



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 4, 2025 – 07:24 pm BST

PDB ID : 9I2T / pdb_00009i2t
Title : Alpha-Methylacyl-CoA racemase from Mycobacterium tuberculosis
Authors : Mojanaga, O.O.; Acharya, K.R.; Lloyd, M.D.
Deposited on : 2025-01-22
Resolution : 2.40 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 : 4-5-2 with Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

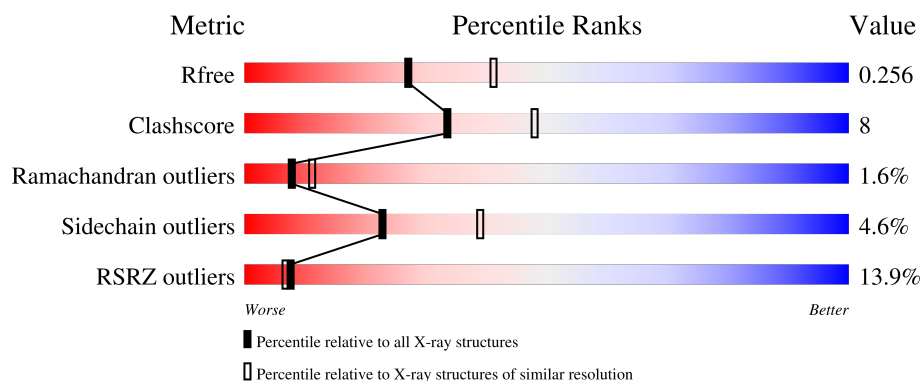
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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	364	<div> <div>7%</div> <div>79%</div> <div>17%</div> <div>..</div> </div>
1	B	364	<div> <div>5%</div> <div>81%</div> <div>15%</div> <div>...</div> </div>
1	C	364	<div> <div>15%</div> <div>71%</div> <div>23%</div> <div>..</div> </div>
1	D	364	<div> <div>15%</div> <div>76%</div> <div>18%</div> <div>..</div> </div>
1	E	364	<div> <div>24%</div> <div>71%</div> <div>24%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	364	
1	G	364	
1	H	364	
1	I	364	
1	J	364	
1	K	364	
1	L	364	

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	ACT	A	402	-	-	X	-
2	ACT	B	401	-	-	X	-
2	ACT	C	401	-	-	X	-
2	ACT	H	401	-	-	X	-
2	ACT	I	401	-	-	X	-
2	ACT	J	401	-	-	X	-
2	ACT	L	401	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33058 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 Alpha-methylacyl-CoA racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	2	0
			2685	1684	481	504	16			
1	B	355	Total	C	N	O	S	0	1	0
			2686	1685	482	503	16			
1	C	355	Total	C	N	O	S	0	2	0
			2691	1687	482	506	16			
1	D	354	Total	C	N	O	S	0	1	0
			2682	1683	481	502	16			
1	E	354	Total	C	N	O	S	0	2	0
			2685	1684	481	504	16			
1	F	354	Total	C	N	O	S	0	1	0
			2680	1682	481	501	16			
1	G	353	Total	C	N	O	S	0	2	0
			2679	1681	480	502	16			
1	H	355	Total	C	N	O	S	0	1	0
			2690	1689	482	503	16			
1	I	355	Total	C	N	O	S	0	1	0
			2688	1686	482	504	16			
1	J	354	Total	C	N	O	S	0	1	0
			2682	1683	481	502	16			
1	K	355	Total	C	N	O	S	0	1	0
			2688	1686	482	504	16			
1	L	355	Total	C	N	O	S	0	1	0
			2688	1686	482	504	16			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	361	GLY	-	expression tag	UNP O06543
A	362	SER	-	expression tag	UNP O06543
A	363	GLY	-	expression tag	UNP O06543
A	364	CYS	-	expression tag	UNP O06543
B	361	GLY	-	expression tag	UNP O06543

