



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2023 – 12:58 PM EDT

PDB ID : 2QQ2  
Title : Crystal structure of C-terminal domain of Human acyl-CoA thioesterase 7  
Authors : Busam, R.; Lehtio, L.; Arrowsmith, C.H.; Berglund, H.; Collins, R.; Dahlgren, L.G.; Herman, M.D.; Edwards, A.; Flodin, S.; Flores, A.; Graslund, S.; Hammarstrom, M.; Hallberg, B.M.; Holmberg-Schiavone, L.; Johansson, I.; Kallas, A.; Karlberg, T.; Kotenyova, T.; Moche, M.; Nordlund, P.; Nyman, T.; Sagemark, J.; Stenmark, P.; Sundstrom, M.; Thorsell, A.G.; Tresaugues, L.; van den Berg, S.; Weigelt, J.; Welin, M.; Persson, C.; Structural Genomics Consortium (SGC)  
Deposited on : 2007-07-26  
Resolution : 2.80 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](mailto: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>.

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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 : 2.35  
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)

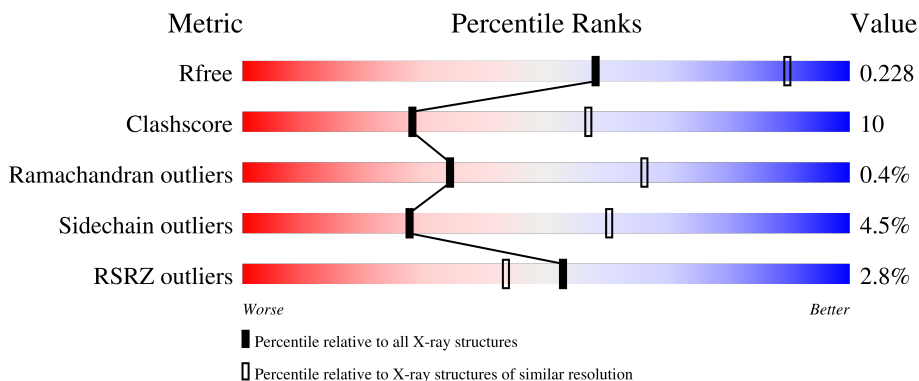
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	193	 4% 61% 18% 19%
1	B	193	 4% 60% 19% 19%
1	C	193	 4% 65% 13% 19%

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
 Validation Pipeline (wwPDB-VP) : 2.35

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Mol	Chain	Length	Quality of chain
1	D	193	<p>3% 64% 15% 21%</p>
1	E	193	<p>2% 62% 12% 22%</p>
1	F	193	<p>2% 63% 13% 23%</p>
1	G	193	<p>2% 63% 12% 23%</p>
1	H	193	<p>3% 63% 14% 21%</p>
1	I	193	<p>6% 65% 13% 20%</p>
1	J	193	<p>2% 63% 11% 26%</p>
1	K	193	<p>2% 63% 16% 19%</p>
1	L	193	<p>2% 64% 14% 20%</p>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14037 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 Cytosolic acyl coenzyme A thioester hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	156	1188	745	210	225	8	0	0	0
1	B	156	1199	749	212	230	8	0	0	0
1	C	157	1199	751	214	226	8	0	0	0
1	D	153	1169	733	203	225	8	0	0	0
1	E	150	1147	718	202	219	8	0	0	0
1	F	149	1143	717	201	217	8	0	0	0
1	G	148	1128	709	196	215	8	0	0	0
1	H	153	1175	736	208	223	8	0	0	0
1	I	154	1187	743	208	228	8	0	0	0
1	J	143	1102	692	193	209	8	0	0	0
1	K	156	1207	754	214	231	8	0	0	0
1	L	154	1193	745	214	226	8	0	0	0

There are 276 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	176	MET	-	expression tag	UNP O00154
A	177	HIS	-	expression tag	UNP O00154
A	178	HIS	-	expression tag	UNP O00154
A	179	HIS	-	expression tag	UNP O00154
A	180	HIS	-	expression tag	UNP O00154

