WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2023 – 11:12 PM EDT

PDB ID	:	6MLK
Title	:	Structure of Thioesterase from DEBS with a thioesterase-specific antibody
Authors	:	Mathews, I.I.; Li, X.; Khosla, C.
Deposited on	:	2018-09-27
Resolution	:	2.45 Å(reported)

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

MolProbity	:	FAILED
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 ⓘ

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

The reported resolution of this entry is 2.45 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 ⓘ

There are 5 unique types of molecules in this entry. The entry contains 5297 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 6-deoxyerythronolide-B synthase EryA3, modules 5 and 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total 1960	C 1237	N 346	O 368	S 9	0	1	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q03133
A	2	ALA	-	expression tag	UNP Q03133
A	3	SER	-	expression tag	UNP Q03133
A	284	SER	-	expression tag	UNP Q03133
A	285	SER	-	expression tag	UNP Q03133
A	286	VAL	-	expression tag	UNP Q03133
A	287	ASP	-	expression tag	UNP Q03133
A	288	LYS	-	expression tag	UNP Q03133
A	289	LEU	-	expression tag	UNP Q03133
A	290	ALA	-	expression tag	UNP Q03133
A	291	ALA	-	expression tag	UNP Q03133
A	292	ALA	-	expression tag	UNP Q03133
A	293	LEU	-	expression tag	UNP Q03133
A	294	GLU	-	expression tag	UNP Q03133
A	295	HIS	-	expression tag	UNP Q03133
A	296	HIS	-	expression tag	UNP Q03133
A	297	HIS	-	expression tag	UNP Q03133
A	298	HIS	-	expression tag	UNP Q03133
A	299	HIS	-	expression tag	UNP Q03133
A	300	HIS	-	expression tag	UNP Q03133

- Molecule 2 is a protein called Light chain of Fab 3A6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	217	Total 1676	C 1051	N 285	O 334	S 6	0	0	0

- Molecule 3 is a protein called Heavy chain of Fab 3A6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	213	Total 1595	C 1017	N 262	O 312	S 4	0	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total 1	Cl 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	12	Total 12	O 12	0	0
5	L	15	Total 15	O 15	0	0
5	H	38	Total 38	O 38	0	0

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

3 Data and refinement statistics ⓘ

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	172.58Å 172.58Å 159.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.43 – 2.45	Depositor
% Data completeness (in resolution range)	99.8 (38.43-2.45)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.175 , 0.235	Depositor
Wilson B-factor (Å^2)	63.6	Xtriage
Anisotropy	0.189	Xtriage
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5297	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

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.