



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 9, 2016 – 08:46 AM EDT

PDB ID : 5BZ4  
Title : Crystal structure of a T1-like thiolase (CoA-complex) from Mycobacterium smegmatis  
Authors : Janardan, N.; Harijan, R.K.; Kiema, T.R.; Wierenga, R.K.; Murthy, M.R.N.  
Deposited on : 2015-06-11  
Resolution : 2.43 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  
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027457  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

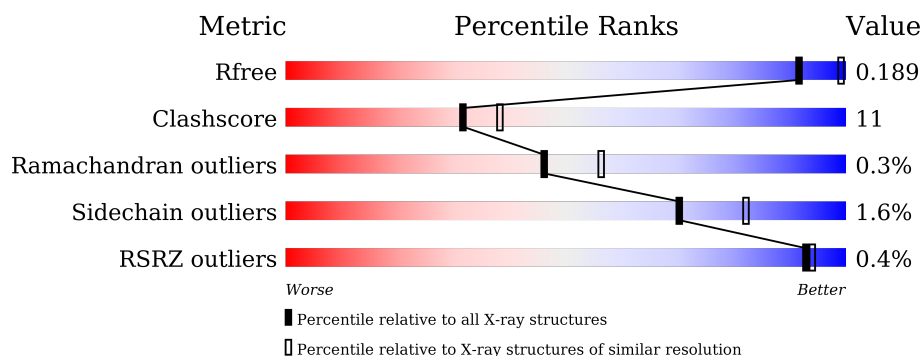
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.43 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))
$R_{free}$	91344	1003 (2.46-2.42)
Clashscore	102246	1071 (2.46-2.42)
Ramachandran outliers	100387	1065 (2.46-2.42)
Sidechain outliers	100360	1065 (2.46-2.42)
RSRZ outliers	91569	1005 (2.46-2.42)

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. 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	407	<div> <div style="width: 76%;">76%</div> <div style="width: 22%;">22%</div> <div style="width: 2%;">.</div> </div>
1	B	407	<div> <div style="width: 77%;">77%</div> <div style="width: 20%;">20%</div> <div style="width: 3%;">..</div> </div>
1	C	407	<div> <div style="width: 77%;">77%</div> <div style="width: 19%;">19%</div> <div style="width: 4%;">..</div> </div>
1	D	407	<div> <div style="width: 76%;">76%</div> <div style="width: 21%;">21%</div> <div style="width: 3%;">.</div> </div>
1	E	407	<div> <div style="width: 76%;">76%</div> <div style="width: 20%;">20%</div> <div style="width: 4%;">..</div> </div>
1	F	407	<div> <div style="width: 78%;">78%</div> <div style="width: 20%;">20%</div> <div style="width: 2%;">.</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	407	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>..</div> </div> </div>
1	H	407	<div> <div></div> <div>78%</div> <div>19%</div> <div>.</div> </div>
1	J	407	<div> <div></div> <div>75%</div> <div>22%</div> <div>.</div> </div>
1	K	407	<div> <div></div> <div>77%</div> <div>20%</div> <div>.</div> </div>
1	L	407	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>..</div> </div> </div>
1	M	407	<div> <div></div> <div>71%</div> <div>27%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	COA	B	501	-	-	-	X
2	COA	D	501	-	-	-	X
2	COA	H	501	-	-	-	X
2	COA	K	501	-	-	-	X

