



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 30, 2021 – 11:06 pm BST

PDB ID : 7NWQ
Title : A carbohydrate binding module family 9 (CBM9) from *Caldicellulosiruptor kristjanssonii* in complex with cellotriose
Authors : Krska, D.; Mazurkewich, S.; Navarro Poulsen, J.; Larsbrink, J.; Lo Leggio, L.
Deposited on : 2021-03-17
Resolution : 2.23 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 : 2.22
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) : 2.22

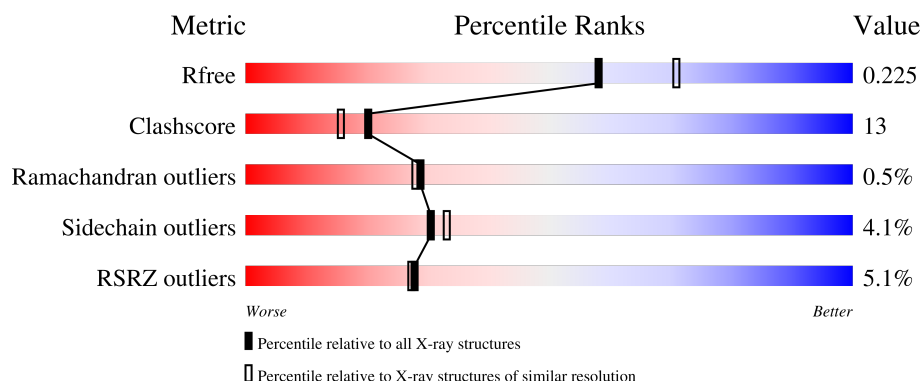
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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 $\leq 5\%$. 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	AAA	215	<div> <div>5%</div> <div>77%</div> <div>13%</div> <div>9%</div> </div>
2	BBB	3	<div> <div>67%</div> <div>33%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BGC	BBB	2	X	-	-	-
3	PEG	AAA	303	-	-	X	-
3	PEG	AAA	305	-	-	X	-
3	PEG	AAA	307	-	-	X	X
4	EDO	AAA	312	-	-	-	X
4	EDO	AAA	316	-	-	-	X
7	1PE	AAA	321	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 1877 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 Beta-xylanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	195	Total	C	N	O	S	0	4	0
			1608	1017	272	316	3			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	1	MET	-	initiating methionine	UNP E4S6E9
AAA	2	GLY	-	expression tag	UNP E4S6E9
AAA	3	SER	-	expression tag	UNP E4S6E9
AAA	4	SER	-	expression tag	UNP E4S6E9
AAA	5	HIS	-	expression tag	UNP E4S6E9
AAA	6	HIS	-	expression tag	UNP E4S6E9
AAA	7	HIS	-	expression tag	UNP E4S6E9
AAA	8	HIS	-	expression tag	UNP E4S6E9
AAA	9	HIS	-	expression tag	UNP E4S6E9
AAA	10	HIS	-	expression tag	UNP E4S6E9
AAA	11	SER	-	expression tag	UNP E4S6E9
AAA	12	SER	-	expression tag	UNP E4S6E9
AAA	13	GLU	-	expression tag	UNP E4S6E9
AAA	14	ASN	-	expression tag	UNP E4S6E9
AAA	15	LEU	-	expression tag	UNP E4S6E9
AAA	16	TYR	-	expression tag	UNP E4S6E9
AAA	17	PHE	-	expression tag	UNP E4S6E9
AAA	18	GLN	-	expression tag	UNP E4S6E9
AAA	19	GLY	-	expression tag	UNP E4S6E9
AAA	20	HIS	-	expression tag	UNP E4S6E9

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	BBB	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

