Full wwPDB X-ray Structure Validation Report (i)

Apr 27, 2024 – 03:06 pm BST

PDB ID	:	6FUV
Title	:	Structure of a manno-oligosaccharide specific solute binding protein, BlMnBP2 from Bifidobacterium animalis subsp. lactis ATCC 27673 in complex with mannotriose
Authors	:	Ejby, M.; Abou Hachem, M.; Guskov, A.; Slotboom, D.J.
Deposited on	:	2018-02-27
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:

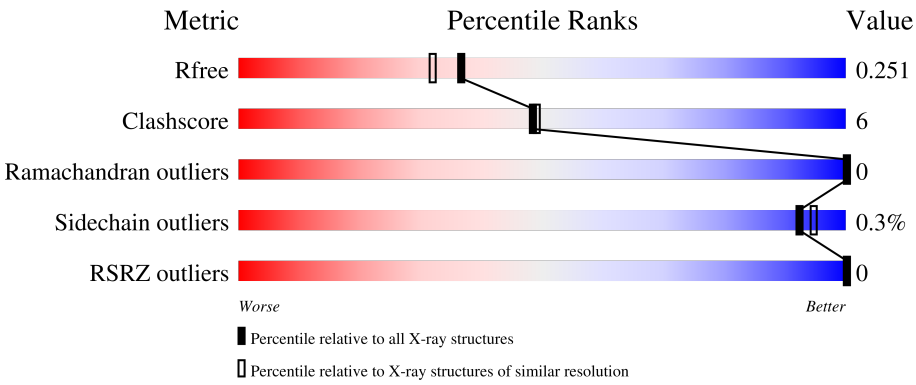
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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	427	88% 12%
2	B	3	33% 67%

2 Entry composition (i)

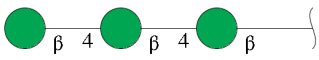
There are 6 unique types of molecules in this entry. The entry contains 7306 atoms, of which 3347 are hydrogens and 0 are deuteriums.

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 Solute Binding Protein, BlMnBP1 in complex with mannotriose.

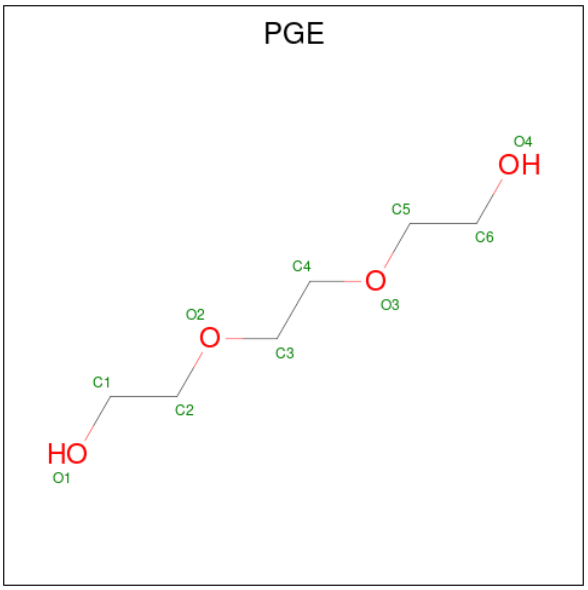
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	427	6560	2117	3198	544	684	17	0	4	0

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



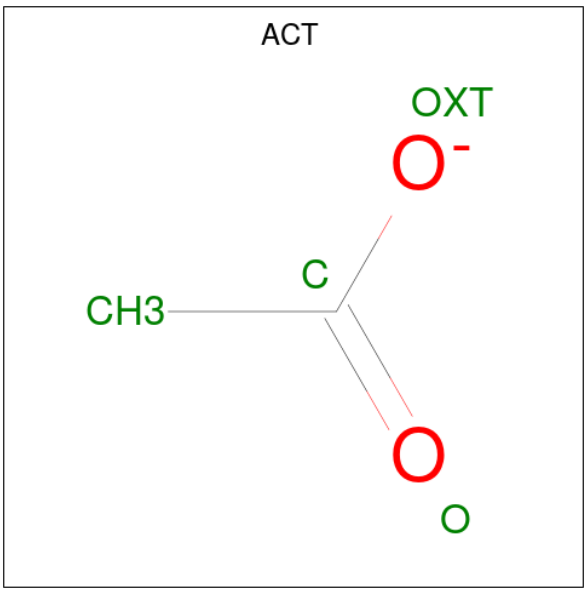
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	H	O			
2	B	3	64	18	30	16	0	0	0

