



Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 12:25 PM GMT

PDB ID : 1XFC
Title : The 1.9 Å crystal structure of alanine racemase from Mycobacterium tuberculosis contains a conserved entryway into the active site
Authors : LeMagueres, P.; Im, H.; Ebalunode, J.; Strych, U.; Benedik, M.J.; Briggs, J.M.; Kohn, H.; Krause, K.L.
Deposited on : 2004-09-14
Resolution : 1.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

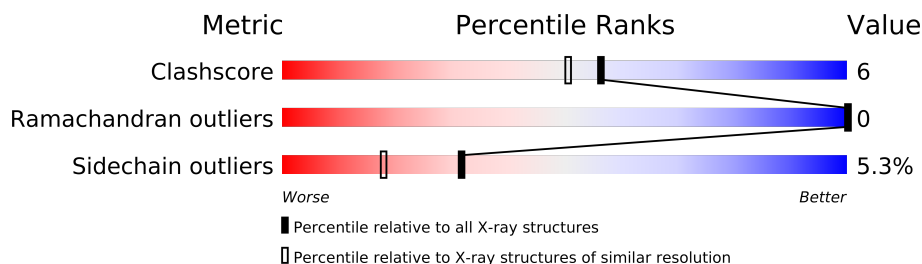
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.90 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))
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	384	
1	B	384	

2 Entry composition i

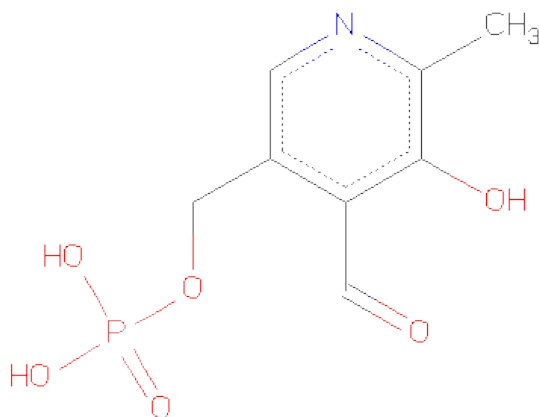
There are 3 unique types of molecules in this entry. The entry contains 5740 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Alanine racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2713	1701	496	502	14			
1	B	356	Total	C	N	O	S	0	0	0
			2647	1659	484	490	14			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	162	Total 162	O 162	0	0
3	B	188	Total 188	O 188	0	0

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	164.78Å 164.78Å 57.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-1.90)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.204 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5740	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.34	0/2762	1.05	8/3758 (0.2%)
1	B	0.33	0/2692	1.04	5/3661 (0.1%)
All	All	0.33	0/5454	1.05	13/7419 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	ARG	NE-CZ-NH1	11.65	126.13	120.30
1	A	310	ARG	CD-NE-CZ	8.94	136.12	123.60
1	A	156	ARG	CD-NE-CZ	8.37	135.32	123.60
1	B	376	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	A	310	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	B	156	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	B	219	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	B	52	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	167	ARG	NE-CZ-NH1	-5.76	117.42	120.30
1	A	310	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	B	156	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	156	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	112	ARG	CD-NE-CZ	5.01	130.62	123.60

