



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2016 – 08:25 PM EDT

PDB ID : 5L72
Title : PI3 kinase delta in complex with N-[6-(5-methanesulfonamido-6-methoxypyridin-3-yl)-1,3-dihydro-2-benzofuran-4-yl]-2-(morpholin-4-yl)acetamide
Authors : Rowland, P.
Deposited on : 2016-06-01
Resolution : 3.06 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : rb-20027939

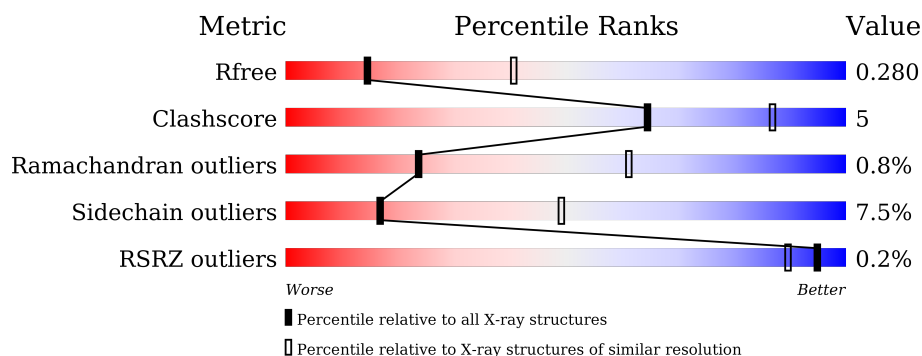
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 3.06 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}	91344	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)

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.

Mol	Chain	Length	Quality of chain
1	A	940	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7225 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.

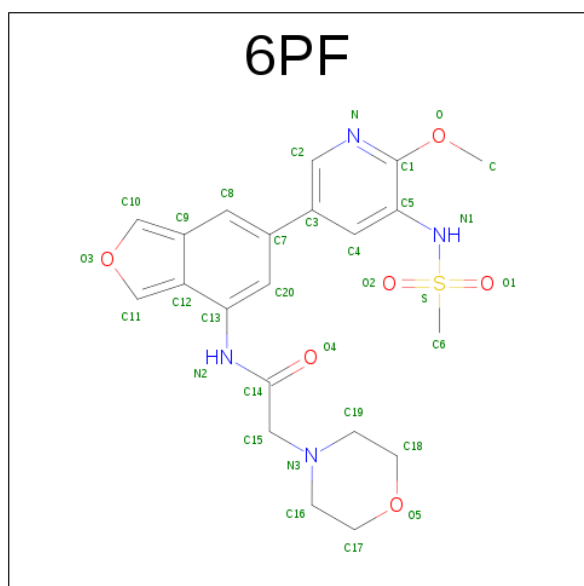
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit delta isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	858	Total	C	N	O	S	0	0	0
			6925	4424	1189	1258	54			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	GLY	-	expression tag	UNP Q3UDT3

- Molecule 2 is N-[6-(5-methanesulfonamido-6-methoxypyridin-3-yl)-1,3-dihydro-2-benzofuran-4-yl]-2-(morpholin-4-yl)acetamide (three-letter code: 6PF) (formula: C₂₁H₂₄N₄O₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			32	21	4	6	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	268	Total 268	O 268	0	0

- Molecule 1: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit delta isoform



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.40Å 64.36Å 115.83Å 90.00° 102.88° 90.00°	Depositor
Resolution (Å)	112.92 – 3.06 112.92 – 3.06	Depositor EDS
% Data completeness (in resolution range)	97.4 (112.92-3.06) 97.4 (112.92-3.06)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 3.07Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.172 , 0.277 0.177 , 0.280	Depositor DCC
R_{free} test set	967 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	55.5	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 99.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7225	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.17% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 6PF

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	0.52	0/7075	0.70	0/9549

There are no bond length outliers.

There are no bond angle outliers.

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	6925	0	6910	71	0
2	A	32	0	0	0	0
3	A	268	0	0	2	0
All	All	7225	0	6910	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 5.

