



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2021 – 12:02 PM EDT

PDB ID : 7N80
Title : Crystal Structure of PI5P4KIIBeta
Authors : Chen, S.; Ha, Y.
Deposited on : 2021-06-11
Resolution : 2.50 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)	:	1.13
EDS	:	2.20
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.20

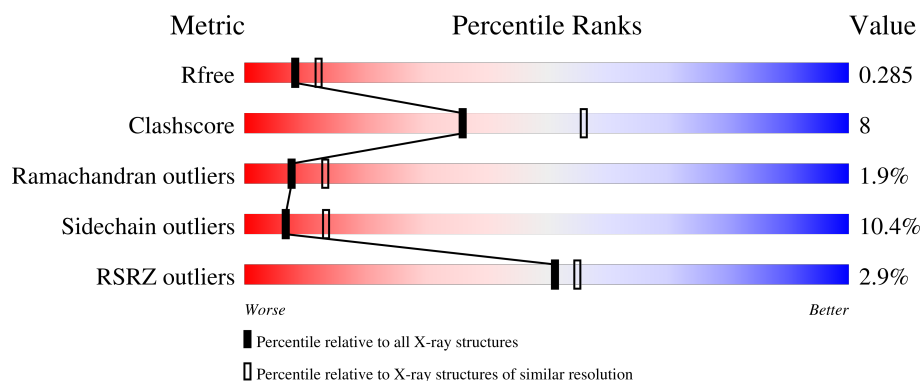
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 $\leq 5\%$. 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	392	<div> <div>2%</div> <div>59%14%•25%</div> </div>
1	B	392	<div> <div>2%</div> <div>56%18%•24%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4702 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 Phosphatidylinositol 5-phosphate 4-kinase type-2 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2293	1474	387	418	14			
1	B	298	Total	C	N	O	S	0	0	0
			2294	1480	383	417	14			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	GLY	-	expression tag	UNP P78356
A	26	PRO	-	expression tag	UNP P78356
A	27	ASN	-	expression tag	UNP P78356
A	28	CYS	-	expression tag	UNP P78356
A	29	ALA	-	expression tag	UNP P78356
A	30	PRO	-	expression tag	UNP P78356
A	31	GLY	-	expression tag	UNP P78356
B	25	GLY	-	expression tag	UNP P78356
B	26	PRO	-	expression tag	UNP P78356
B	27	ASN	-	expression tag	UNP P78356
B	28	CYS	-	expression tag	UNP P78356
B	29	ALA	-	expression tag	UNP P78356
B	30	PRO	-	expression tag	UNP P78356
B	31	GLY	-	expression tag	UNP P78356

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	62	Total	O	0	0
			62	62		
2	B	53	Total	O	0	0
			53	53		

- Molecule 1: Phosphatidylinositol 5-phosphate 4-kinase type-2 beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.73Å 51.20Å 107.08Å 90.00° 94.59° 90.00°	Depositor
Resolution (Å)	40.00 – 2.50 39.41 – 2.47	Depositor EDS
% Data completeness (in resolution range)	87.0 (40.00-2.50) 87.1 (39.41-2.47)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.201 , 0.283 0.204 , 0.285	Depositor DCC
R_{free} test set	1211 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	56.8	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4702	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0/2346	0.79	1/3179 (0.0%)
1	B	0.59	0/2343	0.80	0/3174
All	All	0.60	0/4689	0.80	1/6353 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	LEU	CB-CG-CD1	-5.25	102.08	111.00