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Chain	Residue	Modelled	Actual	Comment	Reference
A	181	HIS	-	expression tag	UNP O00154
A	182	HIS	-	expression tag	UNP O00154
A	183	SER	-	expression tag	UNP O00154
A	184	SER	-	expression tag	UNP O00154
A	185	GLY	-	expression tag	UNP O00154
A	186	VAL	-	expression tag	UNP O00154
A	187	ASP	-	expression tag	UNP O00154
A	188	LEU	-	expression tag	UNP O00154
A	189	GLY	-	expression tag	UNP O00154
A	190	THR	-	expression tag	UNP O00154
A	191	GLU	-	expression tag	UNP O00154
A	192	ASN	-	expression tag	UNP O00154
A	193	LEU	-	expression tag	UNP O00154
A	194	TYR	-	expression tag	UNP O00154
A	195	PHE	-	expression tag	UNP O00154
A	196	GLN	-	expression tag	UNP O00154
A	197	SER	-	expression tag	UNP O00154
A	198	MET	-	expression tag	UNP O00154
B	176	MET	-	expression tag	UNP O00154
B	177	HIS	-	expression tag	UNP O00154
B	178	HIS	-	expression tag	UNP O00154
B	179	HIS	-	expression tag	UNP O00154
B	180	HIS	-	expression tag	UNP O00154
B	181	HIS	-	expression tag	UNP O00154
B	182	HIS	-	expression tag	UNP O00154
B	183	SER	-	expression tag	UNP O00154
B	184	SER	-	expression tag	UNP O00154
B	185	GLY	-	expression tag	UNP O00154
B	186	VAL	-	expression tag	UNP O00154
B	187	ASP	-	expression tag	UNP O00154
B	188	LEU	-	expression tag	UNP O00154
B	189	GLY	-	expression tag	UNP O00154
B	190	THR	-	expression tag	UNP O00154
B	191	GLU	-	expression tag	UNP O00154
B	192	ASN	-	expression tag	UNP O00154
B	193	LEU	-	expression tag	UNP O00154
B	194	TYR	-	expression tag	UNP O00154
B	195	PHE	-	expression tag	UNP O00154
B	196	GLN	-	expression tag	UNP O00154
B	197	SER	-	expression tag	UNP O00154
B	198	MET	-	expression tag	UNP O00154
C	176	MET	-	expression tag	UNP O00154

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Chain	Residue	Modelled	Actual	Comment	Reference
C	177	HIS	-	expression tag	UNP O00154
C	178	HIS	-	expression tag	UNP O00154
C	179	HIS	-	expression tag	UNP O00154
C	180	HIS	-	expression tag	UNP O00154
C	181	HIS	-	expression tag	UNP O00154
C	182	HIS	-	expression tag	UNP O00154
C	183	SER	-	expression tag	UNP O00154
C	184	SER	-	expression tag	UNP O00154
C	185	GLY	-	expression tag	UNP O00154
C	186	VAL	-	expression tag	UNP O00154
C	187	ASP	-	expression tag	UNP O00154
C	188	LEU	-	expression tag	UNP O00154
C	189	GLY	-	expression tag	UNP O00154
C	190	THR	-	expression tag	UNP O00154
C	191	GLU	-	expression tag	UNP O00154
C	192	ASN	-	expression tag	UNP O00154
C	193	LEU	-	expression tag	UNP O00154
C	194	TYR	-	expression tag	UNP O00154
C	195	PHE	-	expression tag	UNP O00154
C	196	GLN	-	expression tag	UNP O00154
C	197	SER	-	expression tag	UNP O00154
C	198	MET	-	expression tag	UNP O00154
D	176	MET	-	expression tag	UNP O00154
D	177	HIS	-	expression tag	UNP O00154
D	178	HIS	-	expression tag	UNP O00154
D	179	HIS	-	expression tag	UNP O00154
D	180	HIS	-	expression tag	UNP O00154
D	181	HIS	-	expression tag	UNP O00154
D	182	HIS	-	expression tag	UNP O00154
D	183	SER	-	expression tag	UNP O00154
D	184	SER	-	expression tag	UNP O00154
D	185	GLY	-	expression tag	UNP O00154
D	186	VAL	-	expression tag	UNP O00154
D	187	ASP	-	expression tag	UNP O00154
D	188	LEU	-	expression tag	UNP O00154
D	189	GLY	-	expression tag	UNP O00154
D	190	THR	-	expression tag	UNP O00154
D	191	GLU	-	expression tag	UNP O00154
D	192	ASN	-	expression tag	UNP O00154
D	193	LEU	-	expression tag	UNP O00154
D	194	TYR	-	expression tag	UNP O00154
D	195	PHE	-	expression tag	UNP O00154