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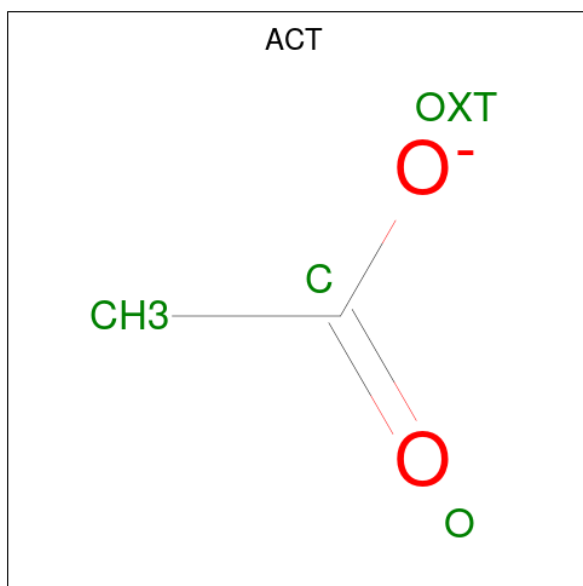
Chain	Residue	Modelled	Actual	Comment	Reference
B	362	SER	-	expression tag	UNP O06543
B	363	GLY	-	expression tag	UNP O06543
B	364	CYS	-	expression tag	UNP O06543
C	361	GLY	-	expression tag	UNP O06543
C	362	SER	-	expression tag	UNP O06543
C	363	GLY	-	expression tag	UNP O06543
C	364	CYS	-	expression tag	UNP O06543
D	361	GLY	-	expression tag	UNP O06543
D	362	SER	-	expression tag	UNP O06543
D	363	GLY	-	expression tag	UNP O06543
D	364	CYS	-	expression tag	UNP O06543
E	361	GLY	-	expression tag	UNP O06543
E	362	SER	-	expression tag	UNP O06543
E	363	GLY	-	expression tag	UNP O06543
E	364	CYS	-	expression tag	UNP O06543
F	361	GLY	-	expression tag	UNP O06543
F	362	SER	-	expression tag	UNP O06543
F	363	GLY	-	expression tag	UNP O06543
F	364	CYS	-	expression tag	UNP O06543
G	361	GLY	-	expression tag	UNP O06543
G	362	SER	-	expression tag	UNP O06543
G	363	GLY	-	expression tag	UNP O06543
G	364	CYS	-	expression tag	UNP O06543
H	361	GLY	-	expression tag	UNP O06543
H	362	SER	-	expression tag	UNP O06543
H	363	GLY	-	expression tag	UNP O06543
H	364	CYS	-	expression tag	UNP O06543
I	361	GLY	-	expression tag	UNP O06543
I	362	SER	-	expression tag	UNP O06543
I	363	GLY	-	expression tag	UNP O06543
I	364	CYS	-	expression tag	UNP O06543
J	361	GLY	-	expression tag	UNP O06543
J	362	SER	-	expression tag	UNP O06543
J	363	GLY	-	expression tag	UNP O06543
J	364	CYS	-	expression tag	UNP O06543
K	361	GLY	-	expression tag	UNP O06543
K	362	SER	-	expression tag	UNP O06543
K	363	GLY	-	expression tag	UNP O06543
K	364	CYS	-	expression tag	UNP O06543
L	361	GLY	-	expression tag	UNP O06543
L	362	SER	-	expression tag	UNP O06543
L	363	GLY	-	expression tag	UNP O06543

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Chain	Residue	Modelled	Actual	Comment	Reference
L	364	CYS	-	expression tag	UNP O06543

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		
2	I	1	Total	C	O	0	0
			4	2	2		
2	J	1	Total	C	O	0	0
			4	2	2		
2	J	1	Total	C	O	0	0
			4	2	2		
2	K	1	Total	C	O	0	0
			4	2	2		
2	L	1	Total	C	O	0	0
			4	2	2		

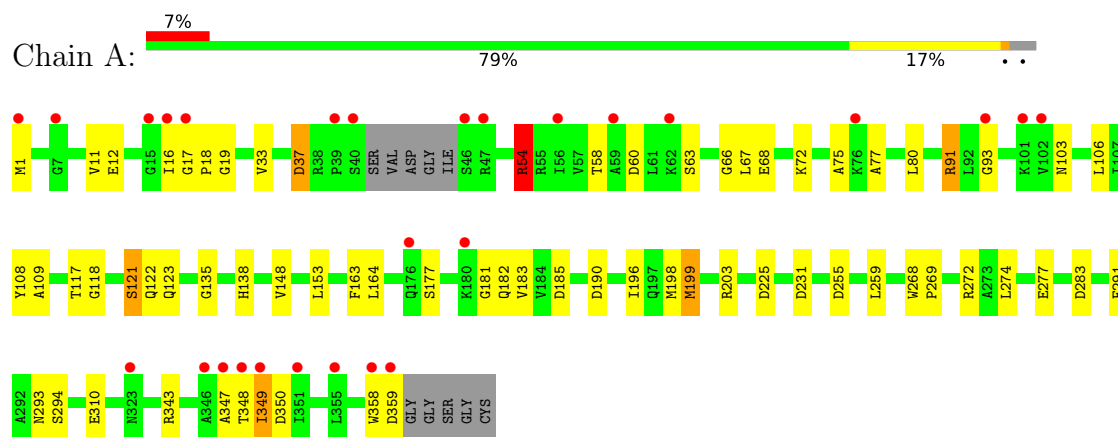
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	94	Total 94	O 94	0	0
3	B	78	Total 78	O 78	0	0
3	C	74	Total 74	O 74	0	0
3	D	48	Total 48	O 48	0	0
3	E	60	Total 60	O 60	0	0
3	F	51	Total 51	O 51	0	0
3	G	53	Total 53	O 53	0	0
3	H	54	Total 54	O 54	0	0
3	I	70	Total 70	O 70	0	0
3	J	60	Total 60	O 60	0	0
3	K	77	Total 77	O 77	0	0
3	L	71	Total 71	O 71	0	0