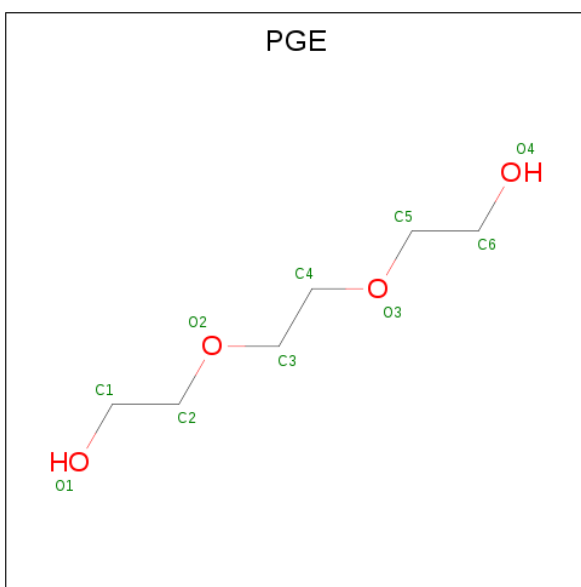


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			4	2	2		
4	AAA	1	Total	C	O	0	0
			4	2	2		
4	AAA	1	Total	C	O	0	0
			4	2	2		
4	AAA	1	Total	C	O	0	0
			4	2	2		
4	AAA	1	Total	C	O	0	0
			4	2	2		
4	AAA	1	Total	C	O	0	0
			4	2	2		
4	AAA	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

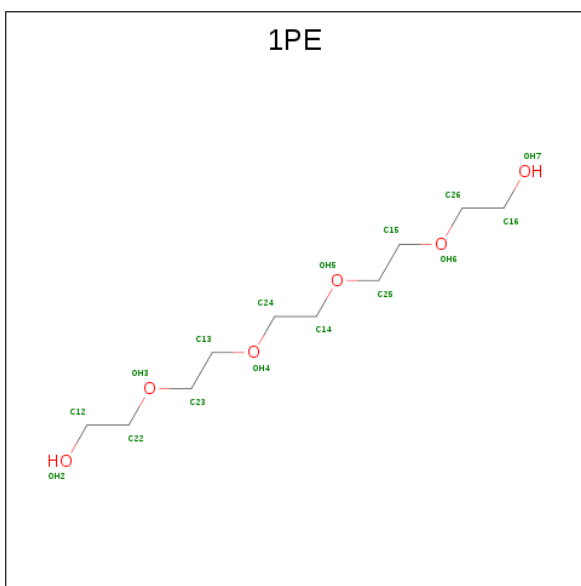
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	3	Total	Ca	0	0
			3	3		

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	AAA	1	Total	C	O	0	0
			10	6	4		
6	AAA	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	AAA	1	Total	C	O	0	0
			16	10	6		

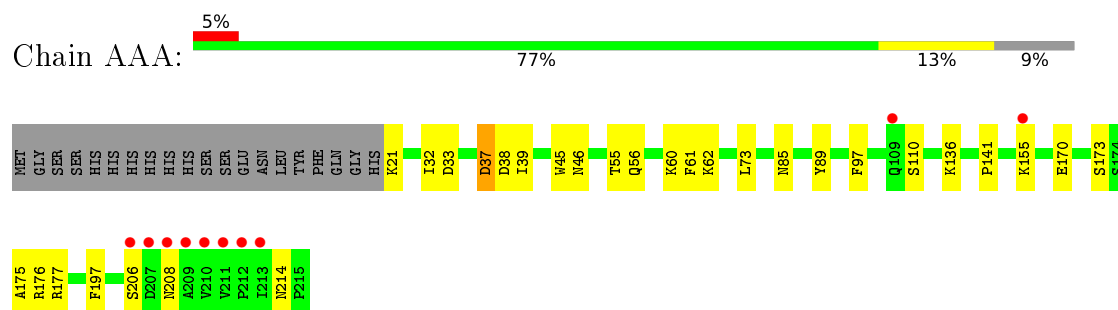
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	111	Total 111	O 111	0	0

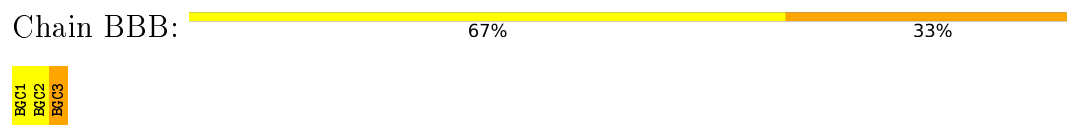
3 Residue-property plots [i](#)