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Chain	Residue	Modelled	Actual	Comment	Reference
D	196	GLN	-	expression tag	UNP O00154
D	197	SER	-	expression tag	UNP O00154
D	198	MET	-	expression tag	UNP O00154
E	176	MET	-	expression tag	UNP O00154
E	177	HIS	-	expression tag	UNP O00154
E	178	HIS	-	expression tag	UNP O00154
E	179	HIS	-	expression tag	UNP O00154
E	180	HIS	-	expression tag	UNP O00154
E	181	HIS	-	expression tag	UNP O00154
E	182	HIS	-	expression tag	UNP O00154
E	183	SER	-	expression tag	UNP O00154
E	184	SER	-	expression tag	UNP O00154
E	185	GLY	-	expression tag	UNP O00154
E	186	VAL	-	expression tag	UNP O00154
E	187	ASP	-	expression tag	UNP O00154
E	188	LEU	-	expression tag	UNP O00154
E	189	GLY	-	expression tag	UNP O00154
E	190	THR	-	expression tag	UNP O00154
E	191	GLU	-	expression tag	UNP O00154
E	192	ASN	-	expression tag	UNP O00154
E	193	LEU	-	expression tag	UNP O00154
E	194	TYR	-	expression tag	UNP O00154
E	195	PHE	-	expression tag	UNP O00154
E	196	GLN	-	expression tag	UNP O00154
E	197	SER	-	expression tag	UNP O00154
E	198	MET	-	expression tag	UNP O00154
F	176	MET	-	expression tag	UNP O00154
F	177	HIS	-	expression tag	UNP O00154
F	178	HIS	-	expression tag	UNP O00154
F	179	HIS	-	expression tag	UNP O00154
F	180	HIS	-	expression tag	UNP O00154
F	181	HIS	-	expression tag	UNP O00154
F	182	HIS	-	expression tag	UNP O00154
F	183	SER	-	expression tag	UNP O00154
F	184	SER	-	expression tag	UNP O00154
F	185	GLY	-	expression tag	UNP O00154
F	186	VAL	-	expression tag	UNP O00154
F	187	ASP	-	expression tag	UNP O00154
F	188	LEU	-	expression tag	UNP O00154
F	189	GLY	-	expression tag	UNP O00154
F	190	THR	-	expression tag	UNP O00154
F	191	GLU	-	expression tag	UNP O00154

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Chain	Residue	Modelled	Actual	Comment	Reference
F	192	ASN	-	expression tag	UNP O00154
F	193	LEU	-	expression tag	UNP O00154
F	194	TYR	-	expression tag	UNP O00154
F	195	PHE	-	expression tag	UNP O00154
F	196	GLN	-	expression tag	UNP O00154
F	197	SER	-	expression tag	UNP O00154
F	198	MET	-	expression tag	UNP O00154
G	176	MET	-	expression tag	UNP O00154
G	177	HIS	-	expression tag	UNP O00154
G	178	HIS	-	expression tag	UNP O00154
G	179	HIS	-	expression tag	UNP O00154
G	180	HIS	-	expression tag	UNP O00154
G	181	HIS	-	expression tag	UNP O00154
G	182	HIS	-	expression tag	UNP O00154
G	183	SER	-	expression tag	UNP O00154
G	184	SER	-	expression tag	UNP O00154
G	185	GLY	-	expression tag	UNP O00154
G	186	VAL	-	expression tag	UNP O00154
G	187	ASP	-	expression tag	UNP O00154
G	188	LEU	-	expression tag	UNP O00154
G	189	GLY	-	expression tag	UNP O00154
G	190	THR	-	expression tag	UNP O00154
G	191	GLU	-	expression tag	UNP O00154
G	192	ASN	-	expression tag	UNP O00154
G	193	LEU	-	expression tag	UNP O00154
G	194	TYR	-	expression tag	UNP O00154
G	195	PHE	-	expression tag	UNP O00154
G	196	GLN	-	expression tag	UNP O00154
G	197	SER	-	expression tag	UNP O00154
G	198	MET	-	expression tag	UNP O00154
H	176	MET	-	expression tag	UNP O00154
H	177	HIS	-	expression tag	UNP O00154
H	178	HIS	-	expression tag	UNP O00154
H	179	HIS	-	expression tag	UNP O00154
H	180	HIS	-	expression tag	UNP O00154
H	181	HIS	-	expression tag	UNP O00154
H	182	HIS	-	expression tag	UNP O00154
H	183	SER	-	expression tag	UNP O00154
H	184	SER	-	expression tag	UNP O00154
H	185	GLY	-	expression tag	UNP O00154
H	186	VAL	-	expression tag	UNP O00154
H	187	ASP	-	expression tag	UNP O00154