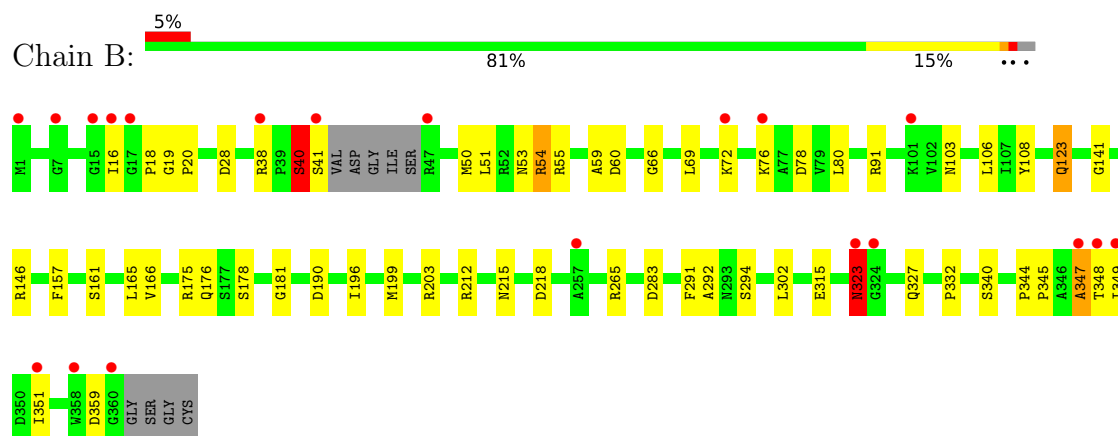
3 Residue-property plots [i](#)

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.

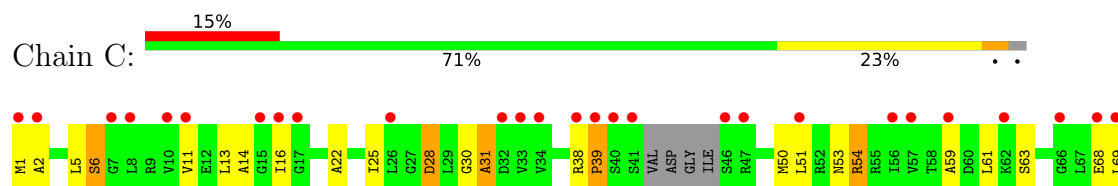
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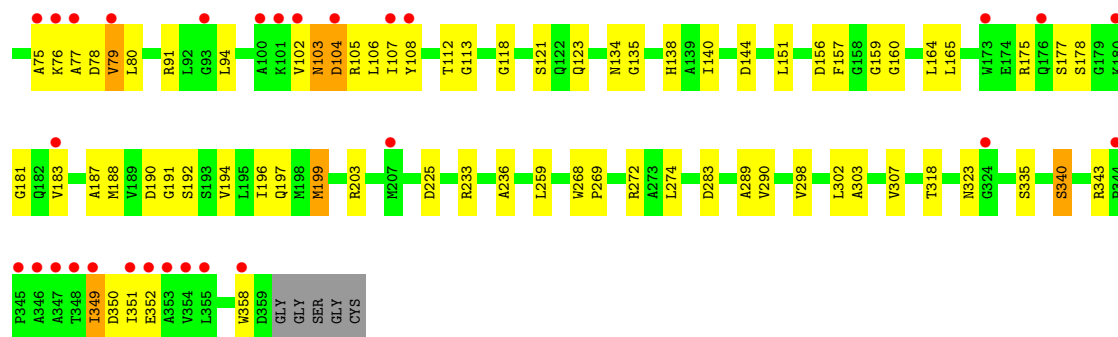


