



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:03 AM UTC

PDB ID : 7ICD / pdb_00007icd
Title : REGULATION OF AN ENZYME BY PHOSPHORYLATION AT THE ACTIVE SITE
Authors : Hurley, J.H.; Dean, A.M.; Sohl, J.L.; Koshlandjunior, D.E.; Stroud, R.M.
Deposited on : 1990-05-30
Resolution : 2.40 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 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 Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

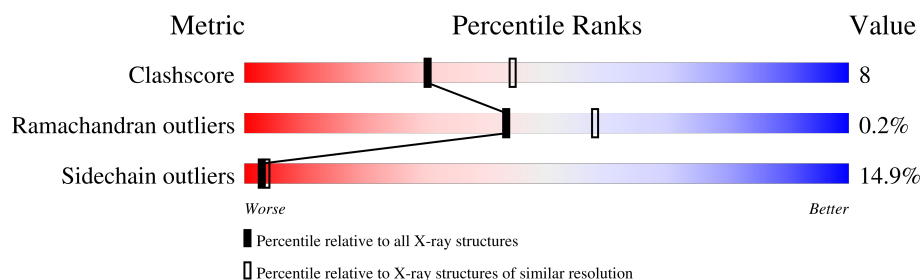
1 Overall quality at a glance

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))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	416	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3216 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 ISOCITRATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	414	3150	2010	531	591	18	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	GLU	SER	conflict	UNP P08200

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	66	Total	O	0	0
			66	66		

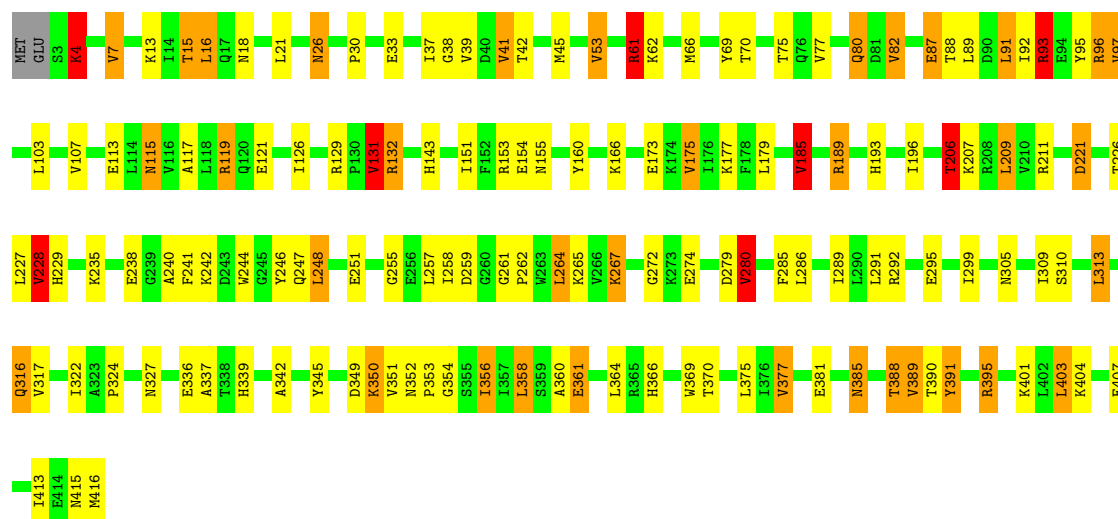
3 Residue-property plots

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: 