## 2 Entry composition

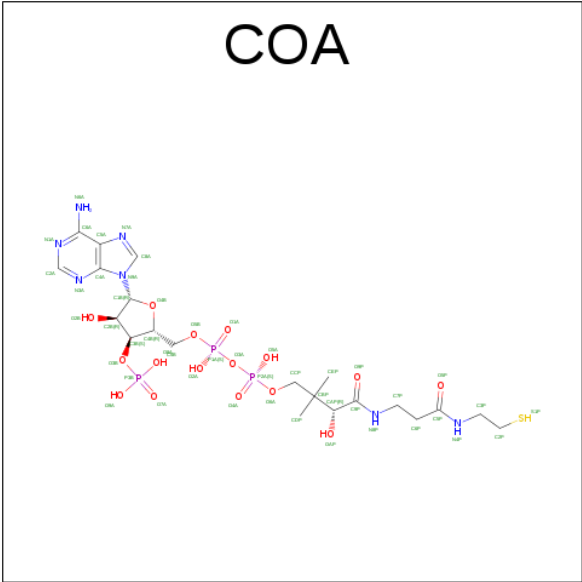
There are 3 unique types of molecules in this entry. The entry contains 36925 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Beta-ketothiolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	1	0
			2912	1802	538	556	16			
1	B	398	Total	C	N	O	S	0	0	0
			2926	1813	537	560	16			
1	C	398	Total	C	N	O	S	0	0	0
			2903	1798	529	560	16			
1	D	397	Total	C	N	O	S	0	0	0
			2923	1811	536	560	16			
1	E	396	Total	C	N	O	S	0	0	0
			2918	1805	536	561	16			
1	F	399	Total	C	N	O	S	0	0	0
			2946	1824	541	565	16			
1	G	402	Total	C	N	O	S	0	0	0
			2956	1829	544	567	16			
1	H	397	Total	C	N	O	S	0	0	0
			2929	1813	539	561	16			
1	J	396	Total	C	N	O	S	0	0	0
			2905	1798	536	555	16			
1	K	400	Total	C	N	O	S	0	0	0
			2943	1821	540	566	16			
1	L	400	Total	C	N	O	S	0	0	0
			2929	1808	541	564	16			
1	M	397	Total	C	N	O	S	0	0	0
			2921	1808	536	561	16			

- Molecule 2 is COENZYME A (three-letter code: COA) (formula:  $C_{21}H_{36}N_7O_{16}P_3S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
2	D	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
2	F	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
2	H	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
2	K	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	141	Total	O	0	0
			141	141		
3	B	167	Total	O	0	0
			167	167		
3	C	147	Total	O	0	0
			147	147		
3	D	145	Total	O	0	0
			145	145		
3	E	110	Total	O	0	0
			110	110		
3	F	114	Total	O	0	0
			114	114		
3	G	121	Total	O	0	0
			121	121		

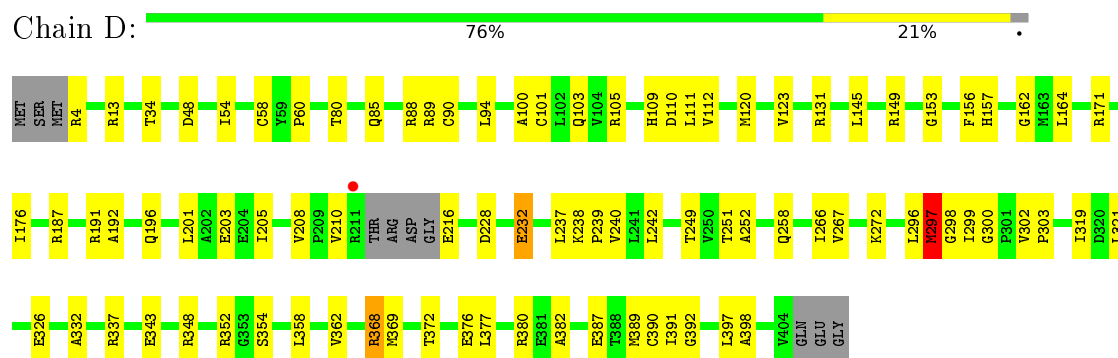
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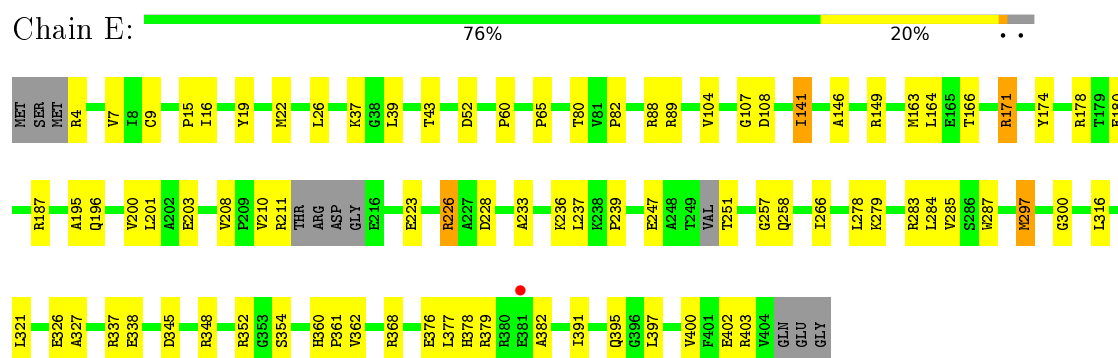
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	159	Total 159	O 159	0	0
3	J	110	Total 110	O 110	0	0
3	K	152	Total 152	O 152	0	0
3	L	106	Total 106	O 106	0	0
3	M	102	Total 102	O 102	0	0



