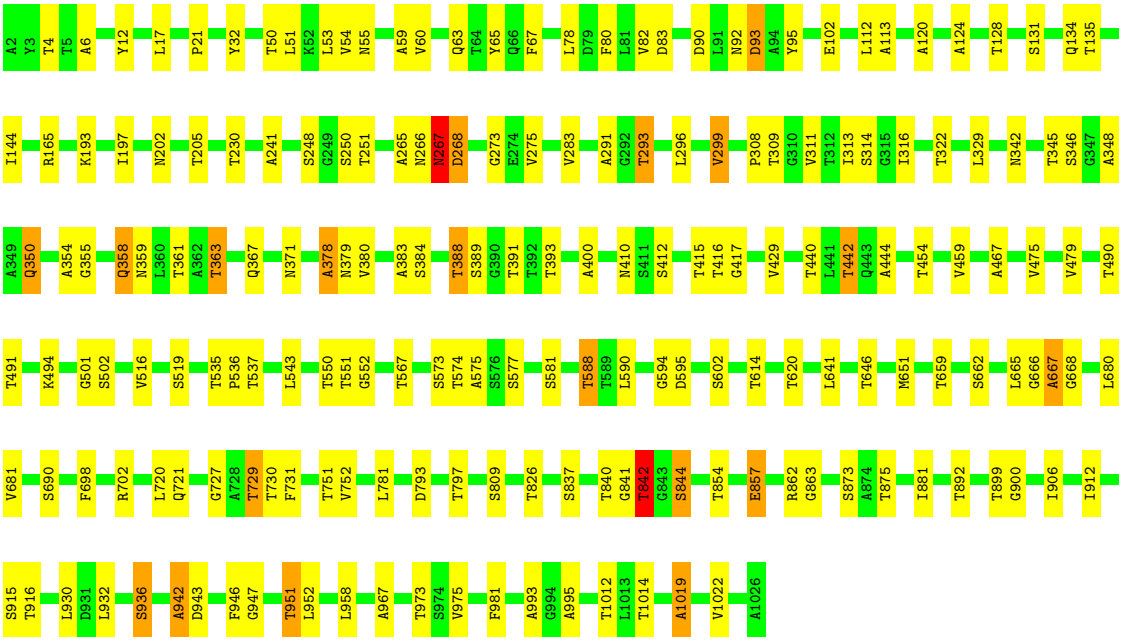
3 Residue-property plots (i)

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. 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. 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: S-layer protein

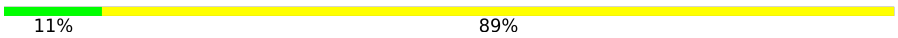
Chain A:





• Molecule 2: 4-acetamido-4,6-dideoxy-alpha-D-mannopyranose-(1-3)-4-acetamido-4,6-dideoxy-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-3)-4-acetamido-4,6-dideoxy-alpha-D-mannopyranose-(1-3)-4-acetamido-4,6-dideoxy-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-3)-4-acetamido-4,6-dideoxy-alpha-D-mannopyranose-(1-3)-4-acetamido-4,6-dideoxy-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose

Chain B:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	51866	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Following Turonova and Briggs NovaCTF	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	3.4	Depositor
Minimum defocus (nm)	-2000	Depositor
Maximum defocus (nm)	-5000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.68	1/6948 (0.0%)	0.93	4/9561 (0.0%)

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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	842	THR	CA-CB	5.33	1.67	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	840	THR	N-CA-C	6.73	129.18	111.00
1	A	32	TYR	CB-CG-CD1	-5.36	117.78	121.00
1	A	900	GLY	N-CA-C	-5.31	99.82	113.10
1	A	793	ASP	CB-CG-OD1	5.26	123.04	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	ARG	Sidechain
1	A	594	GLY	Peptide

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	6888	0	6783	90	0
2	B	111	0	27	0	0
3	A	22	0	0	0	0
All	All	7021	0	6810	90	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 7.