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: Beta-xylanase



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



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 3 2	Depositor
Cell constants a, b, c, α , β , γ	172.49 Å 172.49 Å 172.49 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.52 – 2.23 70.42 – 2.23	Depositor EDS
% Data completeness (in resolution range)	99.7 (70.52-2.23) 99.7 (70.42-2.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.94 (at 2.22 Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.185 , 0.226 0.185 , 0.225	Depositor DCC
R_{free} test set	2000 reflections (9.29%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1877	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 4.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, EDO, BGC, PEG, PGE, 1PE

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	AAA	0.50	0/1645	0.87	1/2237 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	AAA	89	TYR	CB-CG-CD1	-5.43	117.74	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	1608	0	1540	34	0
2	BBB	34	0	30	0	1
3	AAA	49	0	70	23	0
4	AAA	36	0	54	5	0
5	AAA	3	0	0	0	0
6	AAA	20	0	28	1	0
7	AAA	16	0	22	2	0
8	AAA	111	0	0	9	1
All	All	1877	0	1744	44	1

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 13.

All (44) 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:AAA:38:ASP:H	3:AAA:305:PEG:H42	1.03	1.15
1:AAA:38:ASP:N	3:AAA:305:PEG:H42	1.74	1.01
1:AAA:38:ASP:H	3:AAA:305:PEG:C4	1.82	0.92
7:AAA:321:1PE:H142	8:AAA:423:HOH:O	1.73	0.88
4:AAA:310:EDO:H21	8:AAA:503:HOH:O	1.78	0.83
3:AAA:305:PEG:O1	3:AAA:305:PEG:H32	1.86	0.72
1:AAA:177:ARG:HE	3:AAA:303:PEG:H22	1.55	0.71
1:AAA:37:ASP:HA	3:AAA:305:PEG:H41	1.77	0.66
1:AAA:39:ILE:HG23	3:AAA:305:PEG:H21	1.80	0.64
1:AAA:46:ASN:HA	4:AAA:314:EDO:H22	1.80	0.63
1:AAA:60[B]:LYS:HD3	8:AAA:423:HOH:O	2.01	0.60
1:AAA:170[B]:GLU:HG3	1:AAA:170[B]:GLU:O	2.01	0.59
1:AAA:45:TRP:CE2	1:AAA:62:LYS:HE3	2.39	0.57
1:AAA:60[B]:LYS:HE3	8:AAA:406:HOH:O	2.05	0.55
1:AAA:177:ARG:HE	3:AAA:303:PEG:C2	2.18	0.54
1:AAA:38:ASP:CB	3:AAA:305:PEG:H42	2.39	0.53
1:AAA:38:ASP:N	3:AAA:305:PEG:C4	2.57	0.53
3:AAA:304:PEG:H41	4:AAA:316:EDO:H12	1.90	0.52
1:AAA:60[A]:LYS:HG2	7:AAA:321:1PE:H151	1.93	0.51
1:AAA:32:ILE:HG22	1:AAA:136:LYS:HG2	1.92	0.50
1:AAA:55:THR:OG1	1:AAA:170[A]:GLU:OE1	2.26	0.50
1:AAA:110:SER:HA	4:AAA:308:EDO:H11	1.93	0.50
1:AAA:60[A]:LYS:NZ	8:AAA:406:HOH:O	2.44	0.50
3:AAA:307:PEG:H31	8:AAA:496:HOH:O	2.12	0.49
1:AAA:38:ASP:HB3	3:AAA:305:PEG:H42	1.95	0.48
1:AAA:155:LYS:HG3	3:AAA:304:PEG:H32	1.97	0.47
1:AAA:39:ILE:HG12	3:AAA:305:PEG:H11	1.97	0.46
1:AAA:177:ARG:HG2	3:AAA:303:PEG:H22	1.97	0.46
3:AAA:302:PEG:H11	8:AAA:506:HOH:O	2.16	0.45
3:AAA:307:PEG:H31	3:AAA:307:PEG:H11	1.53	0.45
1:AAA:45:TRP:CE2	1:AAA:60[A]:LYS:HD2	2.51	0.44
1:AAA:45:TRP:CD2	1:AAA:60[A]:LYS:HD2	2.53	0.44
1:AAA:141:PRO:HD3	3:AAA:307:PEG:H21	1.99	0.44
1:AAA:39:ILE:CG2	3:AAA:305:PEG:H21	2.46	0.43
1:AAA:37:ASP:CA	3:AAA:305:PEG:H41	2.48	0.43
3:AAA:307:PEG:H11	8:AAA:496:HOH:O	2.19	0.42
1:AAA:85:ASN:HB2	1:AAA:175:ALA:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:45:TRP:CD2	1:AAA:62:LYS:HE3	2.55	0.42
1:AAA:97:PHE:HB3	1:AAA:197:PHE:CZ	2.55	0.42
4:AAA:311:EDO:H22	8:AAA:494:HOH:O	2.20	0.41
1:AAA:61:PHE:HA	1:AAA:73:LEU:O	2.20	0.41
1:AAA:177:ARG:NE	3:AAA:303:PEG:H22	2.31	0.41
1:AAA:33:ASP:HA	1:AAA:136:LYS:HG3	2.03	0.41
6:AAA:320:PGE:H32	6:AAA:320:PGE:H52	1.57	0.40

