



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:35 am GMT

PDB ID : 4KZC  
Title : Structure of PI3K gamma with Imidazopyridine inhibitors  
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Deposited on : 2013-05-29  
Resolution : 3.25 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  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
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

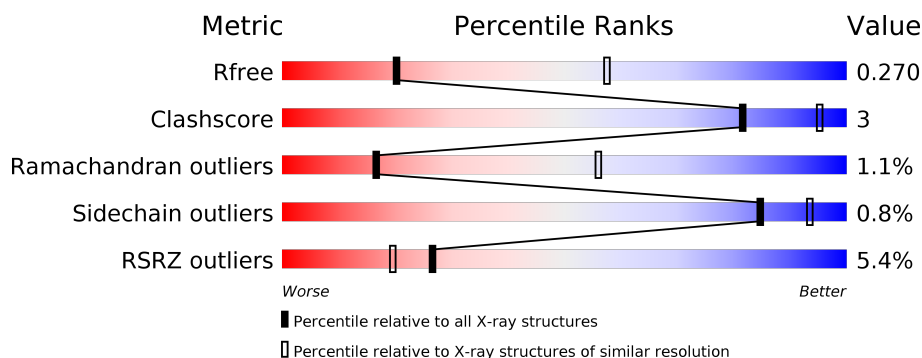
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 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	1852 (3.32-3.20)
Clashscore	112137	2036 (3.32-3.20)
Ramachandran outliers	110173	2000 (3.32-3.20)
Sidechain outliers	110143	1998 (3.32-3.20)
RSRZ outliers	101464	1861 (3.32-3.20)

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  $\geq 3$ , 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	966	<div> <div>5%</div> <div>77%</div> <div>7%</div> <div>15%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	1202	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6282 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.

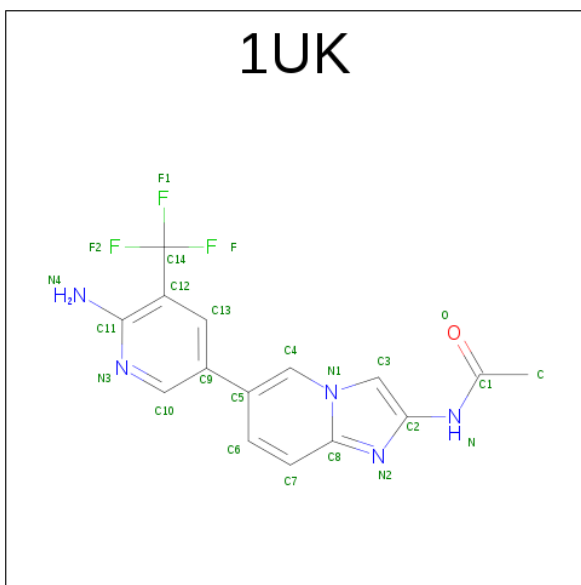
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	821	Total	C	N	O	S	0	0	0
			6253	4005	1063	1153	32			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	EXPRESSION TAG	UNP P48736
A	459	ARG	GLN	ENGINEERED MUTATION	UNP P48736
A	1103	HIS	-	EXPRESSION TAG	UNP P48736
A	1104	HIS	-	EXPRESSION TAG	UNP P48736
A	1105	HIS	-	EXPRESSION TAG	UNP P48736
A	1106	HIS	-	EXPRESSION TAG	UNP P48736
A	1107	HIS	-	EXPRESSION TAG	UNP P48736
A	1108	HIS	-	EXPRESSION TAG	UNP P48736

- Molecule 2 is N-{6-[6-AMINO-5-(TRIFLUOROMETHYL)PYRIDIN-3-YL]IMIDAZO[1,2-A]PYRIDIN-2-YL}ACETAMIDE (three-letter code: 1UK) (formula: C<sub>15</sub>H<sub>12</sub>F<sub>3</sub>N<sub>5</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			24	15	3	5	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.38Å 68.31Å 108.16Å 90.00° 95.24° 90.00°	Depositor
Resolution (Å)	41.42 – 3.25 41.42 – 3.12	Depositor EDS
% Data completeness (in resolution range)	98.5 (41.42-3.25) 98.6 (41.42-3.12)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, $R_{free}$	0.235 , 0.256 0.255 , 0.270	Depositor DCC
$R_{free}$ test set	868 reflections (5.46%)	DCC
Wilson B-factor (Å <sup>2</sup> )	108.1	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 96.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6282	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1UK, 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	0.42	0/6385	0.65	4/8705 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	897	GLY	N-CA-C	6.57	129.51	113.10
1	A	754	ALA	C-N-CA	5.32	135.00	121.70
1	A	546	GLU	C-N-CA	5.25	134.82	121.70
1	A	901	ALA	C-N-CA	5.00	134.21	121.70

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	6253	0	5885	36	0
2	A	24	0	12	0	0
3	A	5	0	0	0	0
All	All	6282	0	5897	36	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 3.

