



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:51 am BST

PDB ID : 4ICD
Title : REGULATION OF ISOCITRATE DEHYDROGENASE BY PHOSPHORYLATION INVOLVES NO LONG-RANGE CONFORMATIONAL CHANGE IN THE FREE ENZYME
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Deposited on : 1989-12-28
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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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) : 2.11

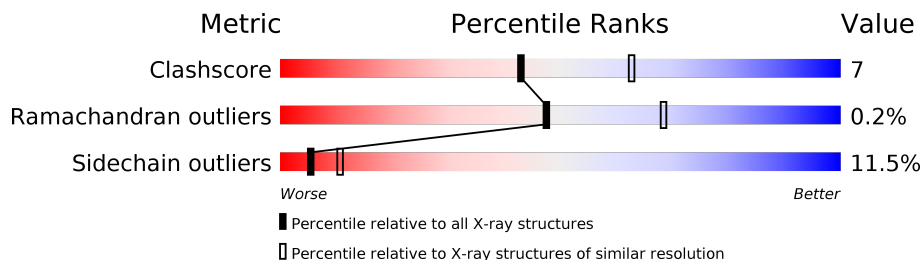
1 Overall quality at a glance i

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 on 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	416	72% 23% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3293 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 PHOSPHORYLATED ISOCITRATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	414	3150	2007	531	593	1	18	0	0	0

- Molecule 2 is water.

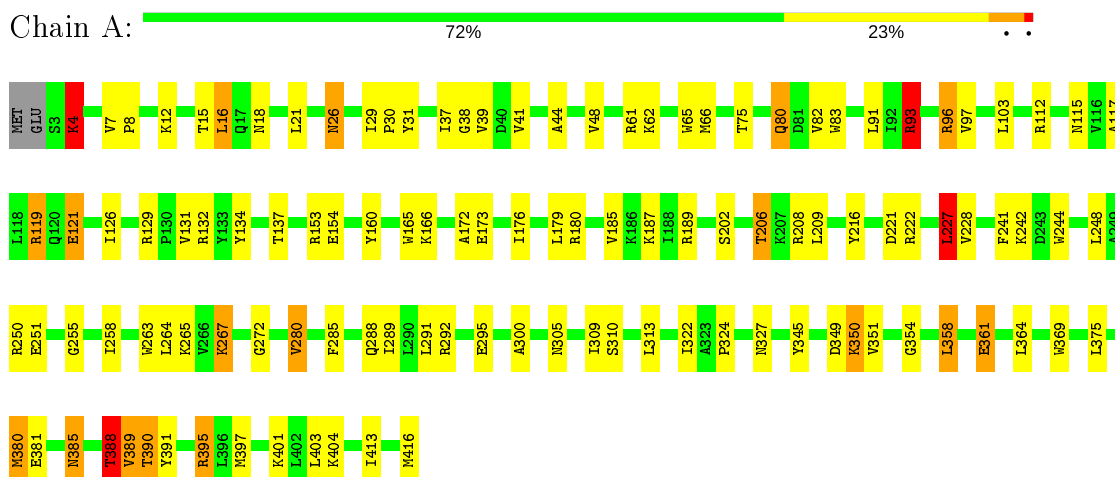
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	143	Total	O	0	0
			143	143		

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 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: PHOSPHORYLATED ISOCITRATE DEHYDROGENASE



4 Data and refinement statistics

Xtrriage (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}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.169 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3293	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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

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	0.81	0/3200	1.50	47/4334 (1.1%)