All (90) 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:265:ALA:HA	1:A:291:ALA:H	1.22	1.04
1:A:230:THR:HG21	1:A:241:ALA:HB1	1.57	0.87
1:A:442:THR:HB	1:A:475:VAL:HB	1.60	0.83
1:A:342:ASN:HD22	1:A:361:THR:HB	1.56	0.71
1:A:51:LEU:O	1:A:54:VAL:HG12	1.91	0.71
1:A:124:ALA:O	1:A:128:THR:OG1	2.09	0.70
1:A:947:GLY:O	1:A:1014:THR:HA	1.94	0.68
1:A:265:ALA:HA	1:A:291:ALA:N	2.04	0.68
1:A:83:ASP:HB2	1:A:92:ASN:HD21	1.58	0.67
1:A:702:ARG:HB2	1:A:721:GLN:HB2	1.77	0.66
1:A:63:GLN:HE22	1:A:205:THR:HB	1.62	0.64
1:A:113:ALA:O	1:A:120:ALA:HA	1.99	0.62
1:A:144:ILE:HG22	1:A:144:ILE:O	2.01	0.60
1:A:841:GLY:H	1:A:844:SER:HG	1.48	0.60
1:A:102:GLU:HA	1:A:202:ASN:HD22	1.67	0.60
1:A:410:ASN:OD1	1:A:412:SER:HB3	2.04	0.57
1:A:501:GLY:HA2	1:A:519:SER:HB3	1.87	0.57
1:A:359:ASN:ND2	1:A:379:ASN:H	2.03	0.57
1:A:416:THR:HG22	1:A:416:THR:O	2.05	0.57
1:A:1019:ALA:HB3	1:A:1022:VAL:HB	1.87	0.57
1:A:440:THR:OG1	1:A:467:ALA:HB2	2.05	0.56
1:A:17:LEU:HD11	1:A:78:LEU:HB3	1.88	0.56
1:A:912:ILE:H	1:A:912:ILE:HD12	1.70	0.56
1:A:313:ILE:HG23	1:A:316:ILE:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:THR:HG21	1:A:241:ALA:CB	2.33	0.54
1:A:12:TYR:CE2	1:A:21:PRO:HB3	2.41	0.54
1:A:841:GLY:N	1:A:844:SER:OG	2.33	0.53
1:A:359:ASN:HD22	1:A:379:ASN:H	1.55	0.53
1:A:12:TYR:CD2	1:A:21:PRO:HB3	2.44	0.53
1:A:265:ALA:CA	1:A:291:ALA:H	2.08	0.53
1:A:273:GLY:HA2	1:A:299:VAL:HG23	1.92	0.52
1:A:354:ALA:HB1	1:A:358:GLN:HE21	1.74	0.51
1:A:367:GLN:NE2	1:A:384:SER:HB3	2.25	0.51
1:A:837:SER:HA	1:A:863:GLY:O	2.11	0.51
1:A:363:THR:HG23	1:A:383:ALA:HB3	1.93	0.51
1:A:416:THR:HB	1:A:444:ALA:HB2	1.92	0.50
1:A:930:LEU:HG	1:A:932:LEU:HD21	1.94	0.50
1:A:942:ALA:O	1:A:943:ASP:CB	2.60	0.50
1:A:102:GLU:HA	1:A:202:ASN:ND2	2.27	0.49
1:A:936:SER:OG	1:A:936:SER:O	2.30	0.49
1:A:55:ASN:O	1:A:59:ALA:HB3	2.14	0.48
1:A:550:THR:HG22	1:A:552:GLY:H	1.77	0.48
1:A:371:ASN:ND2	1:A:391:THR:H	2.11	0.48
1:A:17:LEU:HD12	1:A:82:VAL:HB	1.94	0.48
1:A:80:PHE:C	1:A:80:PHE:CD1	2.86	0.48
1:A:720:LEU:HD13	1:A:731:PHE:CD2	2.48	0.48
