



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:02 PM GMT

PDB ID : 1IG8
Title : Crystal Structure of Yeast Hexokinase PII with the correct amino acid sequence
Authors : Kuser, P.R.; Krauchenco, S.; Antunes, O.A.; Polikarpov, I.
Deposited on : 2001-04-17
Resolution : 2.20 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
<http://wwpdb.org/validation/2016/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 : 1.7 (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

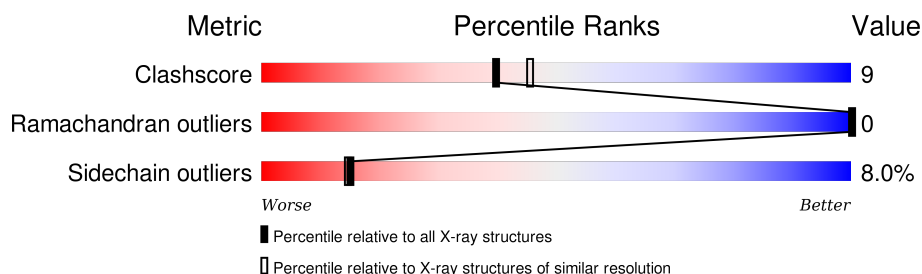
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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. 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	486	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4117 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 hexokinase PII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	469	Total	C	N	O	S	0	0	0
			3671	2337	607	712	15			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

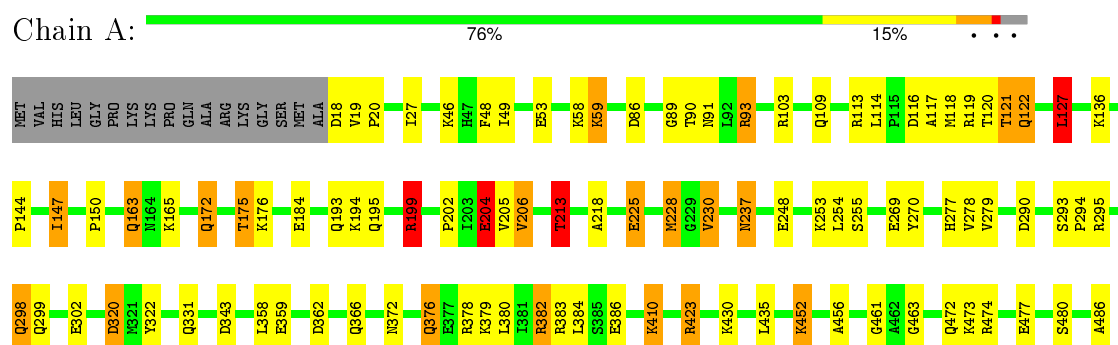
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	441	Total	O	0	0
			441	441		

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: hexokinase PII



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	142.81Å 142.81Å 58.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	13.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (13.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.162 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4117	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.57	0/3749	1.42	35/5075 (0.7%)

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	3

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	423	ARG	CD-NE-CZ	16.55	146.77	123.60
1	A	474	ARG	NE-CZ-NH2	-14.34	113.13	120.30
1	A	199	ARG	CD-NE-CZ	13.16	142.02	123.60
1	A	474	ARG	CD-NE-CZ	13.13	141.98	123.60
1	A	199	ARG	NE-CZ-NH2	12.31	126.45	120.30
1	A	383	ARG	NE-CZ-NH1	10.19	125.39	120.30
1	A	199	ARG	NE-CZ-NH1	-10.02	115.29	120.30
1	A	383	ARG	NE-CZ-NH2	-9.96	115.32	120.30
1	A	382	ARG	NE-CZ-NH2	-8.67	115.97	120.30
1	A	103	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	A	225	GLU	OE1-CD-OE2	8.46	133.46	123.30
1	A	378	ARG	NE-CZ-NH2	8.18	124.39	120.30
1	A	423	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	A	204	GLU	CA-CB-CG	7.35	129.58	113.40
1	A	359	GLU	OE1-CD-OE2	-7.28	114.56	123.30
1	A	103	ARG	NE-CZ-NH2	-7.09	116.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	362	ASP	CB-CG-OD1	6.54	124.19	118.30
1	A	206	VAL	N-CA-CB	-6.53	97.13	111.50
1	A	93	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	A	278	VAL	N-CA-CB	-6.33	97.56	111.50
1	A	86	ASP	CB-CG-OD1	6.27	123.94	118.30
1	A	163	GLN	N-CA-CB	-5.82	100.13	110.60
1	A	322	TYR	CB-CG-CD2	5.77	124.46	121.00
1	A	290	ASP	CB-CG-OD1	5.73	123.46	118.30
1	A	122	GLN	CB-CG-CD	5.47	125.83	111.60
1	A	320	ASP	CB-CG-OD1	-5.46	113.39	118.30
1	A	456	ALA	CB-CA-C	-5.44	101.94	110.10
1	A	474	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	103	ARG	CD-NE-CZ	5.35	131.09	123.60
1	A	127	LEU	CA-CB-CG	5.26	127.39	115.30
1	A	322	TYR	CB-CG-CD1	-5.25	117.85	121.00
1	A	343	ASP	CB-CG-OD1	5.15	122.93	118.30
1	A	378	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	A	228	MET	CA-CB-CG	5.10	121.97	113.30
1	A	302	GLU	OE1-CD-OE2	5.04	129.35	123.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	THR	Mainchain
1	A	213	THR	Mainchain
1	A	279	VAL	Mainchain

