



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 5, 2024 – 06:09 PM JST

PDB ID : 8IVI
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 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 ⓘ 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 : 4.02b-467
Xtrriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

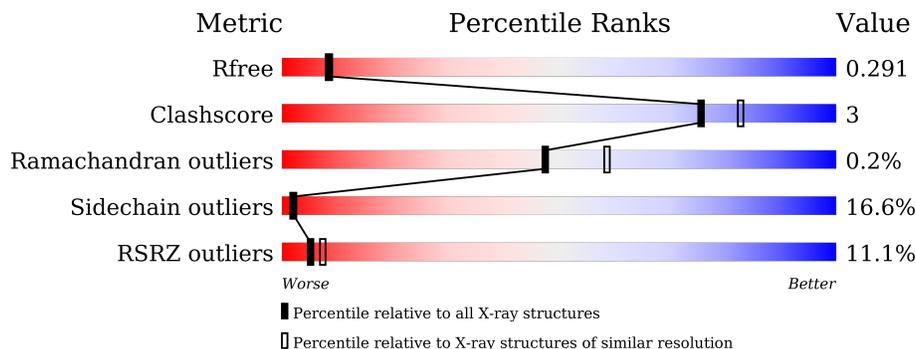
1 Overall quality at a glance

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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	 3% 57% 12% 30%
1	B	591	 13% 54% 13% 31%

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	411	3144	2004	544	585	11	0	0	0
1	B	408	3122	1994	540	577	11	0	0	0

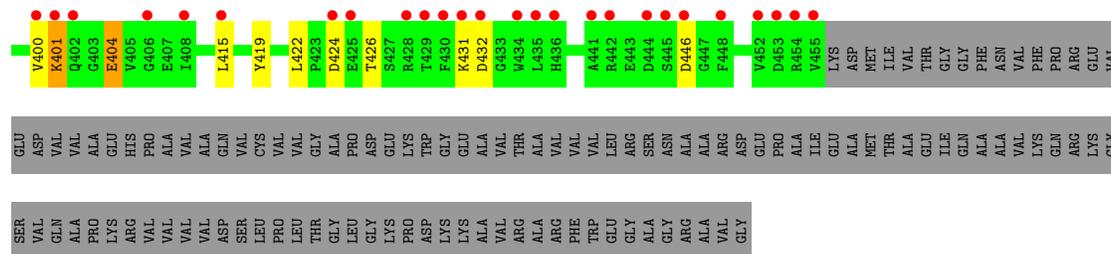
There are 40 discrepancies between the modelled and reference sequences:

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



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 59.50 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.3 (52.50-2.29) 92.4 (59.50-2.29)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.29Å)	Xtrriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.247 , 0.275 0.281 , 0.291	Depositor DCC
R_{free} test set	1987 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	60.9	Xtrriage
Anisotropy	0.383	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6266	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtrriage'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	0.32	0/3215	0.54	1/4378 (0.0%)
1	B	0.31	0/3193	0.54	0/4348
All	All	0.32	0/6408	0.54	1/8726 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	363	MET	N-CA-C	6.40	128.28	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	3144	0	3156	16	0
1	B	3122	0	3140	24	0
All	All	6266	0	6296	39	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.

