



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 28, 2023 – 04:05 AM EDT

PDB ID : 3L3S
Title : Crystal structure of an enoyl-CoA hydrotase/isomerase family protein from *Silicibacter pomeroyi*
Authors : Eswaramoorthy, S.; Silberstein, M.; Burley, S.K.; Swaminathan, S.; New York
SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2009-12-17
Resolution : 2.32 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
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)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

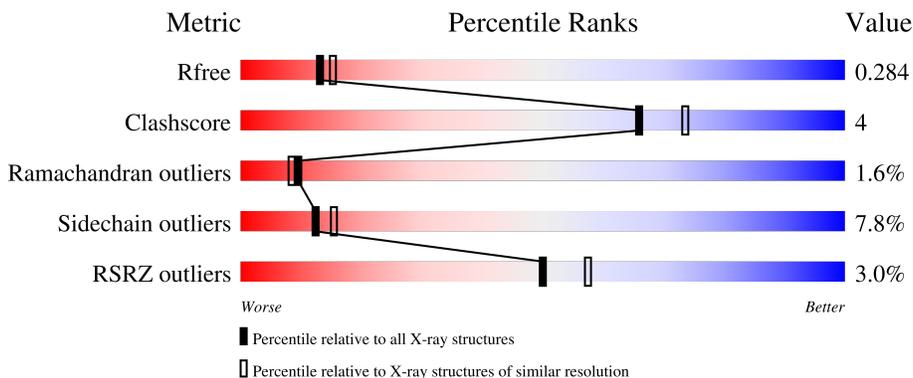
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	263	 75% 12% 12%
1	B	263	 76% 11% 11%
1	C	263	 74% 13% 11%
1	D	263	 75% 12% 12%
1	E	263	 74% 12% 12%

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Mol	Chain	Length	Quality of chain
1	F	263	<p>3% 78% 8% • 12%</p>
1	G	263	<p>3% 74% 12% • 11%</p>
1	H	263	<p>3% 76% 10% • 12%</p>
1	I	263	<p>3% 77% 10% • 11%</p>
1	J	263	<p>3% 75% 13% • 11%</p>
1	K	263	<p>8% 74% 13% • 12%</p>
1	L	263	<p>9% 70% 14% • 12%</p>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 20649 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 Enoyl-CoA hydratase/isomerase family protein.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se				
1	A	232	Total	C	N	O	S	Se	0	0	0	
			1711	1077	311	310	6	7				
1	B	234	Total	C	N	O	S	Se	0	0	0	
			1721	1086	312	310	6	7				
1	C	234	Total	C	N	O	S	Se	0	0	0	
			1722	1085	310	314	6	7				
1	D	232	Total	C	N	O	S	Se	0	0	0	
			1710	1079	308	310	6	7				
1	E	231	Total	C	N	O	S	Se	0	0	0	
			1697	1072	307	305	6	7				
1	F	231	Total	C	N	O	S	Se	0	0	0	
			1701	1074	307	307	6	7				
1	G	233	Total	C	N	O	S	Se	0	0	0	
			1710	1079	309	309	6	7				
1	H	232	Total	C	N	O	S	Se	0	0	0	
			1706	1077	308	308	6	7				
1	I	234	Total	C	N	O	S	Se	0	0	0	
			1718	1083	310	312	6	7				
1	J	233	Total	C	N	O	S	Se	0	0	0	
			1710	1079	309	309	6	7				
1	K	232	Total	C	N	O	S	Se	0	0	0	
			1707	1076	308	310	6	7				
1	L	231	Total	C	N	O	S	Se	0	0	0	
			1702	1073	307	309	6	7				

