



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 1, 2026 – 06:11 PM JST

PDB ID : 9VAG / pdb\_00009vag  
Title : Crystal structure of CoA transferase from *Thermus thermophilus*  
Authors : Yoshida, A.; Yamamoto, H.; Nishiyama, M.  
Deposited on : 2025-06-03  
Resolution : 2.63 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

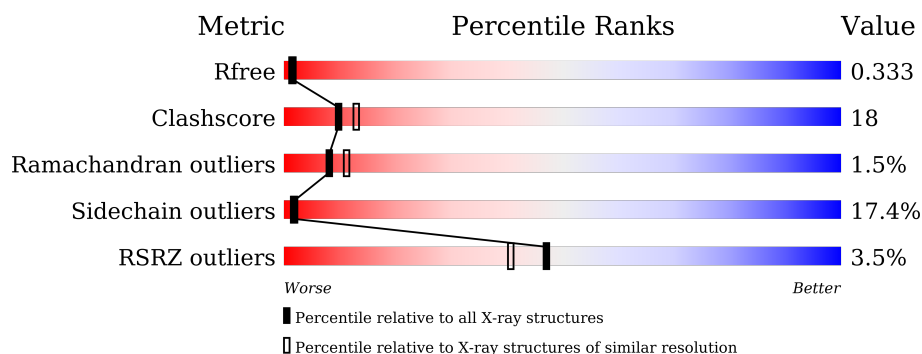
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.63 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))
$R_{free}$	180053	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	450	
1	B	450	
1	C	450	
1	D	450	
1	E	450	
1	F	450	

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Mol	Chain	Length	Quality of chain
1	G	450	<div><div></div><div>5%</div><div>50%</div><div>31%</div><div>11%</div><div>•</div><div>6%</div></div>
1	H	450	<div><div></div><div>2%</div><div>52%</div><div>30%</div><div>9%</div><div>•</div><div>6%</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25802 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-hydroxybutyrate coenzyme A transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	422	Total	C	N	O	S	0	0	0
			3216	2048	574	584	10			
1	H	423	Total	C	N	O	S	0	0	0
			3206	2041	574	581	10			
1	A	426	Total	C	N	O	S	0	3	0
			3277	2086	589	592	10			
1	B	422	Total	C	N	O	S	0	0	0
			3197	2031	574	582	10			
1	C	422	Total	C	N	O	S	0	2	0
			3226	2052	577	587	10			
1	D	423	Total	C	N	O	S	0	0	0
			3217	2050	572	585	10			
1	E	421	Total	C	N	O	S	0	1	0
			3196	2035	571	580	10			
1	G	424	Total	C	N	O	S	0	0	0
			3211	2047	570	584	10			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	445	HIS	-	expression tag	UNP Q72IP9
F	446	HIS	-	expression tag	UNP Q72IP9
F	447	HIS	-	expression tag	UNP Q72IP9
F	448	HIS	-	expression tag	UNP Q72IP9
F	449	HIS	-	expression tag	UNP Q72IP9
F	450	HIS	-	expression tag	UNP Q72IP9
H	445	HIS	-	expression tag	UNP Q72IP9
H	446	HIS	-	expression tag	UNP Q72IP9
H	447	HIS	-	expression tag	UNP Q72IP9
H	448	HIS	-	expression tag	UNP Q72IP9
H	449	HIS	-	expression tag	UNP Q72IP9
H	450	HIS	-	expression tag	UNP Q72IP9
A	445	HIS	-	expression tag	UNP Q72IP9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	446	HIS	-	expression tag	UNP Q72IP9
A	447	HIS	-	expression tag	UNP Q72IP9
A	448	HIS	-	expression tag	UNP Q72IP9
A	449	HIS	-	expression tag	UNP Q72IP9
A	450	HIS	-	expression tag	UNP Q72IP9
B	445	HIS	-	expression tag	UNP Q72IP9
B	446	HIS	-	expression tag	UNP Q72IP9
B	447	HIS	-	expression tag	UNP Q72IP9
B	448	HIS	-	expression tag	UNP Q72IP9
B	449	HIS	-	expression tag	UNP Q72IP9
B	450	HIS	-	expression tag	UNP Q72IP9
C	445	HIS	-	expression tag	UNP Q72IP9
C	446	HIS	-	expression tag	UNP Q72IP9
C	447	HIS	-	expression tag	UNP Q72IP9
C	448	HIS	-	expression tag	UNP Q72IP9
C	449	HIS	-	expression tag	UNP Q72IP9
C	450	HIS	-	expression tag	UNP Q72IP9
D	445	HIS	-	expression tag	UNP Q72IP9
D	446	HIS	-	expression tag	UNP Q72IP9
D	447	HIS	-	expression tag	UNP Q72IP9
D	448	HIS	-	expression tag	UNP Q72IP9
D	449	HIS	-	expression tag	UNP Q72IP9
D	450	HIS	-	expression tag	UNP Q72IP9
E	445	HIS	-	expression tag	UNP Q72IP9
E	446	HIS	-	expression tag	UNP Q72IP9
E	447	HIS	-	expression tag	UNP Q72IP9
E	448	HIS	-	expression tag	UNP Q72IP9
E	449	HIS	-	expression tag	UNP Q72IP9
E	450	HIS	-	expression tag	UNP Q72IP9
G	445	HIS	-	expression tag	UNP Q72IP9
G	446	HIS	-	expression tag	UNP Q72IP9
G	447	HIS	-	expression tag	UNP Q72IP9
G	448	HIS	-	expression tag	UNP Q72IP9
G	449	HIS	-	expression tag	UNP Q72IP9
G	450	HIS	-	expression tag	UNP Q72IP9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total O 1 1	0	0
2	A	11	Total O 11 11	0	0