4 Data and refinement statistics

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) – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.179 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3216	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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	1.13	18/3211 (0.6%)	1.86	70/4351 (1.6%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	193	HIS	CD2-NE2	-8.44	1.28	1.37
1	A	53	VAL	CA-CB	7.07	1.63	1.54
1	A	193	HIS	CG-ND1	-6.82	1.30	1.38
1	A	228	VAL	CA-CB	6.78	1.62	1.54
1	A	229	HIS	CD2-NE2	-6.65	1.30	1.37
1	A	185	VAL	CA-CB	6.54	1.61	1.54
1	A	366	HIS	CD2-NE2	-6.51	1.30	1.37
1	A	280	VAL	CA-CB	6.28	1.64	1.54
1	A	143	HIS	CD2-NE2	-6.15	1.31	1.37
1	A	41	VAL	CA-CB	5.90	1.62	1.54
1	A	175	VAL	CA-CB	5.83	1.62	1.54
1	A	7	VAL	CA-CB	5.79	1.62	1.53
1	A	82	VAL	CA-CB	5.71	1.60	1.53
1	A	377	VAL	CA-CB	5.55	1.61	1.54
1	A	299	ILE	CA-CB	5.55	1.61	1.54
1	A	131	VAL	CA-CB	5.50	1.61	1.54
1	A	206	THR	CA-CB	5.36	1.62	1.53
1	A	339	HIS	CD2-NE2	-5.32	1.31	1.37

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	ASP	N-CA-C	10.41	125.61	110.42
1	A	221	ASP	CA-CB-CG	10.25	122.85	112.60
1	A	389	VAL	N-CA-CB	-9.33	95.11	112.36
1	A	258	ILE	N-CA-C	-9.16	93.44	107.73
1	A	390	THR	N-CA-CB	-8.78	97.80	110.36
1	A	119	ARG	NE-CZ-NH1	-7.77	113.73	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	PRO	CA-C-N	7.60	128.58	119.99
1	A	353	PRO	C-N-CA	7.60	128.58	119.99
1	A	61	ARG	NE-CZ-NH2	7.59	126.03	119.20
1	A	415	ASN	CA-CB-CG	-7.36	105.25	112.60
1	A	189	ARG	NE-CZ-NH2	7.09	125.58	119.20
1	A	196	ILE	N-CA-C	7.05	118.04	107.75
1	A	388	THR	CA-CB-OG1	-6.97	99.14	109.60
1	A	209	LEU	CD1-CG-CD2	6.87	125.92	110.80
1	A	15	THR	CA-CB-OG1	-6.83	99.36	109.60
1	A	119	ARG	NE-CZ-NH2	6.76	125.29	119.20
1	A	228	VAL	O-C-N	6.72	130.52	123.26
1	A	366	HIS	CB-CG-CD2	-6.54	122.69	131.20
1	A	352	ASN	OD1-CG-ND2	-6.53	116.07	122.60
1	A	251	GLU	N-CA-C	6.37	117.88	111.07
1	A	87	GLU	CA-CB-CG	6.16	126.42	114.10
1	A	70	THR	CA-CB-OG1	-6.12	100.42	109.60
