wwPDB X-ray Structure Validation Summary Report (i)

Sep 14, 2020 – 03:51 PM BST

PDB ID	:	6YDC
Title	:	X-ray structure of LPMO
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Deposited on	:	2020-03-20
Resolution	:	2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see references (1)) were used in the production of this report:

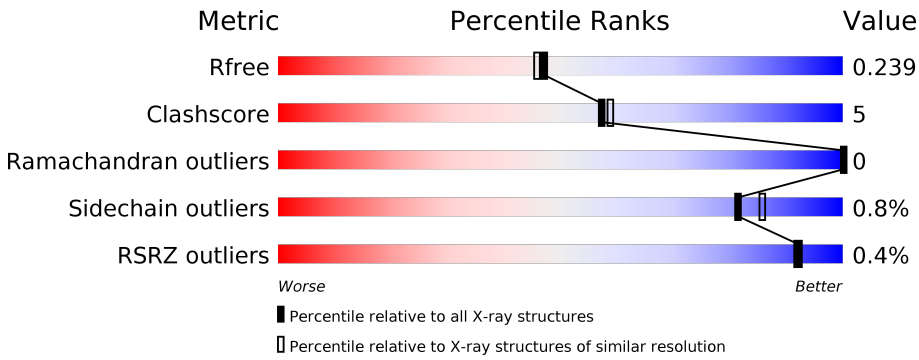
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.4.dev1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.4.dev1

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 on 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	252	81% 8% 11%
1	B	252	79% 9% 11%
1	C	252	78% 10% • 11%
1	D	252	77% 11% 11%
2	E	4	100%
2	F	4	50% 50%

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Mol	Chain	Length	Quality of chain
3	G	3	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8741 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.

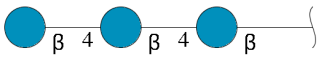
- Molecule 1 is a protein called LPMO lytic polysaccharide monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	224	1785	1145	290	343	7	0	9	0
1	B	224	1781	1142	292	340	7	0	7	0
1	C	224	1787	1148	291	341	7	0	8	0
1	D	224	1779	1143	290	339	7	0	7	0

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	E	4	45	24	21	0	0	0
2	F	4	45	24	21	0	0	0

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

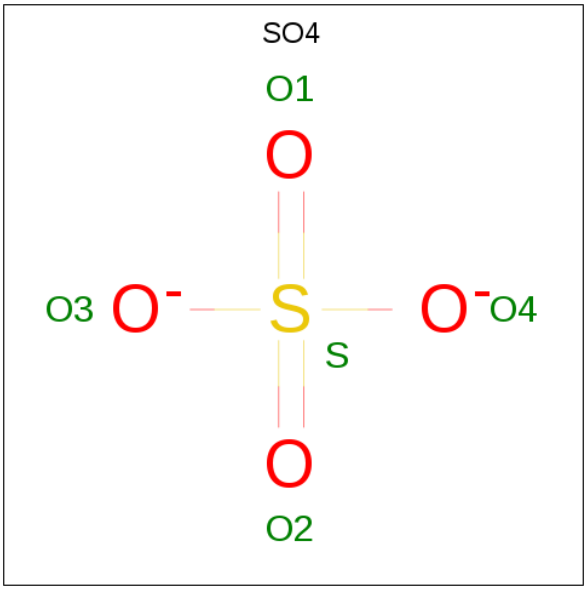


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
3	G	3	34	18	16	0	0	0

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cu 1 1	0	0
4	A	1	Total Cu 1 1	0	0
4	D	1	Total Cu 1 1	0	0
4	C	1	Total Cu 1 1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	1
5	B	1	Total O S 5 4 1	0	1
5	C	1	Total O S 5 4 1	0	1
5	D	1	Total O S 5 4 1	0	1

- Molecule 6 is water.