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	ARG	NE-CZ-NH2	11.13	125.87	120.30
1	A	119	ARG	NE-CZ-NH2	10.04	125.32	120.30
1	A	216	TYR	CB-CG-CD1	-9.70	115.18	121.00
1	A	153	ARG	NE-CZ-NH2	9.25	124.92	120.30
1	A	61	ARG	NE-CZ-NH2	8.64	124.62	120.30
1	A	165	TRP	CD1-CG-CD2	8.48	113.09	106.30
1	A	369	TRP	CD1-CG-CD2	7.83	112.57	106.30
1	A	165	TRP	CE2-CD2-CG	-7.52	101.28	107.30
1	A	189	ARG	NE-CZ-NH2	7.45	124.03	120.30
1	A	244	TRP	CD1-CG-CD2	7.40	112.22	106.30
1	A	65	TRP	CD1-CG-CD2	7.40	112.22	106.30
1	A	189	ARG	NE-CZ-NH1	-7.27	116.67	120.30
1	A	153	ARG	NE-CZ-NH1	-7.10	116.75	120.30
1	A	250	ARG	NE-CZ-NH1	-7.02	116.79	120.30
1	A	244	TRP	CE2-CD2-CG	-6.89	101.78	107.30
1	A	83	TRP	CD1-CG-CD2	6.81	111.75	106.30
1	A	369	TRP	CE2-CD2-CG	-6.72	101.92	107.30
1	A	222	ARG	NE-CZ-NH2	6.67	123.64	120.30
1	A	129	ARG	NE-CZ-NH1	-6.61	116.99	120.30
1	A	380	MET	CG-SD-CE	-6.57	89.69	100.20
1	A	65	TRP	CE2-CD2-CG	-6.54	102.07	107.30
1	A	83	TRP	CE2-CD2-CG	-6.54	102.07	107.30
1	A	180	ARG	NE-CZ-NH1	-6.49	117.05	120.30
1	A	160	TYR	CB-CG-CD2	-6.36	117.19	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	ARG	NE-CZ-NH1	-6.28	117.16	120.30
1	A	389	VAL	N-CA-CB	-6.22	97.82	111.50
1	A	361	GLU	CA-CB-CG	6.21	127.07	113.40
1	A	132	ARG	NE-CZ-NH2	6.01	123.31	120.30
1	A	208	ARG	NE-CZ-NH1	-5.91	117.35	120.30
1	A	263	TRP	CE2-CD2-CG	-5.90	102.58	107.30
1	A	96	ARG	NE-CZ-NH1	-5.81	117.39	120.30
1	A	112	ARG	NE-CZ-NH1	-5.81	117.39	120.30
1	A	165	TRP	CG-CD1-NE1	-5.64	104.46	110.10
1	A	369	TRP	CG-CD1-NE1	-5.60	104.50	110.10
1	A	263	TRP	CD1-CG-CD2	5.59	110.77	106.30
1	A	397	MET	CG-SD-CE	5.58	109.14	100.20
1	A	132	ARG	NE-CZ-NH1	-5.49	117.56	120.30
1	A	4	LYS	CA-CB-CG	-5.47	101.37	113.40
1	A	244	TRP	CG-CD2-CE3	5.46	138.82	133.90
1	A	93	ARG	NE-CZ-NH2	5.37	122.98	120.30
1	A	244	TRP	CG-CD1-NE1	-5.30	104.80	110.10
1	A	390	THR	N-CA-CB	-5.24	100.35	110.30
1	A	31	TYR	CB-CG-CD1	-5.23	117.86	121.00
1	A	388	THR	N-CA-CB	-5.15	100.52	110.30
1	A	227	LEU	CA-CB-CG	5.08	126.99	115.30
1	A	96	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	A	395	ARG	CA-CB-CG	5.01	124.42	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	3150	0	3139	43	0
2	A	143	0	0	2	0
All	All	3293	0	3139	43	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 7.

