

wwPDB X-ray Structure Validation Summary Report (i)

Aug 18, 2022 – 01:13 pm BST

PDB ID : 7PYW

Title : Structure of LPMO (expressed in E.coli) with cellotriose at 5.62x10⁴ Gy Authors : Tandrup, T.; Muderspach, S.J.; Banerjee, S.; Ipsen, J.O.; Rollan, C.H.;

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Deposited on : 2021-10-11

Resolution : 1.40 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : FAILED

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.29

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0267

CCP4 : 7.1.010 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

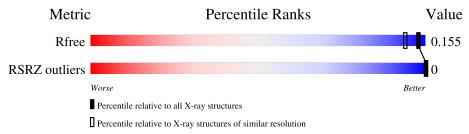
Validation Pipeline (wwPDB-VP) : 2.29

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 1.40 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 $(\# \mathrm{Entries})$	Similar resolution $(\#\text{Entries, resolution range}(\mathring{A}))$			
R_{free}	130704	1714 (1.40-1.40)			
RSRZ outliers	127900	1674 (1.40-1.40)			

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 2439 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 Auxiliary activity 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total 1903	C 1199	N 328	O 373	S 3	0	13	0

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



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace	
2	В	2	Total 23	C 12	O 11	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	
3	Е	3	Total 34	C 18	O 16	0	0	0

• Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

• Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).





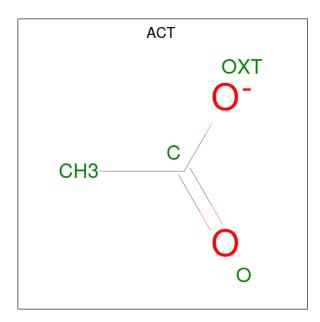
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	1

• Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Cl 2 2	0	0

• Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).





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

• Molecule 8 is water.

\mathbf{Mol}	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	428	Total O 452 452	0	29

 $\operatorname{MolProbity}$ failed to run properly - this section is therefore empty.



3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants	48.84Å 48.84Å 108.79Å	Donositon
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.84 - 1.40	Depositor
Resolution (A)	48.84 - 1.40	EDS
% Data completeness	99.9 (48.84-1.40)	Depositor
(in resolution range)	99.9 (48.84-1.40)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.77 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
D D.	0.137 , 0.153	Depositor
R, R_{free}	0.138 , 0.155	DCC
R_{free} test set	2502 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	13.2	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$< L >=0.51, < L^2>=0.35$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	2439	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.79% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates (i)

5 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	Tuna	Chain	Res	Link	Во	ond leng	ths	Bond angles		
MIOI	Type	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
2	BGC	В	1	2	12,12,12	0.97	0	17,17,17	1.53	2 (11%)
2	BGC	В	2	2	11,11,12	1.38	1 (9%)	15,15,17	1.53	2 (13%)
3	BGC	Е	1	3	12,12,12	0.43	0	17,17,17	0.83	0
3	BGC	Е	2	3	11,11,12	0.78	0	15,15,17	1.04	1 (6%)
3	BGC	Е	3	3	11,11,12	0.65	0	15,15,17	0.70	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	BGC	В	1	2	-	0/2/22/22	0/1/1/1
2	BGC	В	2	2	-	2/2/19/22	0/1/1/1
3	BGC	Е	1	3	-	0/2/22/22	0/1/1/1
3	BGC	Е	2	3	-	0/2/19/22	0/1/1/1
3	BGC	Е	3	3	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	$Ideal(\AA)$
2	В	2	BGC	C2-C3	2.46	1.56	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	В	2	BGC	C1-O5-C5	3.52	116.97	112.19
2	В	1	BGC	O3-C3-C2	-3.41	102.47	110.35
2	В	2	BGC	C1-C2-C3	3.33	113.76	109.67
3	Е	2	BGC	O5-C5-C6	-2.36	103.51	107.20
2	В	1	BGC	O5-C5-C4	2.16	113.62	109.69

There are no chirality outliers.

All (2) torsion outliers are listed below:

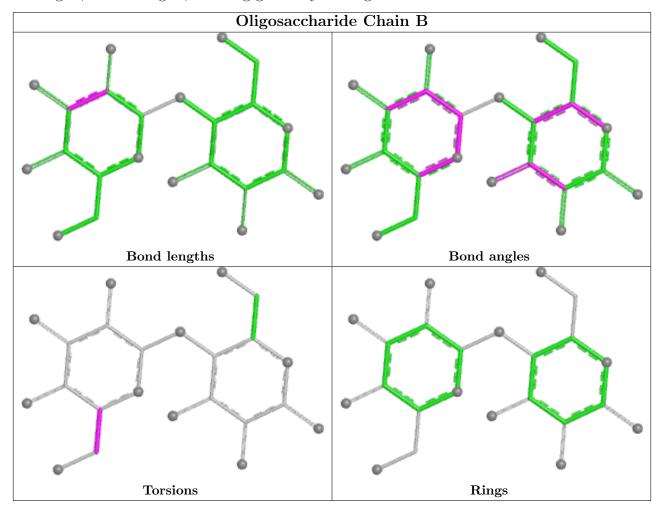
Mo	l C	hain	Res	Type	Atoms
2		В	2	BGC	C4-C5-C6-O6
2		В	2	BGC	O5-C5-C6-O6

There are no ring outliers.