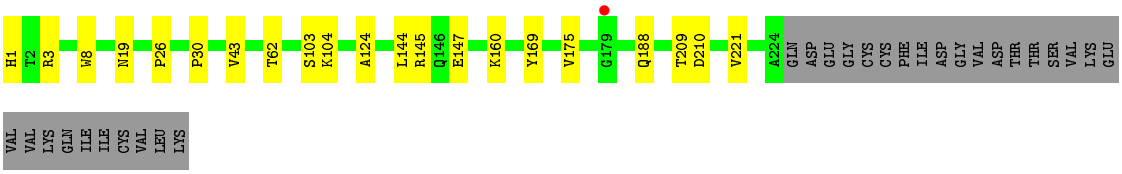
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	355	356	356	0	4
			Total	O		
6	B	377	378	378	0	4
			Total	O		
6	C	337	338	338	0	4
			Total	O		
6	D	387	389	389	0	4

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.

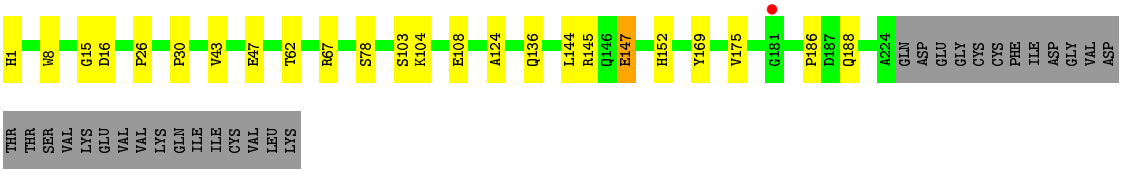
- Molecule 1: LPMO lytic polysaccharide monooxygenase

Chain A:



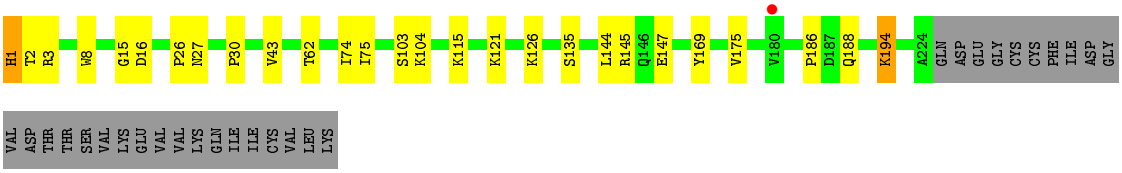
- Molecule 1: LPMO lytic polysaccharide monooxygenase

Chain B:



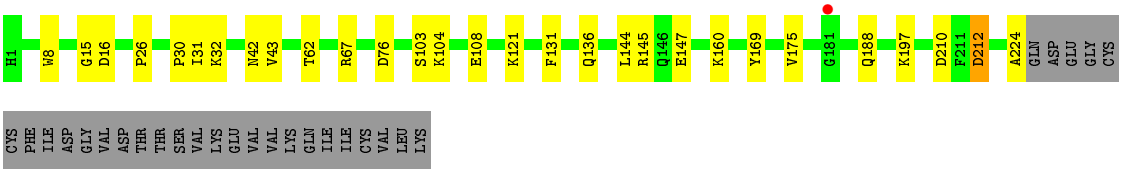
- Molecule 1: LPMO lytic polysaccharide monooxygenase

Chain C:



- Molecule 1: LPMO lytic polysaccharide monooxygenase

Chain D:



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

Chain E: 100%

BGC1 BGC2 BGC3 BGC4

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

Chain F: 50% 50%

BGC1 BGC2 BGC3 BGC4

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

Chain G: 100%

BGC1 BGC2 BGC3

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	39.79Å 120.80Å 136.36Å 90.00° 92.09° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 45.20 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.4 (50.00-2.00) 98.4 (45.20-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 2.00Å)	Xtriage
Refinement program	REFMAC v5.8.0230	Depositor
R, R_{free}	0.215 , 0.262 0.229 , 0.239	Depositor DCC
R_{free} test set	4247 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	19.9	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 45.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.156 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8741	wwPDB-VP
Average B, all atoms (Å^2)	14.0	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 45.59 % 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 1.2927e-04. 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, HIC, SO4, CU