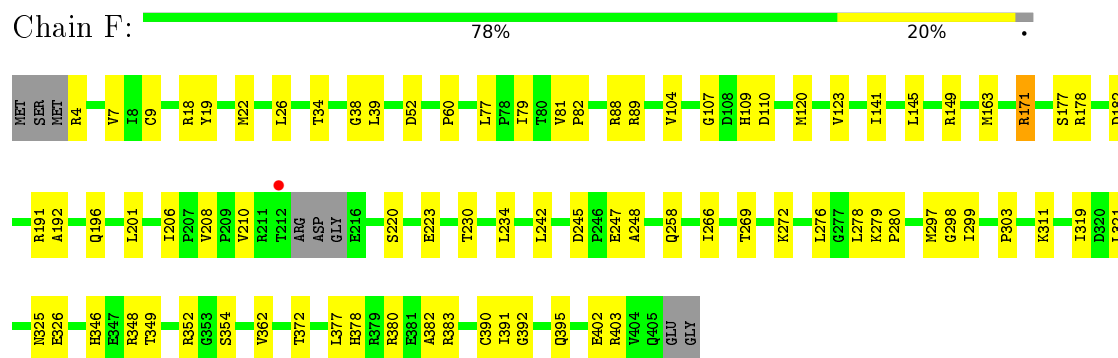
- Molecule 1: Beta-ketothiolase



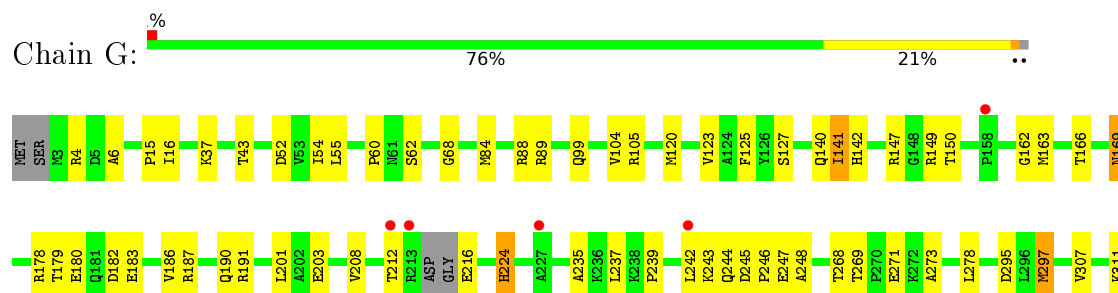
- Molecule 1: Beta-ketothiolase



- Molecule 1: Beta-ketothiolase



- Molecule 1: Beta-ketothiolase

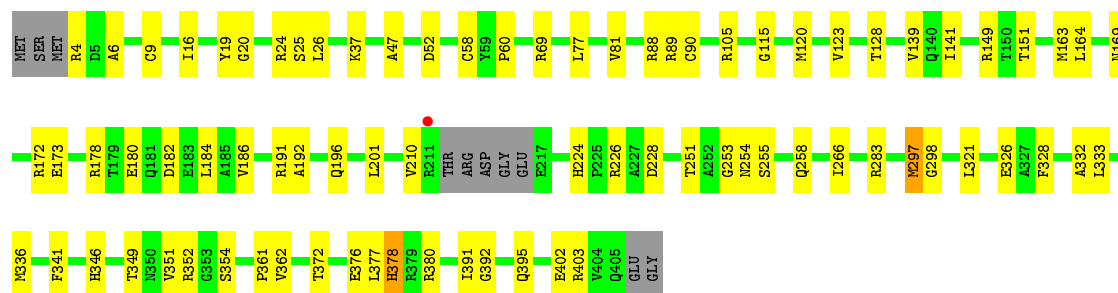






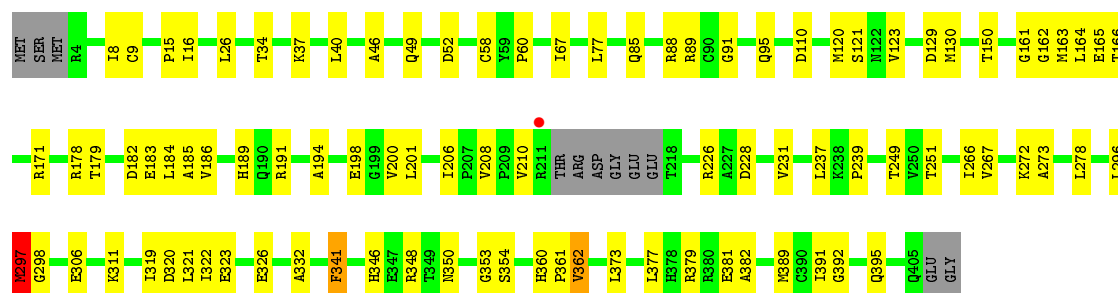
- Molecule 1: Beta-ketothiolase

Chain H: 78% 19%



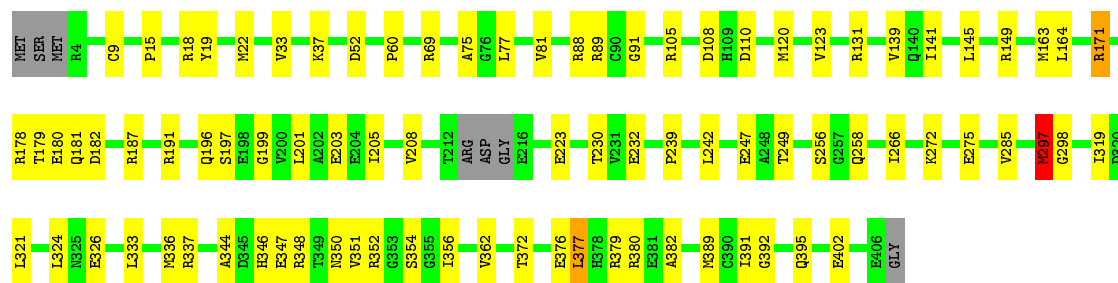
- Molecule 1: Beta-ketothiolase

Chain J: 75% 22%



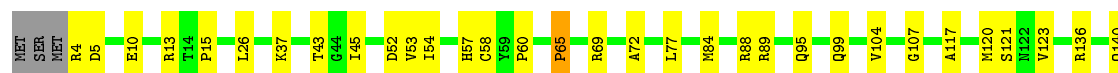
- Molecule 1: Beta-ketothiolase

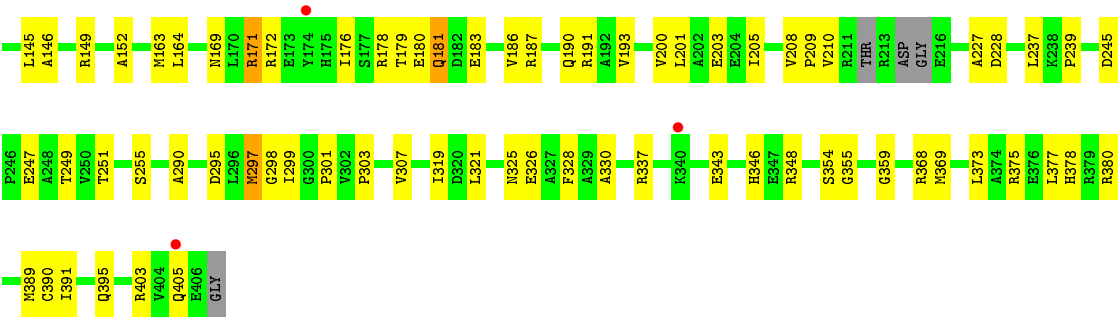
Chain K: 77% 20%



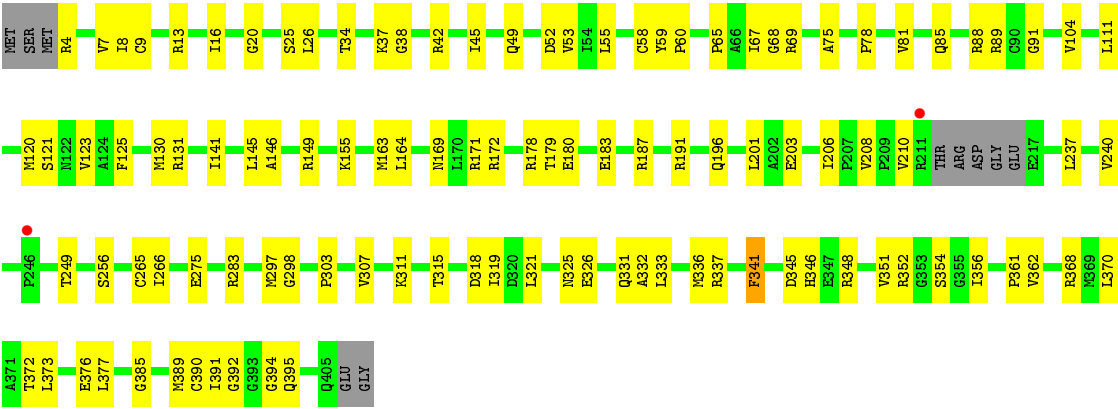
- Molecule 1: Beta-ketothiolase

Chain L: 73% 24%





● Molecule 1: Beta-ketothiolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	190.08Å 190.08Å 265.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.52 – 2.43 47.52 – 2.43	Depositor EDS