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Chain	Residue	Modelled	Actual	Comment	Reference
H	188	LEU	-	expression tag	UNP O00154
H	189	GLY	-	expression tag	UNP O00154
H	190	THR	-	expression tag	UNP O00154
H	191	GLU	-	expression tag	UNP O00154
H	192	ASN	-	expression tag	UNP O00154
H	193	LEU	-	expression tag	UNP O00154
H	194	TYR	-	expression tag	UNP O00154
H	195	PHE	-	expression tag	UNP O00154
H	196	GLN	-	expression tag	UNP O00154
H	197	SER	-	expression tag	UNP O00154
H	198	MET	-	expression tag	UNP O00154
I	176	MET	-	expression tag	UNP O00154
I	177	HIS	-	expression tag	UNP O00154
I	178	HIS	-	expression tag	UNP O00154
I	179	HIS	-	expression tag	UNP O00154
I	180	HIS	-	expression tag	UNP O00154
I	181	HIS	-	expression tag	UNP O00154
I	182	HIS	-	expression tag	UNP O00154
I	183	SER	-	expression tag	UNP O00154
I	184	SER	-	expression tag	UNP O00154
I	185	GLY	-	expression tag	UNP O00154
I	186	VAL	-	expression tag	UNP O00154
I	187	ASP	-	expression tag	UNP O00154
I	188	LEU	-	expression tag	UNP O00154
I	189	GLY	-	expression tag	UNP O00154
I	190	THR	-	expression tag	UNP O00154
I	191	GLU	-	expression tag	UNP O00154
I	192	ASN	-	expression tag	UNP O00154
I	193	LEU	-	expression tag	UNP O00154
I	194	TYR	-	expression tag	UNP O00154
I	195	PHE	-	expression tag	UNP O00154
I	196	GLN	-	expression tag	UNP O00154
I	197	SER	-	expression tag	UNP O00154
I	198	MET	-	expression tag	UNP O00154
J	176	MET	-	expression tag	UNP O00154
J	177	HIS	-	expression tag	UNP O00154
J	178	HIS	-	expression tag	UNP O00154
J	179	HIS	-	expression tag	UNP O00154
J	180	HIS	-	expression tag	UNP O00154
J	181	HIS	-	expression tag	UNP O00154
J	182	HIS	-	expression tag	UNP O00154
J	183	SER	-	expression tag	UNP O00154

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Chain	Residue	Modelled	Actual	Comment	Reference
J	184	SER	-	expression tag	UNP O00154
J	185	GLY	-	expression tag	UNP O00154
J	186	VAL	-	expression tag	UNP O00154
J	187	ASP	-	expression tag	UNP O00154
J	188	LEU	-	expression tag	UNP O00154
J	189	GLY	-	expression tag	UNP O00154
J	190	THR	-	expression tag	UNP O00154
J	191	GLU	-	expression tag	UNP O00154
J	192	ASN	-	expression tag	UNP O00154
J	193	LEU	-	expression tag	UNP O00154
J	194	TYR	-	expression tag	UNP O00154
J	195	PHE	-	expression tag	UNP O00154
J	196	GLN	-	expression tag	UNP O00154
J	197	SER	-	expression tag	UNP O00154
J	198	MET	-	expression tag	UNP O00154
K	176	MET	-	expression tag	UNP O00154
K	177	HIS	-	expression tag	UNP O00154
K	178	HIS	-	expression tag	UNP O00154
K	179	HIS	-	expression tag	UNP O00154
K	180	HIS	-	expression tag	UNP O00154
K	181	HIS	-	expression tag	UNP O00154
K	182	HIS	-	expression tag	UNP O00154
K	183	SER	-	expression tag	UNP O00154
K	184	SER	-	expression tag	UNP O00154
K	185	GLY	-	expression tag	UNP O00154
K	186	VAL	-	expression tag	UNP O00154
K	187	ASP	-	expression tag	UNP O00154
K	188	LEU	-	expression tag	UNP O00154
K	189	GLY	-	expression tag	UNP O00154
K	190	THR	-	expression tag	UNP O00154
K	191	GLU	-	expression tag	UNP O00154
K	192	ASN	-	expression tag	UNP O00154
K	193	LEU	-	expression tag	UNP O00154
K	194	TYR	-	expression tag	UNP O00154
K	195	PHE	-	expression tag	UNP O00154
K	196	GLN	-	expression tag	UNP O00154
K	197	SER	-	expression tag	UNP O00154
K	198	MET	-	expression tag	UNP O00154
L	176	MET	-	expression tag	UNP O00154
L	177	HIS	-	expression tag	UNP O00154
L	178	HIS	-	expression tag	UNP O00154
L	179	HIS	-	expression tag	UNP O00154