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	0.70	0/1858	0.77	1/2538 (0.0%)
1	B	0.69	1/1848 (0.1%)	0.76	0/2522
1	C	0.67	0/1861	0.75	1/2542 (0.0%)
1	D	0.73	1/1846 (0.1%)	0.79	3/2521 (0.1%)
All	All	0.70	2/7413 (0.0%)	0.77	5/10123 (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	B	0	1
1	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	108	GLU	CD-OE1	6.02	1.32	1.25
1	B	147	GLU	CD-OE1	5.30	1.31	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	212	ASP	CB-CA-C	-5.83	98.73	110.40
1	C	3	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	D	210	ASP	CB-CA-C	-5.57	99.27	110.40
1	D	76	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	A	3	ARG	NE-CZ-NH1	-5.23	117.69	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	67	ARG	Sidechain
1	D	67	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1785	0	1709	15	0
1	B	1781	0	1705	17	0
1	C	1787	0	1715	21	0
1	D	1779	0	1706	18	0
2	E	45	0	39	0	0
2	F	45	0	39	1	0
3	G	34	0	30	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
6	A	356	0	0	2	1
6	B	378	0	0	7	0
6	C	338	0	0	6	1
6	D	389	0	0	3	0
All	All	8741	0	6943	70	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 5.

The worst 5 of 70 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:2:THR:HB	1:C:75[B]:ILE:HG23	1.42	1.01
1:A:209[A]:THR:HG22	6:B:503:HOH:O	1.60	0.98
1:C:115:LYS:O	6:C:401:HOH:O	1.81	0.98
1:C:144:LEU:HD12	1:C:175:VAL:HG21	1.46	0.98
1:B:144:LEU:HD12	1:B:175:VAL:HG21	1.45	0.97

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)
6:A:590:HOH:O	6:C:612:HOH:O[2_556]	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	231/252 (92%)	216 (94%)	15 (6%)	0	100	100
1	B	229/252 (91%)	215 (94%)	14 (6%)	0	100	100
1	C	231/252 (92%)	217 (94%)	14 (6%)	0	100	100
1	D	229/252 (91%)	216 (94%)	13 (6%)	0	100	100
All	All	920/1008 (91%)	864 (94%)	56 (6%)	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	195/212 (92%)	194 (100%)	1 (0%)	88 92
1	B	193/212 (91%)	193 (100%)	0	100 100
1	C	195/212 (92%)	193 (99%)	2 (1%)	76 81
1	D	193/212 (91%)	190 (98%)	3 (2%)	62 67
All	All	776/848 (92%)	770 (99%)	6 (1%)	81 86

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	194	LYS
1	D	212	ASP
1	D	160	LYS
1	C	135	SER
1	D	197	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	193	ASN
1	C	188	GLN
1	D	136	GLN
1	B	188	GLN
1	D	14	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	HIC	D	1	1,4	8,11,12	0.97	0	6,14,16	0.75	0
1	HIC	C	1	1,4	8,11,12	1.28	2 (25%)	6,14,16	0.83	0
1	HIC	B	1	1,4	8,11,12	1.20	1 (12%)	6,14,16	0.67	0
1	HIC	A	1	1,4	8,11,12	1.25	1 (12%)	6,14,16	0.87	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
1	HIC	D	1	1,4	-	0/5/6/8	0/1/1/1
1	HIC	C	1	1,4	-	0/5/6/8	0/1/1/1
1	HIC	B	1	1,4	-	0/5/6/8	0/1/1/1
1	HIC	A	1	1,4	-	0/5/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	HIC	CD2-CG	2.46	1.39	1.36
1	A	1	HIC	CD2-CG	2.45	1.39	1.36
1	C	1	HIC	CD2-NE2	-2.20	1.34	1.38
1	C	1	HIC	CD2-CG	2.15	1.39	1.36