1:A:265:ALA:C	1:A:291:ALA:HB3	2.34	0.47
1:A:752:VAL:HB	1:A:781:LEU:HD23	1.96	0.47
1:A:415:THR:HB	1:A:442:THR:O	2.13	0.47
1:A:355:GLY:H	1:A:358:GLN:NE2	2.11	0.47
1:A:144:ILE:O	1:A:144:ILE:CG2	2.62	0.47
1:A:388:THR:OG1	1:A:389:SER:N	2.46	0.47
1:A:131:SER:H	1:A:134:GLN:NE2	2.13	0.47
1:A:641:LEU:HG	1:A:659:THR:HB	1.97	0.47
1:A:345:THR:HG22	1:A:346:SER:N	2.30	0.46
1:A:350:GLN:HE21	1:A:350:GLN:HB2	1.57	0.46
1:A:535:THR:HA	1:A:536:PRO:HD3	1.81	0.46
1:A:854:THR:HB	1:A:857:GLU:CG	2.46	0.45
1:A:267:ASN:HA	1:A:293:THR:OG1	2.16	0.45
1:A:67:PHE:CE1	1:A:197:ILE:HD12	2.52	0.45
1:A:65:TYR:CZ	1:A:112:LEU:HD21	2.53	0.44
1:A:573:SER:HA	1:A:595:ASP:HB3	1.99	0.44
1:A:50:THR:HA	1:A:53:LEU:HD12	1.99	0.44
1:A:308:PRO:HD2	1:A:311:VAL:HG21	1.98	0.44
1:A:429:VAL:HG22	1:A:459:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:THR:HG21	1:A:193:LYS:HB3	2.00	0.43
1:A:4:THR:HG22	1:A:6:ALA:H	1.83	0.43
1:A:666:GLY:O	1:A:667:ALA:C	2.56	0.43
1:A:680:LEU:HB2	1:A:698:PHE:CD1	2.54	0.43
1:A:727:GLY:O	1:A:729:THR:HG22	2.18	0.42
1:A:378:ALA:O	1:A:400:ALA:HB1	2.18	0.42
1:A:581:SER:HA	1:A:602:SER:O	2.18	0.42
1:A:90:ASP:OD1	1:A:93:ASP:HB2	2.20	0.42
1:A:248:SER:C	1:A:267:ASN:HB2	2.40	0.41
1:A:342:ASN:ND2	1:A:361:THR:HB	2.29	0.41
1:A:958:LEU:HB2	1:A:981:PHE:CE2	2.56	0.41
1:A:516:VAL:HB	1:A:543:LEU:HD12	2.02	0.41
1:A:947:GLY:HA3	1:A:1014:THR:O	2.19	0.41
1:A:359:ASN:ND2	1:A:378:ALA:HB3	2.35	0.41
1:A:681:VAL:HG13	1:A:702:ARG:HG2	2.02	0.41
1:A:60:VAL:O	1:A:60:VAL:CG1	2.68	0.41
1:A:881:ILE:HA	1:A:899:THR:O	2.21	0.41
1:A:573:SER:O	1:A:575:ALA:N	2.46	0.41
1:A:967:ALA:HA	1:A:995:ALA:HA	2.03	0.40
1:A:345:THR:HG21	1:A:348:ALA:O	2.21	0.40
1:A:567:THR:HG22	1:A:588:THR:HG22	2.03	0.40
1:A:250:SER:H	1:A:268:ASP:HB3	1.86	0.40
1:A:367:GLN:HE21	1:A:384:SER:HB3	1.83	0.40
1:A:730:THR:HG23	1:A:751:THR:HB	2.04	0.40
1:A:951:THR:O	1:A:952:LEU:HD23	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 PDB entries followed by that with respect to all EM entries.