• Molecule 1: Alpha-methylacyl-CoA racemase

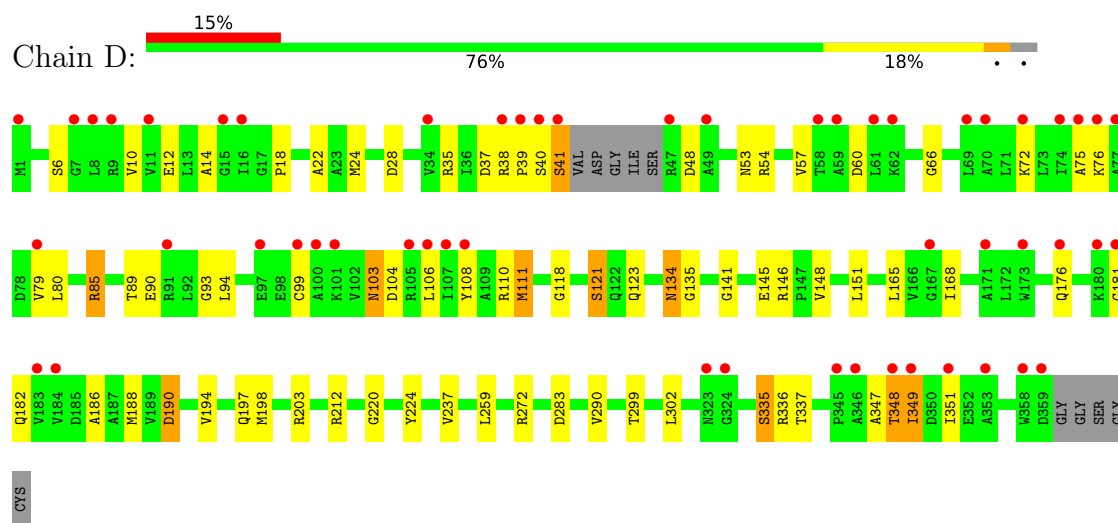


• Molecule 1: Alpha-methylacyl-CoA racemase

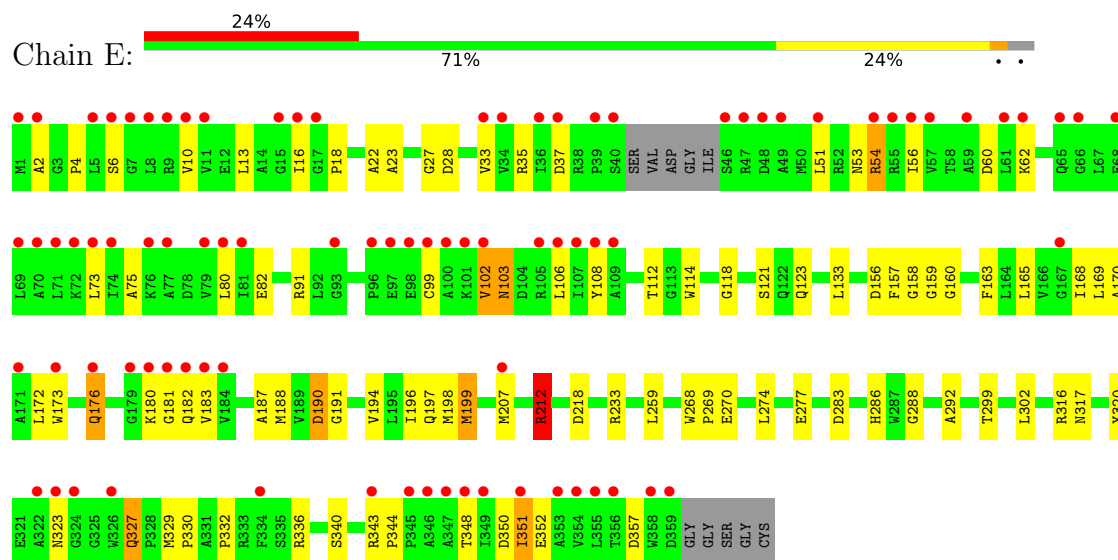




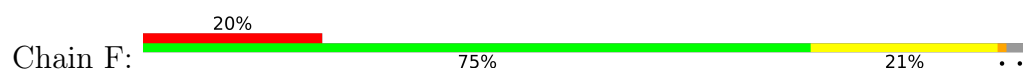
● Molecule 1: Alpha-methylacyl-CoA racemase