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	1	HIC	1	0

5.5 Carbohydrates (i)

11 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	E	1	2	12,12,12	0.89	0	17,17,17	0.51	0
2	BGC	E	2	2	11,11,12	0.89	0	15,15,17	0.62	0
2	BGC	E	3	2	11,11,12	0.54	0	15,15,17	0.65	0
2	BGC	E	4	2	11,11,12	0.48	0	15,15,17	0.65	0
2	BGC	F	1	2	12,12,12	0.86	0	17,17,17	0.53	0
2	BGC	F	2	2	11,11,12	1.36	2 (18%)	15,15,17	0.64	0
2	BGC	F	3	2	11,11,12	0.84	0	15,15,17	0.63	0
2	BGC	F	4	2	11,11,12	0.66	0	15,15,17	0.61	0
3	BGC	G	1	3	12,12,12	0.81	0	17,17,17	1.44	3 (17%)
3	BGC	G	2	3	11,11,12	1.24	1 (9%)	15,15,17	1.34	2 (13%)
3	BGC	G	3	3	11,11,12	0.91	0	15,15,17	1.01	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	BGC	E	1	2	-	0/2/22/22	0/1/1/1
2	BGC	E	2	2	-	2/2/19/22	0/1/1/1
2	BGC	E	3	2	-	0/2/19/22	0/1/1/1
2	BGC	E	4	2	-	2/2/19/22	0/1/1/1
2	BGC	F	1	2	-	0/2/22/22	0/1/1/1
2	BGC	F	2	2	-	2/2/19/22	0/1/1/1
2	BGC	F	3	2	-	1/2/19/22	0/1/1/1
2	BGC	F	4	2	-	0/2/19/22	0/1/1/1
3	BGC	G	1	3	-	0/2/22/22	0/1/1/1
3	BGC	G	2	3	-	2/2/19/22	0/1/1/1
3	BGC	G	3	3	-	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)
3	G	2	BGC	O5-C5	2.90	1.49	1.43
2	F	2	BGC	O5-C1	-2.53	1.39	1.43
2	F	2	BGC	C4-C5	2.35	1.58	1.53

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	1	BGC	C1-O5-C5	-3.55	106.96	113.66
3	G	1	BGC	C6-C5-C4	2.77	119.48	113.00
3	G	1	BGC	O1-C1-C2	2.71	116.66	109.03
3	G	3	BGC	C1-O5-C5	2.40	115.44	112.19
3	G	2	BGC	O3-C3-C2	-2.27	105.64	109.99

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2	BGC	O5-C5-C6-O6
2	F	2	BGC	C4-C5-C6-O6
2	F	2	BGC	O5-C5-C6-O6
2	E	2	BGC	C4-C5-C6-O6
3	G	2	BGC	C4-C5-C6-O6