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	2293	0	2142	37	0
1	B	2294	0	2138	37	0
2	A	62	0	0	8	0
2	B	53	0	0	6	0
All	All	4702	0	4280	71	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 (71) 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:77:ILE:HD11	1:B:77:ILE:HD11	1.27	1.13
1:B:157:VAL:HA	1:B:186:MET:HE1	1.44	0.98
1:A:107:ARG:NH2	2:A:501:HOH:O	2.08	0.83
1:A:157:VAL:HA	1:A:186:MET:HE1	1.60	0.82
1:A:77:ILE:HD11	1:B:77:ILE:CD1	2.10	0.79
1:A:186:MET:N	2:A:502:HOH:O	2.18	0.76
1:A:174:CYS:HB2	1:A:266:ARG:HH11	1.52	0.74
1:A:174:CYS:HB2	1:A:266:ARG:NH1	2.05	0.71
1:A:278:ASP:HB2	1:A:373:PRO:HB2	1.75	0.69
1:A:41:PRO:HA	2:A:504:HOH:O	1.92	0.68
1:A:283:VAL:HG22	1:A:365:MET:HG2	1.74	0.68
1:B:271:LEU:HD21	1:B:370:ILE:HG13	1.76	0.68
1:A:157:VAL:HA	1:A:186:MET:CE	2.29	0.62
1:A:178:THR:HB	1:A:180:LEU:H	1.65	0.62
1:A:251:HIS:HA	1:A:416:THR:HA	1.81	0.62
1:B:157:VAL:HA	1:B:186:MET:CE	2.26	0.61
1:B:190:THR:HG22	2:B:522:HOH:O	2.00	0.60
1:B:157:VAL:HG21	1:B:197:TYR:CD2	2.38	0.59
1:A:372:THR:HB	1:A:373:PRO:HD3	1.84	0.59
1:B:341:GLU:HA	1:B:352:LYS:HZ1	1.67	0.59
1:A:186:MET:HG3	1:A:199:VAL:HG22	1.84	0.58
1:A:357:SER:HB3	1:A:358:PRO:HD2	1.86	0.57
1:B:272:ALA:HB2	1:B:404:SER:HB2	1.88	0.56
1:A:79:VAL:HG22	1:B:77:ILE:HD12	1.86	0.55
1:A:157:VAL:HG21	1:A:197:TYR:CD2	2.42	0.54
1:A:252:VAL:H	1:A:416:THR:HG22	1.73	0.53
1:B:178:THR:HB	1:B:180:LEU:H	1.74	0.53
1:B:252:VAL:HG22	1:B:415:LEU:HD22	1.92	0.52
1:B:368:ILE:O	1:B:369:ASP:HB2	2.10	0.52
1:A:57:LEU:HA	1:A:60:VAL:HG13	1.92	0.51
1:A:201:THR:HG21	2:A:530:HOH:O	2.11	0.51
1:A:161:HIS:HE1	2:A:520:HOH:O	1.94	0.50
1:A:264:LEU:O	1:A:268:VAL:HB	2.12	0.50
1:B:292:GLU:O	1:B:296:MET:HG2	2.12	0.49
1:B:341:GLU:HA	1:B:352:LYS:NZ	2.28	0.49
1:B:54:ILE:HD12	2:B:512:HOH:O	2.12	0.49
1:B:113:ASP:HB2	1:B:116:ASP:OD1	2.13	0.49
1:A:54:ILE:HG21	1:A:118:GLN:HB2	1.95	0.48
1:A:57:LEU:HD13	1:A:104:ARG:HG3	1.96	0.48
1:B:42:ILE:HD11	1:B:196:THR:HG21	1.96	0.47
1:B:86:LYS:HG3	2:B:504:HOH:O	2.15	0.47
1:A:103:PHE:HB3	1:A:184:LEU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:THR:HG22	1:A:267:ASP:OD1	2.16	0.46
1:B:179:LEU:HB2	1:B:367:ILE:HD12	1.96	0.46
1:B:286:HIS:HB3	1:B:362:VAL:HB	1.96	0.46
1:B:51:ASN:HB2	1:B:122:THR:HG21	1.98	0.46
1:A:354:HIS:O	1:A:357:SER:HB2	2.16	0.46
1:B:86:LYS:HE2	1:B:91:SER:OG	2.14	0.46
1:B:218:LYS:HA	1:B:280:SER:HB3	1.97	0.46
1:B:128:ASN:ND2	2:B:503:HOH:O	2.50	0.45
1:B:170:PHE:HB2	1:B:270:PHE:CE1	2.52	0.45
1:A:190:THR:HG22	1:A:195:GLU:HG2	2.00	0.44
1:A:36:PHE:N	2:A:510:HOH:O	2.51	0.43
1:A:371:LEU:HD12	2:A:518:HOH:O	2.18	0.43
1:B:113:ASP:HB3	2:B:549:HOH:O	2.18	0.43
1:B:403:TYR:O	1:B:407:PHE:HB2	2.18	0.43
1:A:350:ALA:HA	1:A:363:TYR:O	2.19	0.43
1:B:81:ASN:O	1:B:91:SER:HB3	2.18	0.43
1:B:252:VAL:HG23	1:B:257:LYS:HB2	2.01	0.43
1:B:185:GLY:HA3	2:B:501:HOH:O	2.19	0.43
1:B:141:THR:HG23	1:B:142:THR:O	2.19	0.42
1:B:170:PHE:HE1	1:B:178:THR:CG2	2.32	0.42
1:B:54:ILE:HG21	1:B:118:GLN:HB2	2.01	0.42
1:B:182:GLN:O	1:B:201:THR:HG22	2.20	0.42
1:A:51:ASN:HB2	1:A:122:THR:HG21	2.01	0.42
1:B:51:ASN:HA	1:B:118:GLN:HE21	1.84	0.42
1:A:368:ILE:HG22	2:A:560:HOH:O	2.20	0.41
1:A:150:LYS:O	1:A:198:MET:HA	2.20	0.41
1:B:206:SER:HA	1:B:347:ASP:OD1	2.20	0.41
1:A:205:PHE:CG	1:A:211:VAL:HG21	2.56	0.41
1:A:170:PHE:HE1	1:A:178:THR:CG2	2.34	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	286/392 (73%)	261 (91%)	20 (7%)	5 (2%)	9	16
1	B	286/392 (73%)	263 (92%)	17 (6%)	6 (2%)	7	11
All	All	572/784 (73%)	524 (92%)	37 (6%)	11 (2%)	8	13