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



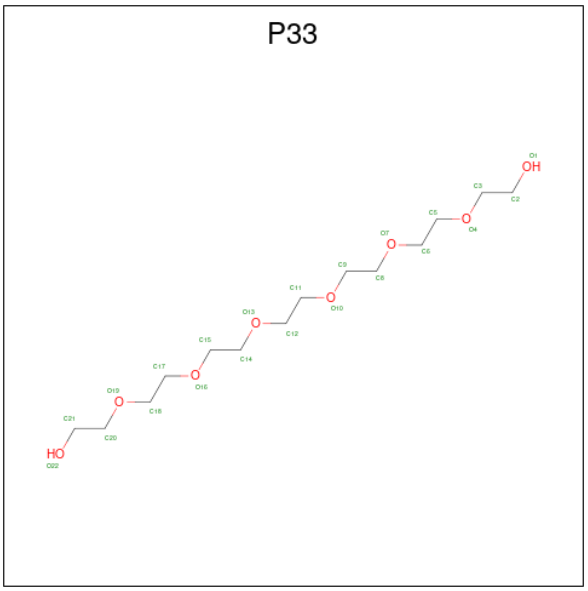
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	A	1	24	6	14	4	0	0
			Total	C	H	O		
3	A	1	24	6	14	4	0	0
			Total	C	H	O		
3	A	1	24	6	14	4	0	0
			Total	C	H	O		
3	A	1	24	6	14	4	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	7	2	3	2	0	0

- Molecule 5 is 3,6,9,12,15,18-HEXAOXAICOSANE-1,20-DIOL (three-letter code: P33) (formula: $C_{14}H_{30}O_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			52	14	30	8		
5	A	1	Total	C	H	O	0	0
			52	14	30	8		

- Molecule 6 is water.

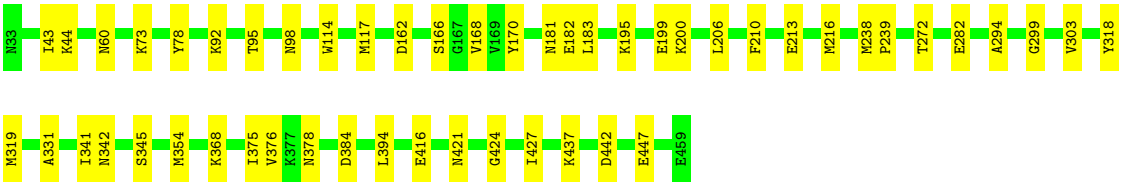
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	475	Total	O	0	0
			475	475		

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: Solute Binding Protein, BlMnBP1 in complex with mannotriose

Chain A:



• Molecule 2: beta-D-mannopyranose-(1-4)-beta-D-mannopyranose-(1-4)-beta-D-mannopyranose

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	52.17Å 64.59Å 133.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.59 – 2.00 40.58 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.4 (40.59-2.00) 90.4 (40.58-2.00)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.178 , 0.251 0.179 , 0.251	Depositor DCC
R_{free} test set	1411 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	21.2	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 56.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7306	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.99% 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: BMA, ACT, P33, PGE

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	0.72	0/3455	0.67	0/4678

There are no bond length outliers.

There are no bond angle outliers.