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MSE	-	expression tag	UNP Q5LQZ3
A	3	SER	-	expression tag	UNP Q5LQZ3
A	4	LEU	-	expression tag	UNP Q5LQZ3
A	257	GLU	-	expression tag	UNP Q5LQZ3
A	258	GLY	-	expression tag	UNP Q5LQZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	259	HIS	-	expression tag	UNP Q5LQZ3
A	260	HIS	-	expression tag	UNP Q5LQZ3
A	261	HIS	-	expression tag	UNP Q5LQZ3
A	262	HIS	-	expression tag	UNP Q5LQZ3
A	263	HIS	-	expression tag	UNP Q5LQZ3
A	264	HIS	-	expression tag	UNP Q5LQZ3
B	2	MSE	-	expression tag	UNP Q5LQZ3
B	3	SER	-	expression tag	UNP Q5LQZ3
B	4	LEU	-	expression tag	UNP Q5LQZ3
B	257	GLU	-	expression tag	UNP Q5LQZ3
B	258	GLY	-	expression tag	UNP Q5LQZ3
B	259	HIS	-	expression tag	UNP Q5LQZ3
B	260	HIS	-	expression tag	UNP Q5LQZ3
B	261	HIS	-	expression tag	UNP Q5LQZ3
B	262	HIS	-	expression tag	UNP Q5LQZ3
B	263	HIS	-	expression tag	UNP Q5LQZ3
B	264	HIS	-	expression tag	UNP Q5LQZ3
C	2	MSE	-	expression tag	UNP Q5LQZ3
C	3	SER	-	expression tag	UNP Q5LQZ3
C	4	LEU	-	expression tag	UNP Q5LQZ3
C	257	GLU	-	expression tag	UNP Q5LQZ3
C	258	GLY	-	expression tag	UNP Q5LQZ3
C	259	HIS	-	expression tag	UNP Q5LQZ3
C	260	HIS	-	expression tag	UNP Q5LQZ3
C	261	HIS	-	expression tag	UNP Q5LQZ3
C	262	HIS	-	expression tag	UNP Q5LQZ3
C	263	HIS	-	expression tag	UNP Q5LQZ3
C	264	HIS	-	expression tag	UNP Q5LQZ3
D	2	MSE	-	expression tag	UNP Q5LQZ3
D	3	SER	-	expression tag	UNP Q5LQZ3
D	4	LEU	-	expression tag	UNP Q5LQZ3
D	257	GLU	-	expression tag	UNP Q5LQZ3
D	258	GLY	-	expression tag	UNP Q5LQZ3
D	259	HIS	-	expression tag	UNP Q5LQZ3
D	260	HIS	-	expression tag	UNP Q5LQZ3
D	261	HIS	-	expression tag	UNP Q5LQZ3
D	262	HIS	-	expression tag	UNP Q5LQZ3
D	263	HIS	-	expression tag	UNP Q5LQZ3
D	264	HIS	-	expression tag	UNP Q5LQZ3
E	2	MSE	-	expression tag	UNP Q5LQZ3
E	3	SER	-	expression tag	UNP Q5LQZ3
E	4	LEU	-	expression tag	UNP Q5LQZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	257	GLU	-	expression tag	UNP Q5LQZ3
E	258	GLY	-	expression tag	UNP Q5LQZ3
E	259	HIS	-	expression tag	UNP Q5LQZ3
E	260	HIS	-	expression tag	UNP Q5LQZ3
E	261	HIS	-	expression tag	UNP Q5LQZ3
E	262	HIS	-	expression tag	UNP Q5LQZ3
E	263	HIS	-	expression tag	UNP Q5LQZ3
E	264	HIS	-	expression tag	UNP Q5LQZ3
F	2	MSE	-	expression tag	UNP Q5LQZ3
F	3	SER	-	expression tag	UNP Q5LQZ3
F	4	LEU	-	expression tag	UNP Q5LQZ3
F	257	GLU	-	expression tag	UNP Q5LQZ3
F	258	GLY	-	expression tag	UNP Q5LQZ3
F	259	HIS	-	expression tag	UNP Q5LQZ3
F	260	HIS	-	expression tag	UNP Q5LQZ3
F	261	HIS	-	expression tag	UNP Q5LQZ3
F	262	HIS	-	expression tag	UNP Q5LQZ3
F	263	HIS	-	expression tag	UNP Q5LQZ3