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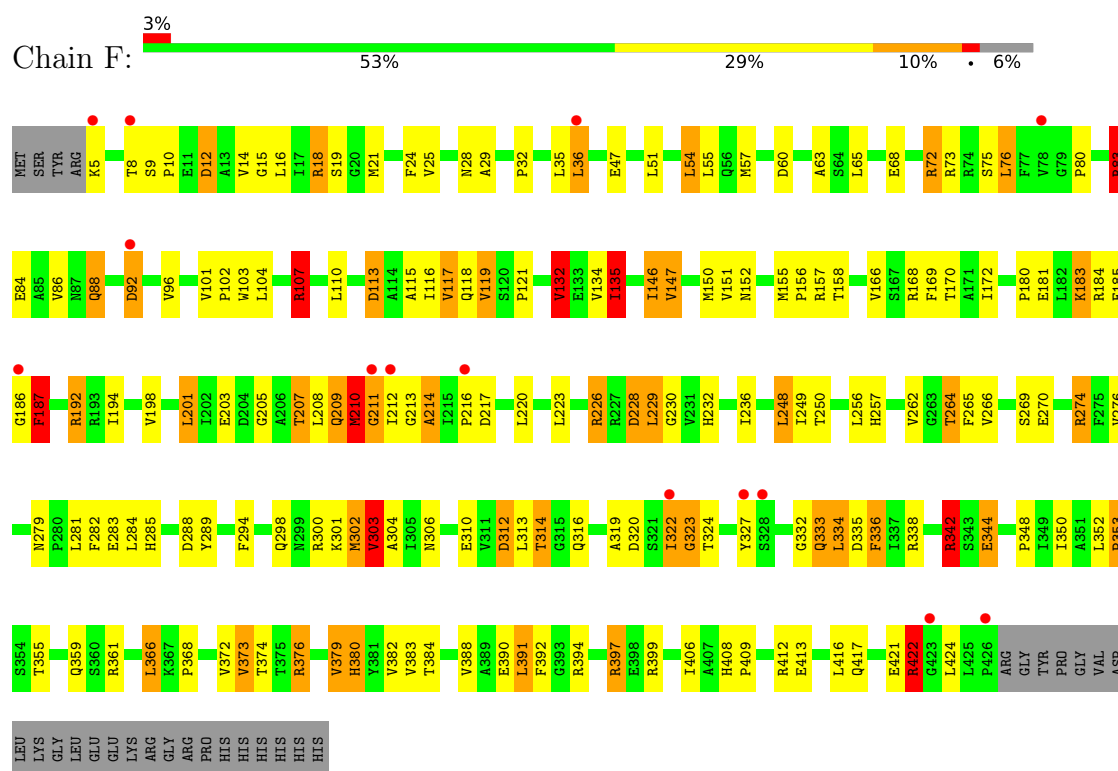
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	13	Total 13	O 13	0	0
2	C	13	Total 13	O 13	0	0
2	D	7	Total 7	O 7	0	0
2	E	8	Total 8	O 8	0	0
2	G	3	Total 3	O 3	0	0