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	A	3362	3198	3183	38	0
2	B	34	30	30	0	0
3	A	40	56	56	8	0
4	A	4	3	3	0	0
5	A	44	60	60	1	0
6	A	475	0	0	16	2
All	All	3959	3347	3332	41	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (41) 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:98[A]:ASN:ND2	6:A:706:HOH:O	2.18	0.77
1:A:378:ASN:HB2	5:A:606:P33:H32	1.72	0.71
1:A:442:ASP:OD2	6:A:701:HOH:O	2.15	0.65
1:A:195:LYS:NZ	6:A:712:HOH:O	2.30	0.64
1:A:199:GLU:OE2	6:A:702:HOH:O	2.15	0.63
3:A:602:PGE:O3	6:A:703:HOH:O	2.15	0.63
1:A:181:ASN:ND2	6:A:713:HOH:O	2.33	0.61
1:A:384:ASP:OD1	6:A:704:HOH:O	2.16	0.60
1:A:416:GLU:HB2	3:A:601:PGE:H62	1.86	0.58
1:A:183:LEU:HG	3:A:605:PGE:H4	1.84	0.57
1:A:368:LYS:HZ2	3:A:603:PGE:H42	1.70	0.56
1:A:166:SER:HA	1:A:299:GLY:HA2	1.87	0.56
1:A:44:LYS:NZ	6:A:710:HOH:O	2.28	0.55
1:A:282:GLU:OE1	6:A:705:HOH:O	2.18	0.55
1:A:182:GLU:HG3	3:A:602:PGE:H4	1.90	0.54
1:A:162:ASP:HA	1:A:375:ILE:HG12	1.88	0.53
1:A:210:PHE:HA	1:A:216[A]:MET:SD	2.51	0.51
1:A:447:GLU:HB3	3:A:601:PGE:H22	1.94	0.49
1:A:181:ASN:HB3	6:A:713:HOH:O	2.11	0.49
1:A:213:GLU:HG2	1:A:424:GLY:HA3	1.94	0.49
1:A:43:ILE:CD1	1:A:354:MET:HG2	2.44	0.48
1:A:331:ALA:HB3	1:A:394:LEU:HD22	1.95	0.48
3:A:602:PGE:H62	6:A:703:HOH:O	2.13	0.48
1:A:342:ASN:HB3	1:A:345:SER:OG	2.14	0.48
1:A:303:VAL:HG21	1:A:318:TYR:HB2	1.97	0.47
1:A:60:ASN:O	1:A:95:THR:HA	2.15	0.47
1:A:200:LYS:HE2	6:A:1080:HOH:O	2.13	0.47
1:A:437:LYS:HE3	6:A:919:HOH:O	2.14	0.47
1:A:341:ILE:HD12	1:A:354:MET:HE2	1.98	0.45
1:A:92:LYS:NZ	6:A:721:HOH:O	2.41	0.45
1:A:168:VAL:HB	1:A:319:MET:HG3	1.97	0.44
1:A:216[B]:MET:HB3	1:A:427:ILE:HB	2.00	0.43
1:A:206:LEU:C	1:A:206:LEU:HD23	2.40	0.43
1:A:206:LEU:O	1:A:272:THR:HA	2.19	0.42
1:A:376:VAL:HG23	6:A:841:HOH:O	2.20	0.42
1:A:238:MET:N	1:A:239:PRO:HD2	2.35	0.42
1:A:170:TYR:HA	1:A:294:ALA:O	2.19	0.41
1:A:73:LYS:HE2	1:A:78:TYR:CE1	2.55	0.41
3:A:605:PGE:H42	6:A:888:HOH:O	2.20	0.41
1:A:114:TRP:CZ3	1:A:117:MET:HG2	2.55	0.41
1:A:73:LYS:HE2	1:A:78:TYR:CD1	2.56	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:910:HOH:O	6:A:1040:HOH:O[4_466]	2.15	0.05
6:A:1080:HOH:O	6:A:1149:HOH:O[3_646]	2.17	0.03

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	429/427 (100%)	418 (97%)	11 (3%)	0	100 100

There are no Ramachandran outliers to report.

