



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:59 PM GMT

PDB ID : 7ICD  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

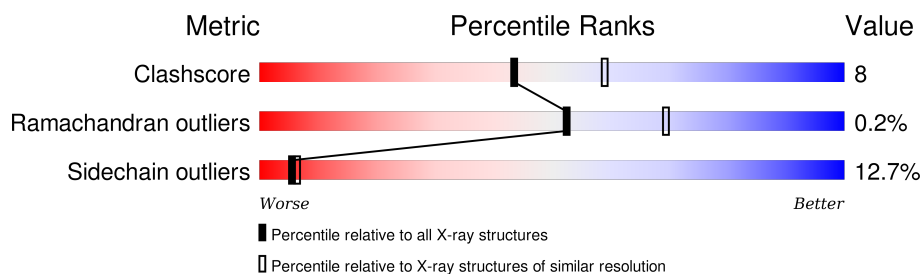
# 1 Overall quality at a glance

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	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	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
1	A	414	Total	C	N	O	S	0	0	0
			3150	2010	531	591	18			

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.

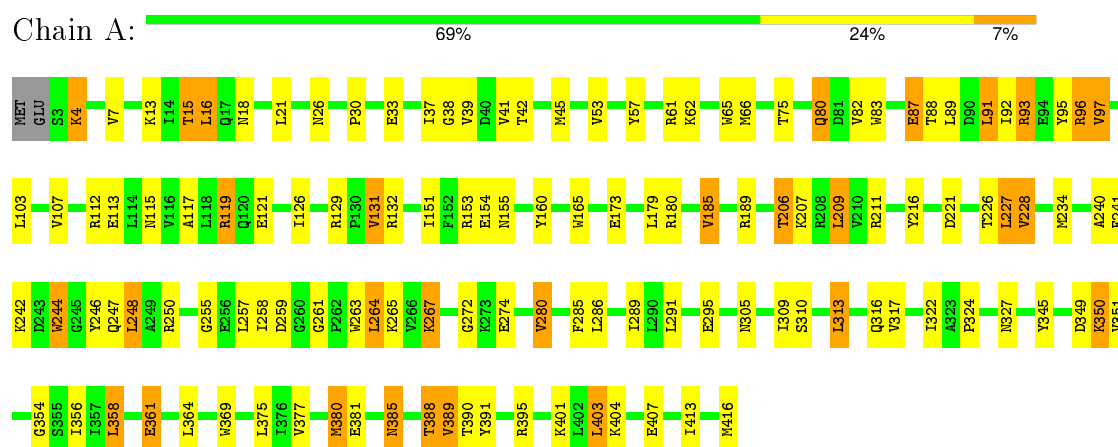
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	66	Total	O	0	0
			66	66		

### 3 Residue-property plots

These plots are drawn for all protein, RNA 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: ISOCITRATE DEHYDROGENASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	27.0	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	0.87	1/3211 (0.0%)	1.57	50/4351 (1.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	TRP	CD1-NE1	-5.24	1.29	1.38

