



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 01:27 am BST

PDB ID : 2NVV  
Title : Crystal Structure of the Putative Acetyl-CoA hydrolase/transferase PG1013 from Porphyromonas gingivalis, Northeast Structural Genomics Target PgR16.  
Authors : Forouhar, F.; Neely, H.; Seetharaman, J.; Yong, W.; Ho, C.K.; Fang, Y.; Cunningham, K.; Ma, L.-C.; Xiao, R.; Liu, J.; Baran, M.C.; Acton, T.B.; Rost, B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2006-11-13  
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](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.

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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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

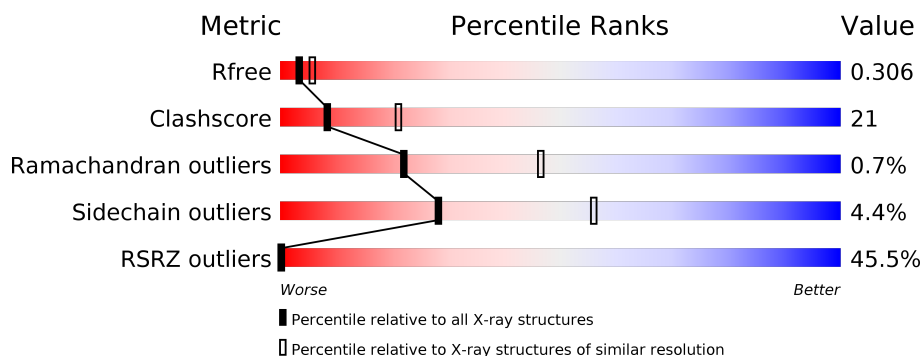
# 1 Overall quality at a glance

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  $\geq 3$ , 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	506	<div> <div>31%</div> <div>65%</div> <div>30%</div> <div>..</div> </div>
1	B	506	<div> <div>36%</div> <div>64%</div> <div>31%</div> <div>..</div> </div>
1	C	506	<div> <div>34%</div> <div>65%</div> <div>30%</div> <div>..</div> </div>
1	D	506	<div> <div>38%</div> <div>65%</div> <div>30%</div> <div>..</div> </div>
1	E	506	<div> <div>61%</div> <div>61%</div> <div>34%</div> <div>..</div> </div>
1	F	506	<div> <div>61%</div> <div>61%</div> <div>34%</div> <div>..</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23178 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 Acetyl-CoA hydrolase/transferase family protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	Se	0	0	0
			3828	2418	672	720	6	12			
1	B	496	Total	C	N	O	S	Se	0	0	0
			3828	2418	672	720	6	12			
1	C	496	Total	C	N	O	S	Se	0	0	0
			3828	2418	672	720	6	12			
1	D	496	Total	C	N	O	S	Se	0	0	0
			3828	2418	672	720	6	12			
1	E	496	Total	C	N	O	S	Se	0	0	0
			3828	2418	672	720	6	12			
1	F	496	Total	C	N	O	S	Se	0	0	0
			3828	2418	672	720	6	12			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
A	57	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
A	168	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
A	170	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
A	243	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
A	281	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
A	294	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
A	372	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
A	373	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
A	397	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
A	408	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
A	488	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
A	497	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
A	499	LEU	-	EXPRESSION TAG	UNP Q7MVN7
A	500	GLU	-	EXPRESSION TAG	UNP Q7MVN7
A	501	HIS	-	EXPRESSION TAG	UNP Q7MVN7
A	502	HIS	-	EXPRESSION TAG	UNP Q7MVN7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	503	HIS	-	EXPRESSION TAG	UNP Q7MVN7
A	504	HIS	-	EXPRESSION TAG	UNP Q7MVN7
A	505	HIS	-	EXPRESSION TAG	UNP Q7MVN7
A	506	HIS	-	EXPRESSION TAG	UNP Q7MVN7
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
B	57	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
B	168	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
B	170	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
B	243	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
B	281	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
B	294	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
B	372	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
B	373	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
B	397	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
B	408	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
B	488	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
B	497	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
B	499	LEU	-	EXPRESSION TAG	UNP Q7MVN7
B	500	GLU	-	EXPRESSION TAG	UNP Q7MVN7
B	501	HIS	-	EXPRESSION TAG	UNP Q7MVN7
B	502	HIS	-	EXPRESSION TAG	UNP Q7MVN7
B	503	HIS	-	EXPRESSION TAG	UNP Q7MVN7
B	504	HIS	-	EXPRESSION TAG	UNP Q7MVN7
B	505	HIS	-	EXPRESSION TAG	UNP Q7MVN7
B	506	HIS	-	EXPRESSION TAG	UNP Q7MVN7
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
C	57	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
