



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 23, 2024 – 05:32 AM EDT

PDB ID : 6FDG  
Title : Novel crystal structure of DHNA-CoA Thioesterase from *Staphylococcus aureus*  
Authors : Murad, A.M.; Betzel, C.; Wrenger, C.  
Deposited on : 2017-12-22  
Resolution : 1.30 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>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

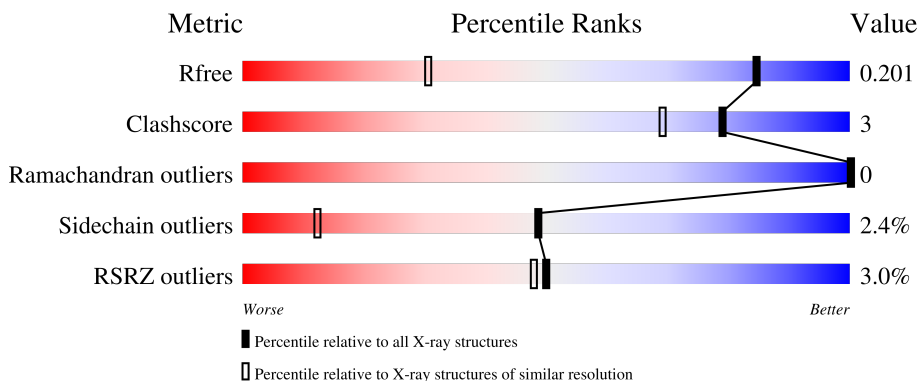
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.30 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	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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  $\geq 3$ , 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	155	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 6%, orange 6%, orange 80%, yellow 80%, yellow 99%, green 99%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>6%</span> <span>80%</span> <span>19%</span> </div> </div>
1	B	155	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, orange 3%, orange 79%, yellow 79%, yellow 94%, green 94%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>79%</span> <span>15%</span> </div> </div>
1	C	155	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, orange 3%, orange 81%, yellow 81%, yellow 98%, green 98%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>81%</span> <span>17%</span> </div> </div>
1	D	155	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, orange 3%, orange 74%, yellow 74%, yellow 95%, green 95%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>74%</span> <span>21%</span> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5483 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 4-hydroxybenzoyl-CoA thioesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	155	Total	C	N	O	S	0	4	0
			1309	847	207	250	5			
1	B	149	Total	C	N	O	S	0	3	0
			1258	817	199	235	7			
1	C	155	Total	C	N	O	S	0	7	0
			1336	861	210	259	6			
1	D	149	Total	C	N	O	S	0	3	0
			1266	821	203	235	7			


- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	82	Total	O	0	0
			82	82		
2	B	71	Total	O	0	0
			71	71		
2	C	85	Total	O	0	0
			85	85		
2	D	76	Total	O	0	0
			76	76		

### 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.

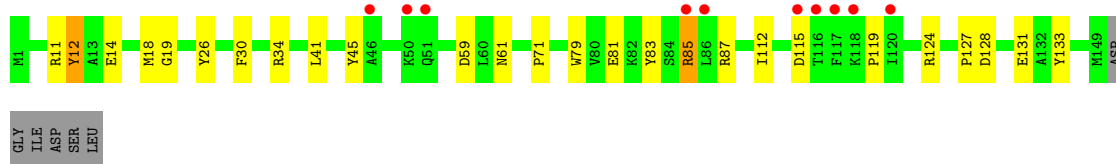
- Molecule 1: 4-hydroxybenzoyl-CoA thioesterase

Chain A: 




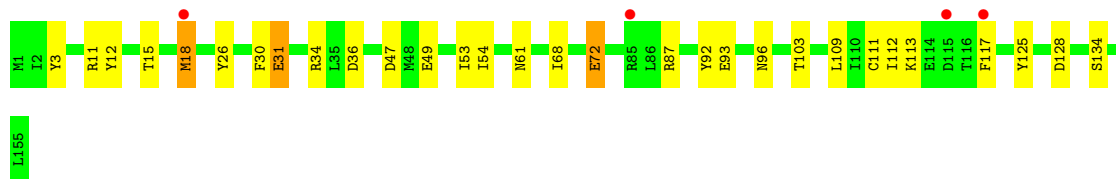
- Molecule 1: 4-hydroxybenzoyl-CoA thioesterase

Chain B: 