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	355/352 (101%)	354 (100%)	1 (0%)	92 95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	421	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	BMA	B	1	2	12,12,12	0.74	0	17,17,17	1.01	0
2	BMA	B	2	2	11,11,12	1.93	3 (27%)	15,15,17	0.97	1 (6%)
2	BMA	B	3	2	11,11,12	1.07	0	15,15,17	1.00	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
2	BMA	B	1	2	-	0/2/22/22	0/1/1/1
2	BMA	B	2	2	-	0/2/19/22	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	BMA	C2-C3	-3.99	1.46	1.52
2	B	2	BMA	O5-C1	-3.41	1.38	1.43
2	B	2	BMA	O5-C5	2.07	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3	BMA	O3-C3-C2	2.50	114.79	109.99
2	B	2	BMA	O2-C2-C3	-2.03	106.08	110.14

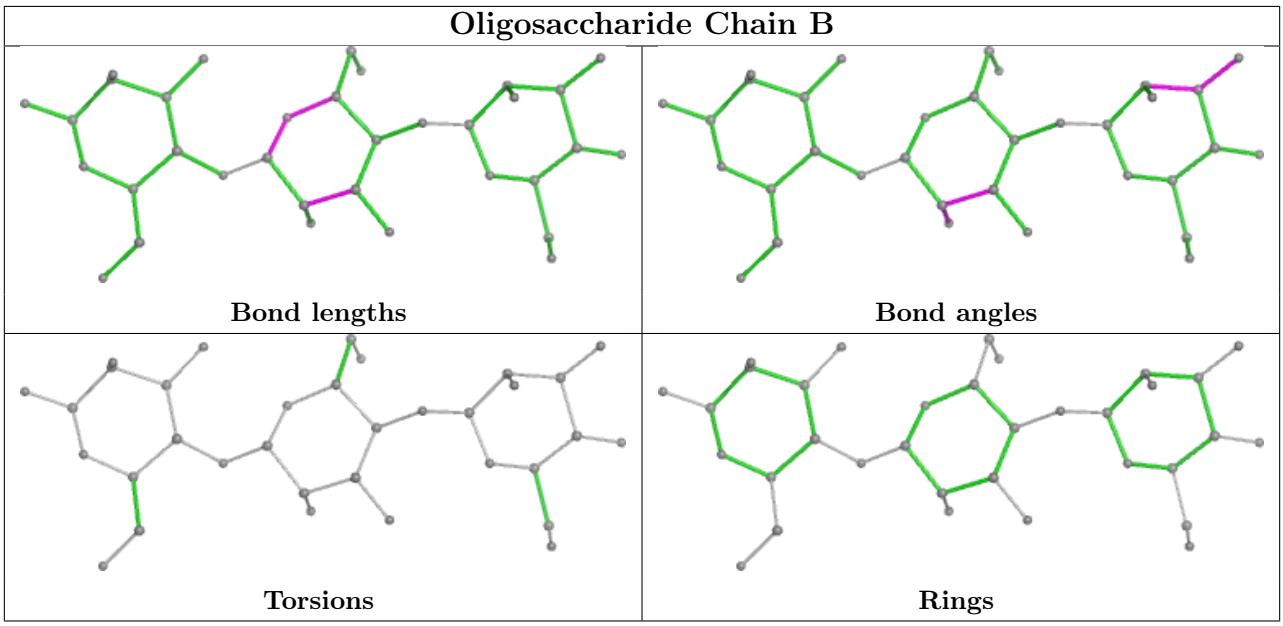
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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



5.6 Ligand geometry (i)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	P33	A	606	-	21,21,21	0.58	0	20,20,20	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	P33	A	607	-	21,21,21	0.57	0	20,20,20	0.62	0
3	PGE	A	603	-	9,9,9	0.28	0	8,8,8	0.60	0
3	PGE	A	602	-	9,9,9	0.38	0	8,8,8	0.31	0
4	ACT	A	604	-	3,3,3	1.02	0	3,3,3	1.71	2 (66%)
3	PGE	A	601	-	9,9,9	0.37	0	8,8,8	0.50	0
3	PGE	A	605	-	9,9,9	0.33	0	8,8,8	0.43	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
5	P33	A	606	-	-	8/19/19/19	-
5	P33	A	607	-	-	5/19/19/19	-
3	PGE	A	603	-	-	6/7/7/7	-
3	PGE	A	602	-	-	3/7/7/7	-
3	PGE	A	601	-	-	5/7/7/7	-
3	PGE	A	605	-	-	5/7/7/7	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	604	ACT	O-C-CH3	-2.11	114.10	122.33
4	A	604	ACT	OXT-C-O	2.06	129.64	122.05