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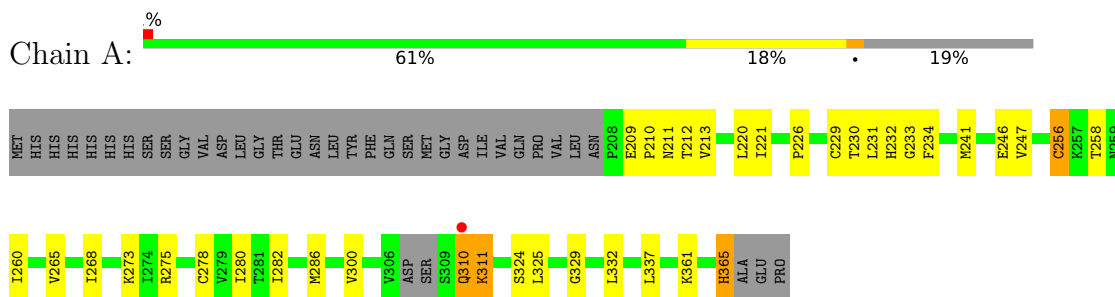
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Chain	Residue	Modelled	Actual	Comment	Reference
L	180	HIS	-	expression tag	UNP O00154
L	181	HIS	-	expression tag	UNP O00154
L	182	HIS	-	expression tag	UNP O00154
L	183	SER	-	expression tag	UNP O00154
L	184	SER	-	expression tag	UNP O00154
L	185	GLY	-	expression tag	UNP O00154
L	186	VAL	-	expression tag	UNP O00154
L	187	ASP	-	expression tag	UNP O00154
L	188	LEU	-	expression tag	UNP O00154
L	189	GLY	-	expression tag	UNP O00154
L	190	THR	-	expression tag	UNP O00154
L	191	GLU	-	expression tag	UNP O00154
L	192	ASN	-	expression tag	UNP O00154
L	193	LEU	-	expression tag	UNP O00154
L	194	TYR	-	expression tag	UNP O00154
L	195	PHE	-	expression tag	UNP O00154
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L	197	SER	-	expression tag	UNP O00154
L	198	MET	-	expression tag	UNP O00154

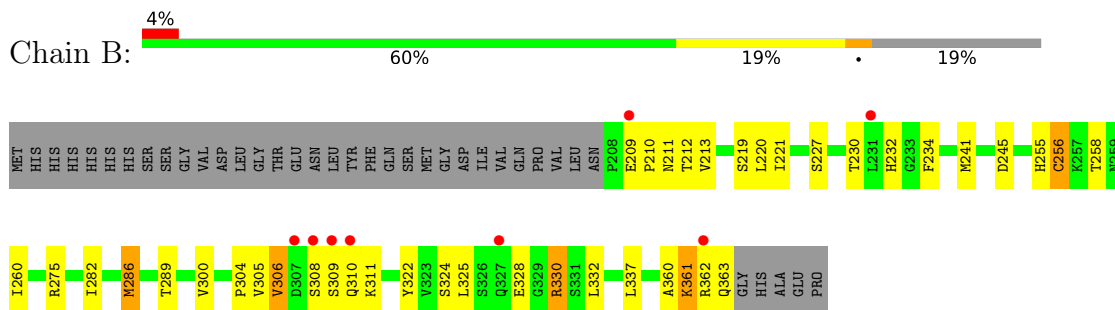
### 3 Residue-property plots [i](#)

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.

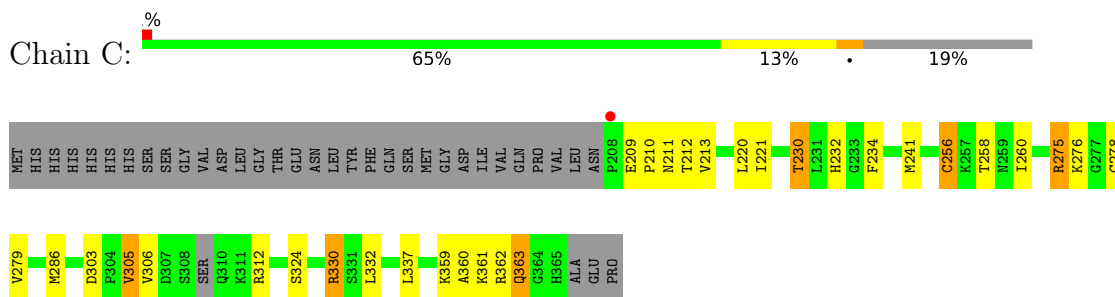
- Molecule 1: Cytosolic acyl coenzyme A thioester hydrolase