All (1) 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)
2:BBB:3:BGC:O2	8:AAA:511:HOH:O[18_655]	2.08	0.12

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	AAA	197/215 (92%)	189 (96%)	7 (4%)	1 (0%)	29 28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	214	ASN

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	AAA	176/190 (93%)	168 (96%)	8 (4%)	27	29

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	21	LYS
1	AAA	37	ASP
1	AAA	56[A]	GLN
1	AAA	56[B]	GLN
1	AAA	173	SER
1	AAA	176	ARG
1	AAA	206	SER
1	AAA	208	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

3 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	BGC	BBB	1	2	12,12,12	0.62	0	17,17,17	1.80	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	BBB	2	2	11,11,12	1.07	1 (9%)	15,15,17	2.58	6 (40%)
2	BGC	BBB	3	2	11,11,12	0.51	0	15,15,17	1.95	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	BGC	BBB	1	2	-	2/2/22/22	0/1/1/1
2	BGC	BBB	2	2	1/1/4/5	2/2/19/22	0/1/1/1
2	BGC	BBB	3	2	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	2	BGC	O4-C4	-2.98	1.36	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	2	BGC	O4-C4-C5	4.92	121.52	109.30
2	BBB	3	BGC	C2-C3-C4	-3.95	104.06	110.89
2	BBB	2	BGC	C1-C2-C3	3.69	114.20	109.67
2	BBB	1	BGC	O5-C5-C4	-3.68	103.01	109.69
2	BBB	2	BGC	O4-C4-C3	3.66	118.80	110.35
2	BBB	3	BGC	O5-C5-C6	3.48	112.66	107.20
2	BBB	2	BGC	O5-C1-C2	-3.39	105.53	110.77
2	BBB	2	BGC	C1-O5-C5	3.26	116.61	112.19
2	BBB	1	BGC	C3-C4-C5	-2.90	105.06	110.24
2	BBB	2	BGC	C3-C4-C5	2.86	115.35	110.24
2	BBB	1	BGC	C6-C5-C4	2.66	119.23	113.00
2	BBB	1	BGC	O2-C2-C1	2.56	115.09	109.16
2	BBB	3	BGC	O3-C3-C2	2.45	114.69	109.99
2	BBB	3	BGC	O4-C4-C5	-2.43	103.26	109.30
2	BBB	3	BGC	C6-C5-C4	-2.41	107.36	113.00
2	BBB	1	BGC	O1-C1-O5	-2.26	103.60	110.38
2	BBB	1	BGC	O3-C3-C2	-2.19	105.28	110.35

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	BBB	2	BGC	C4

All (6) torsion outliers are listed below:

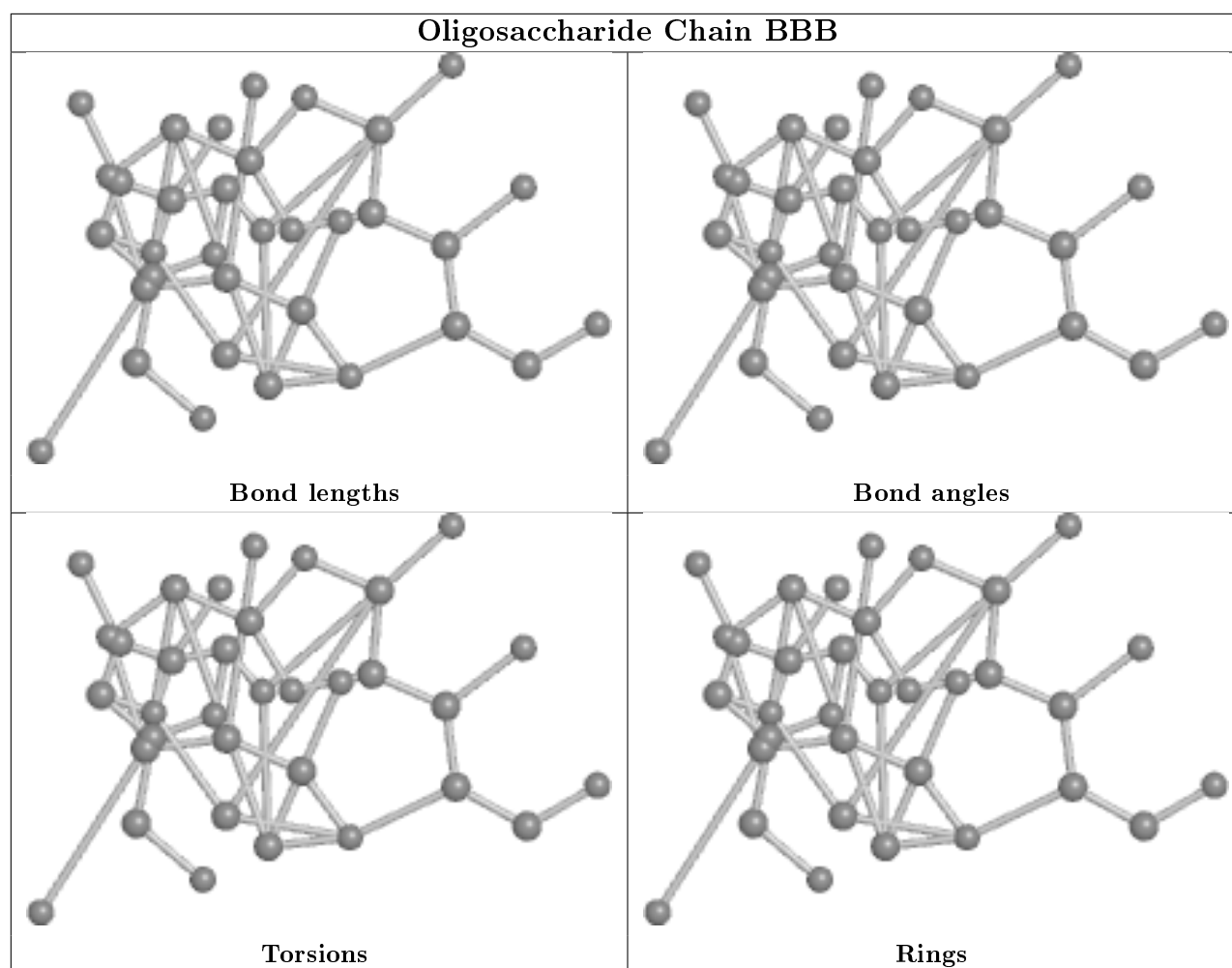
Mol	Chain	Res	Type	Atoms
2	BBB	1	BGC	C4-C5-C6-O6
2	BBB	3	BGC	O5-C5-C6-O6
2	BBB	1	BGC	O5-C5-C6-O6
2	BBB	2	BGC	C4-C5-C6-O6
2	BBB	3	BGC	C4-C5-C6-O6
2	BBB	2	BGC	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	3	BGC	0	1