C	168	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
C	170	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
C	243	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
C	281	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
C	294	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
C	372	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
C	373	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
C	397	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
C	408	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
C	488	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
C	497	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
C	499	LEU	-	EXPRESSION TAG	UNP Q7MVN7
C	500	GLU	-	EXPRESSION TAG	UNP Q7MVN7
C	501	HIS	-	EXPRESSION TAG	UNP Q7MVN7
C	502	HIS	-	EXPRESSION TAG	UNP Q7MVN7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	503	HIS	-	EXPRESSION TAG	UNP Q7MVN7
C	504	HIS	-	EXPRESSION TAG	UNP Q7MVN7
C	505	HIS	-	EXPRESSION TAG	UNP Q7MVN7
C	506	HIS	-	EXPRESSION TAG	UNP Q7MVN7
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
D	57	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
D	168	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
D	170	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
D	243	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
D	281	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
D	294	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
D	372	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
D	373	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
D	397	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
D	408	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
D	488	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
D	497	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
D	499	LEU	-	EXPRESSION TAG	UNP Q7MVN7
D	500	GLU	-	EXPRESSION TAG	UNP Q7MVN7
D	501	HIS	-	EXPRESSION TAG	UNP Q7MVN7
D	502	HIS	-	EXPRESSION TAG	UNP Q7MVN7
D	503	HIS	-	EXPRESSION TAG	UNP Q7MVN7
D	504	HIS	-	EXPRESSION TAG	UNP Q7MVN7
D	505	HIS	-	EXPRESSION TAG	UNP Q7MVN7
D	506	HIS	-	EXPRESSION TAG	UNP Q7MVN7
E	1	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
E	57	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
E	168	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
E	170	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
E	243	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
E	281	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
E	294	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
E	372	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
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E	397	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
E	408	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
E	488	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
E	497	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
E	499	LEU	-	EXPRESSION TAG	UNP Q7MVN7
E	500	GLU	-	EXPRESSION TAG	UNP Q7MVN7
E	501	HIS	-	EXPRESSION TAG	UNP Q7MVN7
E	502	HIS	-	EXPRESSION TAG	UNP Q7MVN7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	503	HIS	-	EXPRESSION TAG	UNP Q7MVN7
E	504	HIS	-	EXPRESSION TAG	UNP Q7MVN7
E	505	HIS	-	EXPRESSION TAG	UNP Q7MVN7
E	506	HIS	-	EXPRESSION TAG	UNP Q7MVN7
F	1	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
F	57	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
F	168	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
F	170	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
F	243	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
F	281	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
F	294	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
F	372	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
F	373	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
F	397	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
F	408	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
F	488	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
F	497	MSE	MET	MODIFIED RESIDUE	UNP Q7MVN7
F	499	LEU	-	EXPRESSION TAG	UNP Q7MVN7
F	500	GLU	-	EXPRESSION TAG	UNP Q7MVN7
F	501	HIS	-	EXPRESSION TAG	UNP Q7MVN7
F	502	HIS	-	EXPRESSION TAG	UNP Q7MVN7
F	503	HIS	-	EXPRESSION TAG	UNP Q7MVN7
F	504	HIS	-	EXPRESSION TAG	UNP Q7MVN7
F	505	HIS	-	EXPRESSION TAG	UNP Q7MVN7
F	506	HIS	-	EXPRESSION TAG	UNP Q7MVN7

