



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 11:28 AM BST

PDB ID : 6LFC
Title : E. coli Thioesterase I mutant DG
Authors : Deng, X.; Chen, L.; Yang, G.
Deposited on : 2019-12-01
Resolution : 2.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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)	:	2.13.1

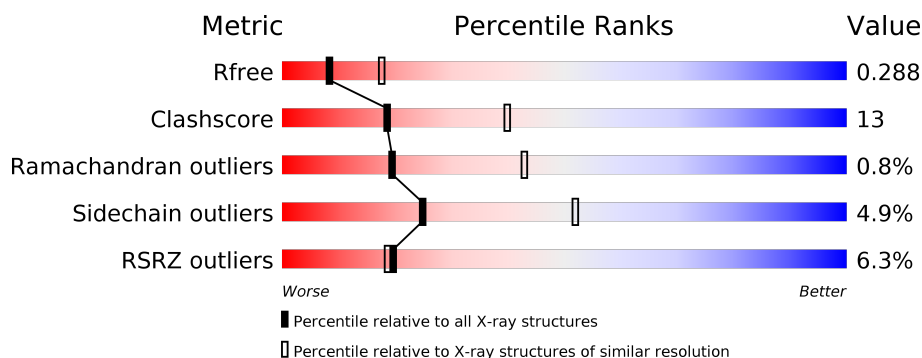
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 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	182	<div> <div>8%</div> <div> <div></div> <div>72%</div> <div>22%</div> <div>• •</div> </div> </div>
1	B	182	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>16%</div> <div>• •</div> </div> </div>
1	C	182	<div> <div>7%</div> <div> <div></div> <div>77%</div> <div>16%</div> <div>• •</div> </div> </div>
1	D	182	<div> <div>7%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>• • •</div> </div> </div>
1	E	182	<div> <div>8%</div> <div> <div></div> <div>67%</div> <div>26%</div> <div>• •</div> </div> </div>
1	F	182	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>• •</div> </div> </div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 8315 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 Acyl-CoA thioesterase I also functions as protease I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	0	0
			1382	883	242	253	4			
1	B	174	Total	C	N	O	S	0	0	0
			1376	880	241	251	4			
1	C	174	Total	C	N	O	S	0	0	0
			1376	880	241	251	4			
1	D	176	Total	C	N	O	S	0	0	0
			1391	888	244	255	4			
1	E	176	Total	C	N	O	S	0	0	0
			1391	888	244	255	4			
1	F	174	Total	C	N	O	S	0	0	0
			1376	880	241	251	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP J7QCR7
A	141	LEU	MET	conflict	UNP J7QCR7
A	142	ASP	GLU	engineered mutation	UNP J7QCR7
A	145	GLY	TYR	engineered mutation	UNP J7QCR7
B	1	MET	-	expression tag	UNP J7QCR7
B	141	LEU	MET	conflict	UNP J7QCR7
B	142	ASP	GLU	engineered mutation	UNP J7QCR7
B	145	GLY	TYR	engineered mutation	UNP J7QCR7
C	1	MET	-	expression tag	UNP J7QCR7
C	141	LEU	MET	conflict	UNP J7QCR7
C	142	ASP	GLU	engineered mutation	UNP J7QCR7
C	145	GLY	TYR	engineered mutation	UNP J7QCR7
D	1	MET	-	expression tag	UNP J7QCR7
D	141	LEU	MET	conflict	UNP J7QCR7
D	142	ASP	GLU	engineered mutation	UNP J7QCR7
D	145	GLY	TYR	engineered mutation	UNP J7QCR7
E	1	MET	-	expression tag	UNP J7QCR7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	141	LEU	MET	conflict	UNP J7QCR7
E	142	ASP	GLU	engineered mutation	UNP J7QCR7
E	145	GLY	TYR	engineered mutation	UNP J7QCR7
F	1	MET	-	expression tag	UNP J7QCR7
F	141	LEU	MET	conflict	UNP J7QCR7
F	142	ASP	GLU	engineered mutation	UNP J7QCR7
F	145	GLY	TYR	engineered mutation	UNP J7QCR7

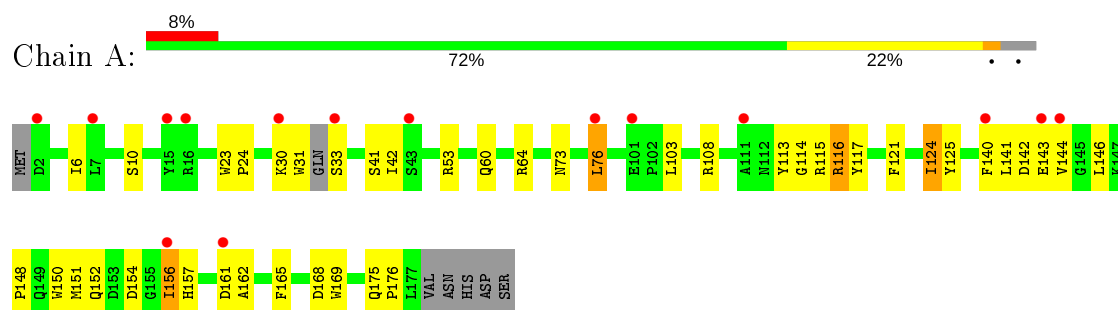
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total O 4 4	0	0
2	B	6	Total O 6 6	0	0
2	C	3	Total O 3 3	0	0
2	D	3	Total O 3 3	0	0
2	E	3	Total O 3 3	0	0
2	F	4	Total O 4 4	0	0