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



5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 3 are monoatomic - leaving 19 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PEG	AAA	304	-	6,6,6	0.26	0	5,5,5	0.27	0
4	EDO	AAA	311	-	3,3,3	0.14	0	2,2,2	0.47	0
4	EDO	AAA	308	-	3,3,3	0.46	0	2,2,2	0.98	0
3	PEG	AAA	305	-	6,6,6	0.50	0	5,5,5	0.99	0
6	PGE	AAA	320	-	9,9,9	0.41	0	8,8,8	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PEG	AAA	301	-	6,6,6	0.16	0	5,5,5	0.09	0
6	PGE	AAA	322	-	9,9,9	0.28	0	8,8,8	0.22	0
4	EDO	AAA	316	-	3,3,3	0.19	0	2,2,2	0.33	0
4	EDO	AAA	312	-	3,3,3	0.28	0	2,2,2	0.60	0
3	PEG	AAA	306	-	6,6,6	0.12	0	5,5,5	0.22	0
4	EDO	AAA	310	-	3,3,3	0.06	0	2,2,2	0.29	0
4	EDO	AAA	313	-	3,3,3	0.23	0	2,2,2	0.76	0
4	EDO	AAA	315	-	3,3,3	0.22	0	2,2,2	0.50	0
3	PEG	AAA	307	-	6,6,6	0.71	0	5,5,5	0.35	0
7	1PE	AAA	321	-	15,15,15	0.31	0	14,14,14	0.24	0
4	EDO	AAA	309	-	3,3,3	0.11	0	2,2,2	0.44	0
4	EDO	AAA	314	-	3,3,3	0.16	0	2,2,2	0.41	0
3	PEG	AAA	302	-	6,6,6	0.26	0	5,5,5	0.15	0
3	PEG	AAA	303	-	6,6,6	0.28	0	5,5,5	0.24	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
3	PEG	AAA	304	-	-	3/4/4/4	-
4	EDO	AAA	311	-	-	1/1/1/1	-
4	EDO	AAA	308	-	-	0/1/1/1	-
3	PEG	AAA	305	-	-	1/4/4/4	-
6	PGE	AAA	320	-	-	2/7/7/7	-
3	PEG	AAA	301	-	-	1/4/4/4	-
6	PGE	AAA	322	-	-	3/7/7/7	-
4	EDO	AAA	316	-	-	1/1/1/1	-
4	EDO	AAA	312	-	-	1/1/1/1	-
3	PEG	AAA	306	-	-	1/4/4/4	-
4	EDO	AAA	310	-	-	0/1/1/1	-
4	EDO	AAA	313	-	-	1/1/1/1	-
4	EDO	AAA	315	-	-	1/1/1/1	-
3	PEG	AAA	307	-	-	3/4/4/4	-
7	1PE	AAA	321	-	-	6/13/13/13	-
4	EDO	AAA	309	-	-	1/1/1/1	-
4	EDO	AAA	314	-	-	0/1/1/1	-
3	PEG	AAA	302	-	-	3/4/4/4	-
3	PEG	AAA	303	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	307	PEG	C1-C2-O2-C3
6	AAA	320	PGE	C3-C4-O3-C5
3	AAA	305	PEG	O2-C3-C4-O4
6	AAA	322	PGE	O3-C5-C6-O4
7	AAA	321	1PE	OH5-C14-C24-OH4
3	AAA	304	PEG	O1-C1-C2-O2
3	AAA	304	PEG	O2-C3-C4-O4
6	AAA	322	PGE	O1-C1-C2-O2
4	AAA	311	EDO	O1-C1-C2-O2
4	AAA	313	EDO	O1-C1-C2-O2
3	AAA	303	PEG	O1-C1-C2-O2
3	AAA	303	PEG	O2-C3-C4-O4
3	AAA	302	PEG	O2-C3-C4-O4
7	AAA	321	1PE	OH2-C12-C22-OH3
3	AAA	307	PEG	O2-C3-C4-O4
3	AAA	304	PEG	C4-C3-O2-C2
3	AAA	301	PEG	C1-C2-O2-C3
3	AAA	303	PEG	C4-C3-O2-C2
3	AAA	307	PEG	O1-C1-C2-O2
3	AAA	302	PEG	C1-C2-O2-C3
4	AAA	309	EDO	O1-C1-C2-O2
7	AAA	321	1PE	C14-C24-OH4-C13
6	AAA	320	PGE	C4-C3-O2-C2
7	AAA	321	1PE	OH4-C13-C23-OH3
4	AAA	315	EDO	O1-C1-C2-O2
6	AAA	322	PGE	O2-C3-C4-O3
3	AAA	306	PEG	C1-C2-O2-C3
7	AAA	321	1PE	C23-C13-OH4-C24
4	AAA	312	EDO	O1-C1-C2-O2
4	AAA	316	EDO	O1-C1-C2-O2
7	AAA	321	1PE	OH6-C15-C25-OH5
3	AAA	302	PEG	O1-C1-C2-O2