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	E	2	Total Zn 2 2	0	0

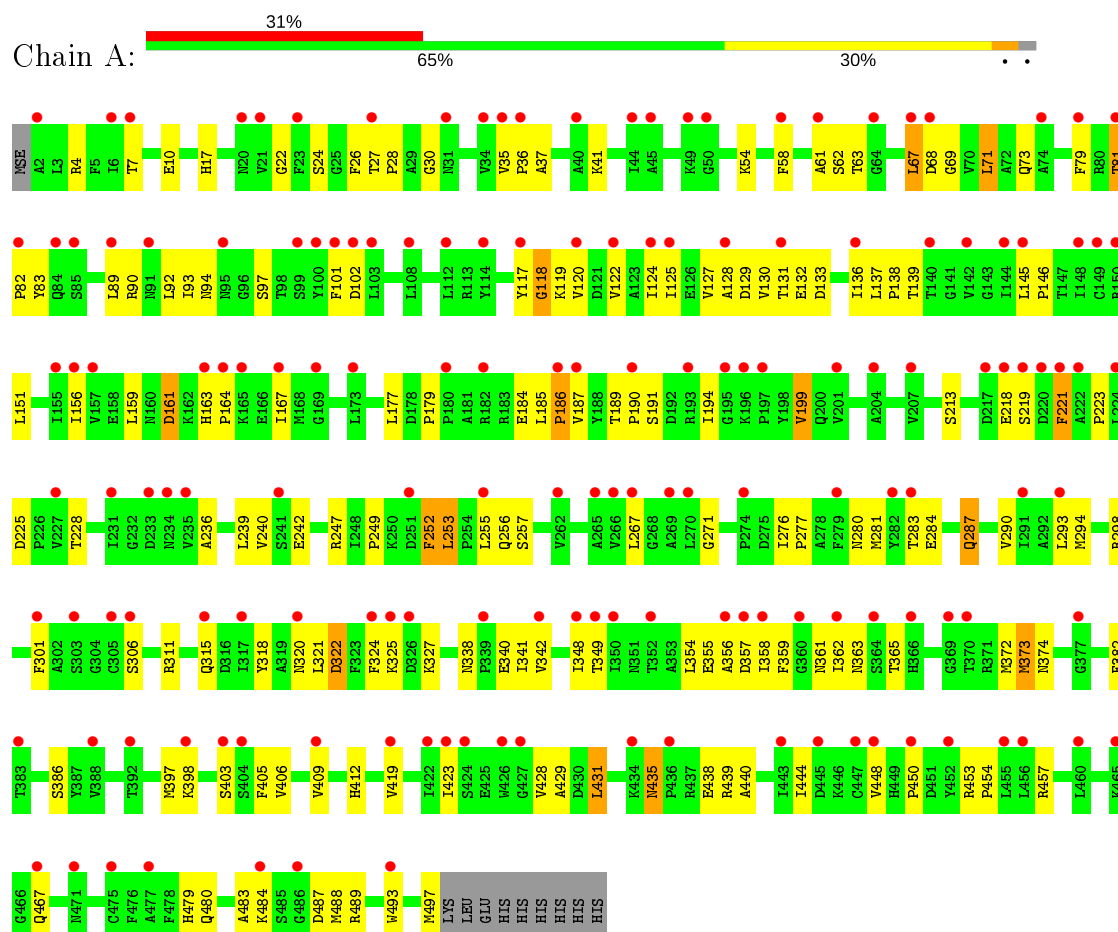
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total 30	O 30	0	0
3	B	22	Total 22	O 22	0	0
3	C	30	Total 30	O 30	0	0
3	D	23	Total 23	O 23	0	0
3	E	52	Total 52	O 52	0	0
3	F	47	Total 47	O 47	0	0

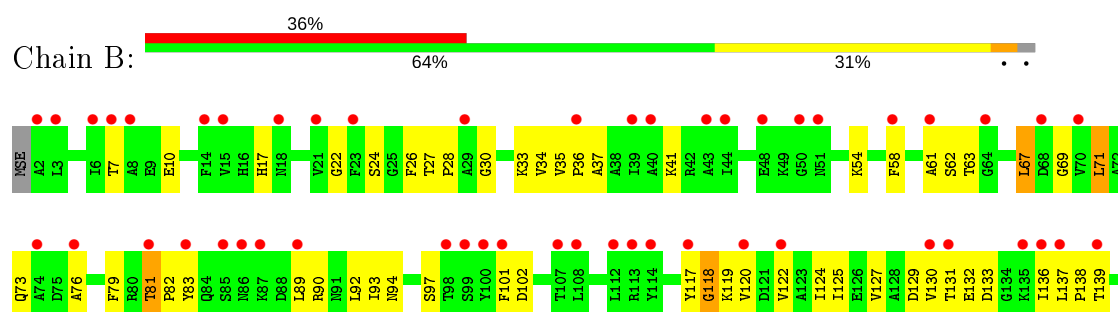
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