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	607	P33	C21-C20-O19-C18
5	A	607	P33	O16-C17-C18-O19
3	A	603	PGE	O2-C3-C4-O3
5	A	606	P33	O13-C14-C15-O16
5	A	607	P33	O13-C14-C15-O16
3	A	601	PGE	O2-C3-C4-O3
3	A	603	PGE	C4-C3-O2-C2
3	A	605	PGE	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
3	A	601	PGE	O1-C1-C2-O2
3	A	602	PGE	O3-C5-C6-O4
3	A	605	PGE	O1-C1-C2-O2
5	A	606	P33	O1-C2-C3-O4
5	A	607	P33	O1-C2-C3-O4
3	A	603	PGE	O3-C5-C6-O4
3	A	603	PGE	O1-C1-C2-O2
3	A	605	PGE	C3-C4-O3-C5
3	A	601	PGE	C1-C2-O2-C3
5	A	606	P33	C21-C20-O19-C18
3	A	605	PGE	C1-C2-O2-C3
3	A	605	PGE	C6-C5-O3-C4
5	A	606	P33	C15-C14-O13-C12
3	A	601	PGE	C4-C3-O2-C2
5	A	606	P33	C2-C3-O4-C5
3	A	603	PGE	C3-C4-O3-C5
5	A	606	P33	C17-C18-O19-C20
5	A	607	P33	O19-C20-C21-O22
5	A	606	P33	C6-C5-O4-C3
5	A	606	P33	C14-C15-O16-C17
3	A	601	PGE	C3-C4-O3-C5
3	A	602	PGE	C6-C5-O3-C4
3	A	603	PGE	C6-C5-O3-C4
3	A	602	PGE	O1-C1-C2-O2

There are no ring outliers.

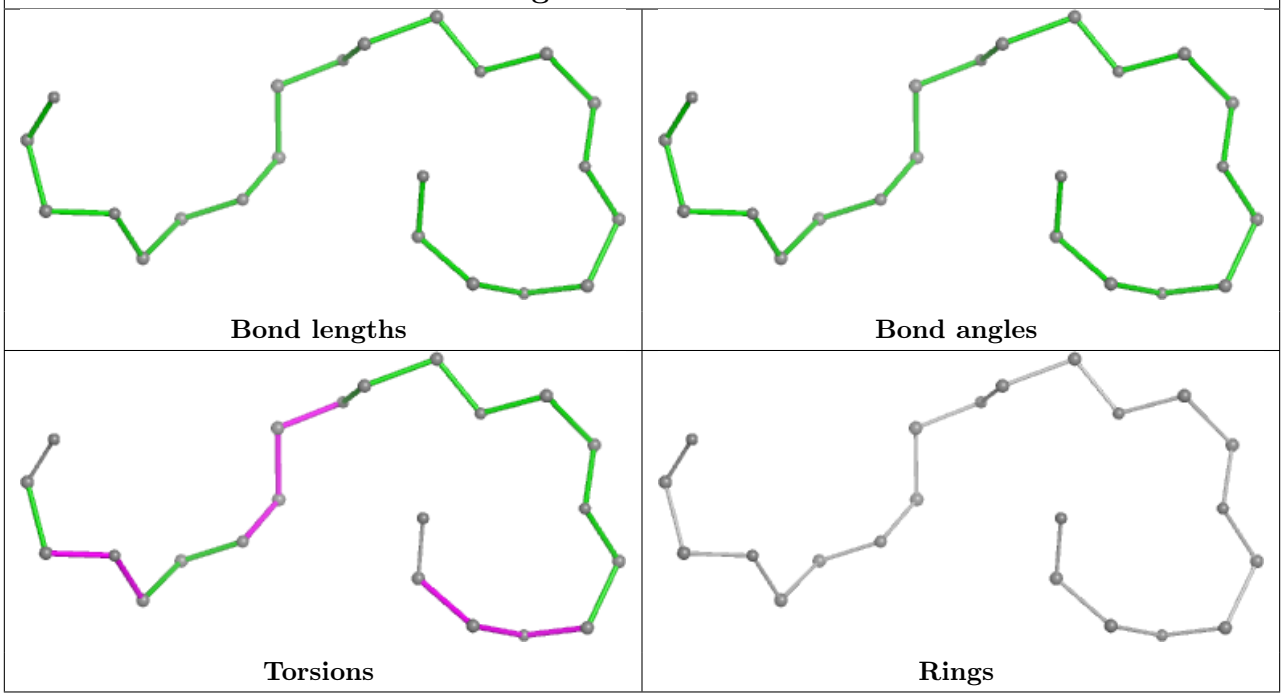
5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	606	P33	1	0
3	A	603	PGE	1	0
3	A	602	PGE	3	0
3	A	601	PGE	2	0
3	A	605	PGE	2	0