% Data completeness (in resolution range)	98.9 (47.52-2.43) 98.9 (47.52-2.43)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.56 (at 2.42Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.161 , 0.188 0.162 , 0.189	Depositor DCC
$R_{free}$ test set	10163 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.1	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 39.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.477 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	36925	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	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 26.17 % 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 2.7670e-03. 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, 0.375 respectively for untwinned datasets, and 0.333, 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: COA

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	0.41	0/2956	0.61	0/4015
1	B	0.47	1/2970 (0.0%)	0.66	4/4029 (0.1%)
1	C	0.43	0/2946	0.63	2/4000 (0.1%)
1	D	0.43	0/2967	0.62	1/4025 (0.0%)
1	E	0.41	0/2961	0.60	0/4016
1	F	0.43	0/2990	0.60	0/4054
1	G	0.42	0/3000	0.63	0/4071
1	H	0.43	0/2973	0.61	1/4033 (0.0%)
1	J	0.41	0/2949	0.61	1/4003 (0.0%)
1	K	0.44	0/2987	0.61	1/4053 (0.0%)
1	L	0.39	0/2972	0.58	0/4030
1	M	0.40	0/2964	0.58	0/4021
All	All	0.42	1/35635 (0.0%)	0.61	10/48350 (0.0%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	297	MET	CG-SD	-5.21	1.67	1.81

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	297	MET	CG-SD-CE	-8.85	86.05	100.20
1	B	297	MET	CG-SD-CE	-7.97	87.45	100.20
1	B	297	MET	CB-CG-SD	7.95	136.24	112.40
1	J	297	MET	CG-SD-CE	-7.78	87.76	100.20
1	H	297	MET	CG-SD-CE	-7.25	88.61	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	180	GLU	Peptide