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	3671	0	3632	64	0
2	A	5	0	0	0	0
3	A	441	0	0	18	1
All	All	4117	0	3632	64	1

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 9.

All (64) 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:237:ASN:HD21	1:A:269:GLU:H	1.15	0.88
1:A:59:LYS:HE3	1:A:59:LYS:H	1.44	0.82
1:A:93:ARG:HE	1:A:109:GLN:NE2	1.85	0.75
1:A:93:ARG:HE	1:A:109:GLN:HE22	1.37	0.73
1:A:175:THR:HG22	1:A:176:LYS:HE2	1.73	0.70
1:A:90:THR:HG23	1:A:113:ARG:HE	1.56	0.69
1:A:193:GLN:NE2	1:A:205:VAL:H	1.94	0.65
1:A:193:GLN:HE22	1:A:205:VAL:H	1.45	0.65
1:A:461:GLY:HA2	3:A:937:HOH:O	1.98	0.64
1:A:237:ASN:ND2	1:A:269:GLU:H	1.94	0.62
1:A:46:LYS:HE3	1:A:46:LYS:HA	1.80	0.62
1:A:118:MET:HE1	1:A:127:LEU:HA	1.82	0.61
1:A:295:ARG:HB3	1:A:298:GLN:HG3	1.83	0.61
1:A:118:MET:HE3	1:A:127:LEU:HD23	1.84	0.59
1:A:410:LYS:HE3	3:A:872:HOH:O	2.03	0.58
1:A:193:GLN:NE2	1:A:205:VAL:HG23	2.18	0.58
1:A:237:ASN:HD21	1:A:269:GLU:N	1.95	0.57
1:A:277:HIS:HD2	3:A:505:HOH:O	1.89	0.56
1:A:293:SER:HB2	1:A:294:PRO:HD2	1.88	0.56
1:A:473:LYS:O	1:A:477:GLU:HG2	2.07	0.55
1:A:194:LYS:HG3	3:A:914:HOH:O	2.07	0.54
1:A:218:ALA:HB2	1:A:463:GLY:HA2	1.90	0.53
1:A:150:PRO:HA	1:A:202:PRO:O	2.09	0.53
1:A:147:ILE:HG12	1:A:202:PRO:HG2	1.91	0.53
1:A:27:ILE:HG12	1:A:380:LEU:HD13	1.91	0.53
1:A:299:GLN:HG2	3:A:652:HOH:O	2.09	0.52
1:A:204:GLU:HG2	3:A:747:HOH:O	2.09	0.51
1:A:118:MET:CE	1:A:127:LEU:HA	2.40	0.51
1:A:120:THR:O	1:A:120:THR:HG22	2.11	0.51
1:A:49:ILE:O	1:A:53:GLU:HG3	2.11	0.51
1:A:184:GLU:HG3	3:A:673:HOH:O	2.11	0.49
1:A:163:GLN:HG2	1:A:165:LYS:O	2.12	0.49
1:A:58:LYS:HG3	1:A:248:GLU:HG2	1.93	0.49
1:A:430:LYS:HE3	3:A:780:HOH:O	2.12	0.49
1:A:331:GLN:NE2	1:A:372:ASN:H	2.11	0.49
1:A:473:LYS:HD2	3:A:862:HOH:O	2.13	0.48
1:A:93:ARG:NE	1:A:109:GLN:HE22	2.07	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ARG:HA	3:A:922:HOH:O	2.12	0.48
1:A:59:LYS:H	1:A:59:LYS:CE	2.22	0.47
1:A:18:ASP:OD2	1:A:379:LYS:HE3	2.14	0.47
1:A:382:ARG:O	1:A:386:GLU:HG3	2.14	0.47
1:A:117:ALA:HA	3:A:894:HOH:O	2.14	0.47
1:A:175:THR:HG23	1:A:176:LYS:HG3	1.98	0.46
1:A:58:LYS:HG3	1:A:248:GLU:OE1	2.15	0.46
