



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:44 AM UTC

PDB ID : 8IVI / pdb_00008ivi
Title : crystal structure of a medium-long chain fatty acyl-CoA ligase
Authors : Li, S.
Deposited on : 2023-03-27
Resolution : 2.29 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

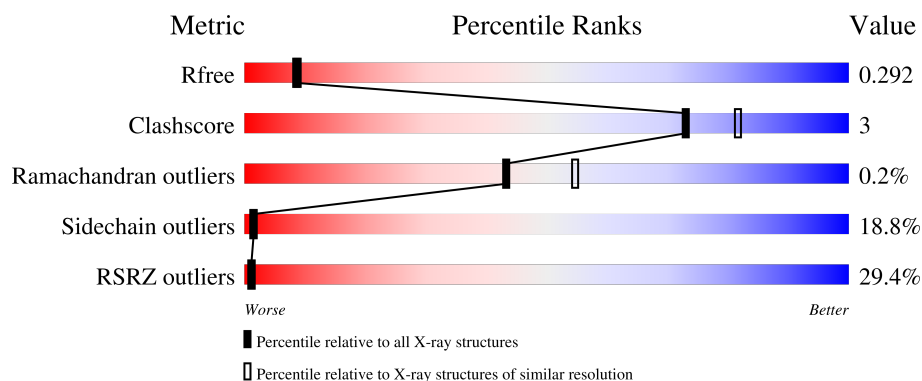
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	591	
1	B	591	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6266 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 Medium/long-chain-fatty-acid--CoA ligase FadD8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3144	2004	544	585	11			
1	B	408	Total	C	N	O	S	0	0	0
			3122	1994	540	577	11			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP O06417
A	-18	GLY	-	expression tag	UNP O06417
A	-17	SER	-	expression tag	UNP O06417
A	-16	SER	-	expression tag	UNP O06417
A	-15	HIS	-	expression tag	UNP O06417
A	-14	HIS	-	expression tag	UNP O06417
A	-13	HIS	-	expression tag	UNP O06417
A	-12	HIS	-	expression tag	UNP O06417
A	-11	HIS	-	expression tag	UNP O06417
A	-10	HIS	-	expression tag	UNP O06417
A	-9	SER	-	expression tag	UNP O06417
A	-8	SER	-	expression tag	UNP O06417
A	-7	GLY	-	expression tag	UNP O06417
A	-6	LEU	-	expression tag	UNP O06417
A	-5	VAL	-	expression tag	UNP O06417
A	-4	PRO	-	expression tag	UNP O06417
A	-3	ARG	-	expression tag	UNP O06417
A	-2	GLY	-	expression tag	UNP O06417
A	-1	SER	-	expression tag	UNP O06417
A	0	HIS	-	expression tag	UNP O06417
B	-19	MET	-	initiating methionine	UNP O06417
B	-18	GLY	-	expression tag	UNP O06417
B	-17	SER	-	expression tag	UNP O06417
B	-16	SER	-	expression tag	UNP O06417
B	-15	HIS	-	expression tag	UNP O06417

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP O06417
B	-13	HIS	-	expression tag	UNP O06417
B	-12	HIS	-	expression tag	UNP O06417
B	-11	HIS	-	expression tag	UNP O06417
B	-10	HIS	-	expression tag	UNP O06417
B	-9	SER	-	expression tag	UNP O06417
B	-8	SER	-	expression tag	UNP O06417
B	-7	GLY	-	expression tag	UNP O06417
B	-6	LEU	-	expression tag	UNP O06417
B	-5	VAL	-	expression tag	UNP O06417
B	-4	PRO	-	expression tag	UNP O06417
B	-3	ARG	-	expression tag	UNP O06417
B	-2	GLY	-	expression tag	UNP O06417
B	-1	SER	-	expression tag	UNP O06417
B	0	HIS	-	expression tag	UNP O06417

