



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 11:24 pm GMT

PDB ID : 2IEW  
Title : Crystal structure of Inositol Phosphate Multikinase Ipk2 from *S. cerevisiae*  
Authors : Holmes, W.; Jogl, G.  
Deposited on : 2006-09-19  
Resolution : 2.00 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  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

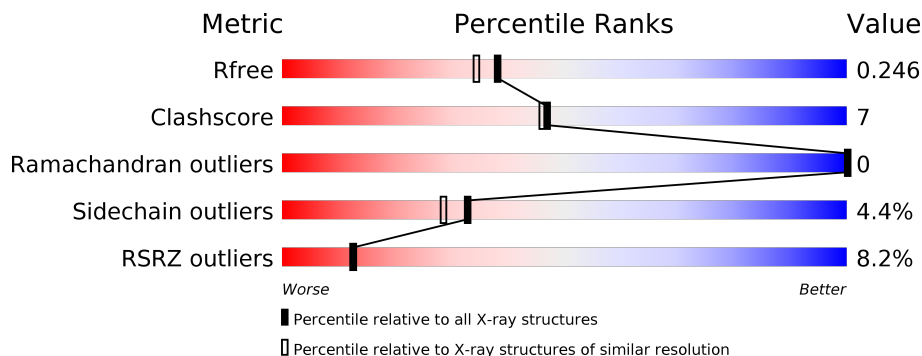
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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.

Mol	Chain	Length	Quality of chain
1	A	363	<div> <div>4%</div> <div>60%</div> <div>11%</div> <div>29%</div> </div>
1	B	363	<div> <div>7%</div> <div>57%</div> <div>12%</div> <div>29%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4676 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 Inositol polyphosphate multikinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			2113	1356	344	403	10			
1	B	256	Total	C	N	O	S	0	0	0
			2091	1342	336	403	10			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	356	LEU	-	CLONING ARTIFACT	UNP P07250
A	357	GLU	-	CLONING ARTIFACT	UNP P07250
A	358	HIS	-	EXPRESSION TAG	UNP P07250
A	359	HIS	-	EXPRESSION TAG	UNP P07250
A	360	HIS	-	EXPRESSION TAG	UNP P07250
A	361	HIS	-	EXPRESSION TAG	UNP P07250
A	362	HIS	-	EXPRESSION TAG	UNP P07250
A	363	HIS	-	EXPRESSION TAG	UNP P07250
B	356	LEU	-	CLONING ARTIFACT	UNP P07250
B	357	GLU	-	CLONING ARTIFACT	UNP P07250
B	358	HIS	-	EXPRESSION TAG	UNP P07250
B	359	HIS	-	EXPRESSION TAG	UNP P07250
B	360	HIS	-	EXPRESSION TAG	UNP P07250
B	361	HIS	-	EXPRESSION TAG	UNP P07250
B	362	HIS	-	EXPRESSION TAG	UNP P07250
B	363	HIS	-	EXPRESSION TAG	UNP P07250

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	273	Total 273	O 273	0	0
3	B	198	Total 198	O 198	0	0

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 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 ( $\text{RSRZ} > 2$ ). 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.

[illegible]

Chain B:

7% 57% 12% 29%

MET ASP THR VAL ASN ASN TYR ARG VAL LEU LEU GLU HIS LYS ALA ALA GLY HIS ASP GLY THR THR LEU LEU ASP GLY D25 I29 F30 K31 F34 I44 Q45 VAL ARG ASP VAL VAL SER SER ARG ARG ARG LYS SER SER SER ASP ALA ASP G58 D59 L62 M66 P67 T68 L73 N74 E75 GLY ALA

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	186.51Å 186.51Å 50.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.00 29.01 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.8 (30.00-2.00) 93.8 (29.01-2.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.41 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.208 , 0.253 0.206 , 0.246	Depositor DCC
$R_{free}$ test set	4868 reflections (8.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.1	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 50.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4676	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.61	2/2155 (0.1%)	0.67	0/2899
1	B	0.51	0/2130	0.62	0/2865
All	All	0.56	2/4285 (0.0%)	0.65	0/5764

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	GLU	CB-CG	7.49	1.66	1.52
1	A	216	GLU	CD-OE1	6.69	1.33	1.25

There are no bond angle outliers.