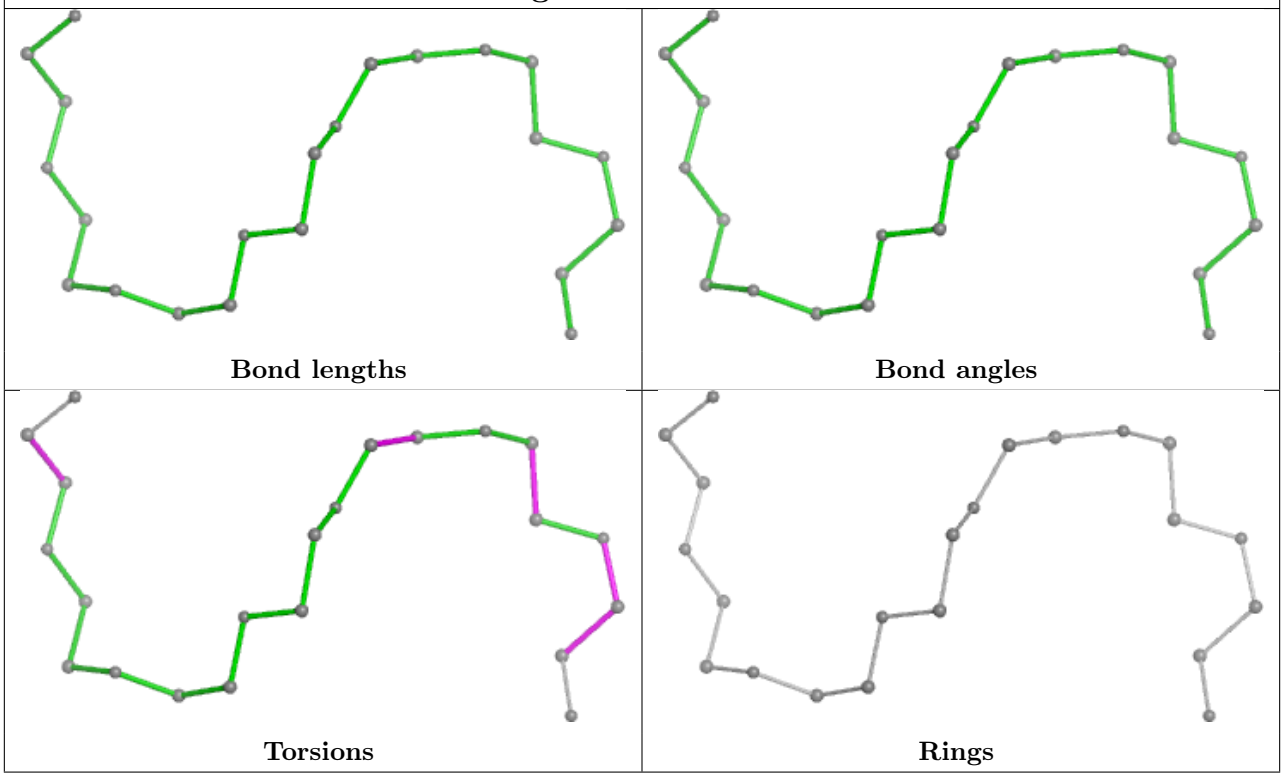
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand P33 A 606



Ligand P33 A 607



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	A	427/427 (100%)	-0.26	0	100	100	12, 20, 33, 45	0

There are no RSRZ outliers to report.

