



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 01:15 AM 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 validation summary 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/ValidationPDFNotes.html>

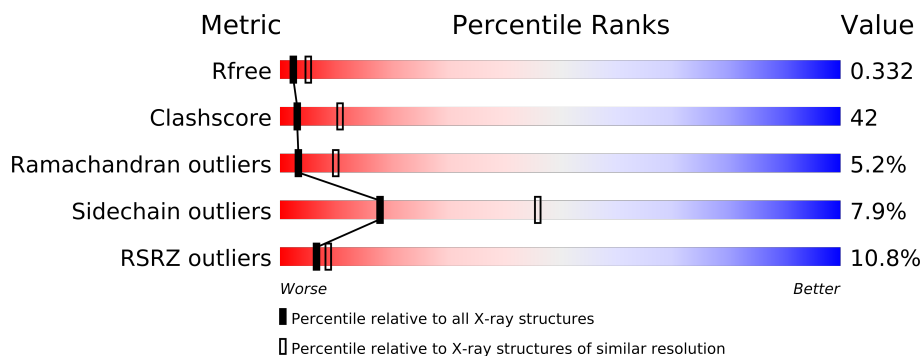
The following versions of software and data (see [references](#)) were used in the production of this report:

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

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}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (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 ≥ 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	966	

2 Entry composition

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

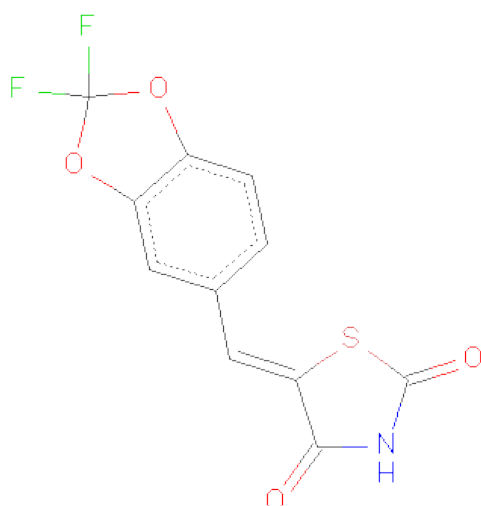
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate3-kinase catalytic subunit, gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	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: C₁₁H₅F₂NO₄S).



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		

V1057	G1058	K1059	N1060	E1061	E1062	D1063	A1064	K1065	K1066	Y1067	F1068	L1069	D1070	Q1071	I1072	E1073	V1074	C1075	R1076	D1077	K1078	G1079	V1080	T1081	V1082	Q1083	F1084	N1085	W1086	F1087	LEU	HIS	HIS	LEU	VAL	LEU	GLY	ILE	LYS	GLN	GLY	GLU	LYS	HIS	SER	ALA	HIS	HIS	HIS	HIS						
F993	Y994	N995	G996	T997	S998	G999	K1000	K1001	T1002	A993	Y994	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	M1034	L1035	M1036	M1039	P1040	Q1041	L1042	T1043	S1044	K1045	E1046	D1047	I1048	E1049	Y1050	T1051	L1055	T1056
Q922	Y925	E926	R927	F928	V929	C932	A933	G934	Y935	C936	Y937	L942	R947	H948	N949	D950	N951	I952	N953	I954	T955	E956	T957	L960	F961	D964	F965	GLY	HIS	ILE	LEU	GLY	ASN	TYR	LYS	SER	PHE	LEU	GLY	ILE	ASN	LYS	F981	R982	V983	V986	L987	T988	P989	D990	F991	L992				
I850	I854	W855	E856	T857	E858	S859	L860	D861	L862	C863	L864	L865	P866	Y867	G868	C869	I870	S871	T872	I876	G877	I881	T886	T887	I888	A889	K890	I891	Q892	Q893	S894	T895	V896	G897	N898	T899	G900	A901	F902	K903	D904	E905	W910	L911	K912	E913	K914	S915	P916	T917	E918	E919	K920	F921		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 2.88Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.257 , 0.352 0.243 , 0.332	Depositor DCC
R_{free} test set	2156 reflections (11.05%)	DCC
Wilson B-factor (Å ²)	72.9	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 88.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 21670 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6273	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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($^{\circ}$)	Ideal($^{\circ}$)
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 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	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

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 42.

The worst 5 of 510 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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	792/966 (82%)	633 (80%)	118 (15%)	41 (5%)	3 10

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 ⓘ

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	643/864 (74%)	592 (92%)	51 (8%)	18 46

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 ⓘ

There are no RNA chains 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 ⓘ

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	-	21,21,21	2.66	7 (33%)	32,32,32	2.19	11 (34%)

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	0/1/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	101	BYM	C16-C15	6.28	1.51	1.39
2	A	101	BYM	C11-C8	4.63	1.47	1.38
2	A	101	BYM	C3-N2	4.31	1.41	1.37
2	A	101	BYM	O10-C14	4.18	1.46	1.39
2	A	101	BYM	O12-C14	3.73	1.45	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	101	BYM	C5-C1-N2	6.38	113.71	110.03
2	A	101	BYM	S4-C3-N2	3.91	112.99	109.29
2	A	101	BYM	C14-O10-C8	-3.60	99.84	105.85
2	A	101	BYM	O12-C9-C8	3.48	112.63	109.70
2	A	101	BYM	C14-O12-C9	-3.35	100.26	105.85

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, 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	812/966 (84%)	0.59	88 (10%) 6 8	16, 60, 104, 135	0

The worst 5 of 88 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	524	CYS	13.2
1	A	523	TYR	11.0
1	A	896	VAL	9.7
1	A	216	ALA	7.5
1	A	148	GLN	7.3

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	BYM	A	101	19/19	0.15	-0.89	39,43,52,63	0

6.5 Other polymers ⓘ

There are no such residues in this entry.