Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2021 – 09:32 AM EDT

PDB ID	:	1IDF
Title	:	ISOCITRATE DEHYDROGENASE K230M MUTANT APO ENZYME
Authors	:	Bolduc, J.M.; Dyer, D.H.; Scott, W.G.; Singer, P.; Sweet, R.M.; Koshland Junior, D.E.; Stoddard, B.L.
Deposited on	:	1995-01-18
Resolution	:	2.50 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
https://www.wwpdb.org/validation/2017/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:

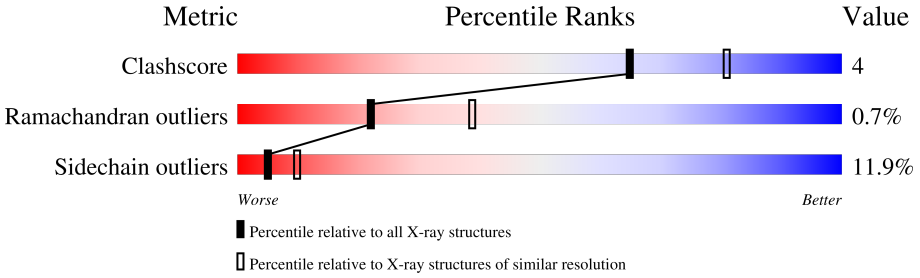
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.50 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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	416	70% 22% 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3217 atoms, of which 22 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 ISOCITRATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	414	3217	2034	22	537	605	19	30	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	230	MET	LYS	engineered mutation	UNP P08200

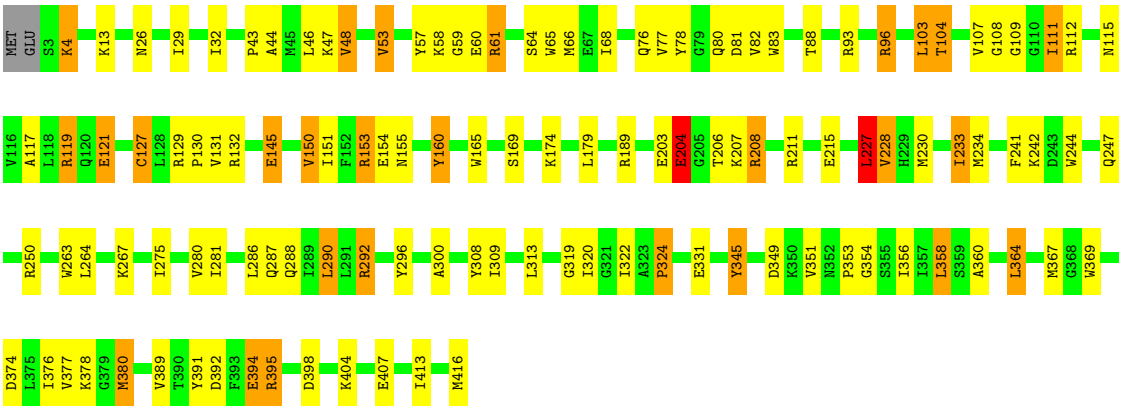
3 Residue-property plots (i)

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. 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. 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: ISOCITRATE DEHYDROGENASE

Chain A: 70% 22% 6%



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	105.10Å 105.10Å 150.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.223 , 0.262	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3217	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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	1.19	7/3256 (0.2%)	1.92	87/4404 (2.0%)

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	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	GLU	CG-CD	6.19	1.61	1.51
1	A	204	GLU	CB-CG	5.86	1.63	1.52
1	A	345	TYR	CB-CG	5.46	1.59	1.51
1	A	244	TRP	CD1-NE1	-5.33	1.28	1.38
1	A	244	TRP	NE1-CE2	-5.18	1.30	1.37
1	A	145	GLU	CD-OE2	-5.16	1.20	1.25
1	A	345	TYR	CA-CB	5.13	1.65	1.53