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:289:GLN:HG2	1:A:677:HIS:CG	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:GLU:HG2	1:A:472:VAL:HG22	1.74	0.68
1:A:194:VAL:HG22	1:A:274:LEU:HB2	1.76	0.67
1:A:385:PRO:HD2	1:A:388:ALA:HB2	1.81	0.63
1:A:331:ARG:HA	1:A:368:GLU:HG3	1.83	0.61
1:A:340:LYS:HE3	1:A:362:GLU:HB3	1.84	0.60
1:A:328:ILE:HD11	1:A:474:TYR:HB2	1.84	0.60
1:A:462:ASN:HD22	1:A:468:ALA:HB2	1.67	0.58
1:A:917:GLY:HA2	1:A:930:VAL:HG23	1.87	0.57
1:A:209:THR:HB	1:A:257:CYS:HB3	1.87	0.57
1:A:702:SER:HB3	1:A:711:THR:HG23	1.87	0.56
1:A:786:GLN:HE22	1:A:988:GLU:HB2	1.72	0.55
1:A:247:HIS:CE1	1:A:740:LEU:HD21	2.43	0.54
1:A:953:PHE:O	1:A:956:PHE:HB3	2.08	0.53
1:A:621:TYR:HE2	3:A:4111:HOH:O	1.90	0.53
1:A:555:TRP:CE3	1:A:561:VAL:HG22	2.44	0.52
1:A:641:ARG:HH12	1:A:737:PRO:HB2	1.74	0.52
1:A:751:PHE:HB3	1:A:759:LEU:HD23	1.92	0.51
1:A:614:GLN:HG3	1:A:981:MET:HG2	1.93	0.50
1:A:194:VAL:HG21	1:A:216:LEU:CD2	2.42	0.50
1:A:256:LEU:HB3	1:A:262:ILE:HG21	1.94	0.50
1:A:700:LYS:HE3	1:A:780:ASN:HD22	1.77	0.49
1:A:289:GLN:HG2	1:A:677:HIS:CD2	2.46	0.49
1:A:583:LEU:HD11	1:A:600:LEU:HD11	1.95	0.48
1:A:759:LEU:O	1:A:777:ILE:HA	2.14	0.48
1:A:943:GLN:HB3	1:A:949:ASN:HB3	1.95	0.48
1:A:684:LYS:HE2	1:A:731:LEU:HB3	1.97	0.47
1:A:163:LEU:HD21	1:A:282:ILE:HG12	1.97	0.47
1:A:325:ILE:HD11	1:A:375:LEU:HD12	1.97	0.46
1:A:752:MET:HG2	1:A:752:MET:H	1.51	0.46
1:A:834:ILE:HD12	1:A:855:LEU:HD11	1.97	0.46
1:A:333:VAL:HG22	1:A:366:CYS:O	2.16	0.45
1:A:423:LEU:HD22	1:A:439:LEU:HD21	1.98	0.45
1:A:968:ARG:HG2	1:A:1002:LEU:O	2.16	0.45
1:A:768:ALA:HB3	1:A:772:GLY:HA3	1.99	0.44
1:A:431:GLN:HB2	1:A:484:TYR:CE1	2.53	0.44
1:A:547:ALA:HA	1:A:550:LEU:HD12	1.99	0.44
1:A:118:SER:OG	1:A:125:LEU:HG	2.18	0.44
1:A:699:VAL:HG21	1:A:759:LEU:HD21	2.00	0.44
1:A:194:VAL:HG21	1:A:216:LEU:HD22	2.00	0.44
1:A:497:HIS:HD2	3:A:4327:HOH:O	2.00	0.44
1:A:523:LEU:HD22	1:A:548:ARG:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:LEU:HD13	1:A:981:MET:HG3	2.00	0.44
1:A:617:GLN:HE22	1:A:620:LYS:NZ	2.16	0.44
1:A:886:THR:HA	1:A:891:ILE:HD12	2.01	0.43
1:A:328:ILE:HB	1:A:472:VAL:HG23	2.01	0.43
1:A:544:GLU:HA	1:A:574:LEU:HD22	2.01	0.43
1:A:645:HIS:CE1	1:A:734:PRO:HA	2.54	0.42
1:A:859:LEU:HD21	1:A:901:ILE:HD11	2.00	0.42
1:A:801:TRP:HE1	1:A:967:LEU:HG	1.84	0.42
1:A:547:ALA:HB1	1:A:587:PHE:CZ	2.54	0.42
1:A:600:LEU:HD22	1:A:603:LEU:HD11	2.01	0.42
1:A:241:LEU:HD13	1:A:274:LEU:HD13	2.02	0.42
1:A:187:ASN:N	1:A:210:LYS:HZ2	2.18	0.41
1:A:676:THR:O	1:A:679:MET:HB3	2.19	0.41
1:A:393:ALA:HB2	1:A:453:LEU:HD13	2.02	0.41
1:A:281:SER:O	1:A:285:MET:HG3	2.21	0.41
1:A:515:LEU:HD22	1:A:545:ALA:HB1	2.01	0.41
1:A:998:LEU:C	1:A:1000:ASP:H	2.24	0.41
1:A:244:ASN:ND2	1:A:273:HIS:HB3	2.36	0.41
1:A:789:LEU:CD1	1:A:981:MET:HG3	2.51	0.41
1:A:285:MET:HA	1:A:288:GLU:HG2	2.03	0.41
1:A:325:ILE:HG13	1:A:375:LEU:HB2	2.02	0.41
1:A:833:THR:HG22	1:A:900:MET:HG2	2.04	0.40
1:A:214:LEU:HD21	1:A:237:GLU:OE2	2.20	0.40
1:A:317:TRP:HH2	1:A:491:ILE:HA	1.85	0.40
1:A:528:LYS:HG2	1:A:552:VAL:HG12	2.04	0.40
1:A:344:GLN:HB2	1:A:395:TYR:CE2	2.56	0.40
1:A:494:LEU:HD21	1:A:559:GLU:HG3	2.03	0.40
1:A:777:ILE:HB	1:A:825:ILE:HB	2.03	0.40
1:A:154:ARG:HD2	1:A:165:TYR:CZ	2.56	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	844/940 (90%)	783 (93%)	54 (6%)	7 (1%)	24	61