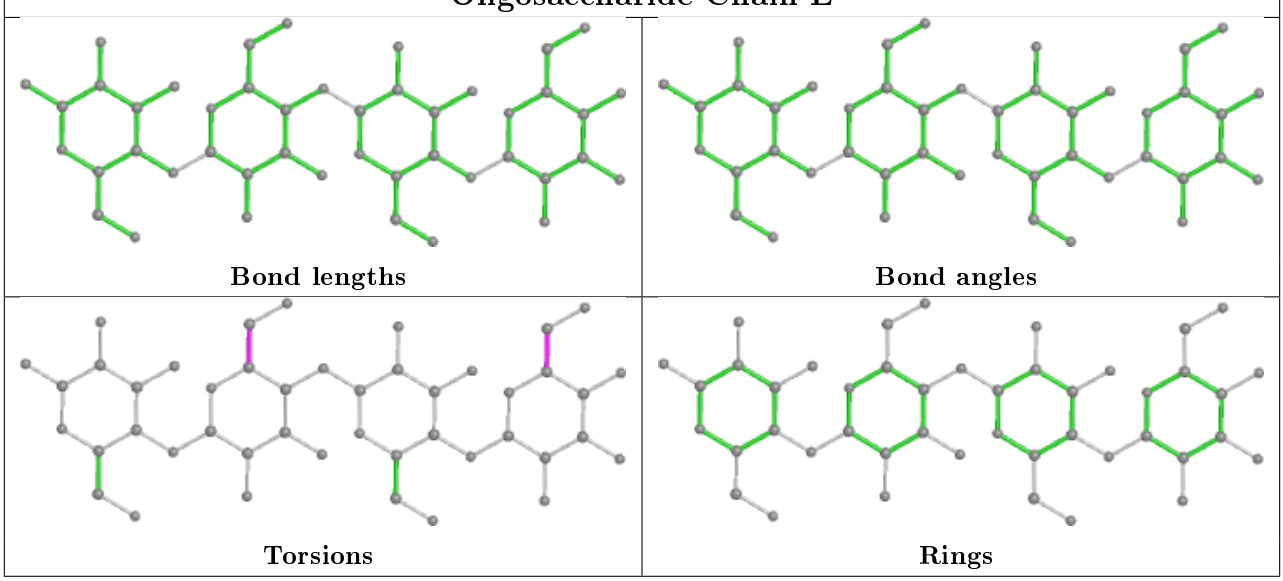
There are no ring outliers.

1 monomer is involved in 1 short contact:

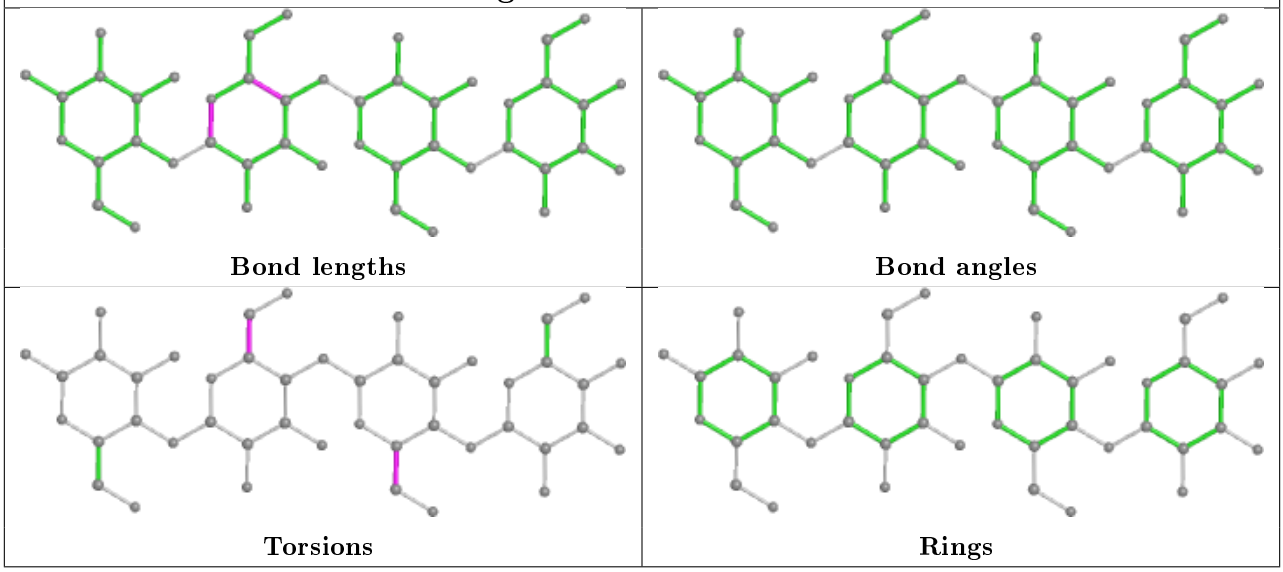
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	BGC	1	0