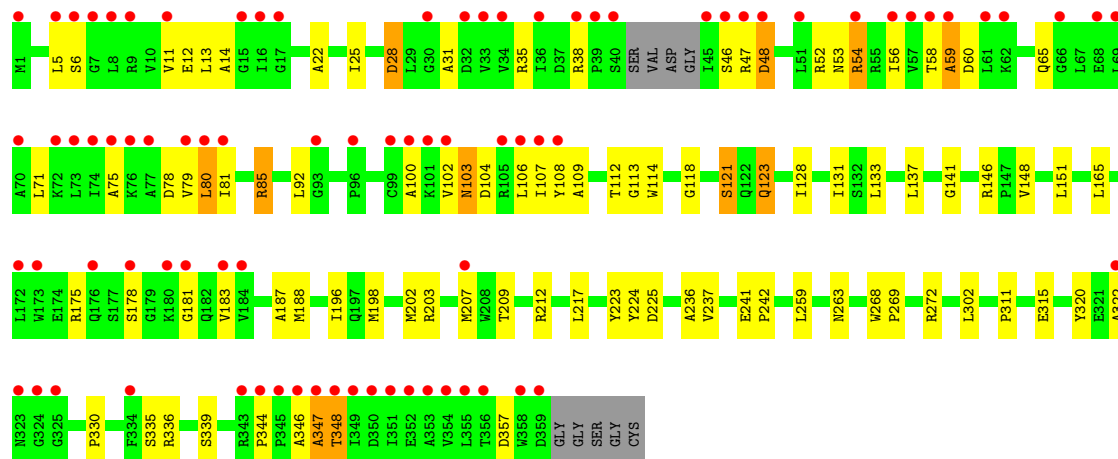


● Molecule 1: Alpha-methylacyl-CoA racemase

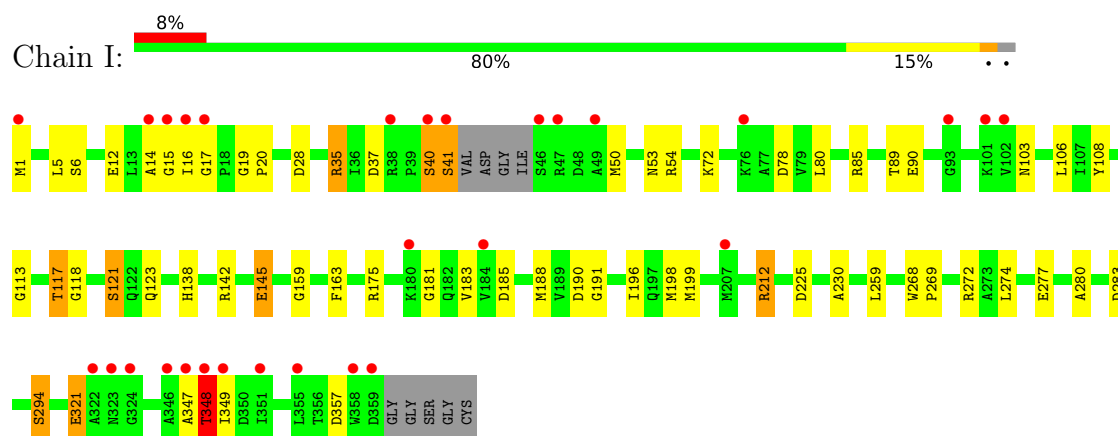


● Molecule 1: Alpha-methylacyl-CoA racemase

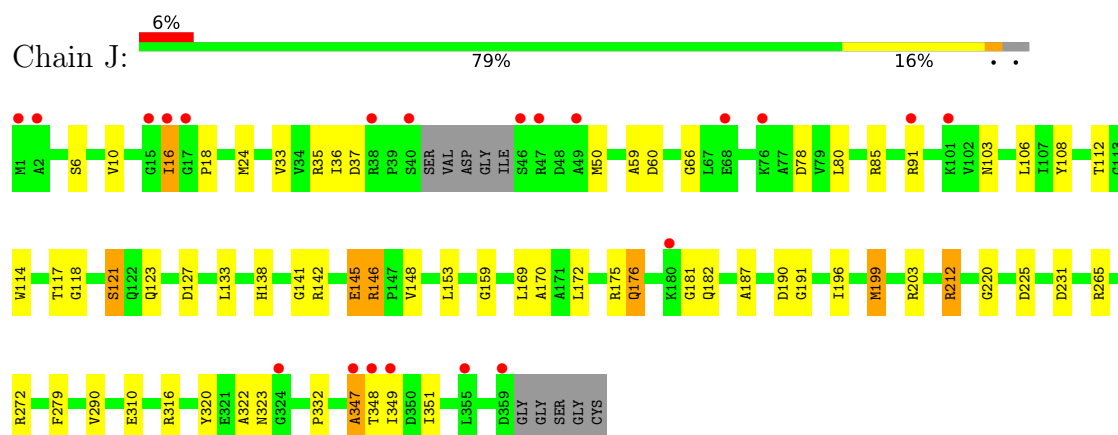




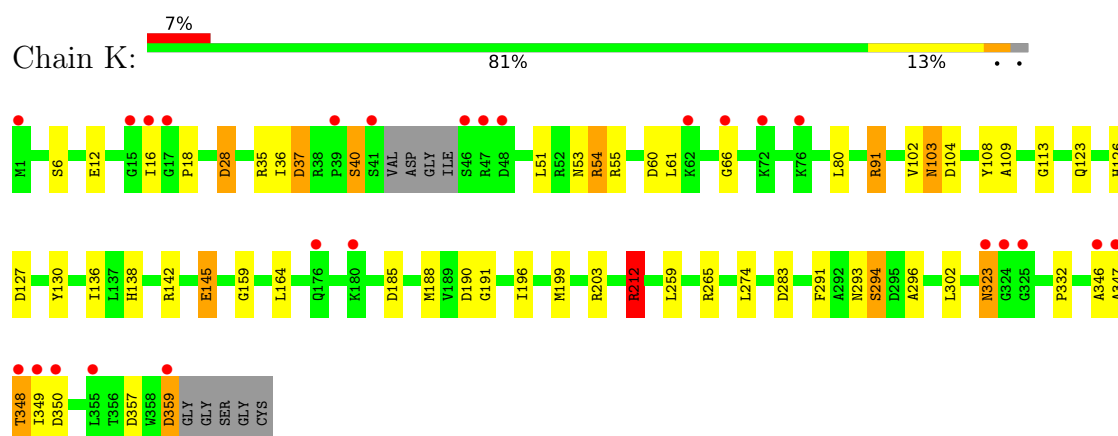
• Molecule 1: Alpha-methylacyl-CoA racemase



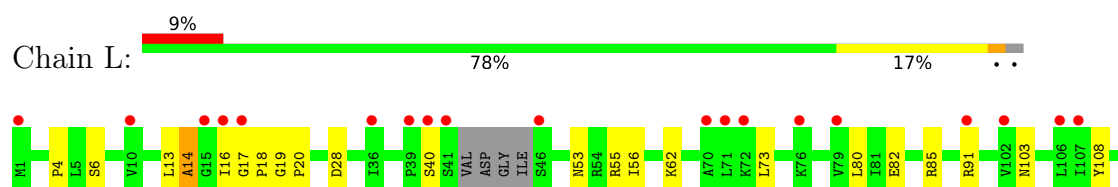
• Molecule 1: Alpha-methylacyl-CoA racemase

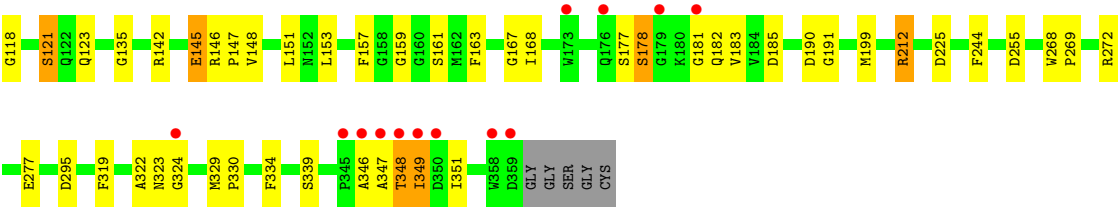


• Molecule 1: Alpha-methylacyl-CoA racemase



• Molecule 1: Alpha-methylacyl-CoA racemase





4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	275.45Å 275.45Å 388.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	224.67 – 2.40 224.67 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (224.67-2.40) 99.9 (224.67-2.40)	Depositor EDS
R_{merge}	0.40	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.88)	Depositor
R, R_{free}	0.212 , 0.250 0.221 , 0.256	Depositor DCC