F	264	HIS	-	expression tag	UNP Q5LQZ3
G	2	MSE	-	expression tag	UNP Q5LQZ3
G	3	SER	-	expression tag	UNP Q5LQZ3
G	4	LEU	-	expression tag	UNP Q5LQZ3
G	257	GLU	-	expression tag	UNP Q5LQZ3
G	258	GLY	-	expression tag	UNP Q5LQZ3
G	259	HIS	-	expression tag	UNP Q5LQZ3
G	260	HIS	-	expression tag	UNP Q5LQZ3
G	261	HIS	-	expression tag	UNP Q5LQZ3
G	262	HIS	-	expression tag	UNP Q5LQZ3
G	263	HIS	-	expression tag	UNP Q5LQZ3
G	264	HIS	-	expression tag	UNP Q5LQZ3
H	2	MSE	-	expression tag	UNP Q5LQZ3
H	3	SER	-	expression tag	UNP Q5LQZ3
H	4	LEU	-	expression tag	UNP Q5LQZ3
H	257	GLU	-	expression tag	UNP Q5LQZ3
H	258	GLY	-	expression tag	UNP Q5LQZ3
H	259	HIS	-	expression tag	UNP Q5LQZ3
H	260	HIS	-	expression tag	UNP Q5LQZ3
H	261	HIS	-	expression tag	UNP Q5LQZ3
H	262	HIS	-	expression tag	UNP Q5LQZ3
H	263	HIS	-	expression tag	UNP Q5LQZ3
H	264	HIS	-	expression tag	UNP Q5LQZ3
I	2	MSE	-	expression tag	UNP Q5LQZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
I	3	SER	-	expression tag	UNP Q5LQZ3
I	4	LEU	-	expression tag	UNP Q5LQZ3
I	257	GLU	-	expression tag	UNP Q5LQZ3
I	258	GLY	-	expression tag	UNP Q5LQZ3
I	259	HIS	-	expression tag	UNP Q5LQZ3
I	260	HIS	-	expression tag	UNP Q5LQZ3
I	261	HIS	-	expression tag	UNP Q5LQZ3
I	262	HIS	-	expression tag	UNP Q5LQZ3
I	263	HIS	-	expression tag	UNP Q5LQZ3
I	264	HIS	-	expression tag	UNP Q5LQZ3
J	2	MSE	-	expression tag	UNP Q5LQZ3
J	3	SER	-	expression tag	UNP Q5LQZ3
J	4	LEU	-	expression tag	UNP Q5LQZ3
J	257	GLU	-	expression tag	UNP Q5LQZ3
J	258	GLY	-	expression tag	UNP Q5LQZ3
J	259	HIS	-	expression tag	UNP Q5LQZ3
J	260	HIS	-	expression tag	UNP Q5LQZ3
J	261	HIS	-	expression tag	UNP Q5LQZ3
J	262	HIS	-	expression tag	UNP Q5LQZ3
J	263	HIS	-	expression tag	UNP Q5LQZ3
J	264	HIS	-	expression tag	UNP Q5LQZ3
K	2	MSE	-	expression tag	UNP Q5LQZ3
K	3	SER	-	expression tag	UNP Q5LQZ3
K	4	LEU	-	expression tag	UNP Q5LQZ3
K	257	GLU	-	expression tag	UNP Q5LQZ3
K	258	GLY	-	expression tag	UNP Q5LQZ3
K	259	HIS	-	expression tag	UNP Q5LQZ3
K	260	HIS	-	expression tag	UNP Q5LQZ3
K	261	HIS	-	expression tag	UNP Q5LQZ3
K	262	HIS	-	expression tag	UNP Q5LQZ3
K	263	HIS	-	expression tag	UNP Q5LQZ3
K	264	HIS	-	expression tag	UNP Q5LQZ3
L	2	MSE	-	expression tag	UNP Q5LQZ3
L	3	SER	-	expression tag	UNP Q5LQZ3
L	4	LEU	-	expression tag	UNP Q5LQZ3
L	257	GLU	-	expression tag	UNP Q5LQZ3
L	258	GLY	-	expression tag	UNP Q5LQZ3
L	259	HIS	-	expression tag	UNP Q5LQZ3
L	260	HIS	-	expression tag	UNP Q5LQZ3
L	261	HIS	-	expression tag	UNP Q5LQZ3
L	262	HIS	-	expression tag	UNP Q5LQZ3
L	263	HIS	-	expression tag	UNP Q5LQZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
L	264	HIS	-	expression tag	UNP Q5LQZ3