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

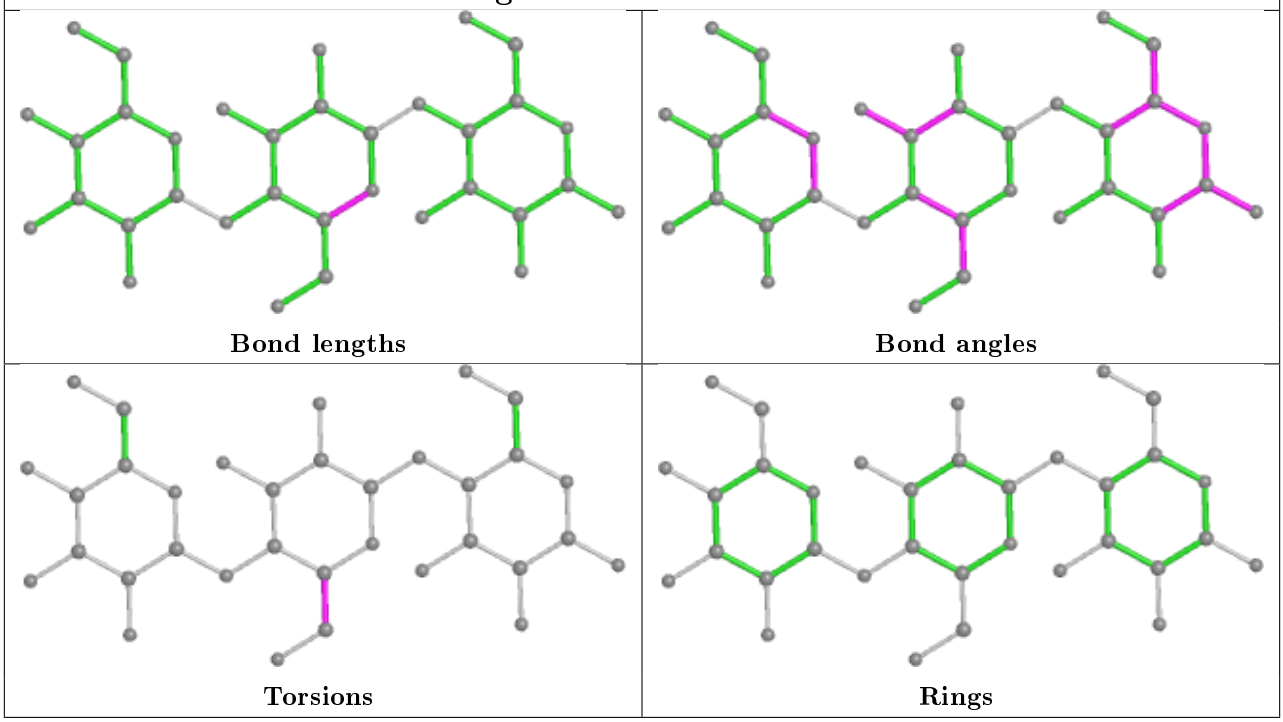
Oligosaccharide Chain E



Oligosaccharide Chain F



Oligosaccharide Chain G



5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
5	SO4	D	302[A]	-	4,4,4	0.39	0	6,6,6	0.67	0
5	SO4	B	306[A]	-	4,4,4	0.37	0	6,6,6	0.54	0
5	SO4	A	306[A]	-	4,4,4	0.29	0	6,6,6	0.16	0
5	SO4	C	303[A]	-	4,4,4	0.40	0	6,6,6	0.19	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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	223/252 (88%)	-0.60	1 (0%)	92	92	8, 12, 17, 28	1 (0%)
1	B	223/252 (88%)	-0.64	1 (0%)	92	92	6, 10, 17, 29	0
1	C	223/252 (88%)	-0.60	1 (0%)	92	92	7, 11, 19, 28	0
1	D	223/252 (88%)	-0.64	1 (0%)	92	92	5, 9, 15, 31	0
All	All	892/1008 (88%)	-0.62	4 (0%)	92	92	5, 10, 17, 31	1 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	181	GLY	2.5