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	2113	0	2090	29	0
1	B	2091	0	2073	31	0
2	A	1	0	0	0	0
3	A	273	0	0	9	0
3	B	198	0	0	11	0
All	All	4676	0	4163	59	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 (59) 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:B:25:ASP:HB2	3:B:559:HOH:O	1.25	1.30
1:A:62:LEU:HD13	1:A:247:MET:HE1	1.62	0.79
1:A:58:GLY:N	3:A:735:HOH:O	2.16	0.78
1:B:330:GLU:HG2	3:B:489:HOH:O	1.91	0.71
1:A:317:SER:N	3:A:674:HOH:O	2.23	0.71
1:A:174:LYS:HG2	1:A:194:ASP:O	1.92	0.70
1:A:62:LEU:HD13	1:A:247:MET:CE	2.21	0.69
1:A:209:GLN:HG2	3:A:600:HOH:O	1.93	0.69
1:B:268:GLU:HG3	3:B:396:HOH:O	1.93	0.68
1:A:278:LYS:HE2	1:A:282:ASP:OD2	1.95	0.65
1:B:317:SER:N	3:B:554:HOH:O	2.33	0.61
1:B:174:LYS:HD2	1:B:179:LEU:HD11	1.84	0.59
1:A:45:GLN:HE22	1:A:69:TYR:H	1.50	0.58
1:B:134:LEU:HD11	1:B:259:LEU:HG	1.86	0.56
1:A:209:GLN:CG	3:A:632:HOH:O	2.55	0.54
1:B:44:ILE:HG22	3:B:382:HOH:O	2.10	0.52
1:A:185:GLU:OE2	3:A:712:HOH:O	2.19	0.51
1:B:112:LYS:HG3	1:B:113:GLN:N	2.26	0.51
1:B:25:ASP:N	1:B:25:ASP:OD1	2.43	0.51
1:B:285:ILE:HG12	1:B:286:ASP:H	1.76	0.49
1:A:209:GLN:HG3	3:A:632:HOH:O	2.11	0.49
1:A:147:LYS:HB3	3:A:656:HOH:O	2.12	0.49
1:A:134:LEU:HD11	1:A:259:LEU:HG	1.94	0.48
1:A:45:GLN:NE2	1:A:69:TYR:H	2.11	0.48
1:B:180:ASN:HB2	3:B:432:HOH:O	2.13	0.48
1:B:62:LEU:HD13	1:B:247:MET:CE	2.43	0.48
1:A:145:LEU:HA	1:A:148:ARG:HB3	1.95	0.47
1:B:44:ILE:CG2	3:B:382:HOH:O	2.62	0.47
1:A:118:GLU:HG3	1:A:284:PHE:CD1	2.50	0.47
1:B:68:THR:HB	1:B:118:GLU:HB3	1.97	0.46
1:B:62:LEU:HD13	1:B:247:MET:HE3	1.97	0.46
1:B:58:GLY:N	3:B:494:HOH:O	2.48	0.46
1:A:209:GLN:HG2	3:A:632:HOH:O	2.15	0.46
1:A:339:GLU:O	1:A:343:GLU:HG3	2.17	0.45
1:A:75:GLU:HB3	1:A:112:LYS:H	1.82	0.44
1:B:66:MET:HG2	1:B:326:PHE:CZ	2.52	0.44
1:B:215:ILE:O	1:B:218:TYR:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:ILE:O	1:B:325:ASP:HB2	2.18	0.44
1:A:238:LYS:HZ3	1:B:59:ASP:CG	2.21	0.44
1:A:132:ILE:O	1:A:258:SER:HA	2.18	0.43
1:A:62:LEU:CD1	1:A:247:MET:CE	2.93	0.43
1:A:332:THR:HB	1:A:335:LYS:HD2	2.00	0.43
1:B:281:ARG:NH1	3:B:409:HOH:O	2.52	0.43
1:B:246:THR:HG22	1:B:247:MET:HE2	2.00	0.43
1:B:167:ILE:O	1:B:203:GLY:HA3	2.19	0.42
1:A:145:LEU:CD2	1:A:148:ARG:HD2	2.50	0.42
1:B:251:GLU:O	1:B:331:ILE:HD12	2.20	0.42
1:A:44:ILE:HG22	1:A:63:CYS:HB3	2.02	0.42
1:B:285:ILE:HG12	1:B:286:ASP:N	2.34	0.41
1:B:261:PHE:N	1:B:261:PHE:CD2	2.88	0.41
1:B:25:ASP:CB	3:B:559:HOH:O	2.13	0.41
1:B:354:LYS:HG2	3:B:442:HOH:O	2.21	0.41
1:B:73:LEU:HB3	1:B:114:TYR:HB2	2.03	0.41
1:B:183:SER:HB3	1:B:185:GLU:OE2	2.21	0.41
1:B:228:ARG:HG2	1:B:270:TRP:CE3	2.56	0.41
1:A:167:ILE:O	1:A:203:GLY:HA3	2.22	0.40
1:A:175:ASN:HB2	1:A:222:PRO:HD3	2.03	0.40
1:A:31:LYS:HE3	3:A:722:HOH:O	2.21	0.40
1:A:32:PRO:HB3	1:A:112:LYS:NZ	2.37	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	250/363 (69%)	248 (99%)	2 (1%)	0	100	100
1	B	248/363 (68%)	242 (98%)	6 (2%)	0	100	100
All	All	498/726 (69%)	490 (98%)	8 (2%)	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	237/327 (72%)	230 (97%)	7 (3%)	46	46
1	B	235/327 (72%)	221 (94%)	14 (6%)	22	17
All	All	472/654 (72%)	451 (96%)	21 (4%)	33	28

