



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 05:38 pm BST

PDB ID : 6ICD
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 : 2.80 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
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) : 2.11

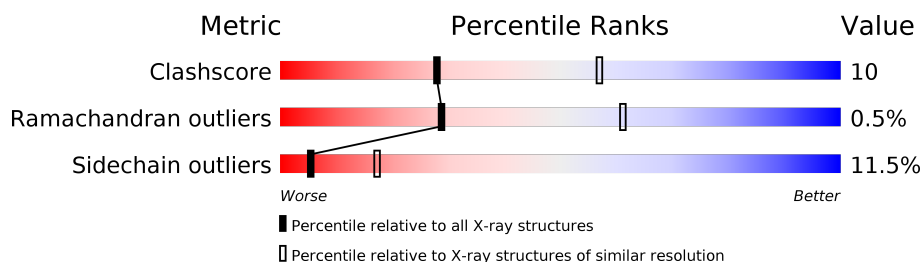
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3150 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
			3149	2009	531	591	18			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	ASP	SER	CONFLICT	UNP P08200

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O	0	0
			1	1		

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) – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.163 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3150	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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	0.90	1/3210 (0.0%)	1.63	54/4350 (1.2%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	VAL	CA-CB	7.21	1.69	1.54

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	TRP	CD1-CG-CD2	9.01	113.51	106.30
1	A	244	TRP	CD1-CG-CD2	8.65	113.22	106.30
1	A	65	TRP	CD1-CG-CD2	8.49	113.09	106.30
1	A	389	VAL	N-CA-CB	-8.46	92.88	111.50
1	A	369	TRP	CD1-CG-CD2	8.29	112.94	106.30
1	A	153	ARG	NE-CZ-NH1	-8.24	116.18	120.30
1	A	65	TRP	CE2-CD2-CG	-8.17	100.76	107.30
1	A	388	THR	N-CA-CB	-7.62	95.81	110.30
1	A	244	TRP	CE2-CD2-CG	-7.61	101.21	107.30
1	A	216	TYR	CB-CG-CD1	-7.56	116.47	121.00
1	A	211	ARG	NE-CZ-NH2	7.52	124.06	120.30
1	A	165	TRP	CE2-CD2-CG	-7.28	101.47	107.30
1	A	65	TRP	CG-CD2-CE3	7.20	140.38	133.90
1	A	361	GLU	CA-CB-CG	7.17	129.17	113.40
1	A	389	VAL	CG1-CB-CG2	7.00	122.11	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	TRP	CE2-CD2-CG	-6.84	101.83	107.30
1	A	129	ARG	NE-CZ-NH1	-6.78	116.91	120.30
1	A	83	TRP	CD1-CG-CD2	6.75	111.70	106.30
1	A	119	ARG	NE-CZ-NH2	6.73	123.67	120.30
1	A	389	VAL	CB-CA-C	6.73	124.19	111.40
1	A	161	ALA	CB-CA-C	-6.67	100.10	110.10
1	A	263	TRP	CD1-CG-CD2	6.64	111.61	106.30
1	A	65	TRP	CB-CG-CD1	-6.63	118.38	127.00
1	A	369	TRP	CE2-CD2-CG	-6.53	102.07	107.30
1	A	15	THR	CA-CB-CG2	6.34	121.28	112.40
1	A	263	TRP	CE2-CD2-CG	-6.19	102.34	107.30
1	A	244	TRP	CG-CD2-CE3	6.14	139.43	133.90
1	A	87	GLU	CA-CB-CG	6.05	126.71	113.40
1	A	112	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	A	369	TRP	CG-CD1-NE1	-5.98	104.12	110.10
1	A	128	LEU	CA-CB-CG	5.94	128.96	115.30
1	A	234	MET	CA-CB-CG	-5.92	103.23	113.30
1	A	388	THR	CA-CB-OG1	-5.91	96.59	109.00
1	A	65	TRP	CG-CD1-NE1	-5.87	104.23	110.10
1	A	244	TRP	CG-CD1-NE1	-5.85	104.25	110.10
1	A	362	MET	CG-SD-CE	5.79	109.46	100.20
1	A	165	TRP	CG-CD1-NE1	-5.77	104.33	110.10
1	A	222	ARG	NE-CZ-NH2	5.59	123.10	120.30
1	A	15	THR	CA-CB-OG1	-5.57	97.30	109.00
1	A	388	THR	CA-CB-CG2	5.49	120.08	112.40
1	A	208	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	A	208	ARG	NE-CZ-NH2	5.40	123.00	120.30
1	A	242	LYS	CB-CG-CD	-5.39	97.58	111.60
1	A	132	ARG	CB-CG-CD	-5.35	97.69	111.60
1	A	97	VAL	CG1-CB-CG2	-5.33	102.38	110.90
1	A	216	TYR	CB-CG-CD2	5.25	124.15	121.00
1	A	83	TRP	CG-CD2-CE3	5.22	138.60	133.90
1	A	244	TRP	CB-CG-CD1	-5.21	120.22	127.00
1	A	227	LEU	CA-CB-CG	5.18	127.22	115.30
1	A	31	TYR	CB-CG-CD1	-5.14	117.91	121.00
1	A	96	ARG	NE-CZ-NH2	5.13	122.86	120.30
1	A	360	ALA	CA-C-N	5.11	128.45	117.20
1	A	132	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	A	160	TYR	CB-CG-CD2	-5.07	117.96	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	57	TYR	Sidechain

