



# wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 07:04 PM GMT

PDB ID : 4ANX  
Title : Complexes of PI3Kgamma with isoform selective inhibitors.  
Authors : Foster, P.G.; Lougheed, J.C.  
Deposited on : 2012-03-22  
Resolution : 2.73 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

---

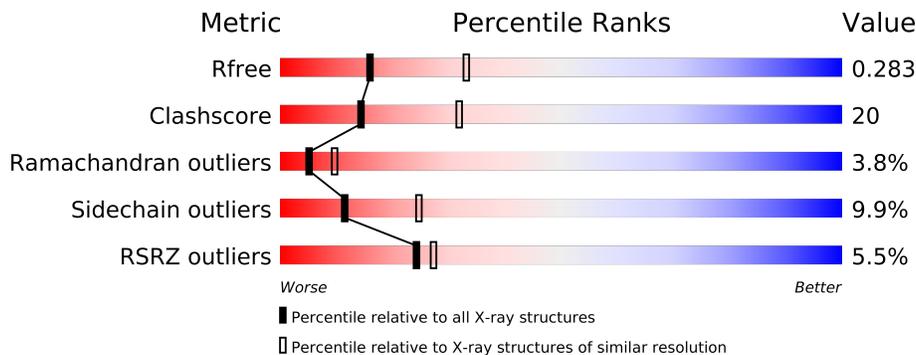
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance i

The reported resolution of this entry is 2.73 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))
$R_{free}$	66092	2164 (2.78-2.70)
Clashscore	79885	2639 (2.78-2.70)
Ramachandran outliers	78287	2594 (2.78-2.70)
Sidechain outliers	78261	2595 (2.78-2.70)
RSRZ outliers	66119	2166 (2.78-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	980	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6828 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

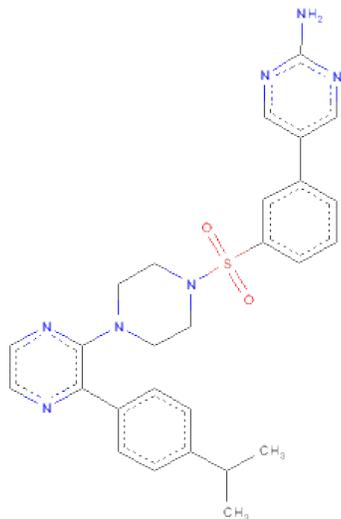
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE3-KINASE CATALYTIC SUBUNIT GAMMA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	833	6757	4334	1153	1235	35	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	MET	-	EXPRESSION TAG	UNP P48736
A	140	LEU	-	EXPRESSION TAG	UNP P48736
A	141	LEU	-	EXPRESSION TAG	UNP P48736
A	142	GLY	-	EXPRESSION TAG	UNP P48736
A	143	SER	-	EXPRESSION TAG	UNP P48736
A	1103	GLU	-	EXPRESSION TAG	UNP P48736
A	1104	PHE	-	EXPRESSION TAG	UNP P48736
A	1105	GLY	-	EXPRESSION TAG	UNP P48736
A	1106	LEU	-	EXPRESSION TAG	UNP P48736
A	1107	VAL	-	EXPRESSION TAG	UNP P48736
A	1108	PRO	-	EXPRESSION TAG	UNP P48736
A	1109	ARG	-	EXPRESSION TAG	UNP P48736
A	1110	GLY	-	EXPRESSION TAG	UNP P48736
A	1111	SER	-	EXPRESSION TAG	UNP P48736
A	1112	GLY	-	EXPRESSION TAG	UNP P48736
A	1113	HIS	-	EXPRESSION TAG	UNP P48736
A	1114	HIS	-	EXPRESSION TAG	UNP P48736
A	1115	HIS	-	EXPRESSION TAG	UNP P48736
A	1116	HIS	-	EXPRESSION TAG	UNP P48736
A	1117	HIS	-	EXPRESSION TAG	UNP P48736
A	1118	HIS	-	EXPRESSION TAG	UNP P48736

