Full wwPDB X-ray Structure Validation Report (i)

Oct 3, 2023 – 07:01 AM EDT

PDB ID	:	6ULW
Title	:	Adenylation, ketoreductase, and pseudo Asub multidomain structure of a keto acid-selecting NRPS module
Authors	:	Alonzo, D.A.; Wang, J.; Chiche-Lapierre, C.; Schmeing, T.M.
Deposited on	:	2019-10-08
Resolution	:	3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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
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 3.40 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 3 unique types of molecules in this entry. The entry contains 74888 atoms, of which 37048 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 Amino acid adenylation domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	1193	18613	5974	9210	1598	1782	49	0	0	0
1	B	1209	18852	6049	9327	1618	1808	50	0	0	0
1	C	1203	18783	6024	9294	1613	1803	49	0	0	0
1	D	1193	18631	5979	9217	1600	1786	49	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1319	ALA	-	expression tag	UNP M5R382
A	1320	ALA	-	expression tag	UNP M5R382
A	1321	ALA	-	expression tag	UNP M5R382
A	1322	GLU	-	expression tag	UNP M5R382
A	1323	ASN	-	expression tag	UNP M5R382
A	1324	LEU	-	expression tag	UNP M5R382
A	1325	TYR	-	expression tag	UNP M5R382
A	1326	PHE	-	expression tag	UNP M5R382
A	1327	GLN	-	expression tag	UNP M5R382
B	1319	ALA	-	expression tag	UNP M5R382
B	1320	ALA	-	expression tag	UNP M5R382
B	1321	ALA	-	expression tag	UNP M5R382
B	1322	GLU	-	expression tag	UNP M5R382
B	1323	ASN	-	expression tag	UNP M5R382
B	1324	LEU	-	expression tag	UNP M5R382
B	1325	TYR	-	expression tag	UNP M5R382
B	1326	PHE	-	expression tag	UNP M5R382
B	1327	GLN	-	expression tag	UNP M5R382
C	1319	ALA	-	expression tag	UNP M5R382
C	1320	ALA	-	expression tag	UNP M5R382
C	1321	ALA	-	expression tag	UNP M5R382

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1322	GLU	-	expression tag	UNP M5R382
C	1323	ASN	-	expression tag	UNP M5R382
C	1324	LEU	-	expression tag	UNP M5R382
C	1325	TYR	-	expression tag	UNP M5R382
C	1326	PHE	-	expression tag	UNP M5R382
C	1327	GLN	-	expression tag	UNP M5R382
D	1319	ALA	-	expression tag	UNP M5R382
D	1320	ALA	-	expression tag	UNP M5R382
D	1321	ALA	-	expression tag	UNP M5R382
D	1322	GLU	-	expression tag	UNP M5R382
D	1323	ASN	-	expression tag	UNP M5R382
D	1324	LEU	-	expression tag	UNP M5R382
D	1325	TYR	-	expression tag	UNP M5R382
D	1326	PHE	-	expression tag	UNP M5R382
D	1327	GLN	-	expression tag	UNP M5R382

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	A	2	2	2	0	0
2	B	2	2	2	0	0
2	C	2	2	2	0	0
2	D	2	2	2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	D	1	1	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	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	141.66Å 143.66Å 431.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.11 – 3.40	Depositor
% Data completeness (in resolution range)	98.6 (49.11-3.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472, REFMAC 5.8.0158	Depositor
R, R_{free}	0.228 , 0.275	Depositor
Wilson B-factor (Å^2)	141.6	Xtriage
Anisotropy	0.390	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.037 for k,h,-l	Xtriage
Total number of atoms	74888	wwPDB-VP
Average B, all atoms (Å^2)	199.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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 (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)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 9 are 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 (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)

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

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

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

5.3 Carbohydrates (i)

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

5.4 Ligands (i)

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

5.5 Other polymers (i)

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