



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 04:58 pm GMT

PDB ID : 2A4Z  
Title : Crystal Structure of human PI3Kgamma complexed with AS604850  
Authors : Camps, M.; Ruckle, T.; Ji, H.; Ardisson, V.; Rintelen, F.; Shaw, J.; Ferrandi, C.; Chabert, C.; Gillieron, C.; Francon, B.; Martin, T.; Gretener, D.; Perrin, D.; Leroy, D.; Vitte, P.-A.; Hirsch, E.; Wymann, M.P.; Cirillo, R.; Schwarz, M.K.; Rommel, C.  
Deposited on : 2005-06-30  
Resolution : 2.90 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](mailto: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.

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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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

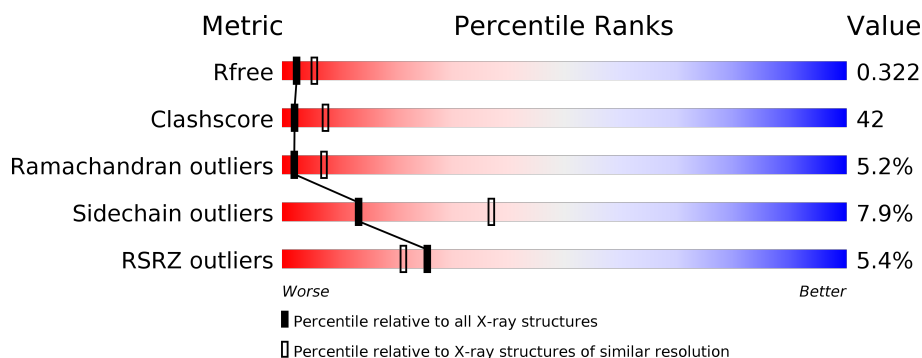
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	111664	1716 (2.90-2.90)
Clashscore	122126	1924 (2.90-2.90)
Ramachandran outliers	120053	1884 (2.90-2.90)
Sidechain outliers	120020	1886 (2.90-2.90)
RSRZ outliers	108989	1669 (2.90-2.90)

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	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6273 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.

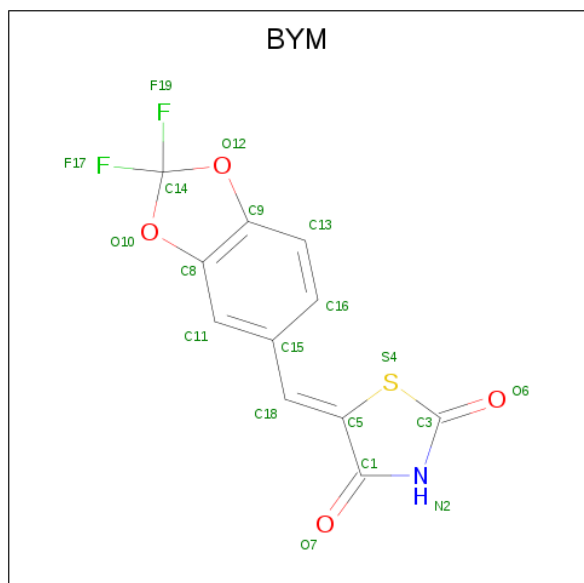
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit, gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	812	6247	4045	1040	1127	35	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	INITIATING METHIONINE	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 (5E)-5-[(2,2-DIFLUORO-1,3-BENZODIOXOL-5-YL)METHYLENE]-1,3-THIAZOLIDINE-2,4-DIONE (three-letter code: BYM) (formula: C<sub>11</sub>H<sub>5</sub>F<sub>2</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			19	11	2	1	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		