1	B	181	GLY	2.3
1	C	180	VAL	2.2
1	A	179	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	HIC	D	1	11/12	0.98	0.08	8,8,9,9	0
1	HIC	C	1	11/12	0.98	0.08	10,11,13,13	0
1	HIC	B	1	11/12	0.98	0.09	8,9,9,9	0
1	HIC	A	1	11/12	0.99	0.07	12,12,14,14	0

6.3 Carbohydrates (i)

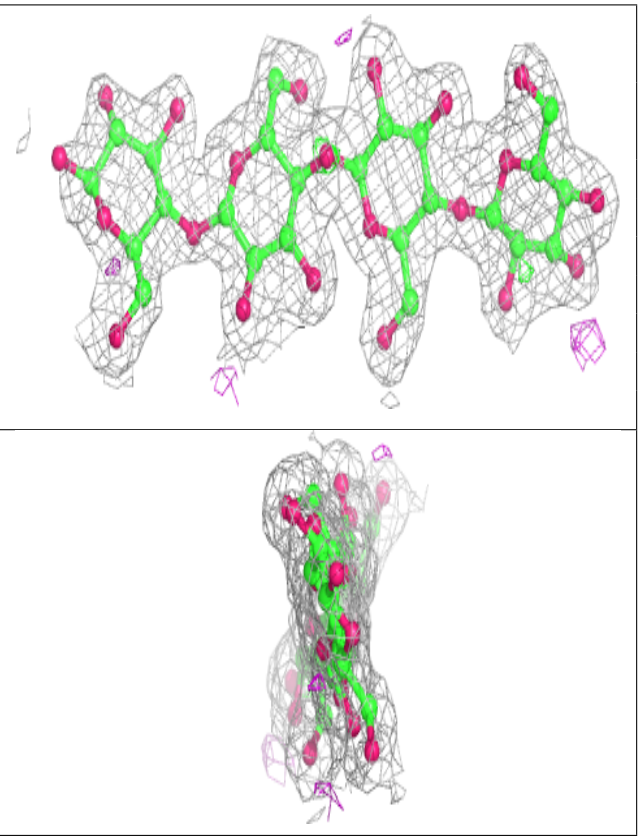
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	F	1	12/12	0.82	0.15	35,42,45,47	12
2	BGC	E	1	12/12	0.90	0.13	41,49,52,61	0
2	BGC	F	2	11/12	0.93	0.13	32,35,41,46	0
3	BGC	G	2	11/12	0.93	0.13	19,21,24,24	0
2	BGC	F	4	11/12	0.93	0.11	34,35,37,40	0
3	BGC	G	3	11/12	0.93	0.17	20,21,22,22	0
2	BGC	E	2	11/12	0.94	0.10	29,32,34,35	0
2	BGC	F	3	11/12	0.94	0.09	29,32,34,35	0
3	BGC	G	1	12/12	0.95	0.09	23,26,27,30	0
2	BGC	E	3	11/12	0.95	0.09	27,29,31,31	0
2	BGC	E	4	11/12	0.96	0.10	31,32,33,34	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.