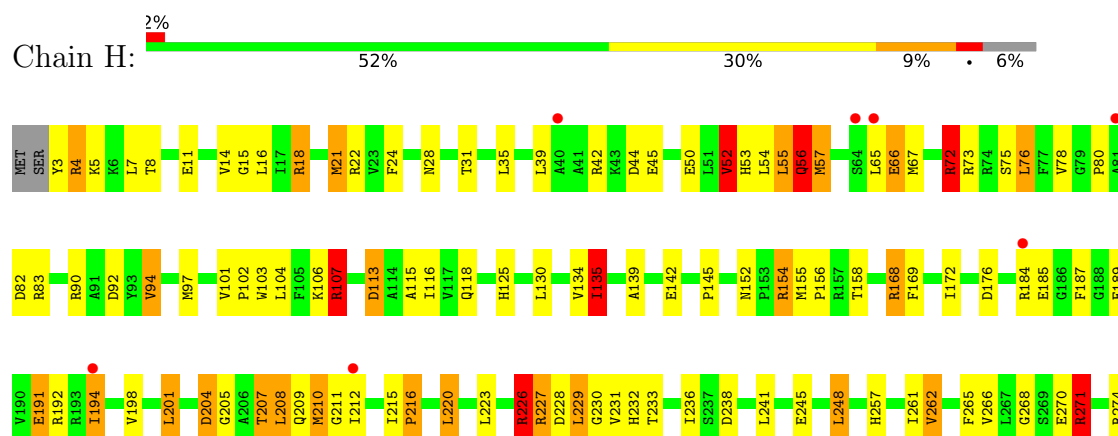
### 3 Residue-property plots [i](#)

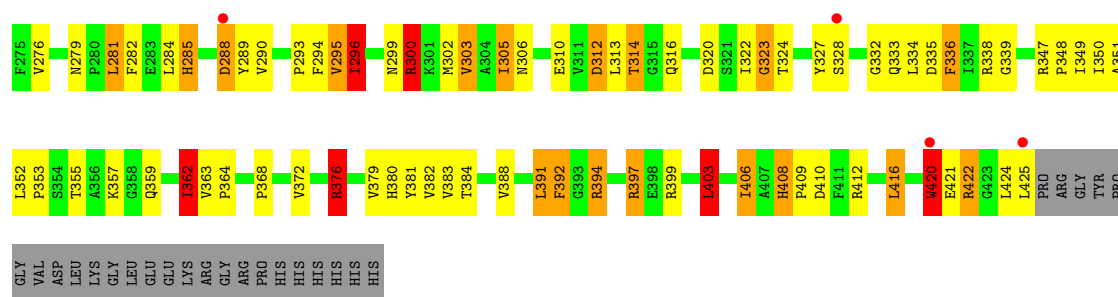
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 4-hydroxybutyrate coenzyme A transferase