## 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	2912	0	2890	78	0
1	B	2926	0	2927	64	0
1	C	2903	0	2878	62	0
1	D	2923	0	2930	62	0
1	E	2918	0	2913	65	0
1	F	2946	0	2954	57	0
1	G	2956	0	2951	70	0
1	H	2929	0	2936	58	0
1	J	2905	0	2900	63	0
1	K	2943	0	2934	66	0
1	L	2929	0	2893	79	0
1	M	2921	0	2919	79	0
2	B	48	0	32	0	0
2	D	48	0	32	8	0
2	F	48	0	32	0	0
2	H	48	0	32	5	0
2	K	48	0	32	1	0
3	A	141	0	0	10	0
3	B	167	0	0	7	0
3	C	147	0	0	6	0
3	D	145	0	0	6	2
3	E	110	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	114	0	0	3	0
3	G	121	0	0	9	0
3	H	159	0	0	12	0
3	J	110	0	0	5	2
3	K	152	0	0	4	0
3	L	106	0	0	7	0
3	M	102	0	0	8	0
All	All	36925	0	35185	756	2

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 11.

The worst 5 of 756 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:C:163:MET:HG2	1:C:297:MET:HE1	1.40	1.02
2:H:501:COA:H71	3:H:670:HOH:O	1.60	0.98
1:L:4:ARG:NH2	1:L:104:VAL:O	1.95	0.98
1:A:166:THR:HG21	1:A:297:MET:HB3	1.51	0.92
1:L:65:PRO:HB3	1:M:89:ARG:HH21	1.37	0.90

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:692:HOH:O	3:J:549:HOH:O[3_654]	1.99	0.21
3:D:603:HOH:O	3:J:502:HOH:O[3_654]	2.13	0.07

## 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	395/407 (97%)	384 (97%)	10 (2%)	1 (0%)	46	56
1	B	394/407 (97%)	379 (96%)	15 (4%)	0	100	100
1	C	394/407 (97%)	380 (96%)	13 (3%)	1 (0%)	46	56
1	D	393/407 (97%)	378 (96%)	14 (4%)	1 (0%)	46	56
1	E	390/407 (96%)	380 (97%)	9 (2%)	1 (0%)	46	56
1	F	395/407 (97%)	383 (97%)	10 (2%)	2 (0%)	34	41
1	G	398/407 (98%)	383 (96%)	13 (3%)	2 (0%)	34	41
1	H	393/407 (97%)	384 (98%)	8 (2%)	1 (0%)	46	56
1	J	392/407 (96%)	380 (97%)	10 (3%)	2 (0%)	34	41
1	K	396/407 (97%)	381 (96%)	14 (4%)	1 (0%)	46	56
1	L	395/407 (97%)	384 (97%)	11 (3%)	0	100	100
1	M	393/407 (97%)	382 (97%)	10 (2%)	1 (0%)	46	56
All	All	4728/4884 (97%)	4578 (97%)	137 (3%)	13 (0%)	46	56

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	362	VAL
1	F	362	VAL
1	J	297	MET
1	M	362	VAL
1	C	297	MET

### 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	293/309 (95%)	291 (99%)	2 (1%)	88	93
1	B	298/309 (96%)	295 (99%)	3 (1%)	82	88
1	C	293/309 (95%)	287 (98%)	6 (2%)	63	77
1	D	299/309 (97%)	294 (98%)	5 (2%)	68	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	298/309 (96%)	292 (98%)	6 (2%)	63	77
1	F	301/309 (97%)	297 (99%)	4 (1%)	76	85
1	G	301/309 (97%)	294 (98%)	7 (2%)	58	73
1	H	300/309 (97%)	295 (98%)	5 (2%)	68	80
1	J	295/309 (96%)	290 (98%)	5 (2%)	68	80
1	K	299/309 (97%)	294 (98%)	5 (2%)	68	80
1	L	294/309 (95%)	286 (97%)	8 (3%)	52	69
1	M	298/309 (96%)	296 (99%)	2 (1%)	88	93
All	All	3569/3708 (96%)	3511 (98%)	58 (2%)	70	82

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	141	ILE
1	G	379	ARG
1	L	228	ASP
1	G	169	ASN
1	G	271	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	103	GLN
1	D	181	GLN
1	K	258	GLN
1	B	99	GLN
1	J	49	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.



## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

5 ligands 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$
2	COA	B	501	-	41,50,50	3.69	11 (26%)	49,75,75	2.13	9 (18%)
2	COA	D	501	-	41,50,50	1.17	3 (7%)	49,75,75	2.14	11 (22%)
2	COA	F	501	-	41,50,50	3.76	11 (26%)	49,75,75	2.31	10 (20%)
2	COA	H	501	-	41,50,50	1.13	2 (4%)	49,75,75	1.43	12 (24%)
2	COA	K	501	-	41,50,50	3.66	10 (24%)	49,75,75	2.57	13 (26%)

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
2	COA	B	501	-	-	0/44/64/64	0/3/3/3
2	COA	D	501	-	-	0/44/64/64	0/3/3/3
2	COA	F	501	-	-	0/44/64/64	0/3/3/3
2	COA	H	501	-	-	0/44/64/64	0/3/3/3
2	COA	K	501	-	-	0/44/64/64	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	COA	C2B-C1B	-14.43	1.30	1.53
2	K	501	COA	C2B-C1B	-14.38	1.30	1.53
2	B	501	COA	C2B-C1B	-14.15	1.31	1.53
2	F	501	COA	C3B-C4B	-5.81	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	501	COA	C3B-C4B	-5.59	1.37	1.52

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	501	COA	N3A-C2A-N1A	-11.13	120.13	128.87
2	F	501	COA	N3A-C2A-N1A	-10.75	120.43	128.87
2	B	501	COA	N3A-C2A-N1A	-10.27	120.80	128.87
2	D	501	COA	N3A-C2A-N1A	-8.43	122.25	128.87
2	K	501	COA	C7P-C6P-C5P	-7.39	99.55	112.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	COA	8	0
2	H	501	COA	5	0
2	K	501	COA	1	0

## 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	398/407 (97%)	-0.67	1 (0%) 94 95	22, 37, 57, 67	0
1	B	398/407 (97%)	-0.74	0 100 100	22, 32, 50, 63	0
1	C	398/407 (97%)	-0.56	4 (1%) 84 85	21, 37, 62, 74	0
1	D	397/407 (97%)	-0.72	1 (0%) 94 95	21, 32, 54, 73	0
1	E	396/407 (97%)	-0.50	1 (0%) 94 95	25, 43, 65, 75	0
1	F	399/407 (98%)	-0.64	1 (0%) 94 95	24, 36, 57, 81	0
1	G	402/407 (98%)	-0.55	6 (1%) 76 77	24, 37, 62, 86	0
1	H	397/407 (97%)	-0.70	1 (0%) 94 95	23, 33, 53, 72	0
1	J	396/407 (97%)	-0.63	1 (0%) 94 95	23, 38, 59, 74	0
1	K	400/407 (98%)	-0.68	0 100 100	21, 33, 58, 73	0
1	L	400/407 (98%)	-0.39	3 (0%) 87 88	24, 46, 75, 82	0
1	M	397/407 (97%)	-0.58	2 (0%) 91 92	27, 41, 61, 75	0
All	All	4778/4884 (97%)	-0.61	21 (0%) 93 94	21, 37, 61, 86	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	212	THR	4.3
1	L	174	TYR	3.3
1	F	212	THR	3.3
1	J	211	ARG	2.9
1	G	212	THR	2.8

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	COA	H	501	48/48	0.77	0.28	7.21	38,57,78,98	0
2	COA	D	501	48/48	0.94	0.31	4.21	20,20,20,20	0
2	COA	B	501	48/48	0.92	0.16	2.64	29,50,73,91	0
2	COA	K	501	48/48	0.92	0.17	2.06	34,58,66,70	0
2	COA	F	501	48/48	0.91	0.16	0.87	39,56,72,78	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.