R_{free} test set	14389 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	49.4	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.004 for -1/2*h+1/2*k-1/2*l, 1/2*h-1/2*k-1/2*l, -h-k 0.006 for -1/2*h-1/2*k+1/2*l, -1/2*h-1/2*k-1/2*l, h-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33058	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: ACT

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	0.58	0/2757	1.14	6/3749 (0.2%)
1	B	0.60	0/2752	1.09	7/3742 (0.2%)
1	C	0.60	0/2763	1.19	10/3757 (0.3%)
1	D	0.60	0/2748	1.17	11/3737 (0.3%)
1	E	0.61	0/2757	1.17	11/3749 (0.3%)
1	F	0.59	0/2746	1.14	5/3734 (0.1%)
1	G	0.59	0/2751	1.16	10/3741 (0.3%)
1	H	0.58	0/2756	1.14	6/3748 (0.2%)
1	I	0.59	0/2754	1.13	8/3745 (0.2%)
1	J	0.59	0/2748	1.11	6/3737 (0.2%)
1	K	0.61	0/2754	1.19	10/3745 (0.3%)
1	L	0.61	0/2754	1.14	8/3745 (0.2%)
All	All	0.60	0/33040	1.15	98/44929 (0.2%)

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	2
1	B	0	2
1	C	0	1
1	D	0	2
1	E	0	2
1	F	0	4
1	H	0	2
1	I	0	3
1	J	0	4
1	K	0	1
1	L	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	25

There are no bond length outliers.