All (36) 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:834:HIS:HB2	1:A:876:ILE:HD12	1.77	0.67
1:A:1045:LYS:O	1:A:1049:GLU:HG2	1.96	0.65
1:A:508:PRO:HG2	1:A:707:ARG:HD3	1.82	0.60
1:A:611:LEU:O	1:A:614:ARG:HG3	2.04	0.58
1:A:754:ALA:HB1	1:A:756:LYS:N	2.19	0.58
1:A:280:TYR:HB3	1:A:282:VAL:HG13	1.86	0.57
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.87	0.57
1:A:1039:MET:HB2	1:A:1042:LEU:HD23	1.89	0.55
1:A:901:ALA:HA	1:A:902:PHE:HB2	1.89	0.55
1:A:645:VAL:HA	1:A:648:LEU:HD12	1.89	0.54
1:A:887:THR:HG22	1:A:890:LYS:H	1.73	0.54
1:A:567:LEU:HD21	1:A:591:LYS:HD3	1.90	0.53
1:A:734:GLN:HB2	1:A:780:PRO:HG2	1.92	0.53
1:A:852:GLU:HG3	1:A:864:LEU:HD12	1.92	0.51
1:A:901:ALA:CA	1:A:902:PHE:HB2	2.42	0.49
1:A:899:THR:HG22	1:A:900:GLY:N	2.29	0.48
1:A:830:ILE:HG23	1:A:878:MET:HB2	1.96	0.48
1:A:370:ILE:HB	1:A:514:MET:HG3	1.97	0.46
1:A:754:ALA:HB1	1:A:755:GLU:C	2.36	0.46
1:A:651:LEU:HD22	1:A:655:ASP:HB3	1.97	0.46
1:A:811:LEU:HB3	1:A:813:LEU:CD1	2.45	0.46
1:A:847:ILE:HG21	1:A:942:LEU:HD21	1.97	0.45
1:A:1042:LEU:N	1:A:1042:LEU:HD22	2.31	0.45
1:A:157:LEU:HD21	1:A:733:THR:HA	1.98	0.45
1:A:917:THR:HG22	1:A:919:GLU:H	1.81	0.45
1:A:693:HIS:CD2	1:A:789:PRO:HG3	2.53	0.44
1:A:802:LYS:HG2	1:A:812:TRP:HB3	1.99	0.43
1:A:727:ALA:O	1:A:731:ASP:HB2	2.17	0.43
1:A:428:LEU:HD22	1:A:465:ASN:HB3	2.01	0.43
1:A:735:GLN:O	1:A:739:ILE:HG12	2.19	0.43
1:A:387:ILE:HG22	1:A:394:LEU:HD12	2.01	0.42
1:A:271:VAL:HG22	1:A:282:VAL:HG12	2.01	0.42
1:A:657:LEU:HG	1:A:691:ILE:HG12	2.02	0.42
1:A:272:LEU:HB3	1:A:305:VAL:CG1	2.50	0.42
1:A:756:LYS:HA	1:A:757:TYR:HA	1.91	0.40
1:A:989:PRO:HA	1:A:992:LEU:HD12	2.04	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	797/966 (82%)	753 (94%)	35 (4%)	9 (1%)	17	56

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	320	LYS
1	A	615	GLU
1	A	778	GLN
1	A	897	GLY
1	A	1043	THR
1	A	900	GLY
1	A	901	ALA
1	A	219	CYS
1	A	916	PRO

### 5.3.2 Protein sidechains [i](#)

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	637/864 (74%)	632 (99%)	5 (1%)	85	93

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	271	VAL
1	A	658	HIS

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Mol	Chain	Res	Type
1	A	707	ARG
1	A	746	THR
1	A	896	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

2 ligands are 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	1UK	A	1201	-	22,26,26	1.07	2 (9%)	26,39,39	0.77	1 (3%)
3	SO4	A	1202	-	4,4,4	0.19	0	6,6,6	0.25	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	1UK	A	1201	-	-	0/12/14/14	0/3/3/3
3	SO4	A	1202	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	1UK	C6-C5	2.89	1.45	1.39
2	A	1201	1UK	C3-C2	3.34	1.41	1.36

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	1UK	C5-C4-N1	-3.06	118.82	121.02

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	821/966 (84%)	0.32	44 (5%) 26 19	60, 112, 169, 201	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	895	THR	5.4
1	A	212	TRP	4.7
1	A	458	VAL	4.0
1	A	228	THR	3.8
1	A	272	LEU	3.5
1	A	1069	LEU	3.5
1	A	381	VAL	3.3
1	A	270	PHE	3.2
1	A	287	ILE	3.0
1	A	235	VAL	3.0
1	A	229	THR	3.0
1	A	869	CYS	2.9
1	A	1004	PRO	2.9
1	A	1075	CYS	2.9
1	A	403	PRO	2.8
1	A	220	ILE	2.8
1	A	313	PRO	2.8
1	A	513	SER	2.7
1	A	232	THR	2.7
1	A	271	VAL	2.5
1	A	224	ILE	2.4
1	A	1089	HIS	2.4
1	A	222	ILE	2.4
1	A	227	SER	2.4
1	A	514	MET	2.4
1	A	922	GLN	2.3
1	A	924	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	382	PHE	2.3
1	A	484	MET	2.2
1	A	930	TYR	2.2
1	A	234	LYS	2.2
1	A	303	ILE	2.2
1	A	545	ALA	2.2
1	A	997	THR	2.1
1	A	226	ARG	2.1
1	A	230	SER	2.1
1	A	995	MET	2.1
1	A	244	ILE	2.1
1	A	404	PHE	2.1
1	A	896	VAL	2.1
1	A	987	LEU	2.1
1	A	240	THR	2.0
1	A	154	LEU	2.0
1	A	357	CYS	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 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( $\text{\AA}^2$ )	Q<0.9
3	SO4	A	1202	5/5	0.93	0.65	8.77	149,149,149,149	0
2	1UK	A	1201	24/24	0.93	0.26	-0.21	83,87,93,94	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.