



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1BO1 / pdb_00001bo1
Title : PHOSPHATIDYLINOSITOL PHOSPHATE KINASE TYPE II BETA
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Deposited on : 1998-08-02
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

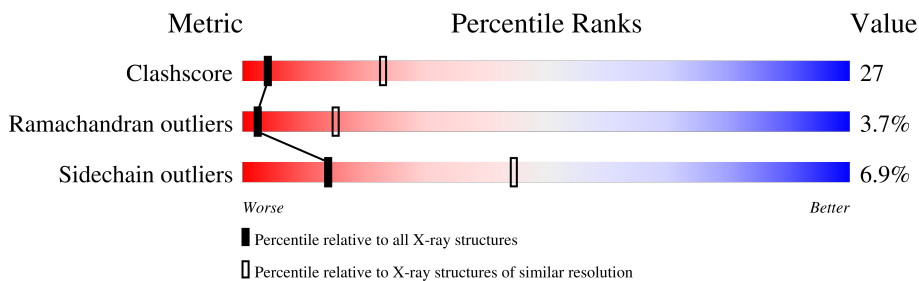
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	416	
1	B	416	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5301 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 PROTEIN (PHOSPHATIDYLINOSITOL PHOSPHATE KINASE IIBETA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2674	1695	454	511	14			
1	B	318	Total	C	N	O	S	0	0	0
			2608	1651	448	494	15			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	13	Total	O	0	0
			13	13		
2	B	6	Total	O	0	0
			6	6		

T221	V228	T222	A291	R301	K229	E225	A226	K230	E230	K231	A232	K233	D234	L235	P236	T237	F238	K239	D240	K241	D242	F243	L244	N245	E246	G247	Q248	K249	L250	H251	V252	S256	K257	F260	K263	L264	K265	R266	D267	V268	E269	F270	L271	A272	Q273	L274	K275	L276	M277	D278	Y279	S280	L281	L282	V283	H286	D287
				A302	ASP	GLU	GLU	CYS	GLY	ASN	ASP	GLY	VAL	GLY	ASN	LEU	LEU	CYS	SER	TYR	GLY	THR	PRO	PRO	PRO	ASP	SER	PRO	GLY	ASN	LEU	LEU	SER	PHE	PRO	ARG	PHE	PHE	GLY	PRO	GLY	GLY	PHE	D343	P344	S345	V346	D347	V348	Y349	A350	M351	K352	S353	H354	S357	
P358	K359	K360	Y363	F364	K365	A366	I367	I368	D369	I370	L371	T372	PRO	TYR	ASP	THR	LYS	LYS	LYS	ALA	ALA	HIS	ALA	ALA	LYS	THR	VAL	LYS	HIS	GLY	ALA	GLY	ALA	GLU	ILE	SER	T397	V398	N399	P400	Y403	S404	R405	R406	F407	N408	E409	F410	M411	S412	N413	I414	L415	T416			

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	109.92Å 182.40Å 106.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 3.00	Depositor
% Data completeness (in resolution range)	94.9 (6.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.229 , 0.299	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5301	wwPDB-VP
Average B, all atoms (Å ²)	48.0	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	0.55	0/2726	1.04	13/3668 (0.4%)
1	B	0.53	0/2660	1.09	23/3580 (0.6%)
All	All	0.54	0/5386	1.07	36/7248 (0.5%)

There are no bond length outliers.

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	399	ASN	CA-C-N	10.69	133.20	119.84
1	B	399	ASN	C-N-CA	10.69	133.20	119.84
1	B	368	ILE	N-CA-C	8.88	127.81	109.34
1	A	368	ILE	N-CA-C	7.83	125.62	109.34
1	B	263	LYS	N-CA-C	-7.55	102.64	111.03

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2674	0	2631	136	0
1	B	2608	0	2572	154	0
2	A	13	0	0	0	0
2	B	6	0	0	1	0
All	All	5301	0	5203	287	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 27.

The worst 5 of 287 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:160:MET:HE1	1:A:164:LEU:HD13	1.52	0.92
1:B:160:MET:HE1	1:B:164:LEU:HD13	1.49	0.91
1:B:212:HIS:HD2	1:B:287:ASP:H	1.20	0.90
1:B:157:VAL:HG21	1:B:197:TYR:CD2	2.07	0.90
1:A:223:ALA:H	1:A:225:GLU:HG2	1.39	0.87

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	318/416 (76%)	268 (84%)	39 (12%)	11 (4%)	3	16
1	B	312/416 (75%)	266 (85%)	34 (11%)	12 (4%)	2	15
All	All	630/832 (76%)	534 (85%)	73 (12%)	23 (4%)	2	15

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	VAL
1	A	232	ALA
1	A	396	SER
1	B	222	VAL
1	B	275	LYS

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	302/374 (81%)	282 (93%)	20 (7%)	15	46
1	B	295/374 (79%)	274 (93%)	21 (7%)	13	43
All	All	597/748 (80%)	556 (93%)	41 (7%)	14	45

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	250	LEU
1	B	354	HIS
1	B	251	HIS
1	B	282	LEU
1	B	370	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	273	GLN
1	B	248	GLN
1	B	51	ASN
1	B	212	HIS
1	A	399	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 [i](#)

There are no oligosaccharides 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.