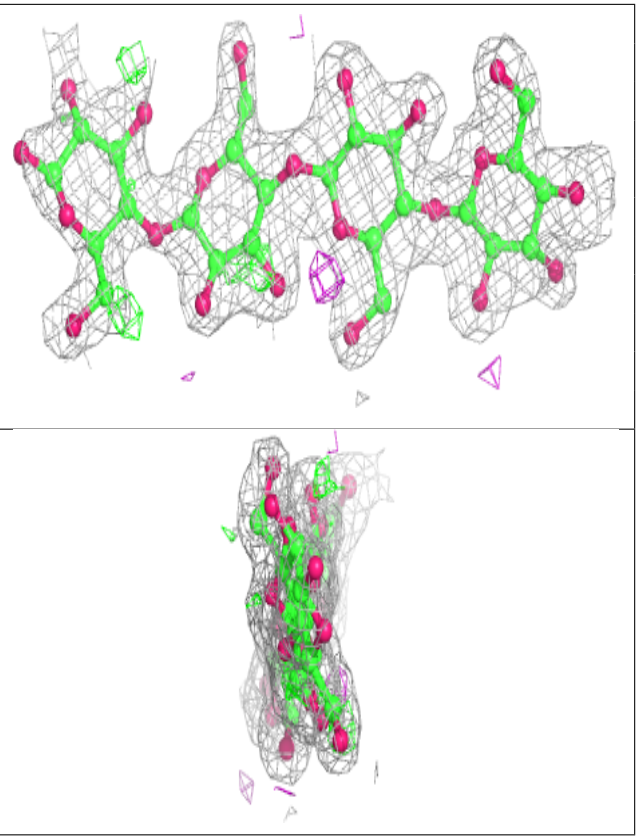
Electron density around Chain E:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



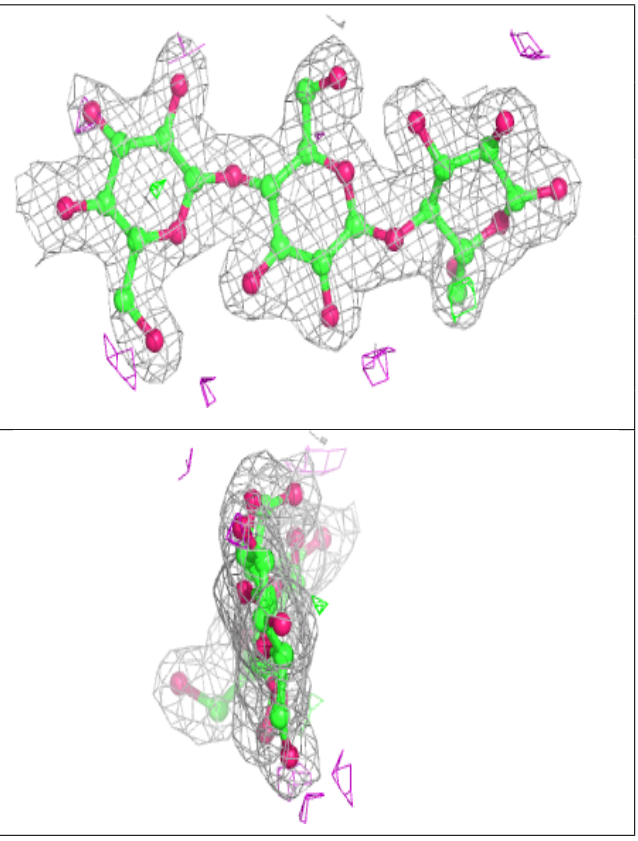
Electron density around Chain F:

$2mF_o$-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 G:

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



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	A	306[A]	5/5	0.94	0.15	32,33,36,36	5
5	SO4	D	302[A]	5/5	0.95	0.19	27,28,28,29	5
5	SO4	C	303[A]	5/5	0.95	0.12	21,23,23,25	5
5	SO4	B	306[A]	5/5	0.96	0.15	25,27,29,29	5
4	CU	C	301	1/1	1.00	0.05	12,12,12,12	0
4	CU	A	301	1/1	1.00	0.05	13,13,13,13	0
4	CU	B	301	1/1	1.00	0.08	9,9,9,9	0
4	CU	D	301	1/1	1.00	0.05	8,8,8,8	0

6.5 Other polymers (i)

There are no such residues in this entry.