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ILE
1	A	141	SER
1	A	145	LEU
1	A	147	LYS
1	A	192	ASP
1	A	285	ILE
1	A	342	ILE
1	B	25	ASP
1	B	29	ILE
1	B	31	LYS
1	B	44	ILE
1	B	45	GLN
1	B	113	GLN
1	B	118	GLU
1	B	147	LYS
1	B	149	GLU
1	B	156	GLU
1	B	185	GLU
1	B	204	ARG
1	B	216	GLU
1	B	331	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	209	GLN
1	A	223	HIS
1	B	45	GLN
1	B	223	HIS

### 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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 [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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	258/363 (71%)	0.04	15 (5%) 24 24	15, 24, 50, 72	0
1	B	256/363 (70%)	0.50	27 (10%) 7 7	20, 35, 64, 87	0
All	All	514/726 (70%)	0.27	42 (8%) 12 12	15, 30, 61, 87	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	285	ILE	11.7
1	B	286	ASP	9.6
1	B	191	ALA	8.3
1	A	191	ALA	8.2
1	B	284	PHE	7.6
1	B	111	SER	7.1
1	B	145	LEU	7.0
1	A	286	ASP	5.3
1	B	282	ASP	5.0
1	B	283	ASP	4.8
1	B	75	GLU	4.1
1	B	156	GLU	4.0
1	A	111	SER	3.9
1	A	285	ILE	3.9
1	B	192	ASP	3.4
1	A	192	ASP	3.4
1	A	112	LYS	3.4
1	B	146	GLU	3.4
1	A	360	HIS	3.2
1	B	113	GLN	3.1
1	B	184	LEU	3.0
1	B	74	ASN	3.0
1	B	197	PHE	2.8
1	B	45	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	190	GLU	2.7
1	A	145	LEU	2.7
1	B	150	ARG	2.6
1	A	75	GLU	2.5
1	B	144	SER	2.5
1	A	190	GLU	2.5
1	A	282	ASP	2.4
1	B	201	LEU	2.3
1	B	348	LEU	2.2
1	B	193	SER	2.2
1	B	274	ASN	2.2
1	A	146	GLU	2.2
1	B	34	PHE	2.2
1	A	147	LYS	2.2
1	A	283	ASP	2.2
1	B	272	LEU	2.1
1	A	197	PHE	2.1
1	B	180	ASN	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	A	501	1/1	0.99	0.11	1.55	31,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.