All (39) 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
1:B:68:PHE:HE1	1:B:278:GLU:HB2	1.70	0.54
1:A:61:HIS:HB3	1:A:64:LYS:HB3	1.92	0.52
1:A:386:LEU:HD22	1:B:56:GLY:HA3	1.93	0.51
1:A:213:VAL:HG13	1:A:230:ILE:HG23	1.92	0.51
1:A:306:PRO:HG3	1:A:335:ALA:HB1	1.94	0.49
1:A:401:LYS:HB2	1:A:401:LYS:HE2	1.56	0.49
1:B:141:LEU:HD22	1:B:146:ILE:HG13	1.94	0.49
1:B:213:VAL:HG13	1:B:230:ILE:HG23	1.95	0.49
1:B:69:LEU:HD22	1:B:109:PRO:HD3	1.96	0.48
1:B:225:LYS:HB2	1:B:225:LYS:HE3	1.30	0.46
1:B:208:LEU:HD22	1:B:212:GLN:HG2	1.98	0.45
1:A:328:THR:HG23	1:A:370:LYS:HD3	1.98	0.45
1:B:376:LYS:H	1:B:376:LYS:HG3	1.45	0.45
1:A:390:VAL:HG22	1:A:410:VAL:HG13	1.97	0.45
1:B:294:ILE:HA	1:B:299:ILE:HB	1.99	0.45
1:B:174:ILE:HB	1:B:188:ALA:HB2	1.99	0.44
1:B:171:LEU:HD23	1:B:171:LEU:HA	1.89	0.44
1:A:313:LEU:HD11	1:A:344:ALA:HB2	1.98	0.44
1:B:104:LEU:HB3	1:B:151:ILE:HG22	2.00	0.43
1:A:104:LEU:HB3	1:A:151:ILE:HG22	1.99	0.43
1:B:101:VAL:HG21	1:B:125:ARG:HH21	1.84	0.43
1:A:298:ARG:HD3	1:A:325:SER:HB3	2.00	0.42
1:B:340:ARG:HE	1:B:340:ARG:HB3	1.43	0.42
1:B:401:LYS:HE2	1:B:401:LYS:HB2	1.77	0.42
1:B:211:ASP:HA	1:B:232:THR:HB	2.02	0.42
1:A:275:LYS:HB3	1:A:275:LYS:HE3	1.59	0.42
1:B:354:GLN:HB3	1:B:368:LEU:HB2	2.01	0.42
1:A:171:LEU:HD12	1:A:171:LEU:HA	1.90	0.42
1:A:410:VAL:HB	1:A:415:LEU:HD11	2.01	0.42
1:B:79:LEU:HD12	1:B:79:LEU:HA	1.83	0.41
1:A:337:ASN:HA	1:A:338:PRO:HD2	1.95	0.41
1:B:141:LEU:HB2	1:B:168:VAL:HG21	2.02	0.41
1:B:400:VAL:HB	1:B:404:GLU:HB3	2.03	0.41
1:B:341:LEU:HB3	1:B:378:LEU:HD22	2.03	0.40

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%)	47	58
1	B	404/591 (68%)	369 (91%)	34 (8%)	1 (0%)	47	58
All	All	811/1182 (69%)	764 (94%)	45 (6%)	2 (0%)	47	58

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%)	282 (85%)	50 (15%)	3	2
1	B	329/466 (71%)	269 (82%)	60 (18%)	1	1
All	All	661/932 (71%)	551 (83%)	110 (17%)	2	2

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ARG
1	A	50	ASN
1	A	54	LEU
1	A	59	LYS

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Mol	Chain	Res	Type
1	A	69	LEU
1	A	72	THR
1	A	73	ARG
1	A	74	LEU
1	A	82	ARG
1	A	84	SER
1	A	110	GLU
1	A	125	ARG
1	A	131	LEU
1	A	133	SER
1	A	147	SER
1	A	148	SER
1	A	159	GLU
1	A	167	GLN
1	A	169	ASP
1	A	177	ILE
1	A	185	LYS
1	A	187	VAL
1	A	189	VAL
1	A	199	GLN
1	A	201	GLN
1	A	204	VAL
1	A	211	ASP
1	A	217	THR
1	A	222	THR
1	A	227	LYS
1	A	232	THR
1	A	254	ARG
1	A	258	CYS
1	A	259	THR
1	A	284	LYS
1	A	289	GLU
1	A	292	ARG
1	A	307	SER
1	A	309	LEU
1	A	336	ILE
1	A	359	SER
1	A	373	HIS
1	A	377	ARG
1	A	395	GLU
1	A	401	LYS
1	A	410	VAL

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Mol	Chain	Res	Type
1	A	428	ARG
1	A	431	LYS
1	A	453	ASP
1	A	456	LYS
1	B	46	SER
1	B	54	LEU
1	B	59	LYS
1	B	66	VAL
1	B	72	THR
1	B	84	SER
1	B	101	VAL
1	B	125	ARG
1	B	131	LEU
1	B	133	SER
1	B	134	LEU
1	B	147	SER
1	B	156	MET
1	B	159	GLU
1	B	166	GLU
1	B	167	GLN
1	B	171	LEU
1	B	173	GLN
1	B	182	ASP
1	B	189	VAL
1	B	194	GLU
1	B	197	LYS
1	B	204	VAL
1	B	207	ASP
1	B	217	THR
1	B	225	LYS
1	B	227	LYS
1	B	229	VAL
1	B	258	CYS
1	B	259	THR
1	B	278	GLU
1	B	280	ILE
1	B	281	VAL
1	B	282	LEU
1	B	284	LYS
1	B	291	LEU
1	B	292	ARG
1	B	293	ILE