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	153	ARG	NE-CZ-NH2	-14.04	113.28	120.30
1	A	61	ARG	NE-CZ-NH1	12.05	126.32	120.30
1	A	230	MET	CG-SD-CE	10.03	116.25	100.20
1	A	208	ARG	NE-CZ-NH1	9.71	125.16	120.30
1	A	250	ARG	NE-CZ-NH1	9.57	125.08	120.30
1	A	280	VAL	CG1-CB-CG2	-8.91	96.64	110.90
1	A	107	VAL	CA-C-N	-8.87	98.46	116.20
1	A	244	TRP	CD1-CG-CD2	8.66	113.23	106.30
1	A	244	TRP	CE2-CD2-CG	-8.55	100.46	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	287	GLN	N-CA-CB	-8.54	95.22	110.60
1	A	103	LEU	CA-CB-CG	8.24	134.26	115.30
1	A	150	VAL	CG1-CB-CG2	-8.03	98.06	110.90
1	A	65	TRP	CE2-CD2-CG	-7.95	100.94	107.30
1	A	65	TRP	CD1-CG-CD2	7.64	112.41	106.30
1	A	165	TRP	CD1-CG-CD2	7.54	112.33	106.30
1	A	96	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	A	244	TRP	CG-CD2-CE3	7.52	140.67	133.90
1	A	83	TRP	CE2-CD2-CG	-7.50	101.30	107.30
1	A	153	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	A	287	GLN	CA-CB-CG	7.47	129.83	113.40
1	A	83	TRP	CD1-CG-CD2	7.41	112.23	106.30
1	A	165	TRP	CE2-CD2-CG	-7.40	101.38	107.30
1	A	211	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	A	160	TYR	CB-CG-CD1	-7.25	116.65	121.00
1	A	129	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	A	389	VAL	N-CA-CB	-7.10	95.89	111.50
1	A	66	MET	CG-SD-CE	7.05	111.48	100.20
1	A	104	THR	CA-C-N	-6.88	102.07	117.20
1	A	380	MET	CG-SD-CE	-6.76	89.39	100.20
1	A	13	LYS	CA-CB-CG	6.73	128.21	113.40
1	A	319	GLY	CA-C-O	-6.68	108.57	120.60
1	A	267	LYS	CA-CB-CG	6.64	128.02	113.40
1	A	263	TRP	CD1-CG-CD2	6.64	111.61	106.30
1	A	119	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	263	TRP	CE2-CD2-CG	-6.60	102.02	107.30
1	A	369	TRP	CD1-CG-CD2	6.59	111.57	106.30
1	A	308	TYR	CB-CG-CD2	-6.56	117.07	121.00
1	A	290	LEU	CA-CB-CG	6.43	130.09	115.30
1	A	46	LEU	CA-CB-CG	6.43	130.08	115.30
1	A	104	THR	O-C-N	6.33	132.83	122.70
1	A	165	TRP	CG-CD2-CE3	6.32	139.58	133.90
1	A	65	TRP	CG-CD2-CE3	6.23	139.51	133.90
1	A	47	LYS	CA-CB-CG	6.22	127.08	113.40
1	A	107	VAL	O-C-N	6.20	133.74	123.20
1	A	369	TRP	CE2-CD2-CG	-6.20	102.34	107.30
1	A	319	GLY	CA-C-N	6.13	130.69	117.20
1	A	4	LYS	N-CA-C	6.09	127.44	111.00
1	A	345	TYR	CB-CG-CD1	6.04	124.63	121.00
1	A	244	TRP	CB-CG-CD1	-6.03	119.16	127.00
1	A	394	GLU	CA-C-N	6.01	130.41	117.20
1	A	82	VAL	CA-CB-CG2	-6.00	101.89	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	111	ILE	CA-CB-CG2	-5.99	98.91	110.90
1	A	228	VAL	CA-C-N	-5.99	104.03	117.20
1	A	227	LEU	CA-CB-CG	5.95	128.99	115.30
1	A	378	LYS	CB-CG-CD	5.92	127.01	111.60
1	A	107	VAL	CG1-CB-CG2	-5.70	101.79	110.90
1	A	250	ARG	CG-CD-NE	5.66	123.68	111.80
1	A	107	VAL	CA-CB-CG2	-5.63	102.45	110.90
1	A	244	TRP	CG-CD1-NE1	-5.60	104.50	110.10
1	A	267	LYS	CA-C-N	5.54	129.40	117.20
1	A	377	VAL	CA-C-N	5.54	129.39	117.20
1	A	112	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	292	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	108	GLY	O-C-N	5.50	132.56	123.20
1	A	376	ILE	CA-C-N	5.50	129.30	117.20
1	A	151	ILE	CG1-CB-CG2	-5.50	99.30	111.40
1	A	331	GLU	CA-CB-CG	5.49	125.48	113.40
1	A	108	GLY	C-N-CA	5.46	133.77	122.30
1	A	127	CYS	N-CA-C	-5.44	96.32	111.00
1	A	395	ARG	CB-CG-CD	5.43	125.71	111.60
1	A	4	LYS	CA-C-N	5.40	129.07	117.20
1	A	287	GLN	CB-CA-C	5.38	121.17	110.40
1	A	374	ASP	CA-CB-CG	5.36	125.19	113.40
1	A	165	TRP	CB-CG-CD1	-5.32	120.08	127.00
1	A	132	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	A	65	TRP	CB-CG-CD1	-5.29	120.12	127.00
1	A	169	SER	CA-CB-OG	5.18	125.20	111.20
1	A	145	GLU	CA-CB-CG	5.18	124.79	113.40
1	A	76	GLN	CA-C-N	-5.17	105.81	117.20
1	A	364	LEU	CA-C-N	5.17	128.56	117.20
1	A	360	ALA	CA-C-N	5.14	128.51	117.20
1	A	349	ASP	CA-CB-CG	5.12	124.66	113.40
1	A	211	ARG	CA-CB-CG	5.10	124.62	113.40
1	A	132	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	53	VAL	CA-C-N	5.08	128.38	117.20
1	A	174	LYS	CB-CG-CD	5.05	124.73	111.60
1	A	215	GLU	CA-CB-CG	5.01	124.42	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	296	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	345	TYR	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	3195	22	3218	26	0
All	All	3195	22	3218	26	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 4.