- Molecule 2 is water.

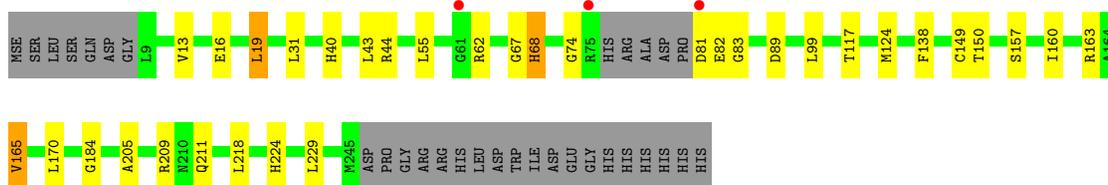
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	5	Total O 5 5	0	0
2	B	20	Total O 20 20	0	0
2	C	19	Total O 19 19	0	0
2	D	16	Total O 16 16	0	0
2	E	14	Total O 14 14	0	0
2	F	20	Total O 20 20	0	0
2	G	8	Total O 8 8	0	0
2	H	9	Total O 9 9	0	0
2	I	6	Total O 6 6	0	0
2	J	3	Total O 3 3	0	0
2	K	10	Total O 10 10	0	0
2	L	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.

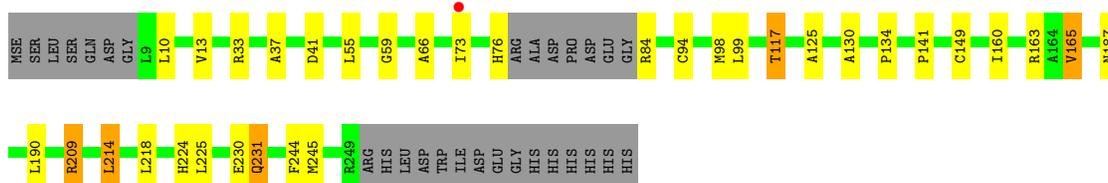
- Molecule 1: Enoyl-CoA hydratase/isomerase family protein

Chain A: 



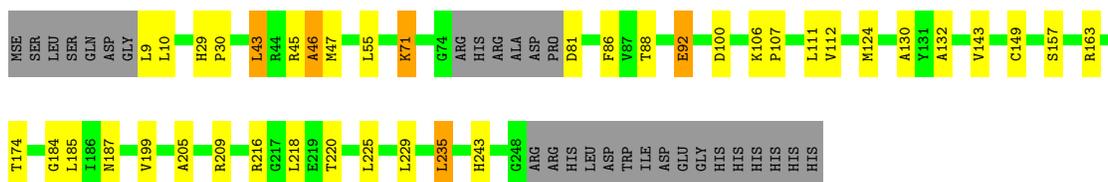
- Molecule 1: Enoyl-CoA hydratase/isomerase family protein

Chain B: 



- Molecule 1: Enoyl-CoA hydratase/isomerase family protein

Chain C: 



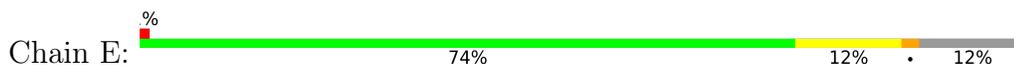
- Molecule 1: Enoyl-CoA hydratase/isomerase family protein

Chain D: 

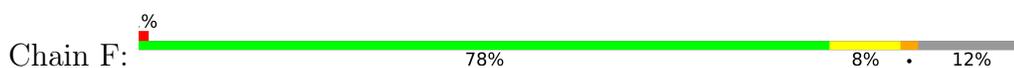




- Molecule 1: Enoyl-CoA hydratase/isomerase family protein



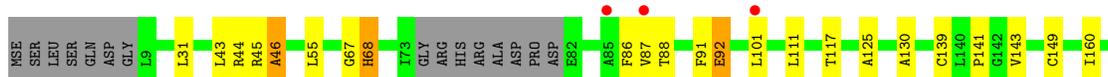
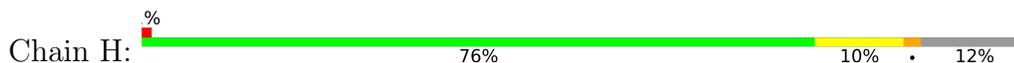
- Molecule 1: Enoyl-CoA hydratase/isomerase family protein



