



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 10:09 AM GMT

PDB ID : 3DMY
Title : Crystal Structure of a predicated acyl-CoA synthetase from E.coli
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Deposited on : 2008-07-01
Resolution : 2.07 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

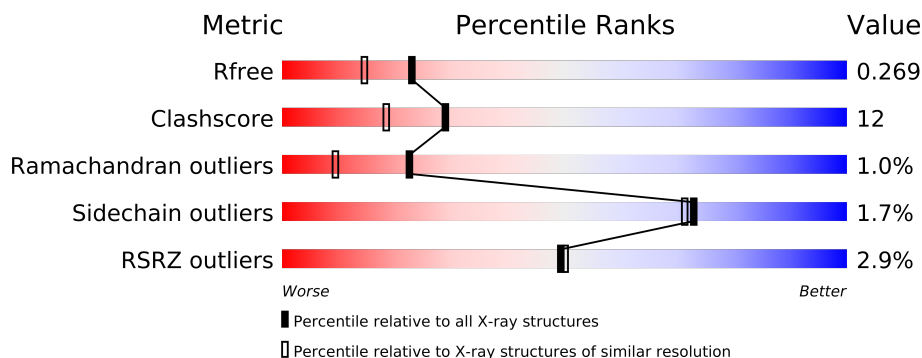
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.07 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1224 (2.08-2.04)
Clashscore	79885	1390 (2.08-2.04)
Ramachandran outliers	78287	1381 (2.08-2.04)
Sidechain outliers	78261	1381 (2.08-2.04)
RSRZ outliers	66119	1225 (2.08-2.04)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	480	
1	B	480	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6952 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Protein fdrA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	Se	0	0	0
			3299	2073	581	628	7	10			
1	B	446	Total	C	N	O	S	Se	0	0	0
			3291	2069	580	625	7	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	556	GLY	-	expression tag	UNP Q47208
A	557	HIS	-	expression tag	UNP Q47208
A	558	PRO	-	expression tag	UNP Q47208
A	559	HIS	-	expression tag	UNP Q47208
A	560	HIS	-	expression tag	UNP Q47208
A	561	HIS	-	expression tag	UNP Q47208
B	556	GLY	-	expression tag	UNP Q47208
B	557	HIS	-	expression tag	UNP Q47208
B	558	PRO	-	expression tag	UNP Q47208
B	559	HIS	-	expression tag	UNP Q47208
B	560	HIS	-	expression tag	UNP Q47208
B	561	HIS	-	expression tag	UNP Q47208

- Molecule 2 is water.

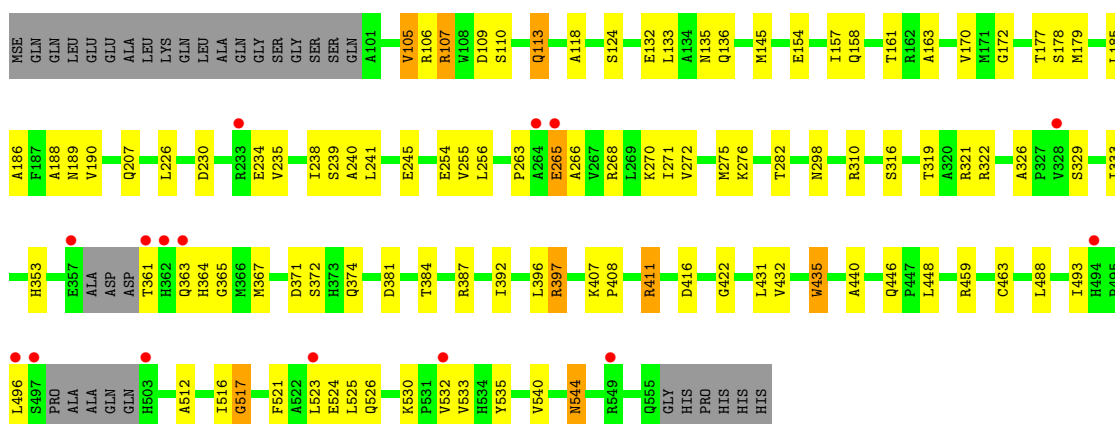
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	167	Total	O	0	0
			167	167		
2	B	195	Total	O	0	0
			195	195		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