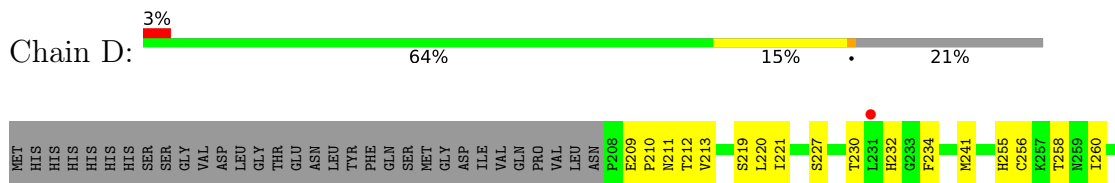
- Molecule 1: Cytosolic acyl coenzyme A thioester hydrolase



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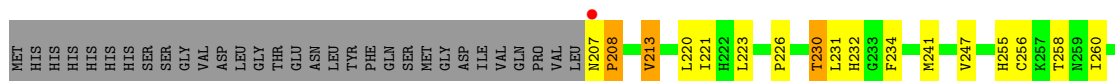


- Molecule 1: Cytosolic acyl coenzyme A thioester hydrolase

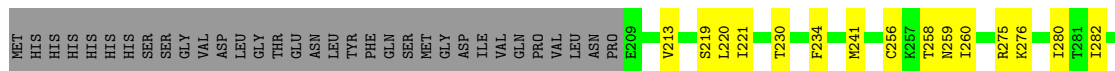




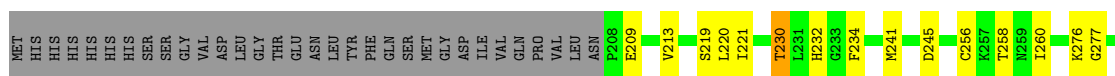
- Molecule 1: Cytosolic acyl coenzyme A thioester hydrolase



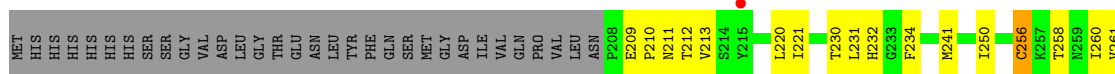
- Molecule 1: Cytosolic acyl coenzyme A thioester hydrolase