- Molecule 1: Enoyl-CoA hydratase/isomerase family protein

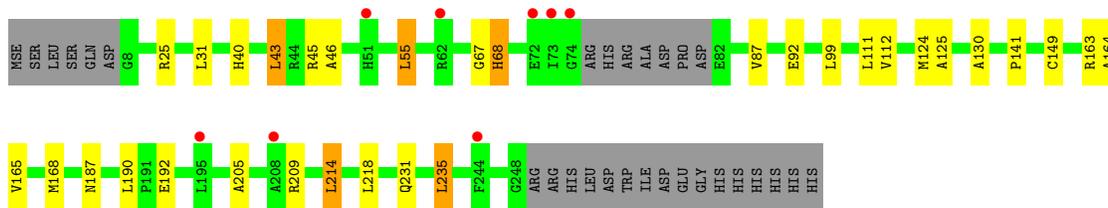


- Molecule 1: Enoyl-CoA hydratase/isomerase family protein

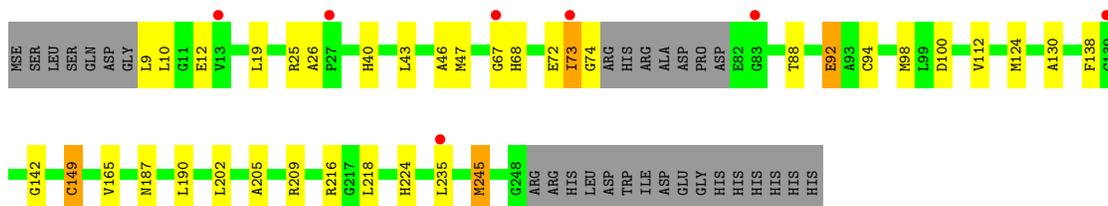
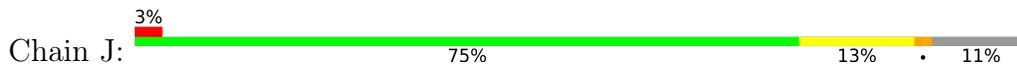


- Molecule 1: Enoyl-CoA hydratase/isomerase family protein

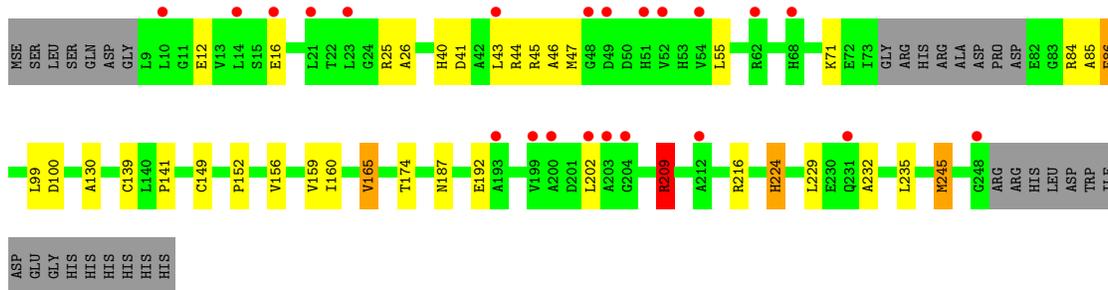
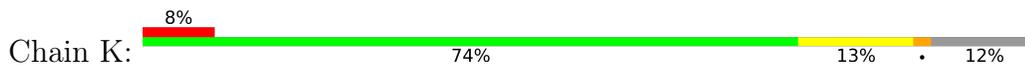