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	1023/1025 (100%)	948 (93%)	61 (6%)	14 (1%)	11 46

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	574	THR
1	A	936	SER
1	A	942	ALA
1	A	1019	ALA
1	A	267	ASN
1	A	667	ALA
1	A	946	PHE
1	A	993	ALA
1	A	417	GLY
1	A	378	ALA
1	A	502	SER
1	A	842	THR
1	A	665	LEU
1	A	668	GLY

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 PDB entries followed by that with respect to all EM entries.

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	698/698 (100%)	642 (92%)	56 (8%)	12 37

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	ASP
1	A	95	TYR
1	A	251	THR
1	A	266	ASN
1	A	267	ASN
1	A	268	ASP
1	A	275	VAL
1	A	283	VAL
1	A	293	THR
1	A	296	LEU
1	A	299	VAL

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Mol	Chain	Res	Type
1	A	309	THR
1	A	314	SER
1	A	322	THR
1	A	329	LEU
1	A	350	GLN
1	A	358	GLN
1	A	363	THR
1	A	380	VAL
1	A	388	THR
1	A	393	THR
1	A	442	THR
1	A	454	THR
1	A	479	VAL
1	A	490	THR
1	A	491	THR
1	A	494	LYS
1	A	537	THR
1	A	551	THR
1	A	577	SER
1	A	588	THR
1	A	590	LEU
1	A	614	THR
1	A	620	THR
1	A	646	THR
1	A	651	MET
1	A	662	SER
1	A	690	SER
1	A	729	THR
1	A	797	THR
1	A	809	SER
1	A	826	THR
1	A	842	THR
1	A	844	SER
1	A	857	GLU
1	A	862	ARG
1	A	873	SER
1	A	875	THR
1	A	892	THR
1	A	906	ILE
1	A	915	SER
1	A	916	THR
1	A	951	THR

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Mol	Chain	Res	Type
1	A	973	THR
1	A	975	VAL
1	A	1012	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	89	ASN
1	A	111	ASN
1	A	134	GLN
1	A	202	ASN
1	A	237	ASN
1	A	266	ASN
1	A	267	ASN
1	A	342	ASN
1	A	350	GLN
1	A	358	GLN
1	A	359	ASN
1	A	367	GLN
1	A	371	ASN
1	A	685	ASN
1	A	709	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

9 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	BMA	B	1	2	11,11,12	1.11	2 (18%)	15,15,17	1.72	3 (20%)
2	MRH	B	2	2	12,13,14	0.37	0	15,18,20	1.25	3 (20%)
2	MRH	B	3	2	12,13,14	0.54	0	15,18,20	1.41	3 (20%)
2	BMA	B	4	2	11,11,12	1.08	0	15,15,17	2.47	8 (53%)
2	MRH	B	5	2	12,13,14	0.43	0	15,18,20	1.43	2 (13%)
2	MRH	B	6	2	12,13,14	0.66	0	15,18,20	1.34	3 (20%)
2	BMA	B	7	2	11,11,12	1.01	1 (9%)	15,15,17	2.10	3 (20%)
2	MRH	B	8	2	12,13,14	0.49	0	15,18,20	1.27	2 (13%)
2	MRH	B	9	2	12,13,14	0.39	0	15,18,20	0.75	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	BMA	B	1	2	-	0/2/19/22	0/1/1/1
2	MRH	B	2	2	-	2/4/21/24	0/1/1/1
2	MRH	B	3	2	-	4/4/21/24	0/1/1/1
2	BMA	B	4	2	-	0/2/19/22	0/1/1/1
2	MRH	B	5	2	-	2/4/21/24	0/1/1/1
2	MRH	B	6	2	-	0/4/21/24	0/1/1/1
2	BMA	B	7	2	-	0/2/19/22	0/1/1/1
2	MRH	B	8	2	-	2/4/21/24	0/1/1/1
2	MRH	B	9	2	-	0/4/21/24	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	7	BMA	C2-C3	2.45	1.56	1.52
2	B	1	BMA	C2-C3	2.15	1.55	1.52
2	B	1	BMA	O5-C1	2.06	1.47	1.43