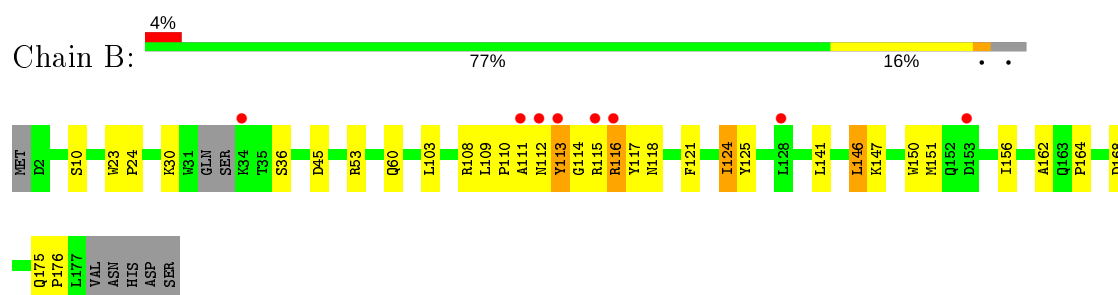
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

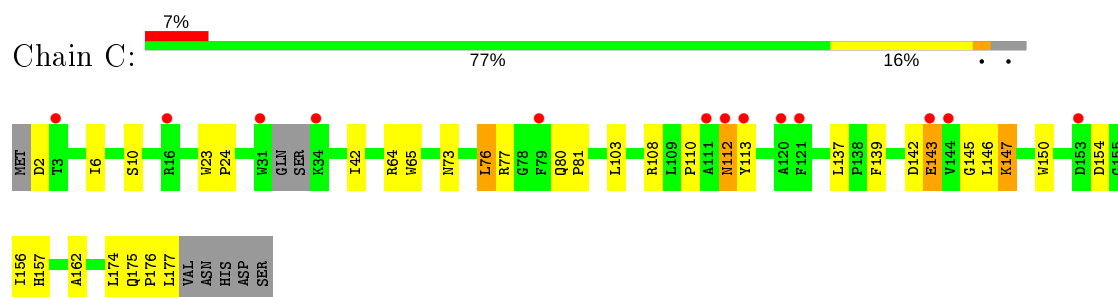
- Molecule 1: Acyl-CoA thioesterase I also functions as protease I



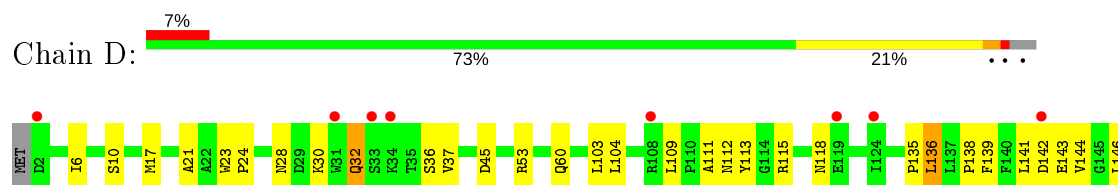
- Molecule 1: Acyl-CoA thioesterase I also functions as protease I

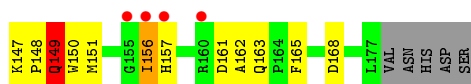


- Molecule 1: Acyl-CoA thioesterase I also functions as protease I

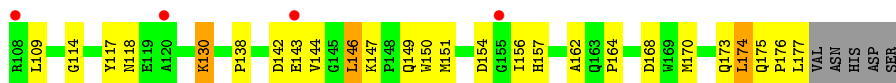
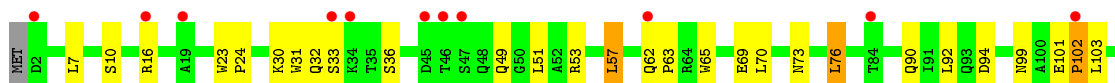


- Molecule 1: Acyl-CoA thioesterase I also functions as protease I

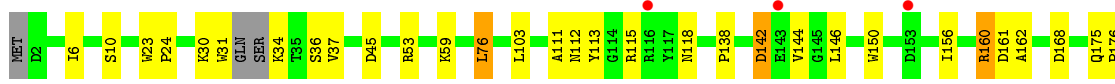
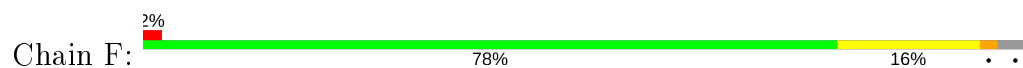