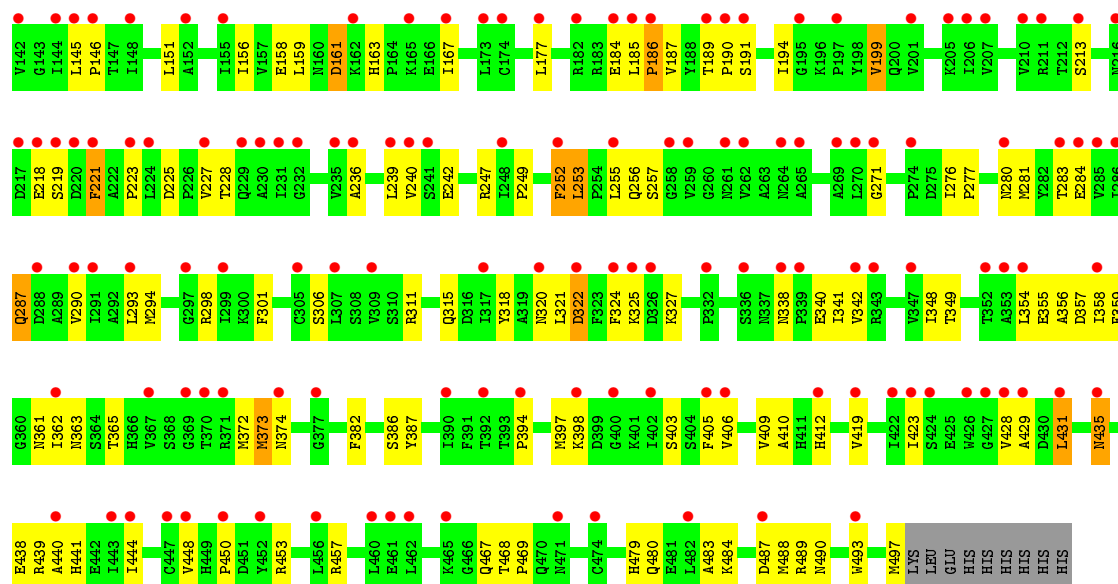
- Molecule 1: Acetyl-CoA hydrolase/transferase family protein



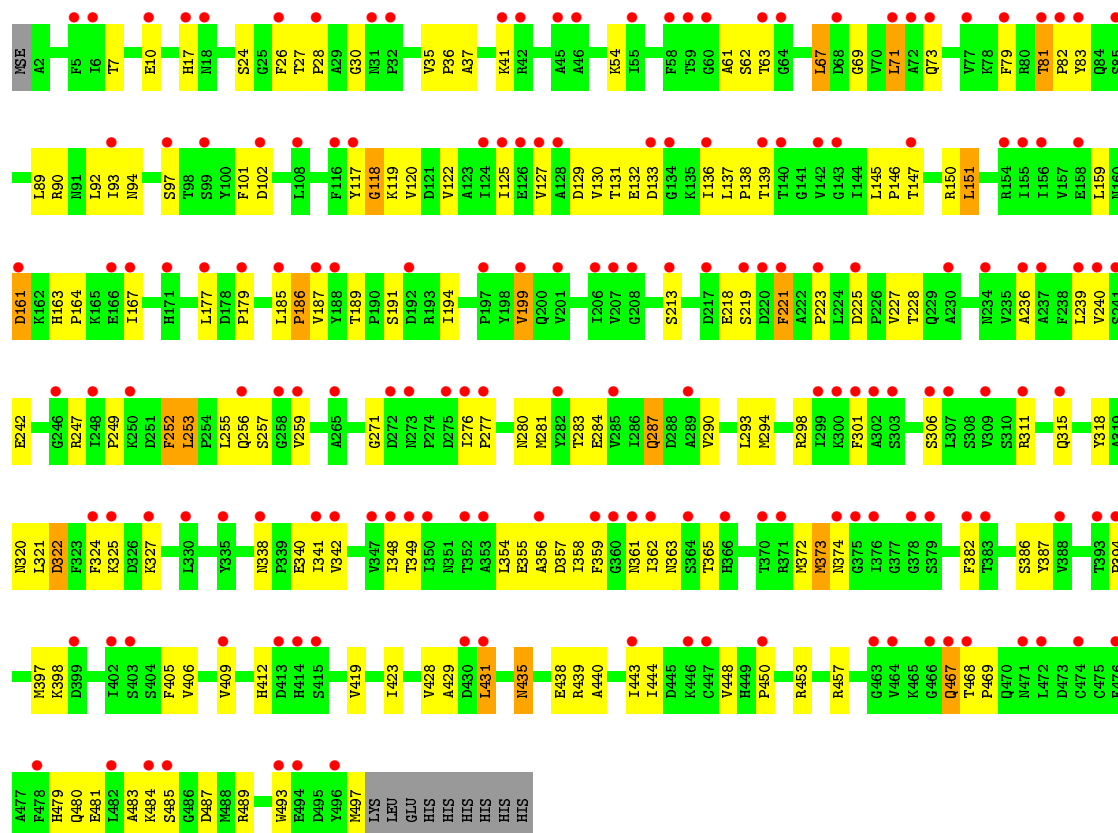
- Molecule 1: Acetyl-CoA hydrolase/transferase family protein