- Molecule 2 is 5-{3-[(4-{3-[4-(1-METHYLETHYL)PHENYL]PYRAZIN-2-YL}PIPERAZIN-1-YL)SULFONYL]PHENYL}PYRIMIDIN-2-AMINE (three-letter code: 534) (formula: C<sub>27</sub>H<sub>29</sub>N<sub>7</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	37	27	7	2	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total	O	0	0
			34	34		





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.42Å 68.53Å 106.26Å 90.00° 95.26° 90.00°	Depositor
Resolution (Å)	32.60 – 2.73 32.60 – 2.73	Depositor EDS
% Data completeness (in resolution range)	99.5 (32.60-2.73) 99.5 (32.60-2.73)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 2.72Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.225 , 0.282 0.226 , 0.283	Depositor DCC
$R_{free}$ test set	1375 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	70.0	Xtrriage
Anisotropy	0.034	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 43.5	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Outliers	0 of 27394 reflections	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6828	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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: 534

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	0.67	2/6901 (0.0%)	0.79	5/9334 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	967	HIS	C-N	-5.82	1.20	1.34
1	A	435	CYS	CB-SG	-5.02	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	575	LEU	CA-CB-CG	6.71	130.72	115.30
1	A	210	TYR	N-CA-C	6.59	128.80	111.00
1	A	967	HIS	O-C-N	-6.08	112.97	122.70
1	A	777	SER	CB-CA-C	5.51	120.58	110.10
1	A	1077	ASP	C-N-CA	5.43	135.28	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	209	GLU	Peptide
1	A	210	TYR	Peptide
1	A	777	SER	Peptide
1	A	965	PHE	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6757	0	6789	266	0
2	A	37	0	29	4	0
3	A	34	0	0	4	0
All	All	6828	0	6818	266	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

The worst 5 of 266 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:967:HIS:H	1:A:968:ILE:HA	1.07	1.11
1:A:775:GLN:HE22	1:A:798:ILE:HD11	1.21	1.02
1:A:827:THR:HG22	1:A:883:LYS:NZ	1.81	0.95
1:A:561:THR:HG22	1:A:591:LYS:NZ	1.81	0.95
1:A:967:HIS:N	1:A:968:ILE:HA	1.73	0.94

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	819/980 (84%)	703 (86%)	85 (10%)	31 (4%)	5 10

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	SER
1	A	211	LEU
1	A	217	ASN
1	A	778	GLN
1	A	905	GLU

### 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	749/874 (86%)	675 (90%)	74 (10%)	11 25

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	721	LEU
1	A	773	ASN
1	A	1007	GLN
1	A	729	LEU
1	A	753	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	658	HIS
1	A	734	GLN
1	A	1071	GLN
1	A	673	HIS
1	A	710	GLN

### 5.3.3 RNA [i](#)

There are no RNA chains 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	534	A	2088	-	41,41,41	2.23	8 (19%)	59,59,59	2.26	19 (32%)

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	534	A	2088	-	-	0/28/38/38	0/5/5/5

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2088	534	C5-C3	-9.56	1.38	1.48
2	A	2088	534	O2-S1	6.09	1.51	1.43
2	A	2088	534	O1-S1	5.42	1.50	1.43
2	A	2088	534	C21-C19	-3.21	1.40	1.49

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2088	534	C4-N3	2.69	1.43	1.36

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2088	534	C15-S1-N4	-5.85	99.86	107.29
2	A	2088	534	O1-S1-N4	5.22	112.04	106.71
2	A	2088	534	C6-N3-C9	5.09	122.13	111.67
2	A	2088	534	O2-S1-O1	-4.82	110.77	119.38
2	A	2088	534	N6-C23-N5	-4.06	120.50	124.57

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	833/980 (85%)	0.29	46 (5%) <span style="border: 1px solid red; padding: 2px;">24</span> <span style="border: 1px solid red; padding: 2px;">27</span>	39, 70, 106, 120	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	378	ASP	6.8
1	A	900	GLY	5.8
1	A	896	VAL	5.7
1	A	376	ASN	5.2
1	A	375	ARG	5.0

### 6.2 Non-standard residues in protein, DNA, RNA chains

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

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	534	A	2088	37/37	0.14	-1.07	61,66,70,71	0

## 6.5 Other polymers

There are no such residues in this entry.