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	3149	0	3141	62	0
2	A	1	0	0	0	0
All	All	3150	0	3141	62	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 (62) 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:267:LYS:HE2	1:A:272:GLY:HA2	1.62	0.81
1:A:401:LYS:HE3	1:A:403:LEU:HD11	1.70	0.72
1:A:154:GLU:HA	1:A:209:LEU:HD13	1.71	0.72
1:A:237:THR:O	1:A:240:ALA:HB3	2.02	0.60
1:A:322:ILE:HG22	1:A:354:GLY:HA3	1.84	0.60
1:A:289:ILE:HD12	1:A:313:LEU:HD13	1.82	0.59
1:A:119:ARG:HD3	1:A:327:ASN:OD1	2.03	0.59
1:A:75:THR:HB	1:A:80:GLN:HA	1.84	0.58
1:A:29:ILE:HD12	1:A:97:VAL:HG22	1.85	0.57
1:A:129:ARG:HB2	1:A:151:ILE:HB	1.86	0.57
1:A:285:PHE:HZ	1:A:299:ILE:HD12	1.69	0.56
1:A:250:ARG:HG3	1:A:264:LEU:HD21	1.88	0.56
1:A:285:PHE:CZ	1:A:299:ILE:HD12	2.42	0.55
1:A:120:GLN:HE22	1:A:161:ALA:HA	1.72	0.54
1:A:4:LYS:NZ	1:A:4:LYS:HB2	2.22	0.54
1:A:26:ASN:HA	1:A:62:LYS:O	2.09	0.53
1:A:304:LEU:O	1:A:307:ASP:HB3	2.09	0.52
1:A:285:PHE:CD2	1:A:309:ILE:HD12	2.43	0.52
1:A:30:PRO:HA	1:A:66:MET:O	2.09	0.52
1:A:167:ALA:HA	1:A:194:CYS:O	2.10	0.51
1:A:288:GLN:HB3	1:A:296:TYR:HE2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LEU:O	1:A:93:ARG:HB2	2.11	0.50
1:A:16:LEU:HD23	1:A:96:ARG:HH21	1.76	0.50
1:A:305:ASN:O	1:A:309:ILE:HG12	2.11	0.50
1:A:137:THR:HG22	1:A:393:PHE:CE2	2.47	0.49
1:A:288:GLN:HB3	1:A:296:TYR:CE2	2.47	0.48
1:A:113:ASP:HB3	1:A:116:VAL:HB	1.95	0.47
1:A:240:ALA:HB1	1:A:244:TRP:CZ3	2.49	0.47
1:A:285:PHE:HD2	1:A:309:ILE:HD12	1.77	0.47
1:A:288:GLN:HE22	1:A:292:ARG:HD3	1.79	0.47
1:A:404:LYS:HB2	1:A:407:GLU:HG3	1.96	0.47
1:A:35:ASP:OD2	1:A:72:GLU:HB3	2.14	0.47
1:A:49:VAL:O	1:A:53:VAL:HG13	2.14	0.47
1:A:322:ILE:HA	1:A:355:SER:N	2.30	0.47
1:A:206:THR:HB	1:A:241:PHE:CD2	2.50	0.46
1:A:257:LEU:HA	1:A:264:LEU:HD12	1.97	0.46
1:A:57:TYR:CG	1:A:61:ARG:HD3	2.50	0.46
1:A:206:THR:O	1:A:210:VAL:HG23	2.16	0.46
1:A:265:LYS:HG2	1:A:274:GLU:HB3	1.98	0.46
1:A:280:VAL:CG2	1:A:285:PHE:HB2	2.47	0.45