All (43) 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:16:LEU:HD23	1:A:96:ARG:HD2	1.72	0.71
1:A:401:LYS:HE3	1:A:403:LEU:HD11	1.75	0.67
1:A:288:GLN:HE22	1:A:292:ARG:HD3	1.67	0.59
1:A:154:GLU:HA	1:A:209:LEU:HD13	1.83	0.59
1:A:305:ASN:O	1:A:309:ILE:HG12	2.02	0.58
1:A:4:LYS:HB2	1:A:4:LYS:NZ	2.19	0.58
1:A:267:LYS:HE2	1:A:272:GLY:HA2	1.86	0.57
1:A:134:TYR:O	1:A:137:THR:HG23	2.05	0.57
1:A:117:ALA:O	1:A:121:GLU:HB2	2.06	0.55
1:A:115:ASN:O	1:A:119:ARG:HG3	2.07	0.55
1:A:401:LYS:HE3	1:A:403:LEU:CD1	2.38	0.54
1:A:26:ASN:HA	1:A:62:LYS:O	2.07	0.54
1:A:258:ILE:HD11	1:A:265:LYS:HG3	1.89	0.54
1:A:206:THR:HB	1:A:241:PHE:CD2	2.43	0.53
1:A:37:ILE:HB	1:A:351:VAL:HG21	1.90	0.53
1:A:202:SER:O	1:A:206:THR:HG23	2.10	0.52
1:A:16:LEU:HD22	1:A:21:LEU:HD23	1.91	0.52
1:A:44:ALA:O	1:A:48:VAL:HG13	2.10	0.52
1:A:227:LEU:HD12	1:A:300:ALA:HB3	1.94	0.50
1:A:179:LEU:O	1:A:185:VAL:HG13	2.12	0.49
1:A:289:ILE:HD12	1:A:313:LEU:HD13	1.95	0.49
1:A:381:GLU:O	1:A:385:ASN:HB2	2.14	0.48
1:A:126:ILE:O	1:A:327:ASN:HA	2.16	0.46
1:A:280:VAL:HG22	1:A:285:PHE:HB2	1.97	0.46
1:A:30:PRO:HA	1:A:66:MET:O	2.17	0.45
1:A:413:ILE:O	1:A:416:MET:HB2	2.17	0.44
1:A:322:ILE:HG22	1:A:354:GLY:HA3	2.01	0.43
1:A:38:GLY:HA2	1:A:41:VAL:HG22	2.00	0.43
1:A:30:PRO:HD2	1:A:97:VAL:O	2.19	0.42
1:A:93:ARG:HD2	2:A:550:HOH:O	2.19	0.42
1:A:388:THR:HG21	2:A:471:HOH:O	2.20	0.42
1:A:29:ILE:HD12	1:A:97:VAL:HG22	2.02	0.42
1:A:358:LEU:HD12	1:A:358:LEU:HA	1.87	0.42
1:A:166:LYS:HE2	1:A:166:LYS:HB3	1.89	0.41
1:A:172:ALA:O	1:A:176:ILE:HG13	2.20	0.41
1:A:291:LEU:O	1:A:292:ARG:HG3	2.20	0.41
1:A:324:PRO:HB3	1:A:358:LEU:HB3	2.03	0.41
1:A:255:GLY:HA2	1:A:265:LYS:O	2.19	0.41
1:A:7:VAL:HA	1:A:8:PRO:HD3	1.89	0.41
1:A:349:ASP:O	1:A:404:LYS:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:TYR:CD2	1:A:350:LYS:HD2	2.56	0.40
1:A:75:THR:HB	1:A:80:GLN:HA	2.04	0.40
1:A:391:TYR:O	1:A:395:ARG:HG3	2.21	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	411/416 (99%)	397 (97%)	13 (3%)	1 (0%)	47 68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ASN

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	322/337 (96%)	285 (88%)	37 (12%)	5 11

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	12	LYS
1	A	15	THR
1	A	16	LEU
1	A	26	ASN
1	A	39	VAL
1	A	80	GLN
1	A	82	VAL
1	A	91	LEU
1	A	93	ARG
1	A	103	LEU
1	A	121	GLU
1	A	131	VAL
1	A	173	GLU
1	A	187	LYS
1	A	206	THR
1	A	221	ASP
1	A	227	LEU
1	A	228	VAL
1	A	242	LYS
1	A	248	LEU
1	A	251	GLU
1	A	264	LEU
1	A	267	LYS
1	A	280	VAL
1	A	295	GLU
1	A	310	SER
1	A	350	LYS
1	A	358	LEU
1	A	361	GLU
1	A	364	LEU
1	A	375	LEU
1	A	380	MET
1	A	385	ASN
1	A	388	THR
1	A	389	VAL
1	A	390	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	288	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue is 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
1	SEP	A	113	1	8,9,10	1.08	0	8,12,14	5.01	3 (37%)

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
1	SEP	A	113	1	-	3/5/8/10	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	SEP	OG-CB-CA	-12.94	95.56	108.14
1	A	113	SEP	P-OG-CB	5.05	132.21	118.30
1	A	113	SEP	O3P-P-O1P	2.13	119.03	110.68

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	113	SEP	CB-OG-P-O3P
1	A	113	SEP	N-CA-CB-OG
1	A	113	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.