1:A:59:LYS:HE3	1:A:59:LYS:N	2.23	0.46
1:A:213:THR:CG2	3:A:517:HOH:O	2.63	0.46
1:A:144:PRO:HA	3:A:793:HOH:O	2.16	0.46
1:A:116:ASP:HB2	3:A:929:HOH:O	2.16	0.45
1:A:195:GLN:O	1:A:199:ARG:HG3	2.16	0.44
1:A:118:MET:CE	1:A:127:LEU:HD23	2.47	0.44
1:A:452:LYS:HB3	3:A:879:HOH:O	2.18	0.44
1:A:19:VAL:HG12	1:A:20:PRO:O	2.18	0.44
1:A:165:LYS:NZ	1:A:486:ALA:HB1	2.33	0.43
1:A:93:ARG:HH21	1:A:109:GLN:NE2	2.16	0.43
1:A:172:GLN:HE21	1:A:172:GLN:HB3	1.75	0.42
1:A:452:LYS:HE3	3:A:599:HOH:O	2.20	0.42
1:A:93:ARG:HH21	1:A:109:GLN:HE22	1.68	0.42
1:A:213:THR:HG21	3:A:517:HOH:O	2.20	0.41
1:A:89:GLY:O	1:A:119:ARG:NH2	2.53	0.41
1:A:91:ASN:OD1	1:A:113:ARG:HA	2.20	0.41
1:A:218:ALA:HB2	1:A:463:GLY:CA	2.51	0.41
1:A:228:MET:HE2	1:A:230:VAL:HG13	2.01	0.41
1:A:366:GLN:HG2	3:A:875:HOH:O	2.20	0.41
1:A:376:GLN:CD	1:A:376:GLN:H	2.24	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:571:HOH:O	3:A:630:HOH:O[8_454]	2.18	0.02

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	467/486 (96%)	449 (96%)	18 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	398/411 (97%)	366 (92%)	32 (8%)	15	15

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	PHE
1	A	59	LYS
1	A	114	LEU
1	A	121	THR
1	A	122	GLN
1	A	127	LEU
1	A	136	LYS
1	A	147	ILE
1	A	172	GLN
1	A	175	THR
1	A	199	ARG
1	A	204	GLU
1	A	206	VAL
1	A	213	THR
1	A	225	GLU
1	A	230	VAL
1	A	237	ASN
1	A	253	LYS
1	A	254	LEU

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Mol	Chain	Res	Type
1	A	255	SER
1	A	270	TYR
1	A	298	GLN
1	A	320	ASP
1	A	358	LEU
1	A	376	GLN
1	A	384	LEU
1	A	410	LYS
1	A	423	ARG
1	A	435	LEU
1	A	452	LYS
1	A	472	GLN
1	A	480	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	GLN
1	A	172	GLN
1	A	182	ASN
1	A	193	GLN
1	A	237	ASN
1	A	251	GLN
1	A	267	ASN
1	A	275	ASN
1	A	277	HIS
1	A	331	GLN
1	A	372	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 carbohydrates in this entry.

5.6 Ligand geometry

1 ligand 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	$\# Z > 2$
2	SO4	A	501	-	4,4,4	0.83	0	6,6,6	0.61	0

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
2	SO4	A	501	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.