1	A	352	ASN	CB-CG-ND2	6.04	125.47	116.40
1	A	389	VAL	CB-CA-C	6.04	120.50	110.30
1	A	279	ASP	CA-CB-CG	6.00	118.60	112.60
1	A	189	ARG	NE-CZ-NH1	-5.98	115.52	121.50
1	A	115	ASN	CB-CA-C	-5.93	101.57	110.88
1	A	336	GLU	N-CA-C	5.87	118.20	108.99
1	A	189	ARG	CA-CB-CG	5.83	125.76	114.10
1	A	235	LYS	N-CA-C	5.80	117.60	111.28
1	A	7	VAL	CA-C-N	5.76	125.69	119.76
1	A	7	VAL	C-N-CA	5.76	125.69	119.76
1	A	389	VAL	N-CA-C	5.73	118.41	108.90
1	A	388	THR	N-CA-CB	-5.72	100.80	110.46
1	A	15	THR	CA-CB-CG2	5.60	120.03	110.50
1	A	388	THR	CB-CA-C	5.60	120.86	111.22
1	A	388	THR	CA-C-O	5.55	127.03	120.70
1	A	342	ALA	CA-C-N	5.54	125.38	119.28
1	A	342	ALA	C-N-CA	5.54	125.38	119.28
1	A	193	HIS	CB-CG-CD2	-5.53	124.01	131.20
1	A	4	LYS	CA-CB-CG	-5.52	103.06	114.10
1	A	93	ARG	CA-C-N	5.50	127.92	120.44
1	A	93	ARG	C-N-CA	5.50	127.92	120.44
1	A	337	ALA	N-CA-C	-5.49	101.73	109.96
1	A	360	ALA	N-CA-C	-5.49	105.45	111.82
1	A	115	ASN	CA-CB-CG	-5.48	107.12	112.60
1	A	259	ASP	O-C-N	5.48	129.25	123.11
1	A	370	THR	N-CA-C	5.41	117.88	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	391	TYR	N-CA-C	5.38	117.85	111.33
1	A	26	ASN	CB-CG-ND2	5.37	124.46	116.40
1	A	69	TYR	N-CA-C	5.37	117.83	108.76
1	A	153	ARG	NE-CZ-NH1	-5.36	116.14	121.50
1	A	166	LYS	N-CA-C	5.35	117.98	110.23
1	A	96	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	A	262	PRO	N-CD-CG	-5.30	97.44	103.80
1	A	361	GLU	CA-CB-CG	5.26	124.62	114.10
1	A	242	LYS	CB-CG-CD	-5.25	99.22	111.30
1	A	96	ARG	NE-CZ-NH1	-5.24	116.26	121.50
1	A	26	ASN	OD1-CG-ND2	-5.23	117.37	122.60
1	A	238	GLU	CA-C-N	5.20	125.72	120.00
1	A	238	GLU	C-N-CA	5.20	125.72	120.00
1	A	132	ARG	NE-CZ-NH1	-5.18	116.32	121.50
1	A	229	HIS	CB-CG-CD2	-5.17	124.48	131.20
1	A	395	ARG	CA-CB-CG	5.12	124.34	114.10
1	A	131	VAL	CA-C-O	5.11	125.43	120.27
1	A	211	ARG	NE-CZ-NH1	-5.09	116.41	121.50
1	A	370	THR	CA-CB-OG1	-5.06	102.00	109.60
1	A	77	VAL	N-CA-C	-5.03	107.90	112.12
1	A	316	GLN	CA-CB-CG	5.02	124.14	114.10
1	A	390	THR	CB-CA-C	5.01	119.95	109.68