Y1067	F1068	L1069	D1070	Q1071	I1072	E1073	V1074	C1075	R1076	D1077	K1078	G1079	W1080	T1081	V1082	Q1083	F1084	N1085	W1086	F1087	LEU	HIS	LEU	VAL	LEU	GLY	ILE	LYS	GLN	GLY	GLU	LYS	HIS	SER	ALA	HIS	HIS	HIS	HIS																	
S1003	F1004	H1005	F1006	Q1007	K1008	F1009	Q1010	D1011	I1012	C1013	V1014	K1015	A1016	Y1017	L1018	R1021	H1022	H1023	T1024	N1025	L1026	L1027	I1028	I1029	L1030	F1031	S1032	M1033	W1034	L1035	M1036	M1039	P1040	G1041	L1042	T1043	S1044	K1045	E1046	D1047	I1048	E1049	Y1050	I1051	L1055	T1056	V1057	G1058	K1059	N1060	E1061	E1062	D1063	A1064	K1065	K1066
A933	G934	Y935	C936	L942	R947	H948	N949	D950	N951	I952	M953	T954	E956	T957	L960	F961	D964	F965	GLY	HIS	ILE	LEU	GLY	ASN	TYR	LYS	SER	PHE	LEU	GLY	ILE	ASN	LYS	E981	R982	V983	V986	L987	T988	P989	D990	F991	L992	F993	V994	M995	G996	T997	S998	R927	G999	K1000	K1001	T1002		
T857	E858	S859	L860	D861	L862	C863	L864	L865	P866	Y867	G868	C869	I870	S871	T872	I876	G877	T881	T886	T887	I888	A889	K890	I891	Q892	Q893	S894	T895	V896	G897	N898	T899	G900	A901	F902	W910	L911	K912	E913	K914	S915	P916	T917	K920	F921	Q922	V925	E926	R927	F928	V929	C932				

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.35Å 67.65Å 106.39Å 90.00° 95.77° 90.00°	Depositor
Resolution (Å)	19.75 – 2.90 19.75 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.2 (19.75-2.90) 96.2 (19.75-2.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.04 (at 2.88Å)	Xtriage
Refinement program	CNS, CNX 2002	Depositor
R, $R_{free}$	0.257 , 0.352 0.232 , 0.322	Depositor DCC
$R_{free}$ test set	2156 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.9	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 117.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6273	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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: BYM

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	0.36	0/6385	0.62	1/8692 (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	575	LEU	CA-CB-CG	5.98	129.06	115.30

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	6247	0	6012	510	0
2	A	19	0	5	5	0
3	A	7	0	0	3	0
All	All	6273	0	6017	510	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 42.

The worst 5 of 510 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:927:ARG:HH11	1:A:927:ARG:HB2	1.10	1.11
1:A:860:LEU:HD22	1:A:1015:LYS:HD3	1.33	1.05
1:A:184:ARG:NH1	1:A:722:ARG:HB2	1.76	1.01
1:A:474:LEU:HA	1:A:526:PRO:HB3	1.45	0.98
1:A:235:VAL:HG11	1:A:244:ILE:HG12	1.46	0.97

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	792/966 (82%)	633 (80%)	118 (15%)	41 (5%)	<b>2</b> <b>7</b>

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	LYS
1	A	215	ILE
1	A	247	SER
1	A	249	PHE
1	A	406	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	643/864 (74%)	592 (92%)	51 (8%)	13 37

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	619	GLN
1	A	726	THR
1	A	1039	MET
1	A	662	GLN
1	A	731	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	554	GLN
1	A	662	GLN
1	A	949	ASN
1	A	585	HIS
1	A	600	GLN

### 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	BYM	A	101	-	19,21,21	2.55	6 (31%)	30,32,32	3.07	11 (36%)

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	BYM	A	101	-	-	0/2/26/26	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	101	BYM	C9-C8	-2.13	1.33	1.39
2	A	101	BYM	F17-C14	2.12	1.39	1.34
2	A	101	BYM	C13-C9	3.78	1.47	1.39
2	A	101	BYM	C3-N2	3.94	1.41	1.36
2	A	101	BYM	C11-C8	4.91	1.47	1.38

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	101	BYM	C1-N2-C3	-9.77	112.20	117.78
2	A	101	BYM	C14-O10-C8	-6.88	99.84	106.39
2	A	101	BYM	C14-O12-C9	-6.44	100.26	106.39
2	A	101	BYM	O6-C3-N2	-2.94	122.78	125.76
2	A	101	BYM	F19-C14-O12	-2.63	107.80	110.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	101	BYM	5	0

## 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, 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	812/966 (84%)	0.14	44 (5%) 26 21	16, 60, 104, 135	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	524	CYS	9.4
1	A	894	SER	6.1
1	A	523	TYR	5.4
1	A	896	VAL	5.2
1	A	216	ALA	4.9

### 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	BYM	A	101	19/19	0.96	0.14	39,43,52,63	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.