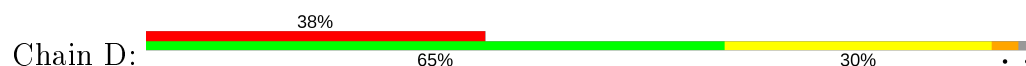


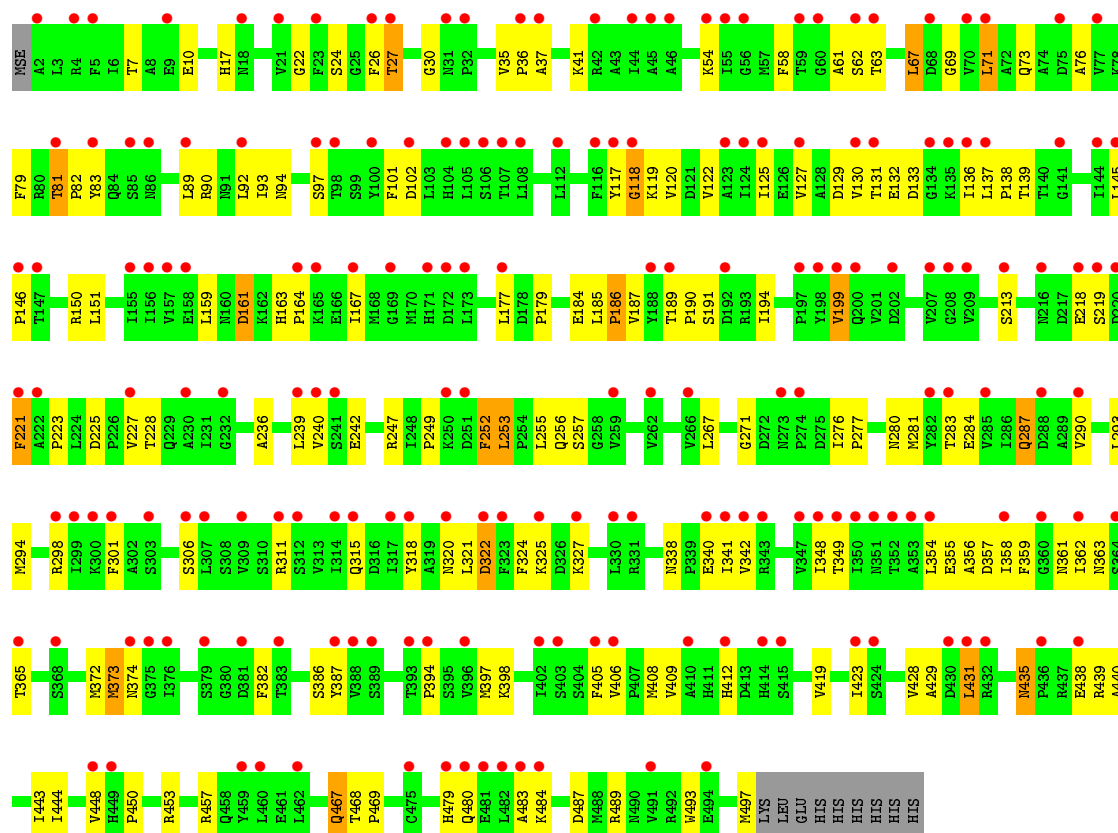


• Molecule 1: Acetyl-CoA hydrolase/transferase family protein

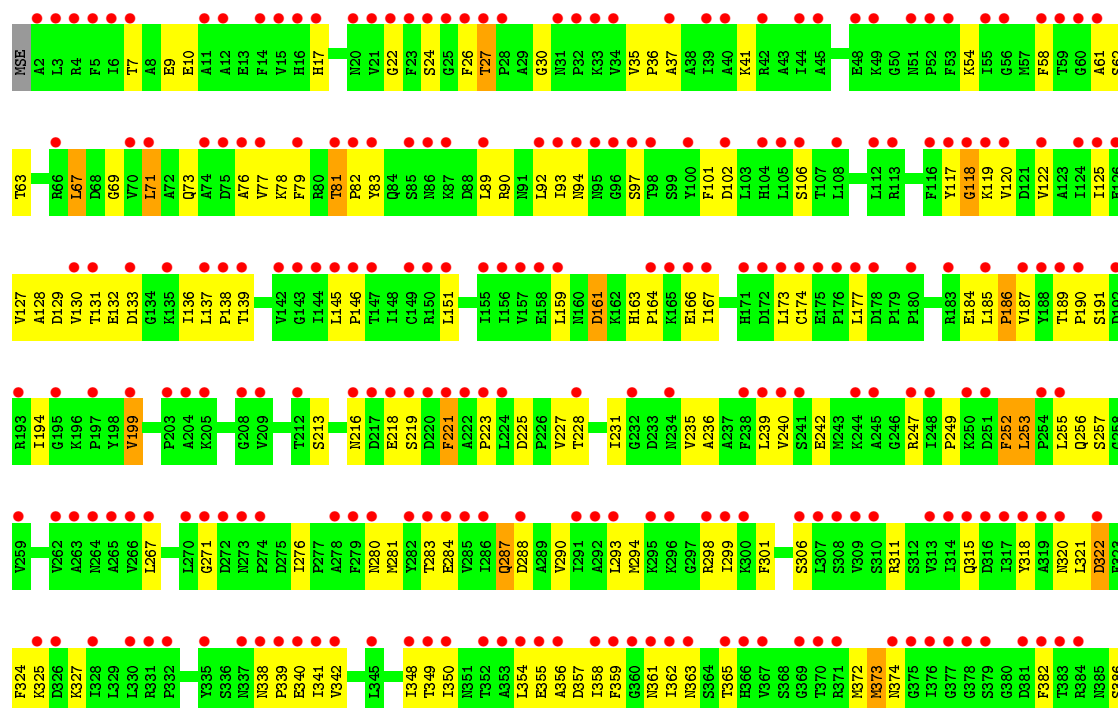


• Molecule 1: Acetyl-CoA hydrolase/transferase family protein





• Molecule 1: Acetyl-CoA hydrolase/transferase family protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.05Å 131.05Å 162.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.95 – 2.70 29.46 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.0 (19.95-2.70) 52.4 (29.46-2.40)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.63 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1, XTALVIEW	Depositor
R, $R_{free}$	0.287 , 0.290 0.307 , 0.306	Depositor DCC
$R_{free}$ test set	8375 reflections (6.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.0	Xtriage
Anisotropy	0.582	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , -5.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l 0.499 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
Reported twinning fraction	0.012 for H, K, L 0.496 for -H, H+K, -L 0.492 for -h,-k,l	Depositor
Outliers	0 of 121779 reflections	Xtriage
$F_o, F_c$ correlation	0.77	EDS
Total number of atoms	23178	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	9.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% 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](#)

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

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	0.38	0/3898	0.66	0/5269
1	B	0.38	0/3898	0.66	0/5269
1	C	0.38	0/3898	0.66	0/5269
1	D	0.38	0/3898	0.66	0/5269
1	E	0.40	0/3898	0.65	0/5269
1	F	0.40	0/3898	0.66	0/5269
All	All	0.39	0/23388	0.66	0/31614

There are no bond length outliers.

