

wwPDB X-ray Structure Validation Summary Report (i)

Dec 19, 2021 – 06:03 am GMT

PDB ID : 7077

Title: Structure of the PL6 family alginate lyase Patl3640 from Pseudoalteromonas

atlantica T6c

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Deposited on : 2021-04-13

Resolution : 2.32 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 : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.24

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)

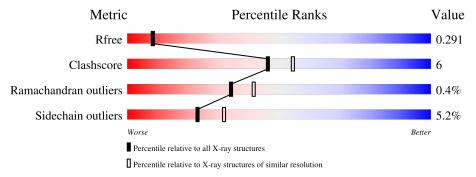
Validation Pipeline (wwPDB-VP) : 2.24

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.32 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)

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%

17% •



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5477 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.

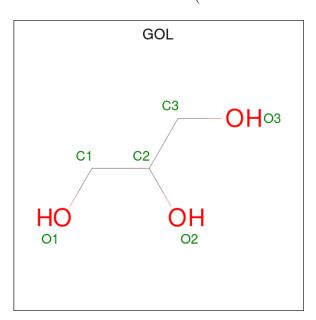
• Molecule 1 is a protein called Poly(Beta-D-mannuronate) lyase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	A	720	Total 5418	C 3384	N 928	O 1093	S 13	0	0	0

There is a discrepancy between the modelled and reference sequences:

C	hain	Residue	Modelled	Actual	Comment	Reference
	A	37	MET	-	initiating methionine	UNP Q15PP6

• Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0

• Molecule 3 is water.



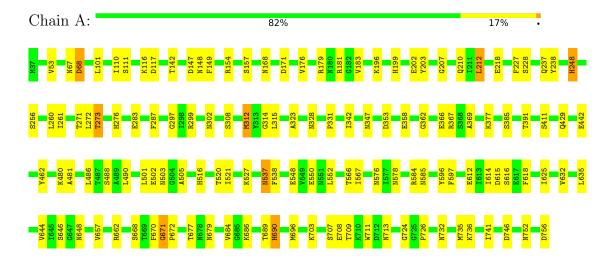
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	53	Total O 53 53	0	0



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. 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: Poly(Beta-D-mannuronate) lyase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	79.53Å 79.53Å 269.47Å	Donositon
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.16 - 2.32	Depositor
Resolution (A)	48.16 - 2.32	EDS
% Data completeness	96.0 (48.16-2.32)	Depositor
(in resolution range)	96.0 (48.16-2.32)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.06 (at 2.32Å)	Xtriage
Refinement program	BUSTER 2.10.3 (29-NOV-2019)	Depositor
R, R_{free}	0.250 , 0.282	Depositor
it, it free	0.260 , 0.291	DCC
R_{free} test set	2190 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å ²)	64.7	Xtriage
Anisotropy	0.570	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$< L >=0.51, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5477	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.85% 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.

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: GOL

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	$\mathbf{lengths}$	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
	1	A	0.42	0/5521	0.65	0/7520

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	5418	0	5100	66	0
2	A	6	0	8	0	0
3	A	53	0	0	1	0
All	All	5477	0	5108	66	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 6.

The worst 5 of 66 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1 Atom-2		$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$	
1:A:736:LYS:HA	1:A:756:ASP:HA	1.56	0.88	

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Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:A:148:ASN:ND2	1:A:179:ARG:NH1	2.37	0.71
1:A:248:HIS:CE1	1:A:668:SER:HA	2.30	0.67
1:A:657:VAL:HG23	1:A:684:VAL:HG11	1.77	0.67
1:A:347:ASN:HD22	1:A:377:LYS:H	1.41	0.65

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 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	Analysed Favoured Al		Outliers	Percentiles	
1	A	718/720 (100%)	676 (94%)	39 (5%)	3 (0%)	34	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	671	GLY
1	A	117	ASP
1	A	741	ILE

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	nalysed Rotameric		Percentiles	
1	A	575/613 (94%)	545 (95%)	30 (5%)	23 32	

5 of 30 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	385	SER
1	A	703	LYS
1	A	442	GLU
1	A	746	ASP
1	A	635	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	603	ASN
1	A	620	ASN
1	A	690	HIS
1	A	648	ASN
1	A	503	ASN

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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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).



7	/[a]	Type	Chain	Res	Link	Bond lengths		Bond angles			
1	Mol	туре	Chain	rtes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
	2	GOL	A	801	-	5,5,5	0.09	0	5,5,5	0.28	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	GOL	A	801	_	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	GOL	O1-C1-C2-C3
2	A	801	GOL	O1-C1-C2-O2

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