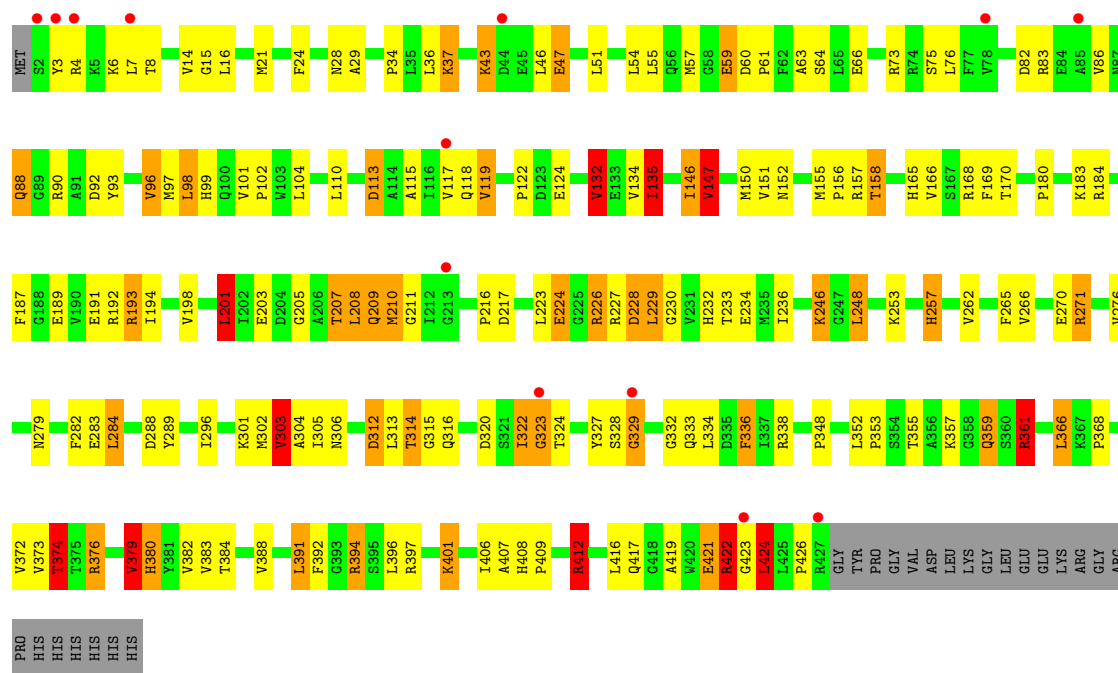


- Molecule 1: 4-hydroxybutyrate coenzyme A transferase

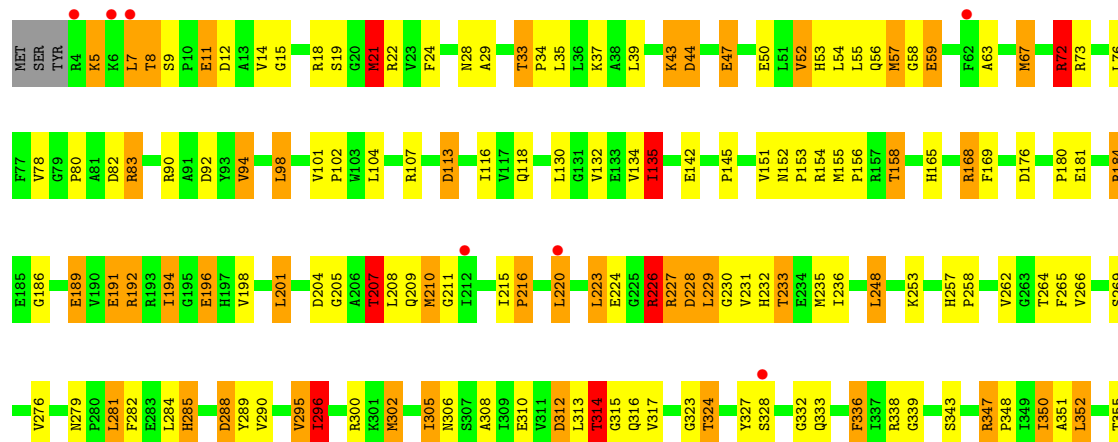




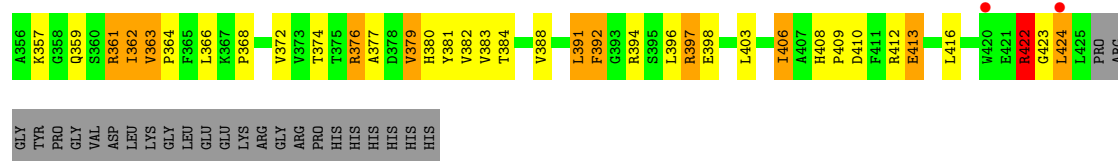
• Molecule 1: 4-hydroxybutyrate coenzyme A transferase