There are no ring outliers.

12 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	304	PEG	2	0
4	AAA	311	EDO	1	0
4	AAA	308	EDO	1	0
3	AAA	305	PEG	12	0
6	AAA	320	PGE	1	0
4	AAA	316	EDO	1	0
4	AAA	310	EDO	1	0
3	AAA	307	PEG	4	0
7	AAA	321	1PE	2	0
4	AAA	314	EDO	1	0
3	AAA	302	PEG	1	0
3	AAA	303	PEG	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	195/215 (90%)	0.44	10 (5%) 28 27	23, 34, 71, 167	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	210	VAL	9.4
1	AAA	209	ALA	8.4
1	AAA	211	VAL	8.0
1	AAA	208	ASN	6.8
1	AAA	207	ASP	4.6
1	AAA	213	ILE	3.0
1	AAA	206	SER	2.8
1	AAA	212	PRO	2.4
1	AAA	109	GLN	2.3
1	AAA	155	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, 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	BGC	BBB	2	11/12	0.90	0.18	37,41,44,45	11
2	BGC	BBB	1	12/12	0.91	0.16	23,30,36,40	12

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BGC	BBB	3	11/12	0.95	0.16	31,35,38,42	11

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
4	EDO	AAA	312	4/4	0.44	0.66	73,79,82,94	0
4	EDO	AAA	313	4/4	0.44	0.38	73,76,82,88	0
7	1PE	AAA	321	16/16	0.44	0.52	56,108,144,158	0
4	EDO	AAA	316	4/4	0.48	0.51	85,85,98,98	0
4	EDO	AAA	309	4/4	0.61	0.27	70,79,84,86	0
6	PGE	AAA	320	10/10	0.68	0.38	72,96,122,140	0
3	PEG	AAA	307	7/7	0.71	0.52	20,22,26,30	7
4	EDO	AAA	308	4/4	0.71	0.22	65,67,70,80	0
4	EDO	AAA	315	4/4	0.72	0.24	61,82,86,89	0
6	PGE	AAA	322	10/10	0.74	0.28	61,80,105,108	0
3	PEG	AAA	301	7/7	0.76	0.23	74,84,98,101	0
3	PEG	AAA	304	7/7	0.76	0.17	69,72,79,87	0
3	PEG	AAA	305	7/7	0.83	0.53	13,16,20,22	7
4	EDO	AAA	310	4/4	0.84	0.34	64,65,71,76	0
3	PEG	AAA	306	7/7	0.84	0.49	74,76,85,88	0
4	EDO	AAA	314	4/4	0.86	0.27	51,55,57,58	0
3	PEG	AAA	302	7/7	0.86	0.16	56,63,83,85	0
3	PEG	AAA	303	7/7	0.87	0.16	38,46,52,55	0
4	EDO	AAA	311	4/4	0.87	0.18	55,57,64,69	0
5	CA	AAA	319	1/1	0.97	0.17	44,44,44,44	1
5	CA	AAA	317	1/1	0.98	0.11	49,49,49,49	0
5	CA	AAA	318	1/1	0.99	0.12	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.