

wwPDB Geometry-Only Validation Summary Report (i)

Jan 11, 2024 – 03:55 pm GMT

PDB ID : 8RBN

Title : Neutron structure of alginate lysase PsPL7C from Paradendryphiella salina

soaked with penta-mannuronic acid

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Deposited on : 2023-12-04

Resolution : 2.10 Å(reported)

This is a wwPDB Geometry-Only 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 : 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

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

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

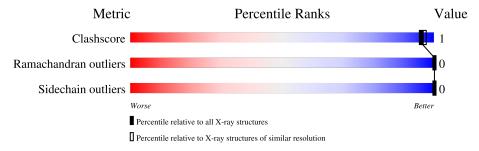
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $NEUTRON\ DIFFRACTION$

The reported resolution of this entry is 2.10 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	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$		
Clashscore	141614	5710 (2.10-2.10)		
Ramachandran outliers	138981	5647 (2.10-2.10)		
Sidechain outliers	138945	5648 (2.10-2.10)		

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	234	98%
2	В	2	100%
3	С	3	100%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4319 atoms, of which 1729 are hydrogens and 631 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 Alginate lyase.

Mol	Chain	Residues		Atoms					ZeroOcc	AltConf	Trace	
1	Λ	231	Total	С	D	Н	N	О	S	108	225	0
1	A	231	3837	1112	374	1689	299	356	7	100	229	

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLU	-	expression tag	UNP A0A7I9C8Z1
A	0	PHE	-	expression tag	UNP A0A7I9C8Z1
A	241	VAL	-	expression tag	UNP A0A7I9C8Z1
A	242	ASP	-	expression tag	UNP A0A7I9C8Z1
A	243	HIS	-	expression tag	UNP A0A7I9C8Z1
A	244	HIS	-	expression tag	UNP A0A7I9C8Z1
A	245	HIS	-	expression tag	UNP A0A7I9C8Z1
A	246	HIS	-	expression tag	UNP A0A7I9C8Z1
A	247	HIS	-	expression tag	UNP A0A7I9C8Z1
A	248	HIS	-	expression tag	UNP A0A7I9C8Z1

• Molecule 2 is an oligosaccharide called 4-deoxy-alpha-L-erythro-hex-4-enopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	9	Total	С	D	Н	О	2	2	0
	Б	2	42	12	3	15	12	3	2	U

• Molecule 3 is an oligosaccharide called beta-D-mannopyranuronic acid-(1-4)-alpha-D-mannopyranuronic acid-(1-4)-beta-D-mannopyranuronic acid.





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	С	3	Total 68	C 18	D 6	H 25	O 19	13	3	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	124	Total 372	D 248	O 124	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.

Note EDS was	not executed.
• Molecule 1: A	Alginate lyase
Chain A:	98%
6LU F0 E78 E78 R132 H1S H1S	
• Molecule 2: 4 c acid	-deoxy-alpha-L-erythro-hex-4-enopyranuronic acid-(1-4)-beta-D-mannopyranuroni
Chain B:	100%
BEW1	
• Molecule 3: b	beta-D-mannopyranuronic acid-(1-4)-alpha-D-mannopyranuronic acid-(1-4)-beta-Donic acid
Chain C:	100%
BEM1 BEM3	



4 Model quality (i)

4.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MAV, BEM, MAW

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	Boı	nd lengths	Bond angles		
IVIOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.83	2/3547 (0.1%)	0.90	2/4821 (0.0%)	

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(\text{\AA})$
1	A	78[A]	GLU	CB-CG	-5.06	1.42	1.52
1	A	78[B]	GLU	CB-CG	-5.06	1.42	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
1	A	132[A]	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	132[B]	ARG	NE-CZ-NH1	6.14	123.37	120.30

There are no chirality outliers.

There are no planarity outliers.

4.2 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	2148	1689	62	0	0
2	В	27	15	0	0	0
3	С	43	25	0	0	0
4	A	372	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2590	1729	62	1	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 1.

All (1) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A + 0 mg 1	Atom-2	Interatomic	Clash	
Atom-1	Atom-2	${ m distance} ({ m \AA})$	overlap (Å)	

There are no symmetry-related clashes.

4.3 Torsion angles (i)

4.3.1 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	452/234 (193%)	438 (97%)	14 (3%)	0	100 100	

There are no Ramachandran outliers to report.

4.3.2 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	377/195 (193%)	377 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.



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

4.3.3 RNA (i)

There are no RNA molecules in this entry.

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)

13 monosaccharides are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

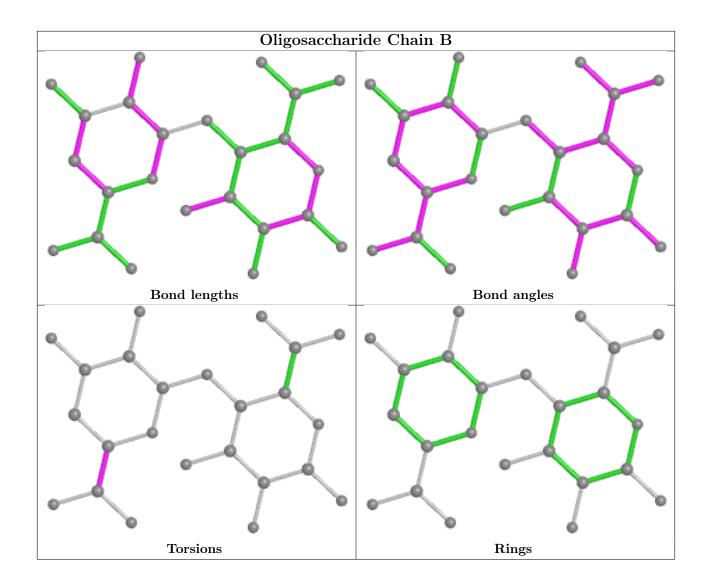
There are no torsion outliers.

There are no ring outliers.

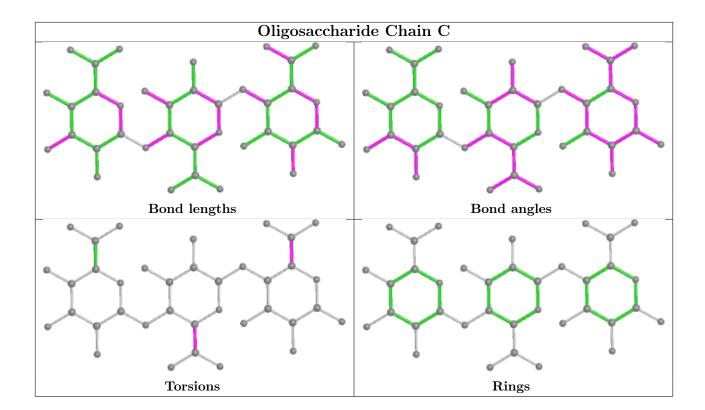
No monomer is involved in short contacts.

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)

There are no ligands in this entry.

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.