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

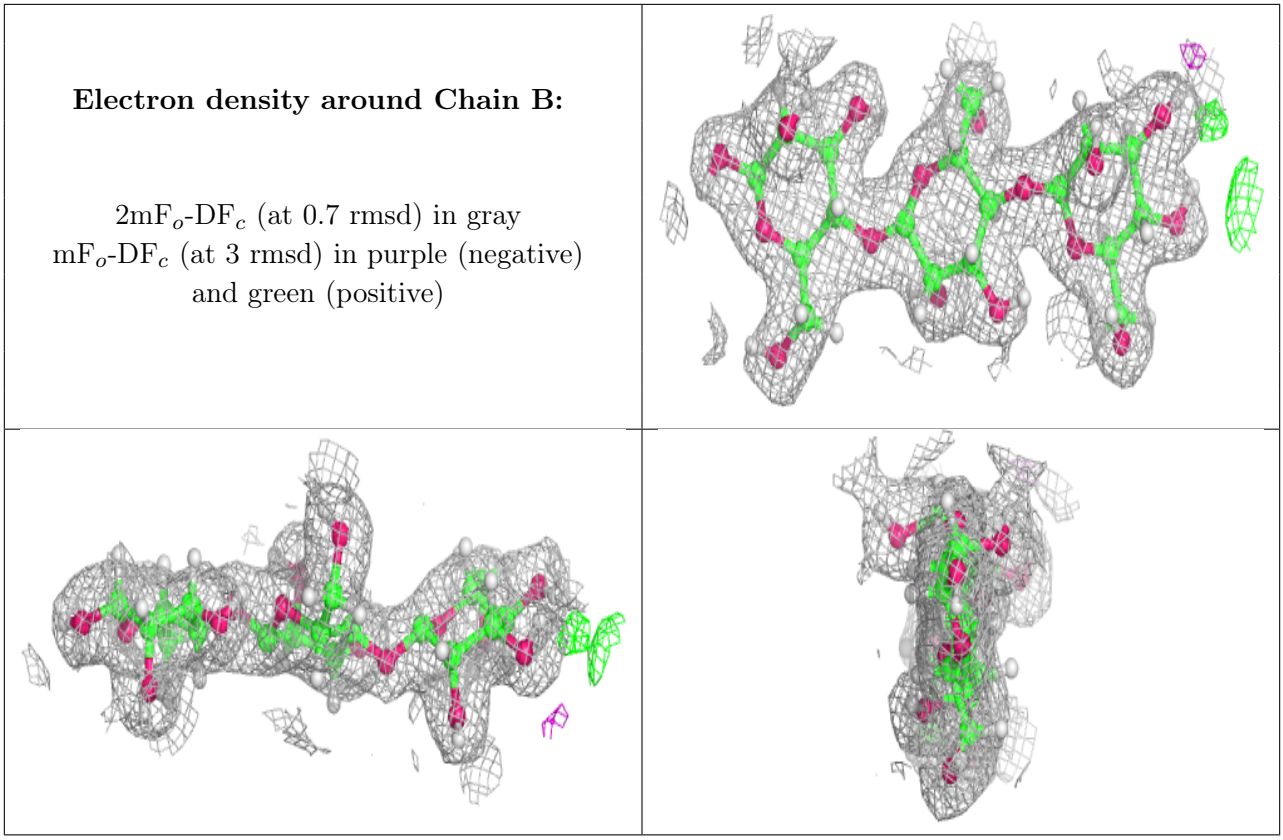
There are no non-standard protein/DNA/RNA residues in this entry.

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	BMA	B	2	11/12	0.96	0.15	14,19,24,25	0
2	BMA	B	1	12/12	0.97	0.13	11,17,21,23	0
2	BMA	B	3	11/12	0.98	0.17	13,18,23,24	0