- Molecule 1: Cytosolic acyl coenzyme A thioester hydrolase

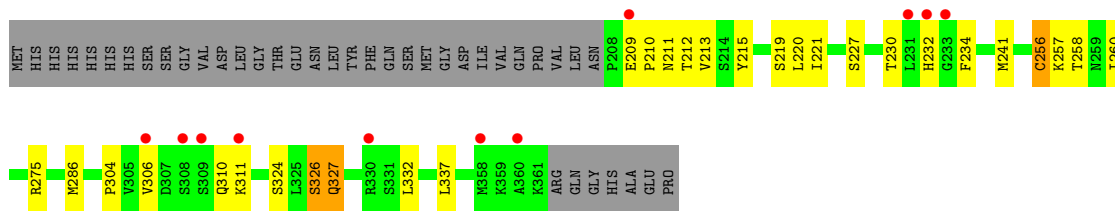


- Molecule 1: Cytosolic acyl coenzyme A thioester hydrolase

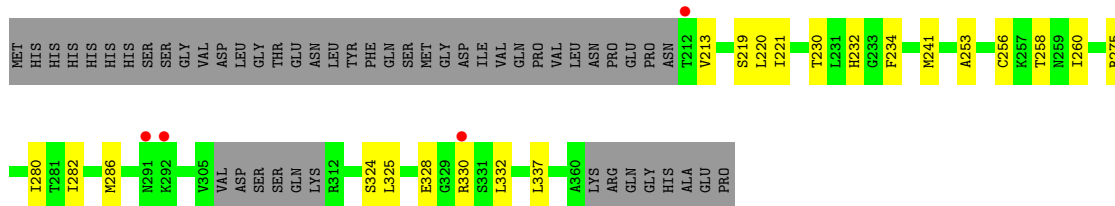


- Molecule 1: Cytosolic acyl coenzyme A thioester hydrolase

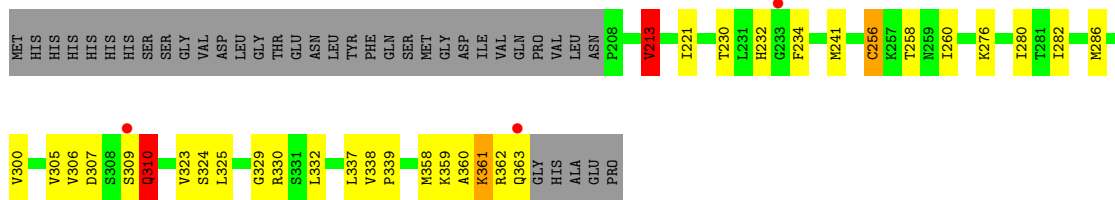




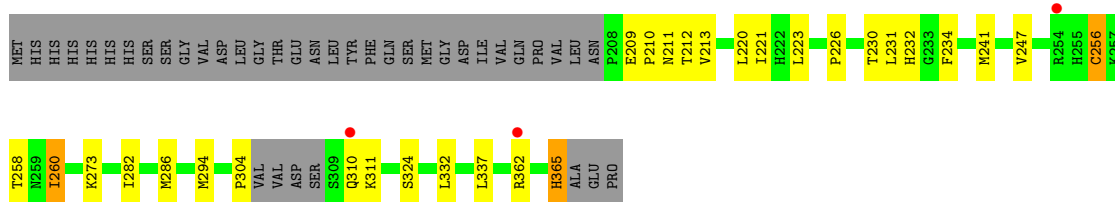
● Molecule 1: Cytosolic acyl coenzyme A thioester hydrolase



● Molecule 1: Cytosolic acyl coenzyme A thioester hydrolase



● Molecule 1: Cytosolic acyl coenzyme A thioester hydrolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.95Å 81.60Å 105.10Å 79.61° 89.70° 74.12°	Depositor
Resolution (Å)	19.87 – 2.80 19.85 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.6 (19.87-2.80) 95.5 (19.85-2.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.41 (at 2.79Å)	Xtrriage
Refinement program	REFMAC 5.3.0032	Depositor
R, $R_{free}$	0.216 , 0.239 0.207 , 0.228	Depositor DCC
$R_{free}$ test set	2984 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	81.7	Xtrriage
Anisotropy	0.165	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 81.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14037	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	1.00	4/1208 (0.3%)	0.78	1/1628 (0.1%)
1	B	0.67	1/1220 (0.1%)	0.67	0/1646
1	C	0.68	2/1219 (0.2%)	0.70	0/1642
1	D	1.05	2/1190 (0.2%)	0.72	1/1607 (0.1%)
1	E	0.71	0/1167	0.69	0/1576
1	F	0.63	1/1162 (0.1%)	0.66	1/1568 (0.1%)
1	G	0.73	1/1148 (0.1%)	0.70	0/1550
1	H	0.57	2/1195 (0.2%)	0.62	0/1612
1	I	0.56	1/1208 (0.1%)	0.64	0/1629
1	J	1.20	3/1120 (0.3%)	0.80	2/1509 (0.1%)
1	K	0.74	2/1228 (0.2%)	0.70	0/1655
1	L	0.66	2/1214 (0.2%)	0.64	1/1633 (0.1%)
All	All	0.79	21/14279 (0.1%)	0.70	6/19255 (0.0%)

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	328	GLU	CD-OE1	23.05	1.51	1.25
1	J	328	GLU	CD-OE1	21.92	1.49	1.25
1	A	365	HIS	C-O	21.61	1.64	1.23
1	J	328	GLU	CD-OE2	21.27	1.49	1.25
1	D	328	GLU	CD-OE2	16.21	1.43	1.25

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	330	ARG	NE-CZ-NH2	-10.38	115.11	120.30
1	J	328	GLU	OE1-CD-OE2	8.50	133.50	123.30
1	D	328	GLU	OE1-CD-OE2	6.42	131.00	123.30
1	A	365	HIS	CA-C-O	-5.79	107.94	120.10
1	F	330	ARG	NE-CZ-NH2	-5.20	117.70	120.30

There are no chirality outliers.



There are no planarity outliers.

## 5.2 Too-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 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	1188	0	1188	35	0
1	B	1199	0	1197	35	0
1	C	1199	0	1201	26	0
1	D	1169	0	1167	24	0
1	E	1147	0	1132	33	0
1	F	1143	0	1142	28	0
1	G	1128	0	1122	24	0
1	H	1175	0	1171	29	0
1	I	1187	0	1193	25	0
1	J	1102	0	1108	16	0
1	K	1207	0	1214	28	0
1	L	1193	0	1196	22	0
All	All	14037	0	14031	277	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 10.