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	85	ARG	CB-CA-C	9.52	124.57	109.52
1	E	190	ASP	CA-CB-CG	7.70	120.30	112.60
1	F	28	ASP	CA-CB-CG	7.50	120.10	112.60
1	F	190	ASP	CA-CB-CG	7.12	119.72	112.60
1	C	144	ASP	CA-CB-CG	7.02	119.62	112.60

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	54	ARG	Sidechain
1	A	91	ARG	Sidechain
1	B	212	ARG	Sidechain
1	B	54	ARG	Peptide
1	C	233	ARG	Sidechain

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	2685	0	2625	36	0
1	B	2686	0	2630	35	0
1	C	2691	0	2630	55	0
1	D	2682	0	2627	41	0
1	E	2685	0	2625	58	0
1	F	2680	0	2625	49	0
1	G	2679	0	2620	56	0
1	H	2690	0	2638	55	0
1	I	2688	0	2632	31	0
1	J	2682	0	2627	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	2688	0	2632	40	0
1	L	2688	0	2632	34	0
2	A	8	0	6	5	0
2	B	4	0	3	3	0
2	C	4	0	3	5	0
2	E	4	0	3	0	0
2	H	4	0	3	5	0
2	I	4	0	3	2	0
2	J	8	0	6	5	0
2	K	4	0	3	1	0
2	L	4	0	3	4	0
3	A	94	0	0	3	0
3	B	78	0	0	2	0
3	C	74	0	0	2	0
3	D	48	0	0	2	0
3	E	60	0	0	3	0
3	F	51	0	0	2	0
3	G	53	0	0	2	0
3	H	54	0	0	1	0
3	I	70	0	0	2	0
3	J	60	0	0	1	0
3	K	77	0	0	4	0
3	L	71	0	0	1	0
All	All	33058	0	31576	488	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 8.

The worst 5 of 488 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:H:141:GLY:HA3	2:H:401:ACT:H1	1.41	1.01
1:E:16:ILE:O	1:E:18:PRO:HD2	1.72	0.90
1:J:141:GLY:HA3	2:J:401:ACT:H1	1.52	0.90
1:K:91:ARG:HD2	3:K:502:HOH:O	1.74	0.86
2:C:401:ACT:H1	1:D:141:GLY:HA3	1.57	0.85

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	352/364 (97%)	329 (94%)	21 (6%)	2 (1%)	22	33
1	B	352/364 (97%)	324 (92%)	19 (5%)	9 (3%)	4	4
1	C	353/364 (97%)	315 (89%)	31 (9%)	7 (2%)	6	8
1	D	351/364 (96%)	320 (91%)	24 (7%)	7 (2%)	6	8
1	E	352/364 (97%)	322 (92%)	26 (7%)	4 (1%)	12	18
1	F	351/364 (96%)	316 (90%)	32 (9%)	3 (1%)	14	22
1	G	351/364 (96%)	313 (89%)	32 (9%)	6 (2%)	7	10
1	H	352/364 (97%)	314 (89%)	27 (8%)	11 (3%)	3	3
1	I	352/364 (97%)	329 (94%)	19 (5%)	4 (1%)	12	18
1	J	351/364 (96%)	323 (92%)	24 (7%)	4 (1%)	12	18
1	K	352/364 (97%)	330 (94%)	19 (5%)	3 (1%)	14	22
1	L	352/364 (97%)	324 (92%)	21 (6%)	7 (2%)	6	8
All	All	4221/4368 (97%)	3859 (91%)	295 (7%)	67 (2%)	8	11

5 of 67 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	B	348	THR
1	C	31	ALA
1	C	103	ASN
1	D	103	ASN

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	273/277 (99%)	258 (94%)	15 (6%)	18	31
1	B	272/277 (98%)	266 (98%)	6 (2%)	47	67
1	C	274/277 (99%)	259 (94%)	15 (6%)	18	31
1	D	272/277 (98%)	258 (95%)	14 (5%)	20	35
1	E	273/277 (99%)	260 (95%)	13 (5%)	21	37
1	F	271/277 (98%)	259 (96%)	12 (4%)	24	41
1	G	272/277 (98%)	254 (93%)	18 (7%)	14	23
1	H	273/277 (99%)	263 (96%)	10 (4%)	29	48
1	I	273/277 (99%)	260 (95%)	13 (5%)	21	37
1	J	272/277 (98%)	262 (96%)	10 (4%)	29	48
1	K	273/277 (99%)	261 (96%)	12 (4%)	24	41
1	L	273/277 (99%)	262 (96%)	11 (4%)	27	45
All	All	3271/3324 (98%)	3122 (95%)	149 (5%)	23	39