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2713	0	2725	39	0
1	B	2647	0	2672	34	0
2	A	15	0	6	1	0
2	B	15	0	6	1	0
3	A	162	0	0	1	0
3	B	188	0	0	3	0
All	All	5740	0	5409	70	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (70) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:280:ASP:O	1:B:328:PRO:HB3	1.83	0.78
1:A:136:THR:OG1	1:A:138:LEU:HD21	1.84	0.77
1:A:138:LEU:HD22	1:A:172:HIS:O	1.85	0.77
1:B:209:HIS:HB3	1:B:226:LEU:HB3	1.69	0.73
1:A:118:LEU:O	1:A:122:ARG:HD3	1.91	0.71
1:A:22:GLU:O	1:A:26:ARG:HG3	1.92	0.70
1:A:135:ASP:HA	1:A:138:LEU:HD12	1.74	0.68
1:B:307:ASN:HB2	3:B:439:HOH:O	1.92	0.68
1:B:179:PRO:HG3	1:B:214:SER:OG	1.97	0.65
1:A:136:THR:H	1:A:138:LEU:HD11	1.62	0.64
1:B:279:ARG:NH2	1:B:328:PRO:HD3	2.13	0.64
1:A:179:PRO:O	1:A:219:ARG:HD3	1.99	0.62
1:A:264:ARG:O	1:A:267:GLU:HG3	2.02	0.60
1:B:51:THR:O	1:B:55:GLN:HG3	2.01	0.60
1:B:177:ASP:O	1:B:178:LYS:HD3	2.01	0.60
1:B:15:MET:HE3	3:B:526:HOH:O	2.01	0.59
1:A:265:ALA:HB2	1:A:279:ARG:HA	1.85	0.58
1:A:301:ARG:HH11	1:A:301:ARG:HG3	1.68	0.58
1:A:36:GLN:HB2	1:A:226:LEU:CD1	2.34	0.58
1:A:166:LEU:HD13	1:A:205:PHE:CE1	2.39	0.57
1:A:136:THR:H	1:A:138:LEU:CD1	2.18	0.56
1:B:200:GLU:HG3	3:B:527:HOH:O	2.04	0.56
1:B:209:HIS:CG	1:B:226:LEU:HD22	2.40	0.56
1:B:161:GLU:O	1:B:161:GLU:HG3	2.07	0.55
1:A:189:GLN:O	1:A:192:THR:HB	2.07	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:29:ARG:CZ	1:B:61:GLY:HA3	2.37	0.54
1:A:210:LEU:O	1:A:210:LEU:HG	2.08	0.53
1:A:338:GLU:OE2	1:A:340:ILE:HD11	2.09	0.52
1:A:182:SER:HA	1:A:185:ASP:OD1	2.10	0.52
1:A:140:ARG:O	1:B:261:LYS:HE3	2.09	0.52
1:B:176:ALA:O	1:B:214:SER:HB2	2.09	0.52
1:A:279:ARG:NH2	1:A:328:PRO:HD3	2.25	0.52
1:A:369:SER:O	1:A:371:ARG:HG2	2.10	0.52
1:A:135:ASP:HA	1:A:138:LEU:CD1	2.40	0.51
1:A:263:ILE:HD13	1:A:283:LEU:HD11	1.92	0.51
1:B:179:PRO:O	1:B:219:ARG:HD3	2.11	0.50
1:B:26:ARG:O	1:B:30:GLU:OE2	2.29	0.50
1:A:109:SER:HB2	1:A:142:GLY:HA2	1.94	0.48
1:A:36:GLN:HB2	1:A:226:LEU:HD13	1.95	0.48
1:A:139:ASN:O	1:B:261:LYS:HD3	2.14	0.48
1:A:173:MET:HA	1:A:187:GLN:OE1	2.14	0.47
1:B:23:HIS:HE1	1:B:246:GLY:O	1.98	0.47
1:A:371:ARG:HD3	1:B:371:ARG:CD	2.44	0.47
1:B:94:ILE:O	1:B:94:ILE:HG23	2.14	0.47
1:A:38:MET:O	1:A:229:PRO:HD2	2.15	0.46
1:B:42:LYS:NZ	2:B:390:PLP:O3	2.50	0.45
1:A:287:PRO:O	1:A:373:ARG:NH2	2.50	0.45
1:B:29:ARG:NH1	1:B:60:ALA:O	2.50	0.45
1:B:64:GLU:OE2	1:B:167:ARG:NH2	2.50	0.44
1:B:376:ARG:HD3	1:B:378:TYR:OH	2.18	0.44
1:B:15:MET:HE1	1:B:379:ARG:NH2	2.32	0.44
1:B:52:ARG:NH2	1:B:380:GLU:OE2	2.50	0.44
1:B:175:TYR:CE1	1:B:183:ILE:HG21	2.53	0.43
1:A:95:ASP:OD1	1:A:123:ARG:NH2	2.50	0.43
1:A:138:LEU:HD11	1:A:171:SER:OG	2.18	0.43
1:B:259:LEU:HD12	1:B:260:VAL:N	2.34	0.43
1:B:231:ILE:HG13	1:B:236:LEU:HB2	2.00	0.43
1:A:42:LYS:NZ	2:A:390:PLP:O3	2.51	0.43
1:A:11:LEU:HD23	1:A:11:LEU:HA	1.80	0.43
1:B:177:ASP:N	1:B:177:ASP:OD1	2.51	0.42
1:A:236:LEU:HD11	1:A:367:VAL:HG11	2.01	0.42
1:A:259:LEU:HA	1:A:335:GLU:CG	2.50	0.42
1:B:281:THR:OG1	1:B:282:ASN:N	2.53	0.42
1:A:169:LEU:HD13	1:A:205:PHE:CE2	2.56	0.41
1:B:290:TYR:HA	1:B:294:VAL:O	2.21	0.41
1:B:283:LEU:HB3	1:B:323:MET:CE	2.51	0.41
1:A:138:LEU:HD13	3:A:476:HOH:O	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:221:ASP:OD1	1:B:221:ASP:N	2.54	0.41
1:A:76:LEU:HD22	1:A:81:ILE:HG13	2.03	0.40
1:A:101:LEU:HD23	1:A:101:LEU:HA	1.89	0.40

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	362/384 (94%)	351 (97%)	11 (3%)	0	100	100
1	B	352/384 (92%)	339 (96%)	13 (4%)	0	100	100
All	All	714/768 (93%)	690 (97%)	24 (3%)	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	275/292 (94%)	256 (93%)	19 (7%)	22	10
1	B	270/292 (92%)	260 (96%)	10 (4%)	45	32
All	All	545/584 (93%)	516 (95%)	29 (5%)	32	18

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU

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Mol	Chain	Res	Type
1	A	37	LEU
1	A	126	ARG
1	A	138	LEU
1	A	151	MET
1	A	157	GLN
1	A	159	MET
1	A	166	LEU
1	A	169	LEU
1	A	173	MET
1	A	181	ASP
1	A	190	ARG
1	A	199	ARG
1	A	204	ARG
1	A	254	LYS
1	A	269	VAL
1	A	279	ARG
1	A	363	HIS
1	A	373	ARG
1	B	30	GLU
1	B	122	ARG
1	B	123	ARG
1	B	161	GLU
1	B	180	ASP
1	B	254	LYS
1	B	262	SER
1	B	279	ARG
1	B	363	HIS
1	B	373	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	GLN
1	A	201	GLN
1	A	307	ASN
1	A	321	GLN
1	B	23	HIS
1	B	31	HIS
1	B	36	GLN
1	B	184	ASN
1	B	353	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

2 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	PLP	A	390	1	14,15,16	1.81	2 (14%)	20,22,23	0.91	0
2	PLP	B	390	1	14,15,16	1.58	2 (14%)	20,22,23	0.94	0

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	PLP	A	390	1	-	0/6/6/8	0/1/1/1
2	PLP	B	390	1	-	0/6/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	390	PLP	C3-C2	-5.72	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	390	PLP	C3-C2	-4.71	1.37	1.40
2	B	390	PLP	P-O2P	-2.25	1.46	1.54
2	A	390	PLP	P-O2P	-2.03	1.47	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.