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Mol	Chain	Res	Type
1	B	298	ARG
1	B	307	SER
1	B	334	SER
1	B	340	ARG
1	B	341	LEU
1	B	358	GLN
1	B	360	GLU
1	B	368	LEU
1	B	375	GLU
1	B	376	LYS
1	B	379	THR
1	B	386	LEU
1	B	394	ASP
1	B	396	HIS
1	B	401	LYS
1	B	404	GLU
1	B	415	LEU
1	B	422	LEU
1	B	424	ASP
1	B	431	LYS
1	B	432	ASP
1	B	446	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	119	GLN
1	B	358	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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

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	411/591 (69%)	0.55	15 (3%) 42 49	48, 65, 84, 109	0
1	B	408/591 (69%)	1.17	76 (18%) 1 1	58, 81, 114, 127	0
All	All	819/1182 (69%)	0.86	91 (11%) 5 7	48, 72, 106, 127	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	377	ARG	6.6
1	B	333	ALA	6.2
1	B	334	SER	6.1
1	B	43	LEU	5.2
1	B	348	PHE	4.8
1	B	431	LYS	4.8
1	B	394	ASP	4.7
1	B	323	LEU	4.7
1	B	434	TRP	4.5
1	B	430	PHE	4.4
1	A	45	ARG	4.4
1	B	393	LEU	4.2
1	B	402	GLN	4.2
1	B	335	ALA	4.1
1	B	322	ASP	4.0
1	B	452	VAL	3.9
1	B	396	HIS	3.9
1	B	316	PRO	3.8
1	B	455	VAL	3.5
1	B	184	LEU	3.5
1	B	293	ILE	3.5
1	B	415	LEU	3.4
1	B	436	HIS	3.4
1	A	69	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	223	THR	3.4
1	B	401	LYS	3.4
1	B	442	ARG	3.3
1	B	428	ARG	3.3
1	B	292	ARG	3.3
1	B	445	SER	3.2
1	B	406	GLY	3.2
1	B	400	VAL	3.1
1	B	185	LYS	3.1
1	B	346	ARG	3.1
1	B	131	LEU	3.0
1	B	302	THR	3.0
1	A	298	ARG	3.0
1	B	326	LEU	2.9
1	B	224	GLY	2.9
1	B	149	LEU	2.8
1	B	304	LEU	2.8
1	B	446	ASP	2.8
1	B	67	LEU	2.8
1	B	432	ASP	2.8
1	B	312	LEU	2.8
1	A	289	GLU	2.7
1	B	425	GLU	2.7
1	A	304	LEU	2.7
1	B	378	LEU	2.7
1	B	186	HIS	2.7
1	B	172	GLN	2.7
1	B	448	PHE	2.7
1	B	363	MET	2.6
1	A	457	ASP	2.6
1	B	397	GLY	2.6
1	A	46	SER	2.6
1	B	256	LEU	2.5
1	B	168	VAL	2.5
1	B	356	TYR	2.5
1	A	59	LYS	2.5
1	A	309	LEU	2.5
1	B	374	ASP	2.4
1	A	93	LEU	2.4
1	B	362	PRO	2.4
1	B	444	ASP	2.4
1	B	280	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	328	THR	2.3
1	B	454	ARG	2.3
1	B	282	LEU	2.3
1	B	288	ALA	2.3
1	B	294	ILE	2.3
1	B	408	ILE	2.3
1	B	101	VAL	2.2
1	A	199	GLN	2.2
1	B	395	GLU	2.2
1	B	73	ARG	2.2
1	B	441	ALA	2.2
1	B	103	LEU	2.2
1	A	455	VAL	2.2
1	B	435	LEU	2.2
1	B	429	THR	2.1
1	B	341	LEU	2.1
1	B	226	PRO	2.1
1	B	453	ASP	2.1
1	B	360	GLU	2.1
1	A	203	LEU	2.1
1	B	206	ALA	2.1
1	A	177	ILE	2.1
1	B	68	PHE	2.0
1	B	134	LEU	2.0
1	B	424	ASP	2.0

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 monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.