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	3143	53	0
2	A	66	0	0	0	0
All	All	3216	0	3143	53	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.

All (53) 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:401:LYS:HE3	1:A:403:LEU:HD11	1.63	0.79
1:A:322:ILE:HG22	1:A:354:GLY:HA3	1.76	0.68
1:A:305:ASN:O	1:A:309:ILE:HG12	1.96	0.66
1:A:154:GLU:HA	1:A:209:LEU:HD13	1.80	0.63
1:A:206:THR:HB	1:A:241:PHE:CD2	2.39	0.57
1:A:16:LEU:HD23	1:A:96:ARG:HD2	1.87	0.56
1:A:115:ASN:O	1:A:119:ARG:HG3	2.05	0.56
1:A:117:ALA:O	1:A:121:GLU:HB2	2.06	0.56
1:A:265:LYS:HD3	1:A:274:GLU:CD	2.32	0.54
1:A:267:LYS:HE2	1:A:272:GLY:HA2	1.90	0.54
1:A:33:GLU:HA	1:A:42:THR:HG21	1.90	0.53
1:A:240:ALA:HB1	1:A:244:TRP:CZ3	2.45	0.52
1:A:255:GLY:HA2	1:A:265:LYS:O	2.10	0.52
1:A:26:ASN:HA	1:A:62:LYS:O	2.10	0.51
1:A:226:THR:HG22	1:A:228:VAL:HG12	1.92	0.51
1:A:16:LEU:HD23	1:A:96:ARG:HH21	1.76	0.50
1:A:30:PRO:HD2	1:A:97:VAL:O	2.11	0.50
1:A:87:GLU:O	1:A:91:LEU:HD22	2.10	0.50
1:A:30:PRO:HA	1:A:66:MET:O	2.12	0.49
1:A:207:LYS:HB3	1:A:248:LEU:HD13	1.94	0.49
1:A:16:LEU:HD22	1:A:21:LEU:HD23	1.94	0.49
1:A:413:ILE:O	1:A:416:MET:HB2	2.12	0.49
1:A:37:ILE:HB	1:A:351:VAL:HG21	1.95	0.48
1:A:75:THR:HB	1:A:80:GLN:HA	1.95	0.48
1:A:126:ILE:O	1:A:327:ASN:HA	2.14	0.48
1:A:207:LYS:HD3	1:A:248:LEU:HB2	1.94	0.48
1:A:61:ARG:HH11	1:A:369:TRP:CD1	2.31	0.48
1:A:345:TYR:CD2	1:A:350:LYS:HD2	2.49	0.48
1:A:129:ARG:HB2	1:A:151:ILE:HB	1.97	0.47
1:A:179:LEU:O	1:A:185:VAL:HG13	2.14	0.47
1:A:289:ILE:HD12	1:A:313:LEU:HD13	1.97	0.46
1:A:391:TYR:O	1:A:395:ARG:HG3	2.16	0.46
1:A:381:GLU:O	1:A:385:ASN:HB2	2.16	0.46
1:A:265:LYS:HG2	1:A:274:GLU:HB3	1.97	0.45
1:A:119:ARG:HD2	1:A:155:ASN:ND2	2.32	0.45
1:A:401:LYS:HE3	1:A:403:LEU:CD1	2.41	0.45
1:A:280:VAL:HG22	1:A:285:PHE:HB2	1.98	0.45
1:A:324:PRO:HB3	1:A:358:LEU:HB3	1.99	0.44
1:A:350:LYS:HD3	1:A:391:TYR:CE2	2.53	0.44
1:A:45:MET:SD	1:A:45:MET:C	3.01	0.44
1:A:349:ASP:O	1:A:404:LYS:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LEU:O	1:A:93:ARG:HB2	2.17	0.43
1:A:4:LYS:HB2	1:A:4:LYS:NZ	2.32	0.43
1:A:88:THR:O	1:A:92:ILE:HG13	2.19	0.43
1:A:38:GLY:HA2	1:A:41:VAL:HG22	2.02	0.42
1:A:403:LEU:HB3	1:A:407:GLU:HB2	2.02	0.41
1:A:246:TYR:HD1	1:A:264:LEU:HD22	1.85	0.41
1:A:257:LEU:HD22	1:A:261:GLY:HA3	2.02	0.41
1:A:131:VAL:HG23	1:A:317:VAL:HG21	2.02	0.40
1:A:13:LYS:HG2	1:A:95:TYR:CE1	2.57	0.40
1:A:45:MET:HB2	1:A:356:ILE:HG23	2.04	0.40
1:A:113:GLU:OE1	1:A:115:ASN:HB2	2.21	0.40
1:A:207:LYS:NZ	1:A:247:GLN:OE1	2.54	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	412/416 (99%)	393 (95%)	18 (4%)	1 (0%)	43	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	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	323/338 (96%)	275 (85%)	48 (15%)	3 3

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	7	VAL
1	A	15	THR
1	A	16	LEU
1	A	39	VAL
1	A	53	VAL
1	A	61	ARG
1	A	80	GLN
1	A	82	VAL
1	A	91	LEU
1	A	93	ARG
1	A	97	VAL
1	A	103	LEU
1	A	107	VAL
1	A	131	VAL
1	A	132	ARG
1	A	160	TYR
1	A	173	GLU
1	A	175	VAL
1	A	177	LYS
1	A	185	VAL
1	A	189	ARG
1	A	206	THR
1	A	221	ASP
1	A	227	LEU
1	A	228	VAL
1	A	248	LEU
1	A	264	LEU
1	A	267	LYS
1	A	280	VAL
1	A	286	LEU
1	A	291	LEU
1	A	292	ARG
1	A	295	GLU
1	A	310	SER
1	A	313	LEU

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Mol	Chain	Res	Type
1	A	316	GLN
1	A	350	LYS
1	A	356	ILE
1	A	358	LEU
1	A	361	GLU
1	A	364	LEU
1	A	375	LEU
1	A	377	VAL
1	A	385	ASN
1	A	388	THR
1	A	389	VAL
1	A	403	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	120	GLN
1	A	143	HIS
1	A	270	ASN
1	A	288	GLN
1	A	316	GLN
1	A	415	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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.