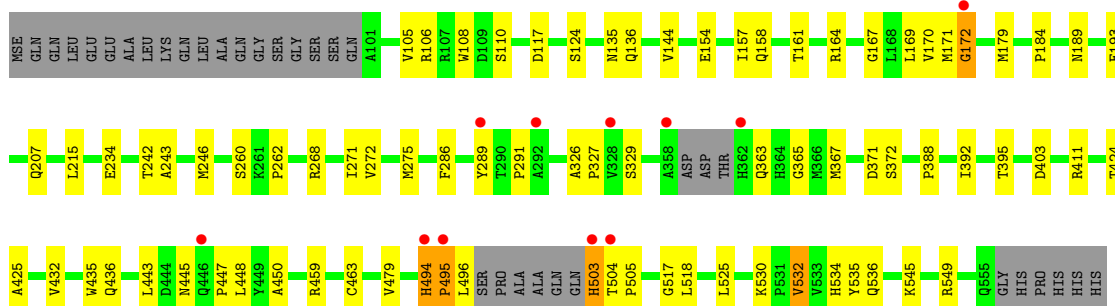
• Molecule 1: Protein fdrA

Chain A:



• Molecule 1: Protein fdrA

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.57Å 107.78Å 153.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.97 – 2.07 48.97 – 1.99	Depositor EDS
% Data completeness (in resolution range)	86.7 (48.97-2.07) 81.6 (48.97-1.99)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.66 (at 1.98Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.237 , 0.270 0.237 , 0.269	Depositor DCC
R_{free} test set	2826 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 29.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	4 of 66699 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6952	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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 lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.32	0/3339	0.62	0/4524
1	B	0.35	0/3331	0.65	0/4513
All	All	0.34	0/6670	0.63	0/9037

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3299	0	3356	88	0
1	B	3291	0	3349	78	0
2	A	167	0	0	14	0
2	B	195	0	0	14	0
All	All	6952	0	6705	165	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

The worst 5 of 165 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:169:LEU:HD22	1:B:246:MSE:HE1	1.41	1.02

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:243:ALA:HA	1:B:246:MSE:HE3	1.42	1.00
1:B:242:THR:HG22	1:B:246:MSE:HE2	1.46	0.95
1:B:108:TRP:HE1	1:B:136:GLN:HE21	1.18	0.92
1:A:263:PRO:HG2	1:A:268:ARG:HB3	1.51	0.91

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	441/480 (92%)	419 (95%)	18 (4%)	4 (1%)	25	11
1	B	440/480 (92%)	418 (95%)	17 (4%)	5 (1%)	21	8
All	All	881/960 (92%)	837 (95%)	35 (4%)	9 (1%)	22	9

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	GLY
1	B	172	GLY
1	B	495	PRO
1	A	265	GLU
1	A	517	GLY

5.3.2 Protein sidechains ⓘ

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	345/359 (96%)	336 (97%)	9 (3%)	59	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	343/359 (96%)	340 (99%)	3 (1%)	87	88
All	All	688/718 (96%)	676 (98%)	12 (2%)	73	71

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	411	ARG
1	A	435	TRP
1	B	503	HIS
1	A	397	ARG
1	A	544	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	526	GLN
1	B	113	GLN
1	B	398	ASN
1	A	536	GLN
1	A	544	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	447/480 (93%)	0.36	15 (3%) 43 43	18, 36, 59, 75	0
1	B	446/480 (92%)	0.25	11 (2%) 54 56	16, 31, 53, 74	0
All	All	893/960 (93%)	0.31	26 (2%) 49 50	16, 33, 58, 75	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	292	ALA	4.9
1	A	361	THR	4.7
1	B	172	GLY	4.4
1	A	496	LEU	4.0
1	A	328	VAL	3.9

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.