Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:27 PM GMT

PDB ID	:	1XAC
Title	:	CHIMERA ISOPROPYLMALATE DEHYDROGENASE BETWEEN BACILLUS SUBTILIS (M) AND THERMUS THERMOPHILUS (T) FROM N-TERMINAL: 20% T MIDDLE 20% M RESIDUAL 60% T, MUTATED AT S82R. LOW TEMPERATURE (100K) STRUCTURE.
Authors	:	Nagata, C.; Moriyama, H.; Tanaka, N.
Deposited on	:	1995-11-09
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

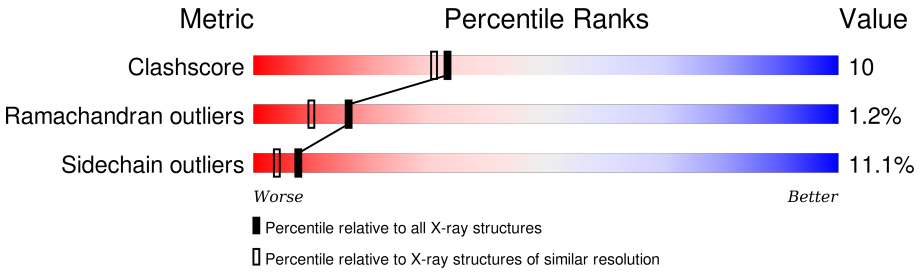
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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. 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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	345	64% 28% 6% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3890 atoms, of which 1035 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 3-ISOPROPYLMALATE DEHYDROGENASE 2T2M6T S82R.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	345	3161	1665	549	450	491	6	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	GLN	GLY	CONFLICT	UNP P00351
A	80	ASN	LEU	CONFLICT	UNP P00351
A	83	GLU	LYS	CONFLICT	UNP P00351
A	84	LEU	ILE	CONFLICT	UNP P00351
A	85	ARG	SER	CONFLICT	UNP P00351
A	88	LYS	THR	CONFLICT	UNP P00351
A	93	ILE	LEU	CONFLICT	UNP P00351
A	96	GLN	SER	CONFLICT	UNP P00351
A	97	LEU	GLN	CONFLICT	UNP P00351
A	106	VAL	ALA	CONFLICT	UNP P00351
A	110	GLU	PRO	CONFLICT	UNP P00351
A	111	SER	GLY	CONFLICT	UNP P00351
A	113	SER	GLU	CONFLICT	UNP P00351
A	114	ASP	ARG	CONFLICT	UNP P00351
A	115	ALA	LEU	CONFLICT	UNP P00351
A	120	LYS	GLU	CONFLICT	UNP P00351
A	122	TYR	ILE	CONFLICT	UNP P00351
A	123	ILE	ALA	CONFLICT	UNP P00351
A	124	ASP	ARG	CONFLICT	UNP P00351
A	125	ASN	GLY	CONFLICT	UNP P00351
A	128	PHE	VAL	CONFLICT	UNP P00351
A	129	VAL	LEU	CONFLICT	UNP P00351

- Molecule 2 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	243	Total 729	H 486	O 243	0	0