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	929	ARG
1	A	197	GLU
1	A	319	LEU
1	A	911	ASP
1	A	854	ALA
1	A	328	ILE
1	A	501	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	760/827 (92%)	703 (92%)	57 (8%)	17	49

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	LEU
1	A	141	THR
1	A	166	SER
1	A	176	ARG
1	A	188	ARG
1	A	206	GLN
1	A	214	LEU
1	A	219	CYS
1	A	246	ARG
1	A	260	GLN
1	A	263	CYS
1	A	264	SER
1	A	267	HIS
1	A	270	LEU

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Mol	Chain	Res	Type
1	A	333	VAL
1	A	334	ASN
1	A	352	GLU
1	A	368	GLU
1	A	376	GLU
1	A	394	LEU
1	A	397	VAL
1	A	416	CYS
1	A	427	ASP
1	A	432	LEU
1	A	453	LEU
1	A	475	LEU
1	A	489	GLU
1	A	500	ARG
1	A	503	ILE
1	A	507	GLU
1	A	509	LEU
1	A	530	LEU
1	A	544	GLU
1	A	548	ARG
1	A	567	LEU
1	A	568	LEU
1	A	712	LYS
1	A	715	MET
1	A	723	THR
1	A	731	LEU
1	A	752	MET
1	A	795	GLN
1	A	809	ARG
1	A	852	LYS
1	A	856	LEU
1	A	870	ARG
1	A	898	ASN
1	A	915	PHE
1	A	933	ILE
1	A	944	GLN
1	A	992	SER
1	A	1004	LEU
1	A	1012	LEU
1	A	1017	VAL
1	A	1029	THR
1	A	1031	VAL

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Mol	Chain	Res	Type
1	A	1032	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	GLN
1	A	193	ASN
1	A	334	ASN
1	A	349	HIS
1	A	431	GLN
1	A	462	ASN
1	A	617	GLN
1	A	780	ASN
1	A	786	GLN
1	A	795	GLN
1	A	838	GLN
1	A	898	ASN
1	A	940	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](#)

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	6PF	A	4000	-	31,35,35	0.76	2 (6%)	37,50,50	0.58	1 (2%)

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	6PF	A	4000	-	-	0/19/27/27	0/3/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4000	6PF	C12-C9	-2.21	1.39	1.46
2	A	4000	6PF	C5-C1	2.50	1.45	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4000	6PF	C12-C13-N2	-2.02	114.64	118.42

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 [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	858/940 (91%)	-0.33	2 (0%) 95 89	23, 55, 93, 136	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	934	LEU	3.0
1	A	323	PHE	2.3

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, 95th 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 ²)	Q<0.9
2	6PF	A	4000	32/32	0.94	0.20	0.36	34,44,81,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.