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	7	BMA	C1-O5-C5	5.28	119.34	112.19
2	B	4	BMA	O4-C4-C5	4.28	119.93	109.30
2	B	4	BMA	C1-O5-C5	-4.02	106.74	112.19
2	B	7	BMA	O4-C4-C5	3.92	119.03	109.30
2	B	1	BMA	C1-O5-C5	3.82	117.37	112.19
2	B	4	BMA	O6-C6-C5	-3.59	98.99	111.29
2	B	1	BMA	C6-C5-C4	-3.22	105.46	113.00
2	B	5	MRH	O5-C1-C2	-3.06	106.04	110.77
2	B	3	MRH	C2-C3-C4	-2.98	108.00	110.63
2	B	3	MRH	C1-C2-C3	2.75	113.05	109.67
2	B	3	MRH	O5-C1-C2	-2.74	106.54	110.77
2	B	4	BMA	C3-C4-C5	2.67	115.00	110.24
2	B	2	MRH	C2-C3-C4	-2.59	108.35	110.63
2	B	6	MRH	O5-C1-C2	-2.58	106.79	110.77
2	B	6	MRH	C1-C2-C3	2.56	112.81	109.67
2	B	7	BMA	C3-C4-C5	-2.50	105.78	110.24
2	B	4	BMA	O2-C2-C3	2.43	115.02	110.14
2	B	4	BMA	O5-C5-C4	2.43	116.75	110.83
2	B	8	MRH	C1-C2-C3	2.40	112.62	109.67
2	B	6	MRH	C2-C3-C4	-2.31	108.59	110.63
2	B	1	BMA	C1-C2-C3	-2.30	106.83	109.67
2	B	4	BMA	O3-C3-C2	-2.27	105.66	109.99
2	B	2	MRH	C3-C4-N4	-2.24	106.38	110.62
2	B	5	MRH	C1-C2-C3	2.21	112.38	109.67
2	B	8	MRH	O5-C1-C2	-2.12	107.50	110.77
2	B	2	MRH	O2-C2-C3	-2.05	106.03	110.14
2	B	4	BMA	O5-C1-C2	-2.00	107.68	110.77

There are no chirality outliers.

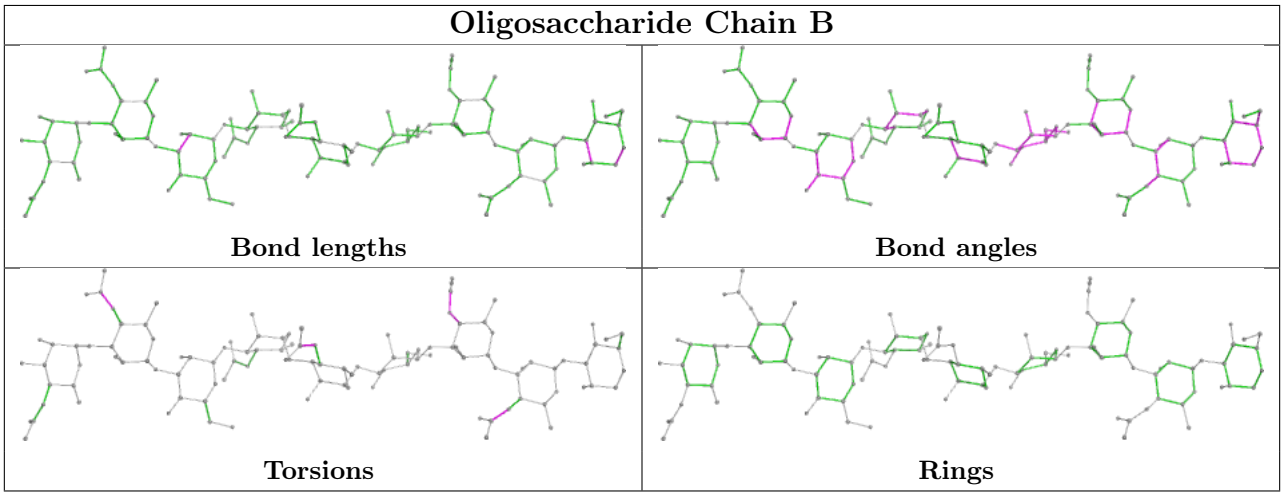
All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	8	MRH	C8-C7-N4-C4
2	B	8	MRH	O7-C7-N4-C4
2	B	3	MRH	C8-C7-N4-C4
2	B	3	MRH	O7-C7-N4-C4
2	B	2	MRH	C8-C7-N4-C4
2	B	5	MRH	C8-C7-N4-C4
2	B	3	MRH	C5-C4-N4-C7
2	B	3	MRH	C3-C4-N4-C7
2	B	2	MRH	O7-C7-N4-C4
2	B	5	MRH	O7-C7-N4-C4

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

Of 22 ligands modelled in this entry, 22 are monoatomic - leaving 0 for Mogul analysis.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10388. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.