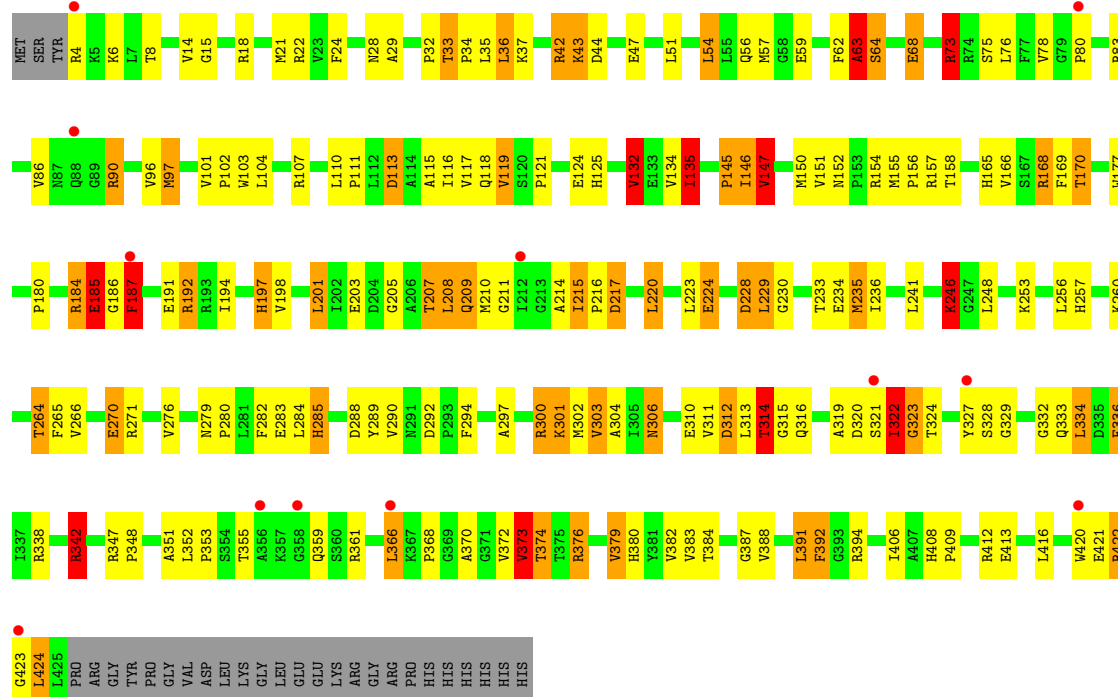
• Molecule 1: 4-hydroxybutyrate coenzyme A transferase