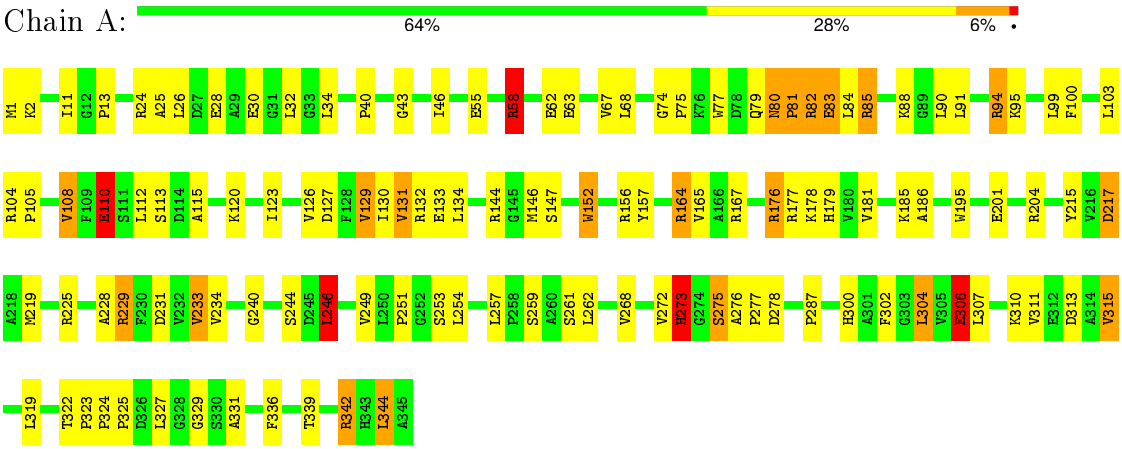
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

- Molecule 1: 3-ISOPROPYLMALATE DEHYDROGENASE 2T2M6T S82R

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	77.30Å 77.30Å 157.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.10)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.200 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3890	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

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	1.17	4/2668 (0.1%)	1.91	69/3621 (1.9%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	GLU	CB-CG	5.52	1.62	1.52
1	A	28	GLU	CG-CD	5.17	1.59	1.51
1	A	77	TRP	CD2-CE2	-5.15	1.35	1.41
1	A	77	TRP	CG-CD2	-5.03	1.35	1.43

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	ARG	NE-CZ-NH2	-13.30	113.65	120.30
1	A	204	ARG	NE-CZ-NH2	-10.22	115.19	120.30
1	A	77	TRP	CD1-CG-CD2	9.48	113.89	106.30
1	A	195	TRP	CD1-CG-CD2	8.18	112.85	106.30
1	A	215	TYR	CB-CG-CD1	-8.15	116.11	121.00
1	A	152	TRP	CE2-CD2-CG	-7.95	100.94	107.30
1	A	77	TRP	CE2-CD2-CG	-7.87	101.00	107.30
1	A	195	TRP	CE2-CD2-CG	-7.75	101.10	107.30
1	A	77	TRP	CG-CD2-CE3	7.71	140.84	133.90
1	A	152	TRP	CG-CD2-CE3	7.69	140.82	133.90
1	A	85	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	A	306	GLU	CB-CG-CD	7.45	134.33	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	94	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	A	104	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	A	58	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	A	219	MET	CG-SD-CE	-7.26	88.59	100.20
1	A	152	TRP	CD1-CG-CD2	7.24	112.09	106.30
1	A	164	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	A	156	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	A	273	HIS	CA-CB-CG	7.14	125.74	113.60
1	A	24	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	A	82	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	A	233	VAL	CG1-CB-CG2	-6.79	100.04	110.90
1	A	126	VAL	CG1-CB-CG2	-6.68	100.21	110.90
1	A	82	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	A	179	HIS	CB-CA-C	-6.52	97.36	110.40
1	A	179	HIS	N-CA-CB	6.48	122.27	110.60