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	336	PHE
1	A	358	PRO
1	B	132	GLN
1	B	296	MET
1	A	337	PHE
1	B	358	PRO
1	A	143	TYR
1	B	293	GLN
1	B	33	VAL
1	A	339	PRO
1	B	338	GLY

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	235/351 (67%)	218 (93%)	17 (7%)	14	28
1	B	234/351 (67%)	202 (86%)	32 (14%)	3	7
All	All	469/702 (67%)	420 (90%)	49 (10%)	7	13

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	VAL
1	A	77	ILE
1	A	104	ARG
1	A	113	ASP
1	A	127	ILE

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Mol	Chain	Res	Type
1	A	137	THR
1	A	141	THR
1	A	173	GLU
1	A	174	CYS
1	A	178	THR
1	A	192	ASP
1	A	254	GLU
1	A	256	SER
1	A	268	VAL
1	A	282	LEU
1	A	289	ASP
1	A	372	THR
1	B	35	LEU
1	B	40	GLU
1	B	60	VAL
1	B	64	VAL
1	B	76	LYS
1	B	85	ASN
1	B	92	ARG
1	B	109	ARG
1	B	115	GLN
1	B	141	THR
1	B	154	SER
1	B	159	GLU
1	B	165	LYS
1	B	174	CYS
1	B	177	ASN
1	B	178	THR
1	B	190	THR
1	B	201	THR
1	B	210	THR
1	B	268	VAL
1	B	273	GLN
1	B	275	LYS
1	B	280	SER
1	B	296	MET
1	B	300	GLU
1	B	351	MET
1	B	352	LYS
1	B	365	MET
1	B	372	THR
1	B	398	VAL

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Mol	Chain	Res	Type
1	B	399	ASN
1	B	410	PHE

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

Mol	Chain	Res	Type
1	A	402	GLN
1	B	85	ASN
1	B	273	GLN
1	B	408	ASN

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 monosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q<0.9
1	A	294/392 (75%)	0.00	8 (2%) 54 58	36, 59, 105, 148	0
1	B	298/392 (76%)	0.12	9 (3%) 50 53	38, 62, 110, 135	0
All	All	592/784 (75%)	0.06	17 (2%) 51 55	36, 60, 108, 148	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	358	PRO	4.8
1	B	219	GLY	4.6
1	A	414	ILE	4.0
1	A	416	THR	4.0
1	B	345	SER	3.7
1	A	411	MET	3.6
1	B	411	MET	3.5
1	A	413	ASN	3.3
1	B	33	VAL	3.3
1	B	403	TYR	2.7
1	A	67	MET	2.5
1	B	289	ASP	2.4
1	B	354	HIS	2.4
1	B	278	ASP	2.3
1	B	413	ASN	2.3
1	A	415	LEU	2.1
1	A	412	SER	2.0

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 monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.