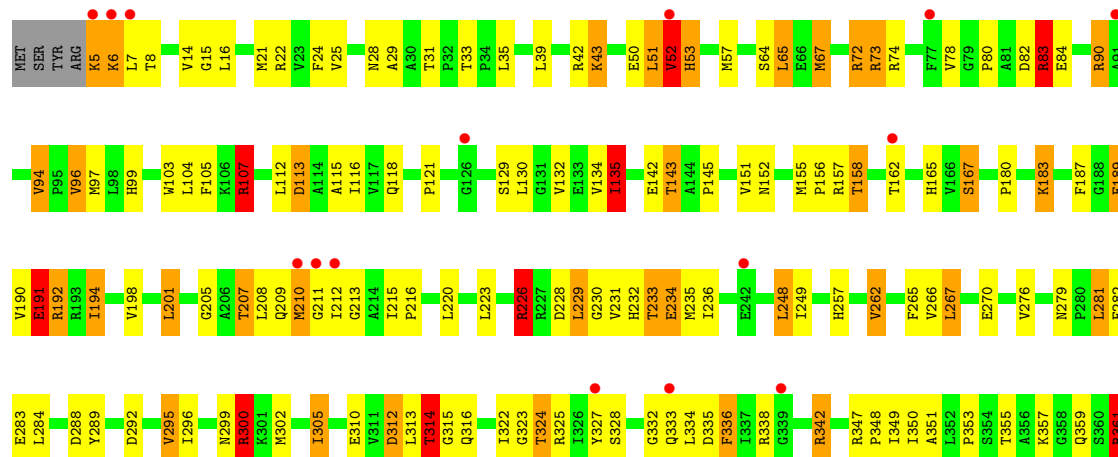


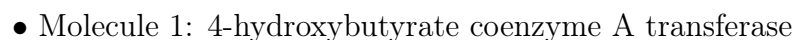
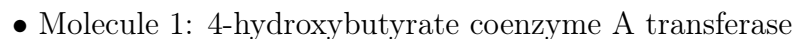


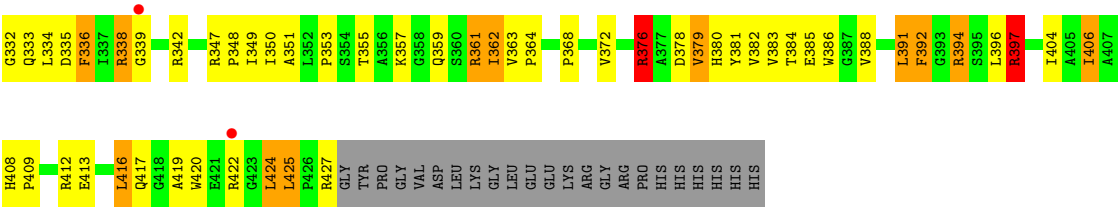
• Molecule 1: 4-hydroxybutyrate coenzyme A transferase



• Molecule 1: 4-hydroxybutyrate coenzyme A transferase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.34Å 147.38Å 171.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.26 – 2.63 47.26 – 2.63	Depositor EDS
% Data completeness (in resolution range)	97.4 (47.26-2.63) 97.4 (47.26-2.63)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, $R_{free}$	0.283 , 0.347 0.275 , 0.333	Depositor DCC
$R_{free}$ test set	5326 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.6	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 33.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.57$ , $\langle L^2 \rangle = 0.41$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	25802	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.18 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.7077e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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	0.97	5/3348 (0.1%)	1.68	66/4547 (1.5%)
1	B	0.96	0/3265	1.66	52/4437 (1.2%)
1	C	0.96	2/3298 (0.1%)	1.72	69/4478 (1.5%)
1	D	0.97	2/3287 (0.1%)	1.67	59/4468 (1.3%)
1	E	0.97	0/3266	1.70	65/4439 (1.5%)
1	F	0.98	1/3286 (0.0%)	1.71	72/4465 (1.6%)
1	G	0.95	1/3281 (0.0%)	1.68	46/4461 (1.0%)
1	H	0.96	1/3275 (0.0%)	1.68	54/4452 (1.2%)
All	All	0.96	12/26306 (0.0%)	1.69	483/35747 (1.4%)

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	A	0	8
1	B	0	9
1	C	0	12
1	D	0	12
1	E	0	12
1	F	0	6
1	G	0	12
1	H	0	11
All	All	0	82

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	322	ILE	C-O	-6.25	1.16	1.24
1	A	422	ARG	NE-CZ	5.94	1.39	1.33
1	F	312	ASP	CG-OD2	5.58	1.35	1.25
1	A	99	HIS	ND1-CE1	5.53	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	99	HIS	CG-CD2	-5.43	1.29	1.35

The worst 5 of 483 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	97	MET	CG-SD-CE	13.98	131.67	100.90
1	C	42	ARG	NE-CZ-NH2	13.60	131.44	119.20
1	E	42	ARG	NE-CZ-NH1	-13.38	108.12	121.50
1	C	288	ASP	CA-CB-CG	12.58	125.18	112.60
1	F	288	ASP	CA-CB-CG	12.46	125.06	112.60

There are no chirality outliers.