1	A	181	VAL	CG1-CB-CG2	-6.43	100.61	110.90
1	A	77	TRP	CG-CD1-NE1	-6.29	103.81	110.10
1	A	167	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	A	156	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	215	TYR	CB-CG-CD2	6.09	124.65	121.00
1	A	108	VAL	CA-C-N	-6.08	103.83	117.20
1	A	246	LEU	CB-CG-CD1	-6.06	100.70	111.00
1	A	164	ARG	CB-CG-CD	-6.04	95.89	111.60
1	A	278	ASP	CA-CB-CG	6.04	126.69	113.40
1	A	204	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	58	ARG	CA-CB-CG	6.00	126.61	113.40
1	A	77	TRP	CB-CG-CD1	-5.81	119.44	127.00
1	A	67	VAL	CA-C-N	5.81	129.98	117.20
1	A	229	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	A	268	VAL	CA-C-N	5.67	129.67	117.20
1	A	94	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	164	ARG	CB-CA-C	-5.63	99.14	110.40
1	A	82	ARG	CB-CG-CD	5.55	126.03	111.60
1	A	2	LYS	CG-CD-CE	-5.54	95.27	111.90
1	A	63	GLU	CA-CB-CG	5.54	125.58	113.40
1	A	129	VAL	CG1-CB-CG2	-5.48	102.13	110.90
1	A	152	TRP	NE1-CE2-CD2	5.42	112.72	107.30
1	A	164	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	195	TRP	CG-CD2-CE3	5.42	138.78	133.90
1	A	144	ARG	CA-C-N	5.39	126.99	116.20
1	A	91	LEU	CB-CG-CD1	-5.39	101.83	111.00
1	A	186	ALA	CB-CA-C	-5.38	102.03	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	181	VAL	CA-C-N	5.34	128.95	117.20
1	A	108	VAL	N-CA-C	-5.33	96.61	111.00
1	A	25	ALA	CB-CA-C	-5.33	102.11	110.10
1	A	28	GLU	N-CA-C	-5.26	96.79	111.00
1	A	110	GLU	CA-CB-CG	5.25	124.95	113.40
1	A	40	PRO	CA-C-N	5.24	128.73	117.20
1	A	233	VAL	CA-C-N	5.24	128.73	117.20
1	A	152	TRP	CB-CG-CD1	-5.22	120.21	127.00
1	A	273	HIS	CA-C-N	5.21	126.62	116.20
1	A	126	VAL	CA-CB-CG2	-5.16	103.17	110.90
1	A	342	ARG	N-CA-CB	-5.13	101.37	110.60
1	A	217	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	195	TRP	CB-CG-CD1	-5.07	120.41	127.00
1	A	126	VAL	CA-CB-CG1	5.04	118.46	110.90
1	A	127	ASP	CB-CG-OD1	5.03	122.82	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	80	ASN	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	2612	549	2630	54	0
2	A	243	486	0	12	0
All	All	2855	1035	2630	54	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 10.