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	ARG	NE-CZ-NH1	-13.14	113.73	120.30
1	A	61	ARG	NE-CZ-NH2	11.45	126.03	120.30
1	A	189	ARG	NE-CZ-NH2	10.55	125.58	120.30
1	A	119	ARG	NE-CZ-NH2	9.98	125.29	120.30
1	A	189	ARG	NE-CZ-NH1	-9.56	115.52	120.30
1	A	165	TRP	CD1-CG-CD2	8.86	113.39	106.30
1	A	369	TRP	CD1-CG-CD2	8.58	113.16	106.30
1	A	65	TRP	CD1-CG-CD2	8.36	112.99	106.30
1	A	153	ARG	NE-CZ-NH1	-8.31	116.14	120.30
1	A	96	ARG	NE-CZ-NH1	-8.08	116.26	120.30
1	A	83	TRP	CD1-CG-CD2	8.00	112.70	106.30
1	A	132	ARG	NE-CZ-NH1	-7.97	116.32	120.30
1	A	211	ARG	NE-CZ-NH1	-7.78	116.41	120.30
1	A	165	TRP	CE2-CD2-CG	-7.58	101.23	107.30
1	A	65	TRP	CE2-CD2-CG	-7.47	101.32	107.30
1	A	389	VAL	N-CA-CB	-7.45	95.11	111.50
1	A	96	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	A	83	TRP	CE2-CD2-CG	-7.00	101.70	107.30
1	A	180	ARG	NE-CZ-NH1	-6.72	116.94	120.30
1	A	244	TRP	CE2-CD2-CG	-6.71	101.94	107.30
1	A	369	TRP	CE2-CD2-CG	-6.61	102.01	107.30
1	A	390	THR	N-CA-CB	-6.58	97.80	110.30
1	A	244	TRP	CD1-CG-CD2	6.50	111.50	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	ILE	N-CA-C	-6.50	93.44	111.00
1	A	250	ARG	NE-CZ-NH2	6.34	123.47	120.30
1	A	228	VAL	CA-C-N	-6.00	103.99	117.20
1	A	87	GLU	CA-CB-CG	5.92	126.42	113.40
1	A	369	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	A	93	ARG	NE-CZ-NH2	5.85	123.22	120.30
1	A	132	ARG	NE-CZ-NH2	5.83	123.21	120.30
1	A	165	TRP	CG-CD1-NE1	-5.78	104.32	110.10
1	A	263	TRP	CD1-CG-CD2	5.75	110.90	106.30
1	A	216	TYR	CB-CG-CD1	-5.70	117.58	121.00
1	A	263	TRP	CE2-CD2-CG	-5.68	102.75	107.30
1	A	61	ARG	NE-CZ-NH1	-5.67	117.46	120.30
1	A	189	ARG	CA-CB-CG	5.62	125.76	113.40
1	A	250	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	A	244	TRP	CG-CD2-CE3	5.51	138.86	133.90
1	A	15	THR	CA-CB-CG2	5.45	120.03	112.40
1	A	259	ASP	N-CA-C	5.41	125.61	111.00
1	A	380	MET	CG-SD-CE	-5.39	91.57	100.20
1	A	83	TRP	CG-CD1-NE1	-5.29	104.81	110.10
1	A	112	ARG	NE-CZ-NH2	5.27	122.94	120.30
1	A	209	LEU	CD1-CG-CD2	5.14	125.92	110.50
1	A	227	LEU	CA-CB-CG	5.13	127.10	115.30
1	A	361	GLU	CA-CB-CG	5.10	124.62	113.40
1	A	57	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	A	65	TRP	CG-CD1-NE1	-5.04	105.06	110.10
1	A	234	MET	CG-SD-CE	-5.01	92.18	100.20
1	A	388	THR	N-CA-CB	-5.00	100.80	110.30

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	51	0
2	A	66	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3216	0	3143	51	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 (51) 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:117:ALA:O	1:A:121:GLU:HB2	2.06	0.56
1:A:115:ASN:O	1:A:119:ARG:HG3	2.05	0.56
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:265:LYS:HD3	1:A:274:GLU:CD	2.32	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: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:391:TYR:O	1:A:395:ARG:HG3	2.16	0.46
1:A:289:ILE:HD12	1:A:313:LEU:HD13	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:350:LYS:HD3	1:A:391:TYR:CE2	2.53	0.44
1:A:324:PRO:HB3	1:A:358:LEU:HB3	1.99	0.44
1:A:349:ASP:O	1:A:404:LYS:HB3	2.17	0.44
1:A:89:LEU:O	1:A:93:ARG:HB2	2.17	0.43
1:A:4:LYS:NZ	1:A:4:LYS:HB2	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:113:GLU:OE1	1:A:115:ASN:HB2	2.21	0.40
1:A:45:MET:HB2	1:A:356:ILE:HG23	2.04	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%)	52 69

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%)	282 (87%)	41 (13%)	<b>5</b> <b>6</b>

All (41) 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	80	GLN
1	A	82	VAL
1	A	91	LEU
1	A	97	VAL
1	A	103	LEU
1	A	107	VAL
1	A	131	VAL
1	A	160	TYR
1	A	173	GLU
1	A	185	VAL
1	A	206	THR
1	A	221	ASP
1	A	227	LEU
1	A	242	LYS
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	295	GLU
1	A	310	SER
1	A	313	LEU
1	A	316	GLN

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Mol	Chain	Res	Type
1	A	350	LYS
1	A	358	LEU
1	A	361	GLU
1	A	364	LEU
1	A	375	LEU
1	A	377	VAL
1	A	380	MET
1	A	385	ASN
1	A	388	THR
1	A	389	VAL
1	A	403	LEU

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 ⓘ

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.