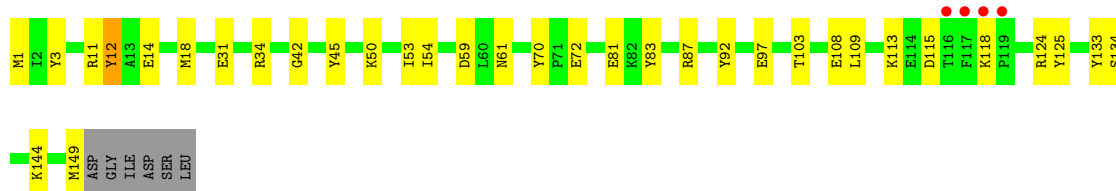
- Molecule 1: 4-hydroxybenzoyl-CoA thioesterase

Chain C: 



- Molecule 1: 4-hydroxybenzoyl-CoA thioesterase

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.61Å 90.78Å 75.38Å 90.00° 92.00° 90.00°	Depositor
Resolution (Å)	75.33 – 1.30 53.57 – 1.30	Depositor EDS
% Data completeness (in resolution range)	97.9 (75.33-1.30) 97.9 (53.57-1.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.178 , 0.198 0.185 , 0.201	Depositor DCC
$R_{free}$ test set	8701 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.1	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 48.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5483	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% 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

### 5.1 Standard geometry

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	1.75	17/1342 (1.3%)	1.59	22/1812 (1.2%)
1	B	1.59	10/1291 (0.8%)	1.43	11/1741 (0.6%)
1	C	1.55	9/1369 (0.7%)	1.45	16/1847 (0.9%)
1	D	1.73	11/1296 (0.8%)	1.56	18/1747 (1.0%)
All	All	1.66	47/5298 (0.9%)	1.51	67/7147 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31[A]	GLU	CD-OE2	13.36	1.40	1.25
1	A	31[B]	GLU	CD-OE2	13.36	1.40	1.25
1	D	12	TYR	CE1-CZ	-13.29	1.21	1.38
1	A	31[A]	GLU	CD-OE1	10.40	1.37	1.25
1	A	31[B]	GLU	CD-OE1	10.40	1.37	1.25

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	128	ASP	CB-CG-OD2	-13.30	106.33	118.30
1	C	34	ARG	NE-CZ-NH1	10.61	125.61	120.30
1	A	31[A]	GLU	OE1-CD-OE2	10.47	135.86	123.30
1	A	31[B]	GLU	OE1-CD-OE2	10.47	135.86	123.30
1	D	11	ARG	NE-CZ-NH2	-9.22	115.69	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	68	ILE	Mainchain

## 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	1309	0	1293	11	0
1	B	1258	0	1253	14	0
1	C	1336	0	1308	8	0
1	D	1266	0	1260	9	0
2	A	82	0	0	0	0
2	B	71	0	0	0	0
2	C	85	0	0	0	0
2	D	76	0	0	0	0
All	All	5483	0	5114	29	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 29 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:54[A]:ILE:HG21	1:B:18[A]:MET:SD	1.96	1.05
1:B:18[A]:MET:HG3	1:D:12:TYR:OH	1.68	0.93
1:A:54[A]:ILE:CG2	1:B:18[A]:MET:SD	2.59	0.89
1:D:59:ASP:OD2	1:D:61:ASN:ND2	2.15	0.79
1:B:12:TYR:OH	1:D:18[A]:MET:HG3	1.83	0.79

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	157/155 (101%)	157 (100%)	0	0	100	100
1	B	149/155 (96%)	147 (99%)	2 (1%)	0	100	100
1	C	159/155 (103%)	158 (99%)	1 (1%)	0	100	100
1	D	149/155 (96%)	146 (98%)	3 (2%)	0	100	100
All	All	614/620 (99%)	608 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	143/139 (103%)	141 (99%)	2 (1%)	67	34
1	B	137/139 (99%)	132 (96%)	5 (4%)	35	4
1	C	146/139 (105%)	142 (97%)	4 (3%)	44	9
1	D	137/139 (99%)	134 (98%)	3 (2%)	52	15
All	All	563/556 (101%)	549 (98%)	14 (2%)	49	10

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	72[A]	GLU
1	C	72[B]	GLU
1	D	118	LYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	D	50	LYS
1	D	103	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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	155/155 (100%)	0.05	0 100 100	15, 22, 36, 44	0
1	B	149/155 (96%)	0.29	10 (6%) 17 15	15, 21, 50, 66	0
1	C	155/155 (100%)	0.14	4 (2%) 56 54	14, 20, 34, 48	0
1	D	149/155 (96%)	0.13	4 (2%) 54 52	14, 21, 39, 49	0
All	All	608/620 (98%)	0.15	18 (2%) 50 48	14, 21, 39, 66	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	116	THR	5.0
1	B	115	ASP	3.9
1	D	116	THR	3.4
1	B	118	LYS	3.3
1	B	117	PHE	3.3

### 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.