ALA	VAL	GLY
ALA	ARG	ASP
GLU	PRO	ALA
ILE	GLU	ALA
GLY	MET	THR
ALA	VAL	GLU
GLU	THR	ILE
GLN	GLY	ALA
ALA	ASN	VAL
VAL	PHE	LYS
LYS	GLN	ARG
GLN	LYS	GLY
SER	VAL	ASP
VAL	GLN	ALA
ALA	PRO	LYS
LYS	ARG	VAL
VAL	PRO	ALA
VAL	VAL	VAL
VAL	ASP	GLN
ASP	VAL	LEU
LEU	PRO	LEU
LEU	THR	GLY
GLY	LEU	GLY
GLY	LYS	GLY
PRO	ASP	LYS
LYS	ALA	VAL
VAL	ARG	ALA
ALA	ARG	PHE
TRP	VAL	TRP
GLU	LEU	GLY
ARG	ALA	GLY
ASN	ALA	ARG
ALA	Y449	
Y450	Y451	
V452	D453	
ALA	R454	
ILE	V455	
LYS		
ASP	D394	
MET	E395	
THR	H396	
VAL	G397	
THR	K398	
GLY	F399	
GLY	V400	
PHE	K401	
ALA	Q402	
ASN	G403	
VAL	E404	
LYS	V405	
GLN	G406	
ARG	E407	
LYS	T408	
GLY	C409	
SER	V410	
VAL	L414	
GLN	L415	
ALA	A416	
PRO	G417	
LYS	G418	
ARG	Y419	
VAL	W420	
VAL	M421	
VAL	L422	
ASP	P423	
SER	D424	
LEU	CYS	
PRO	VAL	
LEU	T426	
THR	S427	
GLY	R428	
LEU	T429	
GLY	F430	
LYS	K431	
PRO	D432	
ASP	G433	
LYS	L435	
LYS	H436	
ALA	D439	
VAL	L440	
ARG	A441	
ALA	R442	
ARG	VAL	
PHE	TRP	
TRP	VAL	
GLU	D444	
LEU	S445	
ARG	D446	
ALA	G447	
GLY	ASN	
ARG	F448	
L386	F387	
A388	R389	
V390	A391	
D392	L392	
L393	D394	
E395	H396	
G397	K398	
F399	V400	
K401	Q402	
G403	E404	
V405	G406	
E407	T408	
C409	V410	
L414	L415	
A416	G417	
G418	Y419	
W420	M421	
L422	P423	
D424	CYS	
VAL	T426	
S427	R428	
T429	F430	
K431	D432	
G433	L435	
H436	D439	
L440	A441	
R442	VAL	
E443	TRP	
D444	S445	
D446	G447	
ASN	F448	
I242	W247	
P250	F253	
M257	C258	
T259	P260	
L261	S262	
H263	A264	
G265	A266	
A267	F268	
E278	M279	
I280	V281	
L282	A283	
K284	A288	
E289	V290	
L291	R292	
I293	I294	
I299	T300	
A301	T302	
M303	L304	
V305	P306	
S307	M308	
L309	L312	
L313	D314	
H315	P316	
D317	S318	
H319	T320	
R321		
P322	S324	
S325	L326	
E327	T328	
V329	Y330	
G332	G333	
A334	S335	
A336	I337	
P338	V339	
R340	L341	
A344	I345	
R346	R347	
F348	G349	
P350	I351	
F352	A353	
Q354	T355	
G357	S358	
E360	A361	
P362	M363	
V364	I365	
T366	V367	
L368	D372	
H373	D374	
E375	R376	
R377	L378	
T379	S380	
C381	G382	
R383		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.23Å 105.00Å 135.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.50 – 2.29 52.50 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.3 (52.50-2.29) 92.4 (52.50-2.29)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.247 , 0.275 0.283 , 0.292	Depositor DCC
R_{free} test set	2000 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	60.9	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6266	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.50	1/3215 (0.0%)	0.85	9/4378 (0.2%)
1	B	0.48	0/3193	0.88	3/4348 (0.1%)
All	All	0.49	1/6408 (0.0%)	0.86	12/8726 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	412	GLY	C-N	5.74	1.38	1.33

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	433	GLY	N-CA-C	-8.29	104.43	115.21
1	A	363	MET	N-CA-C	8.21	128.28	110.80
1	B	152	ASP	N-CA-C	-7.70	99.95	109.65
1	A	152	ASP	N-CA-C	-7.69	99.96	109.65
1	A	359	SER	N-CA-C	-6.99	104.56	113.23

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	3144	0	3156	17	0
1	B	3122	0	3140	24	0
All	All	6266	0	6296	40	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 3.

The worst 5 of 40 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:194:GLU:OE2	1:A:197:LYS:NZ	2.26	0.68
1:B:68:PHE:HB2	1:B:280:ILE:HA	1.79	0.64
1:B:305:VAL:HG22	1:B:308:MET:HG3	1.84	0.60
1:B:419:TYR:H	1:B:426:THR:HG22	1.67	0.58
1:A:65:PRO:HA	1:A:75:THR:HA	1.88	0.56

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	407/591 (69%)	395 (97%)	11 (3%)	1 (0%)	43	55
1	B	404/591 (68%)	369 (91%)	34 (8%)	1 (0%)	43	55
All	All	811/1182 (69%)	764 (94%)	45 (6%)	2 (0%)	43	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	363	MET
1	B	362	PRO

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	332/466 (71%)	277 (83%)	55 (17%)	2	2
1	B	329/466 (71%)	260 (79%)	69 (21%)	1	1
All	All	661/932 (71%)	537 (81%)	124 (19%)	1	1

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	54	LEU
1	B	394	ASP
1	B	159	GLU
1	B	386	LEU
1	B	422	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	HIS
1	A	358	GLN
1	B	421	ASN
1	B	172	GLN
1	B	358	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	411/591 (69%)	1.29	67 (16%) 4 5	48, 65, 84, 109	0
1	B	408/591 (69%)	1.91	174 (42%) 0 0	58, 81, 114, 127	0
All	All	819/1182 (69%)	1.60	241 (29%) 1 1	48, 72, 106, 127	0

The worst 5 of 241 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	335	ALA	6.4
1	A	69	LEU	4.8
1	B	377	ARG	4.6
1	B	348	PHE	4.4
1	B	430	PHE	4.4

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 oligosaccharides 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.