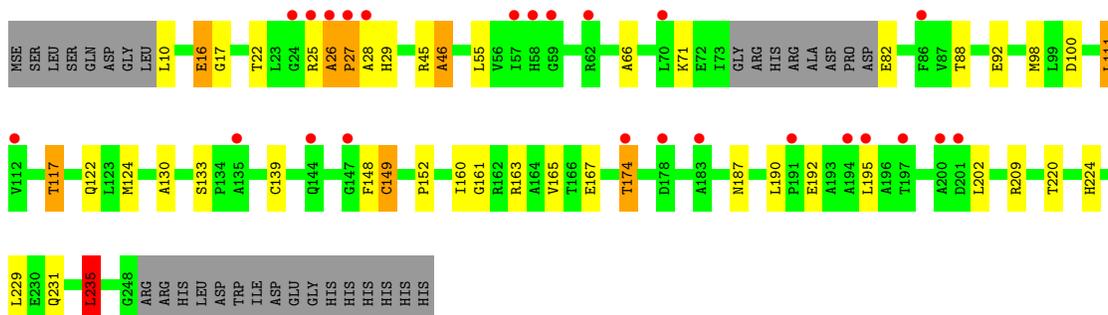
- Molecule 1: Enoyl-CoA hydratase/isomerase family protein



- Molecule 1: Enoyl-CoA hydratase/isomerase family protein



- Molecule 1: Enoyl-CoA hydratase/isomerase family protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.40Å 124.28Å 147.00Å 90.00° 102.44° 90.00°	Depositor
Resolution (Å)	50.00 – 2.32 49.65 – 2.32	Depositor EDS
% Data completeness (in resolution range)	92.3 (50.00-2.32) 75.1 (49.65-2.32)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.32Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.263 , 0.294 0.255 , 0.284	Depositor DCC
R_{free} test set	5005 reflections (3.84%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtrriage
Anisotropy	0.567	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 5.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	20649	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.42% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OCS

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	0.53	0/1725	0.79	0/2335
1	B	0.53	0/1737	0.80	3/2354 (0.1%)
1	C	0.55	0/1737	0.81	1/2353 (0.0%)
1	D	0.55	0/1725	0.81	1/2337 (0.0%)
1	E	0.55	0/1712	0.80	0/2320
1	F	0.54	0/1716	0.78	1/2325 (0.0%)
1	G	0.56	0/1725	0.85	2/2337 (0.1%)
1	H	0.54	0/1721	0.80	1/2332 (0.0%)
1	I	0.57	0/1733	0.80	4/2347 (0.2%)
1	J	0.54	0/1725	0.78	0/2337
1	K	0.55	0/1722	0.82	3/2333 (0.1%)
1	L	0.56	0/1717	0.84	3/2326 (0.1%)
All	All	0.55	0/20695	0.81	19/28036 (0.1%)

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	111	LEU	CA-CB-CG	7.27	132.01	115.30
1	I	235	LEU	CA-CB-CG	5.91	128.90	115.30
1	F	111	LEU	CA-CB-CG	5.80	128.65	115.30
1	L	55	LEU	CA-CB-CG	5.75	128.52	115.30
1	G	55	LEU	CA-CB-CG	5.71	128.42	115.30

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	1711	0	1729	11	0
1	B	1721	0	1737	15	0
1	C	1722	0	1738	24	0
1	D	1710	0	1731	12	0
1	E	1697	0	1720	13	0
1	F	1701	0	1725	11	0
1	G	1710	0	1730	17	0
1	H	1706	0	1727	22	0
1	I	1718	0	1736	11	0
1	J	1710	0	1731	12	0
1	K	1707	0	1722	23	0
1	L	1702	0	1720	20	0
2	A	5	0	0	0	0
2	B	20	0	0	1	0
2	C	19	0	0	2	0
2	D	16	0	0	0	0
2	E	14	0	0	0	0
2	F	20	0	0	1	0
2	G	8	0	0	0	0
2	H	9	0	0	0	0
2	I	6	0	0	0	0
2	J	3	0	0	0	0
2	K	10	0	0	0	0
2	L	4	0	0	0	0
All	All	20649	0	20746	164	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 4.