1:A:131:VAL:HG23	1:A:317:VAL:HG21	2.00	0.44
1:A:257:LEU:HD22	1:A:261:GLY:CA	2.46	0.44
1:A:131:VAL:HG11	1:A:313:LEU:HB3	1.98	0.44
1:A:345:TYR:CD2	1:A:350:LYS:HD2	2.53	0.44
1:A:13:LYS:HG2	1:A:95:TYR:CE1	2.52	0.44
1:A:115:ASN:O	1:A:119:ARG:HG3	2.18	0.43
1:A:71:GLY:O	1:A:74:SER:HB3	2.20	0.42
1:A:179:LEU:O	1:A:183:MET:HB2	2.19	0.42
1:A:116:VAL:O	1:A:120:GLN:HG3	2.20	0.42
1:A:40:ASP:O	1:A:43:PRO:HD2	2.20	0.42
1:A:167:ALA:O	1:A:168:ASP:HB2	2.21	0.41
1:A:12:LYS:HB3	1:A:24:PRO:HG3	2.01	0.41
1:A:287:GLN:O	1:A:291:LEU:HD22	2.20	0.41
1:A:154:GLU:CA	1:A:209:LEU:HD13	2.43	0.41
1:A:350:LYS:HD3	1:A:391:TYR:CD2	2.56	0.41
1:A:28:ILE:HA	1:A:64:SER:O	2.20	0.41
1:A:127:CYS:HB2	1:A:155:ASN:ND2	2.36	0.41
1:A:391:TYR:CG	1:A:392:ASP:N	2.88	0.40
1:A:16:LEU:HD22	1:A:21:LEU:HD23	2.04	0.40
1:A:37:ILE:HB	1:A:351:VAL:HG21	2.04	0.40
1:A:163:ILE:HB	1:A:198:ILE:HB	2.02	0.40
1:A:324:PRO:HB3	1:A:358:LEU:HB3	2.03	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%)	385 (93%)	25 (6%)	2 (0%)	29 61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	80	GLN

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	323/338 (96%)	286 (88%)	37 (12%)	5 17

All (37) 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	25	GLU
1	A	80	GLN

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Mol	Chain	Res	Type
1	A	82	VAL
1	A	91	LEU
1	A	97	VAL
1	A	107	VAL
1	A	131	VAL
1	A	160	TYR
1	A	173	GLU
1	A	187	LYS
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	286	LEU
1	A	291	LEU
1	A	292	ARG
1	A	295	GLU
1	A	311	ASP
1	A	313	LEU
1	A	320	ILE
1	A	350	LYS
1	A	358	LEU
1	A	361	GLU
1	A	364	LEU
1	A	370	THR
1	A	377	VAL
1	A	388	THR
1	A	389	VAL
1	A	390	THR
1	A	395	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	80	GLN
1	A	120	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates 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 ⓘ

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.