- Molecule 1: Acyl-CoA thioesterase I also functions as protease I



- Molecule 1: Acyl-CoA thioesterase I also functions as protease I



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.93 Å 118.23 Å 121.29 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.00 – 2.70 63.13 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (63.00-2.70) 99.9 (63.13-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.69 Å)	Xtriage
Refinement program	REFMAC v1.0	Depositor
R, R_{free}	0.227 , 0.261 0.266 , 0.288	Depositor DCC
R_{free} test set	969 reflections (3.23%)	wwPDB-VP
Wilson B-factor (Å ²)	73.1	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8315	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.17% 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	0.44	0/1415	0.69	0/1923
1	B	0.41	0/1409	0.68	1/1915 (0.1%)
1	C	0.51	1/1409 (0.1%)	0.70	0/1915
1	D	0.50	1/1425 (0.1%)	0.71	1/1938 (0.1%)
1	E	0.63	3/1425 (0.2%)	0.72	1/1938 (0.1%)
1	F	0.42	0/1409	0.67	0/1915
All	All	0.49	5/8492 (0.1%)	0.70	3/11544 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	102	PRO	N-CA	13.41	1.70	1.47
1	C	147	LYS	C-N	8.53	1.50	1.34
1	D	157	HIS	C-N	8.37	1.50	1.34
1	E	101	GLU	C-N	5.82	1.45	1.34
1	E	16	ARG	CZ-NH2	-5.60	1.25	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	102	PRO	CA-N-CD	-8.36	99.80	111.50
1	D	135	PRO	N-CA-C	7.78	132.33	112.10
1	B	113	TYR	CB-CA-C	-5.08	100.24	110.40

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	1382	0	1377	50	0
1	B	1376	0	1372	45	0
1	C	1376	0	1372	30	0
1	D	1391	0	1386	46	0
1	E	1391	0	1386	51	0
1	F	1376	0	1372	26	0
2	A	4	0	0	0	0
2	B	6	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	4	0	0	0	0
All	All	8315	0	8265	219	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 219 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:E:102:PRO:CA	1:E:102:PRO:N	1.70	1.44
1:D:146:LEU:CD1	1:D:151:MET:HE3	1.62	1.29
1:D:146:LEU:HD11	1:D:151:MET:CE	1.65	1.27
1:A:141:LEU:CD2	1:A:169:TRP:CG	2.30	1.14
1:A:141:LEU:HD23	1:A:169:TRP:CG	1.80	1.13

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	171/182 (94%)	165 (96%)	5 (3%)	1 (1%)	25	50
1	B	170/182 (93%)	165 (97%)	5 (3%)	0	100	100
1	C	170/182 (93%)	163 (96%)	6 (4%)	1 (1%)	25	50
1	D	174/182 (96%)	165 (95%)	5 (3%)	4 (2%)	6	16
1	E	174/182 (96%)	162 (93%)	11 (6%)	1 (1%)	25	50
1	F	170/182 (93%)	160 (94%)	9 (5%)	1 (1%)	25	50
All	All	1029/1092 (94%)	980 (95%)	41 (4%)	8 (1%)	19	43

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	32	GLN
1	F	142	ASP
1	A	140	PHE
1	C	143	GLU
1	D	32	GLN

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	146/153 (95%)	138 (94%)	8 (6%)	21	46
1	B	145/153 (95%)	139 (96%)	6 (4%)	30	59
1	C	145/153 (95%)	139 (96%)	6 (4%)	30	59
1	D	147/153 (96%)	141 (96%)	6 (4%)	30	59
1	E	147/153 (96%)	138 (94%)	9 (6%)	18	41
1	F	145/153 (95%)	137 (94%)	8 (6%)	21	46
All	All	875/918 (95%)	832 (95%)	43 (5%)	25	52

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	143	GLU

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Mol	Chain	Res	Type
1	D	149	GLN
1	F	103	LEU
1	D	10	SER
1	D	36	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	157	HIS
1	D	60	GLN
1	F	62	GLN
1	C	90	GLN
1	C	112	ASN

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 [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	175/182 (96%)	0.56	15 (8%) 10 8	36, 56, 73, 90	0
1	B	174/182 (95%)	0.49	8 (4%) 32 31	39, 57, 74, 91	0
1	C	174/182 (95%)	0.59	13 (7%) 14 12	30, 56, 80, 99	0
1	D	176/182 (96%)	0.45	12 (6%) 17 15	40, 57, 77, 96	0
1	E	176/182 (96%)	0.62	15 (8%) 10 9	40, 59, 75, 88	0
1	F	174/182 (95%)	0.41	3 (1%) 70 72	45, 58, 74, 86	0
All	All	1049/1092 (96%)	0.52	66 (6%) 20 19	30, 57, 76, 99	0

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	112	ASN	8.5
1	B	116	ARG	6.6
1	D	156	ILE	5.8
1	E	34	LYS	5.5
1	C	111	ALA	5.4

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 monosaccharides 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.