The worst 5 of 164 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:F:130:ALA:H	1:F:187:ASN:HD22	1.37	0.72
1:B:130:ALA:H	1:B:187:ASN:HD22	1.35	0.71
1:H:44:ARG:HH22	1:K:44:ARG:HH22	1.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:ALA:H	1:D:187:ASN:HD22	1.39	0.68
1:I:130:ALA:H	1:I:187:ASN:HD22	1.41	0.68

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	227/263 (86%)	214 (94%)	9 (4%)	4 (2%)	8 7
1	B	229/263 (87%)	221 (96%)	8 (4%)	0	100 100
1	C	229/263 (87%)	216 (94%)	11 (5%)	2 (1%)	17 19
1	D	227/263 (86%)	216 (95%)	7 (3%)	4 (2%)	8 7
1	E	226/263 (86%)	216 (96%)	5 (2%)	5 (2%)	6 5
1	F	226/263 (86%)	217 (96%)	6 (3%)	3 (1%)	12 12
1	G	228/263 (87%)	218 (96%)	6 (3%)	4 (2%)	8 7
1	H	227/263 (86%)	218 (96%)	5 (2%)	4 (2%)	8 7
1	I	229/263 (87%)	218 (95%)	9 (4%)	2 (1%)	17 19
1	J	228/263 (87%)	213 (93%)	10 (4%)	5 (2%)	6 5
1	K	227/263 (86%)	214 (94%)	9 (4%)	4 (2%)	8 7
1	L	226/263 (86%)	208 (92%)	11 (5%)	7 (3%)	4 2
All	All	2729/3156 (86%)	2589 (95%)	96 (4%)	44 (2%)	9 8

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	GLU
1	D	86	PHE
1	G	46	ALA

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Mol	Chain	Res	Type
1	G	86	PHE
1	K	86	PHE

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	168/188 (89%)	153 (91%)	15 (9%)	9 11
1	B	169/188 (90%)	155 (92%)	14 (8%)	11 13
1	C	170/188 (90%)	161 (95%)	9 (5%)	22 31
1	D	169/188 (90%)	158 (94%)	11 (6%)	17 22
1	E	167/188 (89%)	152 (91%)	15 (9%)	9 11
1	F	168/188 (89%)	159 (95%)	9 (5%)	22 30
1	G	168/188 (89%)	151 (90%)	17 (10%)	7 8
1	H	168/188 (89%)	160 (95%)	8 (5%)	25 35
1	I	169/188 (90%)	155 (92%)	14 (8%)	11 13
1	J	168/188 (89%)	153 (91%)	15 (9%)	9 11
1	K	168/188 (89%)	154 (92%)	14 (8%)	11 13
1	L	168/188 (89%)	152 (90%)	16 (10%)	8 9
All	All	2020/2256 (90%)	1863 (92%)	157 (8%)	12 15

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	47	MSE
1	L	22	THR
1	J	165	VAL
1	K	100	ASP
1	L	190	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	187	ASN
1	J	187	ASN
1	J	68	HIS
1	K	68	HIS
1	D	187	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

12 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OCS	F	149	1	7,8,9	2.05	2 (28%)	6,11,13	3.11	2 (33%)
1	OCS	G	149	1	7,8,9	1.93	2 (28%)	6,11,13	3.84	3 (50%)
1	OCS	H	149	1	7,8,9	2.31	2 (28%)	6,11,13	4.06	3 (50%)
1	OCS	L	149	1	7,8,9	1.75	3 (42%)	6,11,13	4.43	2 (33%)
1	OCS	A	149	1	7,8,9	2.34	2 (28%)	6,11,13	3.57	3 (50%)
1	OCS	J	149	1	7,8,9	2.12	2 (28%)	6,11,13	4.14	2 (33%)
1	OCS	E	149	1	7,8,9	2.05	2 (28%)	6,11,13	3.19	4 (66%)
1	OCS	B	149	1	7,8,9	2.20	2 (28%)	6,11,13	3.73	4 (66%)
1	OCS	K	149	1	7,8,9	2.13	2 (28%)	6,11,13	3.95	3 (50%)
1	OCS	C	149	1	7,8,9	2.12	2 (28%)	6,11,13	3.50	4 (66%)
1	OCS	D	149	1	7,8,9	2.07	2 (28%)	6,11,13	3.36	3 (50%)
1	OCS	I	149	1	7,8,9	1.93	2 (28%)	6,11,13	3.56	4 (66%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OCS	F	149	1	-	3/4/7/9	-
1	OCS	G	149	1	-	4/4/7/9	-
1	OCS	H	149	1	-	2/4/7/9	-
1	OCS	L	149	1	-	4/4/7/9	-
1	OCS	A	149	1	-	3/4/7/9	-
1	OCS	J	149	1	-	2/4/7/9	-
1	OCS	E	149	1	-	4/4/7/9	-
1	OCS	B	149	1	-	2/4/7/9	-
1	OCS	K	149	1	-	4/4/7/9	-
1	OCS	C	149	1	-	3/4/7/9	-
1	OCS	D	149	1	-	4/4/7/9	-
1	OCS	I	149	1	-	4/4/7/9	-