All (54) 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:94:ARG:HD2	1:A:134:LEU:HD13	1.69	0.72
1:A:80:ASN:HB2	1:A:81:PRO:HD3	1.73	0.69
1:A:30:GLU:HB2	1:A:32:LEU:HD13	1.75	0.67
1:A:83:GLU:HA	1:A:88:LYS:HG3	1.77	0.66
1:A:99:LEU:HD13	1:A:261:SER:HB2	1.81	0.63
1:A:323:PRO:HG2	1:A:329:GLY:HA3	1.83	0.60
1:A:257:LEU:HD12	2:A:736:HOH:O	2.01	0.59
1:A:11:ILE:HG12	1:A:275:SER:O	2.04	0.58
1:A:324:PRO:HB3	2:A:609:HOH:O	2.06	0.56
1:A:94:ARG:HD2	1:A:134:LEU:CD1	2.36	0.55
1:A:105:PRO:HB3	1:A:129:VAL:HG22	1.89	0.55
1:A:272:VAL:O	1:A:273:HIS:HB3	2.06	0.54
1:A:132:ARG:HG2	1:A:133:GLU:O	2.09	0.52
1:A:26:LEU:HD21	1:A:344:LEU:HG	1.91	0.52
1:A:322:THR:OG1	1:A:339:THR:HG21	2.11	0.51
1:A:108:VAL:HG22	1:A:251:PRO:HA	1.93	0.51
1:A:225:ARG:HD3	2:A:510:HOH:O	2.12	0.50
1:A:82:ARG:NH2	2:A:525:HOH:O	2.44	0.50
1:A:311:VAL:O	1:A:315:VAL:HG13	2.13	0.49
1:A:342:ARG:HH11	1:A:342:ARG:HG2	1.78	0.48
1:A:85:ARG:HD3	2:A:664:HOH:O	2.13	0.47
1:A:302:PHE:O	1:A:304:LEU:HD13	2.14	0.47
1:A:103:LEU:HD13	1:A:262:LEU:HD22	1.96	0.47
1:A:176:ARG:HH21	1:A:231:ASP:HA	1.79	0.47
1:A:62:GLU:HG3	1:A:62:GLU:O	2.15	0.47
1:A:79:GLN:HG3	1:A:80:ASN:N	2.29	0.46
1:A:130:ILE:HG12	1:A:233:VAL:HB	1.98	0.46
1:A:43:GLY:HA2	1:A:46:ILE:HD12	1.98	0.46
1:A:257:LEU:O	1:A:272:VAL:HG23	2.17	0.45
1:A:90:LEU:HD22	2:A:468:HOH:O	2.16	0.45
1:A:327:LEU:HD12	2:A:535:HOH:O	2.17	0.44
1:A:120:LYS:O	1:A:123:ILE:HG12	2.18	0.44
1:A:225:ARG:NH1	2:A:424:HOH:O	2.49	0.44
1:A:287:PRO:HG2	1:A:336:PHE:HD2	1.83	0.44
1:A:310:LYS:HB3	1:A:310:LYS:HE2	1.73	0.44
1:A:100:PHE:CE1	1:A:164:ARG:HB3	2.52	0.43
1:A:276:ALA:N	1:A:277:PRO:HD3	2.33	0.43
1:A:58:ARG:NH1	2:A:515:HOH:O	2.51	0.43
1:A:112:LEU:HD11	1:A:319:LEU:HD22	2.01	0.42
1:A:99:LEU:HD13	1:A:261:SER:CB	2.48	0.42
1:A:325:PRO:HD3	1:A:331:ALA:O	2.20	0.42
1:A:325:PRO:HA	1:A:329:GLY:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ARG:HG3	1:A:240:GLY:HA3	2.01	0.42
1:A:300:HIS:CE1	2:A:675:HOH:O	2.73	0.42
1:A:113:SER:O	1:A:115:ALA:N	2.53	0.42
1:A:185:LYS:HA	1:A:185:LYS:HD2	1.87	0.42
1:A:246:LEU:O	1:A:249:VAL:HG22	2.18	0.42
1:A:131:VAL:HG22	1:A:234:VAL:HG23	2.02	0.41
1:A:74:GLY:HA2	1:A:75:PRO:HD3	1.85	0.41
1:A:259:SER:HB2	1:A:272:VAL:HG22	2.02	0.41
1:A:68:LEU:HD22	2:A:512:HOH:O	2.21	0.41
1:A:1:MET:HG3	1:A:302:PHE:CE2	2.57	0.40
1:A:120:LYS:HB2	2:A:638:HOH:O	2.21	0.40
1:A:306:GLU:HG2	1:A:307:LEU:N	2.36	0.40

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	343/345 (99%)	316 (92%)	23 (7%)	4 (1%)	16 10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	PRO
1	A	110	GLU
1	A	177	ARG
1	A	228	ALA

5.3.2 Protein sidechains (i)

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	270/270 (100%)	240 (89%)	30 (11%)	8 4

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	PRO
1	A	34	LEU
1	A	55	GLU
1	A	58	ARG
1	A	83	GLU
1	A	84	LEU
1	A	95	LYS
1	A	110	GLU
1	A	131	VAL
1	A	146	MET
1	A	147	SER
1	A	152	TRP
1	A	157	TYR
1	A	165	VAL
1	A	176	ARG
1	A	178	LYS
1	A	201	GLU
1	A	217	ASP
1	A	229	ARG
1	A	244	SER
1	A	246	LEU
1	A	253	SER
1	A	254	LEU
1	A	273	HIS
1	A	275	SER
1	A	304	LEU
1	A	306	GLU
1	A	313	ASP
1	A	315	VAL
1	A	344	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

There are no ligands in this entry.

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.