



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3G7S
Title : Crystal structure of a long-chain-fatty-acid-CoA ligase (FadD1) from Archaeoglobus fulgidus
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Deposited on : 2009-02-10
Resolution : 2.15 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

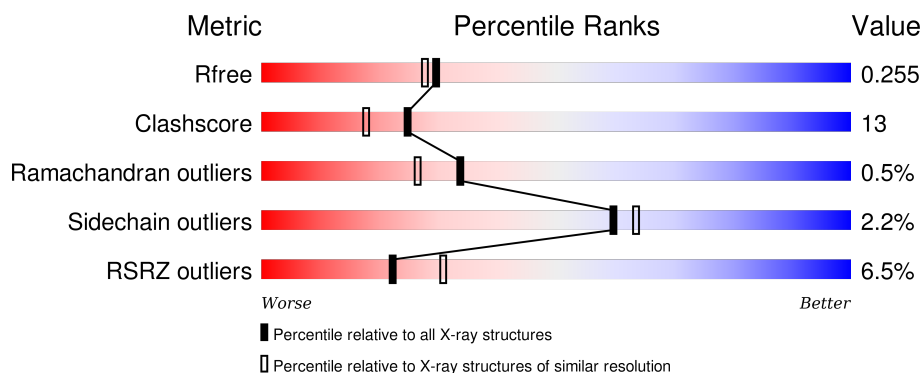
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	549	<div> <div>8%</div> <div>67%</div> <div>22%</div> <div>9%</div> </div>
1	B	549	<div> <div>4%</div> <div>66%</div> <div>22%</div> <div>10%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8080 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 Long-chain-fatty-acid--CoA ligase (FadD-1).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	Se	0	0	0
			3926	2524	641	737	6	18			
1	B	496	Total	C	N	O	S	Se	0	0	0
			3924	2526	641	732	6	19			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	EXPRESSION TAG	UNP O30147
A	0	SER	-	EXPRESSION TAG	UNP O30147
A	1	LEU	-	EXPRESSION TAG	UNP O30147
A	541	GLY	-	EXPRESSION TAG	UNP O30147
A	542	HIS	-	EXPRESSION TAG	UNP O30147
A	543	HIS	-	EXPRESSION TAG	UNP O30147
A	544	HIS	-	EXPRESSION TAG	UNP O30147
A	545	HIS	-	EXPRESSION TAG	UNP O30147
A	546	HIS	-	EXPRESSION TAG	UNP O30147
A	547	HIS	-	EXPRESSION TAG	UNP O30147
B	-1	MSE	-	EXPRESSION TAG	UNP O30147
B	0	SER	-	EXPRESSION TAG	UNP O30147
B	1	LEU	-	EXPRESSION TAG	UNP O30147
B	541	GLY	-	EXPRESSION TAG	UNP O30147
B	542	HIS	-	EXPRESSION TAG	UNP O30147
B	543	HIS	-	EXPRESSION TAG	UNP O30147
B	544	HIS	-	EXPRESSION TAG	UNP O30147
B	545	HIS	-	EXPRESSION TAG	UNP O30147
B	546	HIS	-	EXPRESSION TAG	UNP O30147
B	547	HIS	-	EXPRESSION TAG	UNP O30147

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	92	Total 92	O 92	0	0
2	B	138	Total 138	O 138	0	0

E504	S507	GLY	TYR	LYS	ARG	VAL	E513	E514	V515	E516	F517	L521	P522	ARG	THR	ALA	SER	GLY	LYS	LEU	LEU	ARG	ARG	LEU	LEU	ARG	GLU	LYS	GLU	ALA	GLU	GLY	HIS	HIS	HIS	HIS	HIS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.04Å 105.07Å 182.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.57 – 2.15 48.96 – 2.15	Depositor EDS
% Data completeness (in resolution range)	85.8 (45.57-2.15) 85.9 (48.96-2.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.16Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.256 0.222 , 0.255	Depositor DCC
R_{free} test set	2667 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	22.7	Xtriage
Anisotropy	0.846	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 55377 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8080	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.39	0/3998	0.63	1/5382 (0.0%)
1	B	0.42	0/3995	0.65	1/5376 (0.0%)
All	All	0.40	0/7993	0.64	2/10758 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	ASN	N-CA-C	-5.18	97.01	111.00
1	A	339	CYS	N-CA-C	5.09	124.75	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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	3926	0	3900	101	0
1	B	3924	0	3908	100	0
2	A	92	0	0	3	0
2	B	138	0	0	6	0
All	All	8080	0	7808	200	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 13.

The worst 5 of 200 close contacts within the same asymmetric unit are listed below, sorted by

their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:MSE:HE2	1:A:465:VAL:HG12	1.32	1.07
1:A:457:MSE:HE1	1:A:464:ASP:HA	1.31	1.07
1:A:457:MSE:HE1	1:A:464:ASP:CA	1.95	0.96
1:A:137:LYS:HB3	1:A:138:PRO:HD3	1.48	0.95
1:B:395:TYR:N	1:B:402:ASN:HD21	1.71	0.89

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 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	487/549 (89%)	462 (95%)	21 (4%)	4 (1%)	24	15
1	B	486/549 (88%)	470 (97%)	15 (3%)	1 (0%)	52	51
All	All	973/1098 (89%)	932 (96%)	36 (4%)	5 (0%)	34	26

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	VAL
1	A	339	CYS
1	B	339	CYS
1	A	460	GLU
1	A	188	GLY

5.3.2 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	430/453 (95%)	423 (98%)	7 (2%)	70	76
1	B	430/453 (95%)	418 (97%)	12 (3%)	51	52
All	All	860/906 (95%)	841 (98%)	19 (2%)	60	63

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	131	MSE
1	B	340	PRO
1	B	458	LYS
1	B	2	GLU
1	B	496	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	329	HIS
1	B	119	ASN
1	B	329	HIS
1	A	324	ASN
1	B	331	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	479/549 (87%)	0.52	42 (8%)	12 18	14, 33, 64, 77	0
1	B	477/549 (86%)	0.07	20 (4%)	40 50	13, 25, 61, 72	0
All	All	956/1098 (87%)	0.29	62 (6%)	22 31	13, 29, 63, 77	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	GLY	13.2
1	A	468	ILE	7.2
1	A	190	THR	6.9
1	B	517	PHE	6.3
1	B	521	LEU	5.7

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.