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	149	OCS	OD3-SG	-4.82	1.30	1.45
1	A	149	OCS	OD3-SG	-4.48	1.31	1.45
1	J	149	OCS	OD3-SG	-4.37	1.32	1.45
1	B	149	OCS	OD3-SG	-4.03	1.33	1.45
1	G	149	OCS	OD3-SG	-3.98	1.33	1.45

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	149	OCS	OD1-SG-CB	-7.64	97.86	106.94
1	J	149	OCS	OD1-SG-CB	-7.62	97.89	106.94
1	L	149	OCS	OD2-SG-CB	7.02	116.92	105.74
1	H	149	OCS	OD1-SG-CB	-6.79	98.87	106.94
1	K	149	OCS	OD1-SG-CB	-6.75	98.91	106.94

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	149	OCS	CA-CB-SG-OD2
1	B	149	OCS	CA-CB-SG-OD2
1	C	149	OCS	CA-CB-SG-OD2

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Mol	Chain	Res	Type	Atoms
1	D	149	OCS	N-CA-CB-SG
1	D	149	OCS	CA-CB-SG-OD2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	149	OCS	1	0
1	L	149	OCS	1	0
1	J	149	OCS	1	0
1	E	149	OCS	1	0

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	224/263 (85%)	0.11	3 (1%) 77 81	14, 36, 52, 62	0
1	B	226/263 (85%)	-0.18	1 (0%) 92 95	15, 28, 46, 55	0
1	C	226/263 (85%)	-0.06	0 100 100	15, 30, 47, 56	0
1	D	224/263 (85%)	0.05	2 (0%) 84 88	15, 33, 49, 59	0
1	E	223/263 (84%)	-0.03	2 (0%) 84 88	18, 34, 49, 58	0
1	F	223/263 (84%)	0.01	2 (0%) 84 88	17, 31, 45, 58	0
1	G	225/263 (85%)	0.12	7 (3%) 49 56	20, 35, 51, 66	0
1	H	224/263 (85%)	0.27	3 (1%) 77 81	20, 40, 54, 65	0
1	I	226/263 (85%)	0.18	8 (3%) 44 51	16, 38, 52, 59	0
1	J	225/263 (85%)	0.25	7 (3%) 49 56	20, 38, 53, 59	0
1	K	224/263 (85%)	0.57	22 (9%) 7 10	21, 46, 60, 66	0
1	L	223/263 (84%)	0.78	24 (10%) 5 8	21, 50, 61, 63	0
All	All	2693/3156 (85%)	0.17	81 (3%) 50 57	14, 36, 55, 66	0

The worst 5 of 81 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	27	PRO	6.0
1	H	85	ALA	5.5
1	G	248	GLY	5.3
1	L	27	PRO	4.4
1	L	197	THR	3.9

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	OCS	K	149	9/10	0.91	0.14	35,36,40,40	0
1	OCS	L	149	9/10	0.91	0.09	46,48,51,51	0
1	OCS	I	149	9/10	0.92	0.12	34,36,45,46	0
1	OCS	B	149	9/10	0.94	0.13	32,35,41,42	0
1	OCS	D	149	9/10	0.95	0.14	29,32,36,36	0
1	OCS	E	149	9/10	0.95	0.14	30,30,39,40	0
1	OCS	G	149	9/10	0.95	0.12	25,33,42,43	0
1	OCS	F	149	9/10	0.96	0.11	30,32,38,38	0
1	OCS	J	149	9/10	0.96	0.11	36,37,46,46	0
1	OCS	A	149	9/10	0.97	0.11	25,28,32,33	0
1	OCS	H	149	9/10	0.97	0.09	34,34,38,40	0
1	OCS	C	149	9/10	0.98	0.11	22,23,35,36	0

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.