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	321	GLU
1	L	177	SER
1	J	121	SER
1	K	145	GLU
1	D	349	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	286	HIS
1	J	197	GLN
1	H	327	GLN
1	J	116	GLN
1	J	308	HIS

5.3.3 RNA ⓘ

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](#)

11 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	ACT	E	401	-	3,3,3	1.00	0	3,3,3	0.91	0
2	ACT	J	401	-	3,3,3	0.86	0	3,3,3	0.93	0
2	ACT	J	402	-	3,3,3	1.03	0	3,3,3	0.68	0
2	ACT	A	402	-	3,3,3	0.65	0	3,3,3	1.09	0
2	ACT	B	401	-	3,3,3	0.91	0	3,3,3	0.85	0
2	ACT	K	401	-	3,3,3	1.13	0	3,3,3	0.86	0
2	ACT	A	401	-	3,3,3	1.10	0	3,3,3	0.70	0
2	ACT	L	401	-	3,3,3	1.06	0	3,3,3	0.61	0
2	ACT	H	401	-	3,3,3	0.85	0	3,3,3	0.99	0
2	ACT	C	401	-	3,3,3	0.91	0	3,3,3	0.86	0
2	ACT	I	401	-	3,3,3	1.09	0	3,3,3	0.87	0

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.

10 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	401	ACT	4	0
2	J	402	ACT	1	0
2	A	402	ACT	4	0
2	B	401	ACT	3	0
2	K	401	ACT	1	0
2	A	401	ACT	1	0
2	L	401	ACT	4	0
2	H	401	ACT	5	0
2	C	401	ACT	5	0
2	I	401	ACT	2	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, 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	354/364 (97%)	0.12	27 (7%)	21 19	30, 50, 98, 136	2 (0%)
1	B	355/364 (97%)	0.13	20 (5%)	31 28	31, 51, 97, 152	1 (0%)
1	C	355/364 (97%)	0.57	56 (15%)	6 5	31, 55, 115, 138	2 (0%)
1	D	354/364 (97%)	0.56	53 (14%)	6 6	31, 55, 111, 141	1 (0%)
1	E	354/364 (97%)	0.93	86 (24%)	2 2	31, 61, 121, 147	2 (0%)
1	F	354/364 (97%)	0.75	72 (20%)	3 3	31, 58, 118, 158	1 (0%)
1	G	353/364 (96%)	0.93	86 (24%)	2 2	32, 61, 116, 153	2 (0%)
1	H	355/364 (97%)	0.84	83 (23%)	2 2	32, 61, 128, 156	1 (0%)
1	I	355/364 (97%)	0.27	29 (8%)	19 17	33, 53, 96, 137	1 (0%)
1	J	354/364 (97%)	0.21	21 (5%)	29 27	32, 50, 99, 148	1 (0%)
1	K	355/364 (97%)	0.19	25 (7%)	24 22	32, 50, 106, 142	1 (0%)
1	L	355/364 (97%)	0.28	32 (9%)	17 15	32, 52, 101, 159	1 (0%)
All	All	4253/4368 (97%)	0.48	590 (13%)	7 7	30, 55, 112, 159	16 (0%)

The worst 5 of 590 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	16	ILE	9.1
1	E	16	ILE	8.1
1	A	16	ILE	7.7
1	D	16	ILE	7.5
1	J	16	ILE	7.4

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](#)

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
2	ACT	L	401	4/4	0.85	0.22	65,86,90,93	0
2	ACT	H	401	4/4	0.88	0.20	73,91,94,95	0
2	ACT	J	402	4/4	0.92	0.14	64,69,70,70	0
2	ACT	J	401	4/4	0.92	0.17	71,94,95,96	0
2	ACT	E	401	4/4	0.93	0.16	67,69,72,76	0
2	ACT	C	401	4/4	0.94	0.18	74,78,86,94	0
2	ACT	B	401	4/4	0.94	0.19	68,78,82,85	0
2	ACT	I	401	4/4	0.95	0.10	42,54,56,57	0
2	ACT	A	402	4/4	0.96	0.21	54,63,63,67	0
2	ACT	K	401	4/4	0.97	0.09	53,53,63,64	0
2	ACT	A	401	4/4	0.97	0.09	52,55,56,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.