All (26) 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:413:ILE:O	1:A:416:MET:HG2	2.01	0.60
1:A:119:ARG:HD2	1:A:155:ASN:ND2	2.18	0.59
1:A:115:ASN:O	1:A:119:ARG:HG3	2.04	0.58
1:A:322:ILE:HG22	1:A:354:GLY:HA3	1.87	0.56
1:A:44:ALA:O	1:A:48:VAL:HG13	2.08	0.53
1:A:207:LYS:NZ	1:A:247:GLN:HE21	2.06	0.52
1:A:206:THR:CG2	1:A:241:PHE:HD2	2.25	0.50
1:A:203:GLU:HG3	1:A:207:LYS:HE3	1.95	0.48
1:A:228:VAL:HG21	1:A:309:ILE:HD11	1.95	0.48
1:A:227:LEU:HD12	1:A:300:ALA:HB3	1.96	0.48
1:A:288:GLN:HE22	1:A:292:ARG:HD2	1.79	0.48
1:A:404:LYS:HB2	1:A:407:GLU:HG3	1.96	0.48
1:A:68:ILE:HD12	1:A:88:THR:HG23	1.97	0.46
1:A:32:ILE:HG13	1:A:68:ILE:HG13	1.99	0.45
1:A:204:GLU:O	1:A:208:ARG:HG2	2.17	0.44
1:A:324:PRO:HB3	1:A:358:LEU:HB3	2.00	0.43
1:A:233:ILE:HG22	1:A:234:MET:HG3	2.01	0.43
1:A:57:TYR:O	1:A:59:GLY:N	2.52	0.43
1:A:127:CYS:SG	1:A:153:ARG:HD3	2.59	0.43
1:A:117:ALA:O	1:A:121:GLU:HB2	2.19	0.42
1:A:353:PRO:O	1:A:356:ILE:HG22	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ARG:O	1:A:96:ARG:HD2	2.20	0.41
1:A:130:PRO:HA	1:A:150:VAL:HA	2.02	0.41
1:A:29:ILE:HD11	1:A:367:MET:CE	2.51	0.41
1:A:206:THR:HG22	1:A:241:PHE:HD2	1.84	0.41
1:A:77:VAL:HG12	1:A:78:TYR:CE1	2.56	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	412/416 (99%)	383 (93%)	26 (6%)	3 (1%)	22 39

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	58	LYS
1	A	109	GLY

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	336/338 (99%)	296 (88%)	40 (12%)	5 10

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	43	PRO
1	A	48	VAL
1	A	53	VAL
1	A	60	GLU
1	A	61	ARG
1	A	64	SER
1	A	80	GLN
1	A	81	ASP
1	A	103	LEU
1	A	104	THR
1	A	111	ILE
1	A	121	GLU
1	A	131	VAL
1	A	145	GLU
1	A	154	GLU
1	A	160	TYR
1	A	179	LEU
1	A	189	ARG
1	A	204	GLU
1	A	227	LEU
1	A	233	ILE
1	A	242	LYS
1	A	264	LEU
1	A	275	ILE
1	A	281	ILE
1	A	286	LEU
1	A	290	LEU
1	A	313	LEU
1	A	320	ILE
1	A	324	PRO
1	A	351	VAL
1	A	358	LEU
1	A	364	LEU
1	A	380	MET
1	A	391	TYR
1	A	392	ASP
1	A	394	GLU
1	A	395	ARG
1	A	398	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	ASN
1	A	247	GLN
1	A	288	GLN
1	A	327	ASN

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 monosaccharides 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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.