The worst 5 of 277 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:G:311:LYS:N	1:G:311:LYS:CA	1.69	1.52
1:A:365:HIS:C	1:A:365:HIS:O	1.64	1.34
1:H:261:VAL:HG22	1:H:325:LEU:HD11	1.22	1.17
1:E:256:CYS:HB3	1:E:258:THR:HG22	1.24	1.16
1:G:256:CYS:HB3	1:G:258:THR:HG22	1.18	1.15

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	152/193 (79%)	144 (95%)	7 (5%)	1 (1%)	22	53
1	B	154/193 (80%)	146 (95%)	5 (3%)	3 (2%)	8	26
1	C	153/193 (79%)	143 (94%)	10 (6%)	0	100	100
1	D	151/193 (78%)	141 (93%)	10 (7%)	0	100	100
1	E	146/193 (76%)	140 (96%)	5 (3%)	1 (1%)	22	53
1	F	145/193 (75%)	139 (96%)	6 (4%)	0	100	100
1	G	144/193 (75%)	138 (96%)	6 (4%)	0	100	100
1	H	149/193 (77%)	142 (95%)	7 (5%)	0	100	100
1	I	152/193 (79%)	142 (93%)	9 (6%)	1 (1%)	22	53
1	J	139/193 (72%)	134 (96%)	5 (4%)	0	100	100
1	K	154/193 (80%)	144 (94%)	8 (5%)	2 (1%)	12	36
1	L	150/193 (78%)	143 (95%)	7 (5%)	0	100	100
All	All	1789/2316 (77%)	1696 (95%)	85 (5%)	8 (0%)	34	66

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	309	SER
1	B	361	LYS
1	K	361	LYS
1	A	311	LYS
1	B	306	VAL

### 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	131/168 (78%)	126 (96%)	5 (4%)	33	67
1	B	134/168 (80%)	127 (95%)	7 (5%)	23	55
1	C	132/168 (79%)	123 (93%)	9 (7%)	16	42
1	D	131/168 (78%)	128 (98%)	3 (2%)	50	82
1	E	126/168 (75%)	119 (94%)	7 (6%)	21	51
1	F	127/168 (76%)	120 (94%)	7 (6%)	21	52
1	G	125/168 (74%)	120 (96%)	5 (4%)	31	65
1	H	130/168 (77%)	125 (96%)	5 (4%)	33	67
1	I	134/168 (80%)	128 (96%)	6 (4%)	27	60
1	J	123/168 (73%)	119 (97%)	4 (3%)	38	72
1	K	136/168 (81%)	128 (94%)	8 (6%)	19	49
1	L	133/168 (79%)	128 (96%)	5 (4%)	33	67
All	All	1562/2016 (78%)	1491 (96%)	71 (4%)	27	60

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	332	LEU
1	K	260	ILE
1	K	332	LEU
1	E	213	VAL
1	D	332	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	365	HIS
1	J	291	ASN
1	H	327	GLN
1	H	291	ASN
1	I	327	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	156/193 (80%)	-0.18	1 (0%) 89 86	65, 83, 108, 122	0
1	B	156/193 (80%)	-0.12	8 (5%) 28 19	65, 84, 110, 119	0
1	C	157/193 (81%)	-0.25	1 (0%) 89 86	65, 83, 107, 122	0
1	D	153/193 (79%)	-0.13	5 (3%) 46 36	65, 83, 110, 132	0
1	E	150/193 (77%)	-0.11	3 (2%) 65 56	65, 83, 104, 111	0
1	F	149/193 (77%)	0.00	4 (2%) 54 44	65, 83, 102, 111	0
1	G	148/193 (76%)	0.16	4 (2%) 54 44	65, 83, 101, 111	0
1	H	153/193 (79%)	0.00	5 (3%) 46 36	65, 83, 104, 111	0
1	I	154/193 (79%)	0.14	11 (7%) 16 9	65, 83, 107, 111	0
1	J	143/193 (74%)	0.16	4 (2%) 53 43	65, 83, 102, 111	0
1	K	156/193 (80%)	-0.18	3 (1%) 66 59	65, 83, 108, 130	0
1	L	154/193 (79%)	-0.09	3 (1%) 66 59	65, 83, 104, 111	0
All	All	1829/2316 (78%)	-0.05	52 (2%) 53 43	65, 83, 107, 132	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	231	LEU	4.9
1	D	309	SER	4.2
1	I	309	SER	4.0
1	K	363	GLN	3.8
1	H	327	GLN	3.7

### 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 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.