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



6.4 Ligands (i)

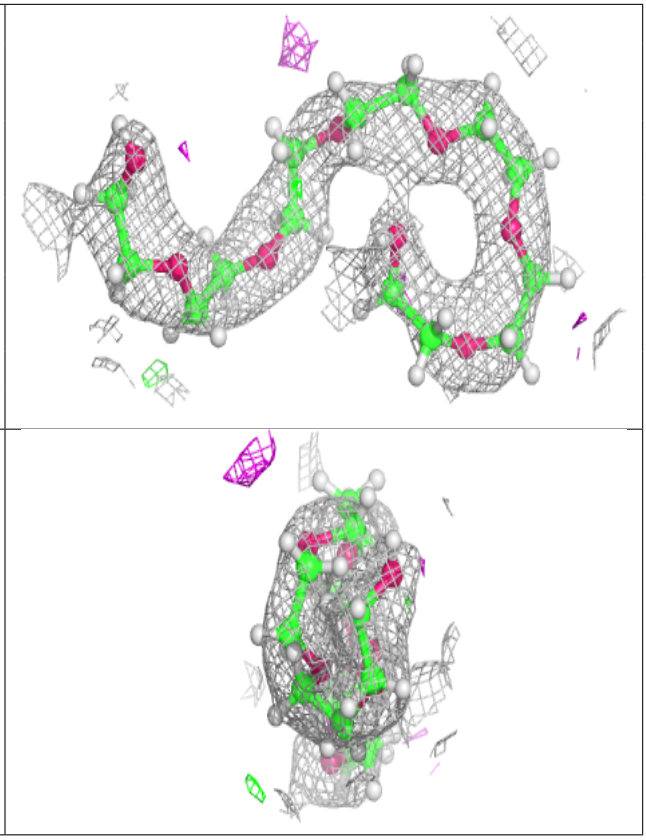
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PGE	A	605	10/10	0.86	0.18	24,39,49,51	0
3	PGE	A	602	10/10	0.89	0.15	25,35,47,47	0
3	PGE	A	603	10/10	0.91	0.24	19,34,45,56	0
3	PGE	A	601	10/10	0.91	0.17	30,39,51,53	0
5	P33	A	606	22/22	0.93	0.18	25,38,47,52	0
5	P33	A	607	22/22	0.96	0.15	19,27,38,46	0
4	ACT	A	604	4/4	0.97	0.11	22,26,30,33	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

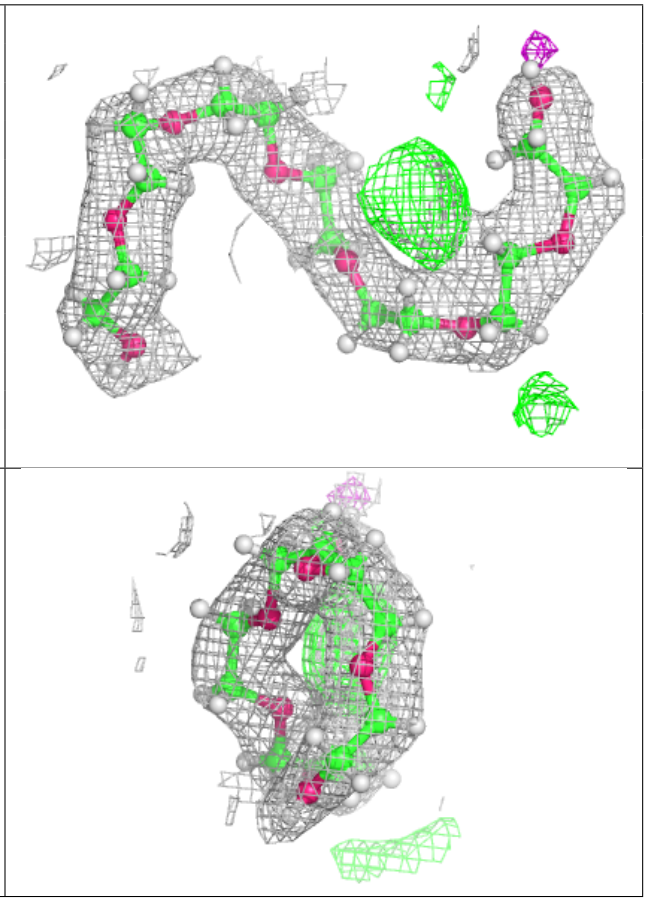
Electron density around P33 A 606:

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



Electron density around P33 A 607:

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



6.5 Other polymers (i)

There are no such residues in this entry.