There are no bond angle outliers.

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	3828	0	3808	155	0
1	B	3828	0	3808	154	0
1	C	3828	0	3808	150	0
1	D	3828	0	3808	154	0
1	E	3828	0	3808	173	0
1	F	3828	0	3808	191	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
3	A	30	0	0	10	0
3	B	22	0	0	9	0
3	C	30	0	0	2	0
3	D	23	0	0	2	0
3	E	52	0	0	20	0
3	F	47	0	0	30	0
All	All	23178	0	22848	957	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 21.

The worst 5 of 957 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:298:ARG:HB2	3:A:516:HOH:O	1.58	1.03
1:F:419:VAL:HG12	3:F:517:HOH:O	1.67	0.94
1:E:136:ILE:HB	1:E:199:VAL:HG13	1.50	0.93
1:F:136:ILE:HB	1:F:199:VAL:HG13	1.51	0.92
1:A:94:ASN:HD21	1:A:372:MSE:H	1.18	0.91

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	494/506 (98%)	458 (93%)	33 (7%)	3 (1%)	25 50
1	B	494/506 (98%)	462 (94%)	29 (6%)	3 (1%)	25 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	494/506 (98%)	460 (93%)	31 (6%)	3 (1%)	25	50
1	D	494/506 (98%)	461 (93%)	29 (6%)	4 (1%)	19	43
1	E	494/506 (98%)	461 (93%)	29 (6%)	4 (1%)	19	43
1	F	494/506 (98%)	460 (93%)	30 (6%)	4 (1%)	19	43
All	All	2964/3036 (98%)	2762 (93%)	181 (6%)	21 (1%)	22	46

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	GLY
1	A	221	PHE
1	B	118	GLY
1	B	221	PHE
1	C	118	GLY

### 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	416/413 (101%)	398 (96%)	18 (4%)	29	57
1	B	416/413 (101%)	398 (96%)	18 (4%)	29	57
1	C	416/413 (101%)	397 (95%)	19 (5%)	27	54
1	D	416/413 (101%)	397 (95%)	19 (5%)	27	54
1	E	416/413 (101%)	398 (96%)	18 (4%)	29	57
1	F	416/413 (101%)	398 (96%)	18 (4%)	29	57
All	All	2496/2478 (101%)	2386 (96%)	110 (4%)	28	56

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	287	GLN
1	D	159	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	239	LEU
1	C	373	MSE
1	D	67	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 109 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	467	GLN
1	D	264	ASN
1	F	280	ASN
1	C	479	HIS
1	D	51	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.



## 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	484/506 (95%)	1.75	159 (32%) 0 0	6, 7, 18, 30	0
1	B	484/506 (95%)	1.82	184 (38%) 0 0	6, 7, 18, 30	0
1	C	484/506 (95%)	1.75	170 (35%) 0 0	6, 7, 18, 30	0
1	D	484/506 (95%)	1.91	191 (39%) 0 0	6, 7, 18, 30	0
1	E	484/506 (95%)	2.58	310 (64%) 0 0	6, 7, 18, 30	0
1	F	484/506 (95%)	2.62	307 (63%) 0 0	6, 7, 18, 30	0
All	All	2904/3036 (95%)	2.07	1321 (45%) 0 0	6, 7, 18, 30	0

The worst 5 of 1321 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	427	GLY	8.4
1	F	134	GLY	7.5
1	F	232	GLY	7.2
1	C	85	SER	6.9
1	F	299	ILE	6.8

### 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 carbohydrates in this entry.

## 6.4 Ligands [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	ZN	D	507	1/1	0.85	0.10	17,17,17,17	0
2	ZN	E	508	1/1	0.86	0.10	25,25,25,25	0
2	ZN	A	507	1/1	0.87	0.09	16,16,16,16	0
2	ZN	B	507	1/1	0.89	0.09	20,20,20,20	0
2	ZN	C	507	1/1	0.94	0.10	18,18,18,18	0
2	ZN	E	507	1/1	0.97	0.07	15,15,15,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.