wwPDB X-ray Structure Validation Summary Report (i)

Oct 2, 2023 – 12:21 AM EDT

PDB ID	:	6MFZ
Title	:	Crystal structure of dimodular LgrA in a condensation state
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Deposited on	:	2018-09-12
Resolution	:	6.00 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 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	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
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)	:	2.35.1

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 6.00 Å.

There are no overall percentile quality scores available for this entry.

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

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18882 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 Linear gramicidin synthase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1789	Total	C	N	O	S	0	0	0
			14226	9089	2430	2649	58			
1	B	585	Total	C	N	O	S	0	0	0
			4648	2958	797	871	22			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q70LM7
A	0	ALA	-	expression tag	UNP Q70LM7
A	1	MET	-	expression tag	UNP Q70LM7
A	2	GLY	-	expression tag	UNP Q70LM7
A	1804	ALA	-	expression tag	UNP Q70LM7
A	1805	ALA	-	expression tag	UNP Q70LM7
A	1806	ALA	-	expression tag	UNP Q70LM7
A	1807	GLU	-	expression tag	UNP Q70LM7
A	1808	ASN	-	expression tag	UNP Q70LM7
A	1809	LEU	-	expression tag	UNP Q70LM7
A	1810	TYR	-	expression tag	UNP Q70LM7
A	1811	PHE	-	expression tag	UNP Q70LM7
A	1812	GLN	-	expression tag	UNP Q70LM7
B	-1	GLY	-	expression tag	UNP Q70LM7
B	0	ALA	-	expression tag	UNP Q70LM7
B	1	MET	-	expression tag	UNP Q70LM7
B	2	GLY	-	expression tag	UNP Q70LM7
B	1804	ALA	-	expression tag	UNP Q70LM7
B	1805	ALA	-	expression tag	UNP Q70LM7
B	1806	ALA	-	expression tag	UNP Q70LM7
B	1807	GLU	-	expression tag	UNP Q70LM7
B	1808	ASN	-	expression tag	UNP Q70LM7
B	1809	LEU	-	expression tag	UNP Q70LM7
B	1810	TYR	-	expression tag	UNP Q70LM7
B	1811	PHE	-	expression tag	UNP Q70LM7

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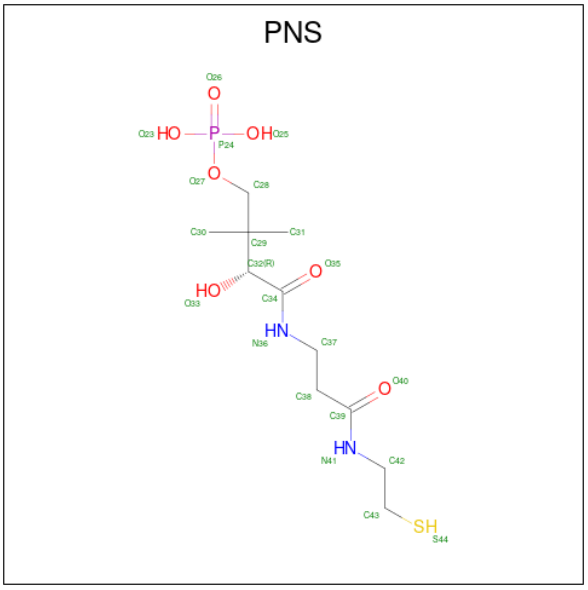
Chain	Residue	Modelled	Actual	Comment	Reference
B	1812	GLN	-	expression tag	UNP Q70LM7

- Molecule 2 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula: $C_{11}H_{23}N_2O_7PS$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 4 3 1	0	0
2	A	1	Total O P 4 3 1	0	0

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

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	213.60Å 262.75Å 249.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.63 – 6.00	Depositor
% Data completeness (in resolution range)	99.9 (78.63-6.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 6.18Å)	Xtriage
Refinement program	PHENIX (dev_3494: ???)	Depositor
R, R_{free}	0.255 , 0.279	Depositor
Wilson B-factor (Å^2)	216.9	Xtriage
Anisotropy	0.457	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18882	wwPDB-VP
Average B, all atoms (Å^2)	343.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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.

4 Model quality

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

2 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	$\#\|Z\| > 2$
2	PNS	A	1902	1	0,3,21	-	-	0,3,29	-	-
2	PNS	A	1901	1	0,3,21	-	-	0,3,29	-	-

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

5.1 Protein, DNA and RNA chains

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

5.2 Non-standard residues in protein, DNA, RNA chains

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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