5 of 82 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	107	ARG	Sidechain
1	F	157	ARG	Sidechain
1	F	18	ARG	Sidechain
1	F	184	ARG	Sidechain
1	F	83	ARG	Sidechain

## 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	3277	0	3288	99	0
1	B	3197	0	3198	126	0
1	C	3226	0	3238	122	0
1	D	3217	0	3232	115	0
1	E	3196	0	3187	114	0
1	F	3216	0	3234	123	0
1	G	3211	0	3214	141	0
1	H	3206	0	3210	123	0
2	A	11	0	0	1	0
2	B	13	0	0	3	0
2	C	13	0	0	1	0
2	D	7	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	8	0	0	1	0
2	G	3	0	0	0	0
2	H	1	0	0	0	0
All	All	25802	0	25801	907	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 18.

The worst 5 of 907 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:139:ALA:O	1:G:143:THR:HG22	1.44	1.16
1:B:423:GLY:O	1:B:424:LEU:HG	1.47	1.12
1:A:333:GLN:HE21	1:A:374:THR:CG2	1.64	1.10
1:H:399:ARG:O	1:H:403:LEU:HD22	1.51	1.09
1:C:333:GLN:HE21	1:C:374:THR:CG2	1.66	1.08

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	427/450 (95%)	392 (92%)	29 (7%)	6 (1%)	9	12
1	B	420/450 (93%)	378 (90%)	37 (9%)	5 (1%)	10	15
1	C	422/450 (94%)	385 (91%)	29 (7%)	8 (2%)	6	8
1	D	421/450 (94%)	382 (91%)	33 (8%)	6 (1%)	9	12
1	E	420/450 (93%)	383 (91%)	31 (7%)	6 (1%)	9	12
1	F	420/450 (93%)	383 (91%)	31 (7%)	6 (1%)	9	12
1	G	422/450 (94%)	382 (90%)	32 (8%)	8 (2%)	6	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	421/450 (94%)	383 (91%)	31 (7%)	7 (2%)	7	9
All	All	3373/3600 (94%)	3068 (91%)	253 (8%)	52 (2%)	8	11

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	135	ILE
1	F	323	GLY
1	H	55	LEU
1	H	56	GLN
1	H	135	ILE

### 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	337/362 (93%)	280 (83%)	57 (17%)	2	2
1	B	328/362 (91%)	270 (82%)	58 (18%)	2	2
1	C	333/362 (92%)	277 (83%)	56 (17%)	2	2
1	D	333/362 (92%)	272 (82%)	61 (18%)	2	1
1	E	327/362 (90%)	274 (84%)	53 (16%)	2	2
1	F	333/362 (92%)	280 (84%)	53 (16%)	2	2
1	G	330/362 (91%)	264 (80%)	66 (20%)	1	1
1	H	329/362 (91%)	272 (83%)	57 (17%)	2	2
All	All	2650/2896 (92%)	2189 (83%)	461 (17%)	2	2

5 of 461 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	54	LEU
1	G	296	ILE
1	D	25	VAL
1	G	248	LEU

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Mol	Chain	Res	Type
1	G	33	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	316	GLN
1	E	28	ASN
1	C	359	GLN
1	D	257	HIS
1	E	232	HIS

### 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 oligosaccharides 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	426/450 (94%)	0.46	13 (3%) 51 45	19, 48, 87, 112	3 (0%)
1	B	422/450 (93%)	0.44	9 (2%) 63 59	25, 47, 82, 124	0
1	C	422/450 (93%)	0.48	12 (2%) 55 50	19, 45, 78, 113	2 (0%)
1	D	423/450 (94%)	0.54	17 (4%) 42 35	27, 48, 86, 119	0
1	E	421/450 (93%)	0.46	20 (4%) 35 29	19, 45, 75, 125	1 (0%)
1	F	422/450 (93%)	0.47	14 (3%) 49 43	21, 48, 78, 117	0
1	G	424/450 (94%)	0.65	23 (5%) 31 26	28, 50, 85, 123	0
1	H	423/450 (94%)	0.50	11 (2%) 57 52	27, 49, 79, 120	0
All	All	3383/3600 (93%)	0.50	119 (3%) 47 41	19, 48, 82, 125	6 (0%)

The worst 5 of 119 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	212	ILE	4.6
1	G	328	SER	4.5
1	F	212	ILE	4.4
1	G	82	ASP	4.3
1	D	212	ILE	4.3

### 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 oligosaccharides 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.