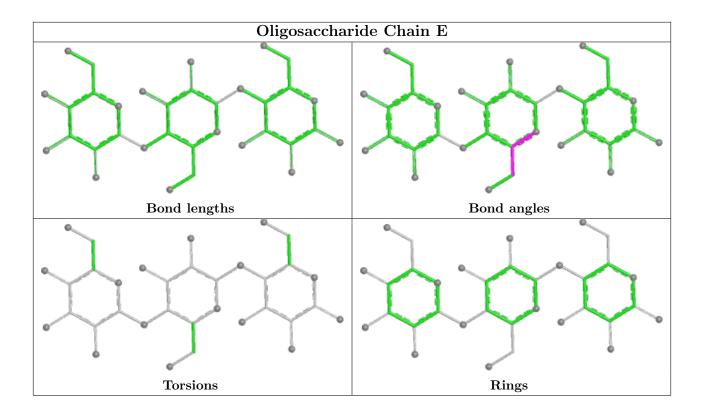


No monomer is involved in short contacts.

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







4.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Res	Link	В	Bond lengths			Bond angles		
MIOI	Type		nes	LillK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2								
5	SO4	A	303	-	4,4,4	0.40	0	6,6,6	0.14	0								
5	SO4	A	305[A]	-	4,4,4	0.38	0	6,6,6	0.20	0								
7	ACT	A	308	-	3,3,3	1.00	0	3,3,3	0.77	0								
5	SO4	A	302	-	4,4,4	0.36	0	6,6,6	0.44	0								
5	SO4	A	304	-	4,4,4	0.33	0	6,6,6	0.34	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.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



5 Fit of model and data (i)

5.1 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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	$\langle { m RSRZ} \rangle$	# RSRZ > 2	$OWAB(Å^2)$	Q < 0.9
1	A	235/235 (100%)	-0.09	0 100 100	9, 12, 19, 38	0

There are no RSRZ outliers to report.

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

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

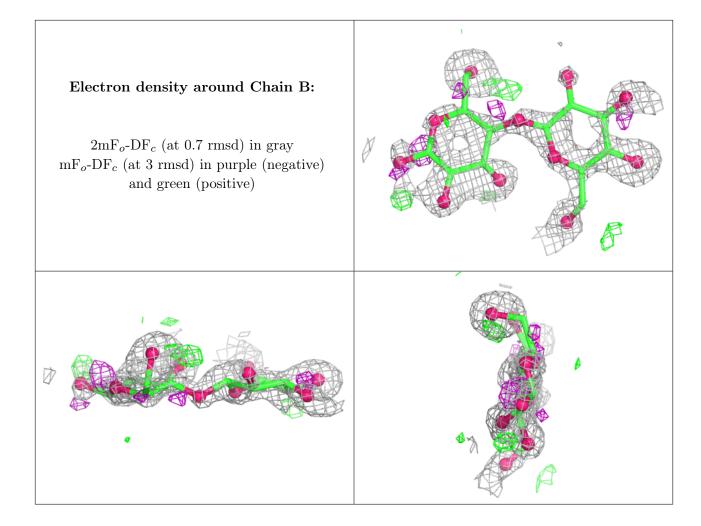
5.3 Carbohydrates (i)

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

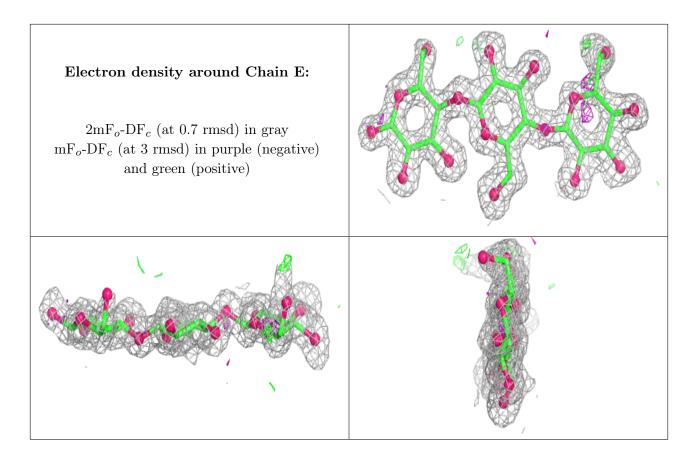
Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B-factors}({f \AA}^2)$	Q < 0.9
2	BGC	В	1	12/12	0.74	0.30	24,40,46,47	0
3	BGC	Ε	3	11/12	0.80	0.15	21,25,32,39	0
2	BGC	В	2	11/12	0.81	0.31	22,40,45,48	0
3	BGC	Е	2	11/12	0.85	0.14	17,23,26,27	0
3	BGC	Ε	1	12/12	0.91	0.17	17,23,34,45	0

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.









5.4 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
5	SO4	A	305[A]	5/5	0.75	0.35	15,16,22,23	5
7	ACT	A	308	4/4	0.79	0.24	29,49,50,51	0
5	SO4	A	304	5/5	0.88	0.15	21,22,23,24	5
5	SO4	A	303	5/5	0.94	0.15	19,33,36,36	5
6	CL	A	307	1/1	0.95	0.07	32,32,32,32	0
5	SO4	A	302	5/5	0.98	0.09	17,18,24,24	5
6	CL	A	306	1/1	0.99	0.05	17,17,17,17	1
4	CU	A	301	1/1	1.00	0.07	11,11,11,11	0

5.5 Other polymers (i)

There are no such residues in this entry.

