



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 10:10 PM EST

PDB ID : 5I4U  
Title : The crystal structure of PI3Kdelta with compound 34  
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Deposited on : 2016-02-12  
Resolution : 2.37 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

<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	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
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-20028442

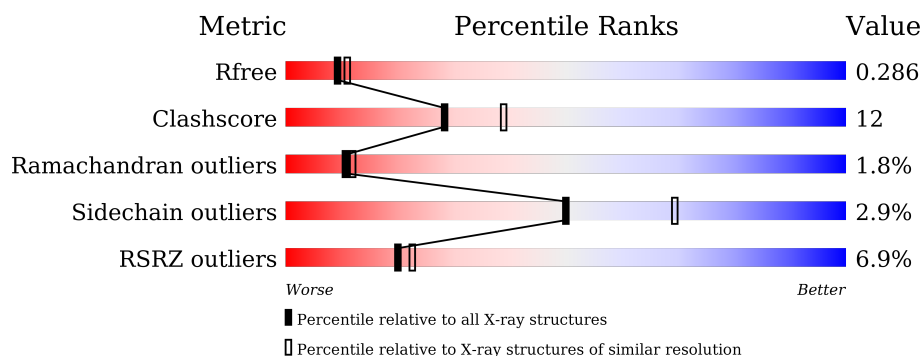
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.37 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	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)

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	939	<div> <div>6%</div> <div>65%</div> <div>20%</div> <div>..</div> <div>13%</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6681 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.

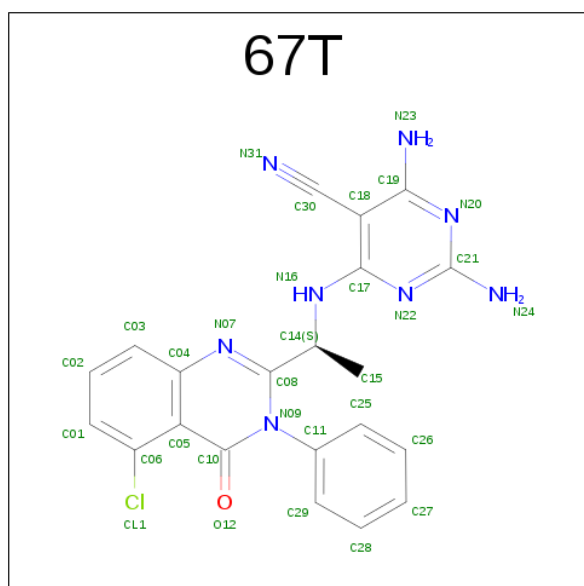
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit delta isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	815	Total	C	N	O	S	0	0	0
			6566	4210	1115	1187	54			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	508	GLN	-	insertion	UNP O35904

- Molecule 2 is 2,4-diamino-6-[[[(1S)-1-(5-chloro-4-oxo-3-phenyl-3,4-dihydroquinazolin-2-yl)ethyl]amino]pyrimidine-5-carbonitrile (three-letter code: 67T) (formula: C<sub>21</sub>H<sub>17</sub>ClN<sub>8</sub>O).



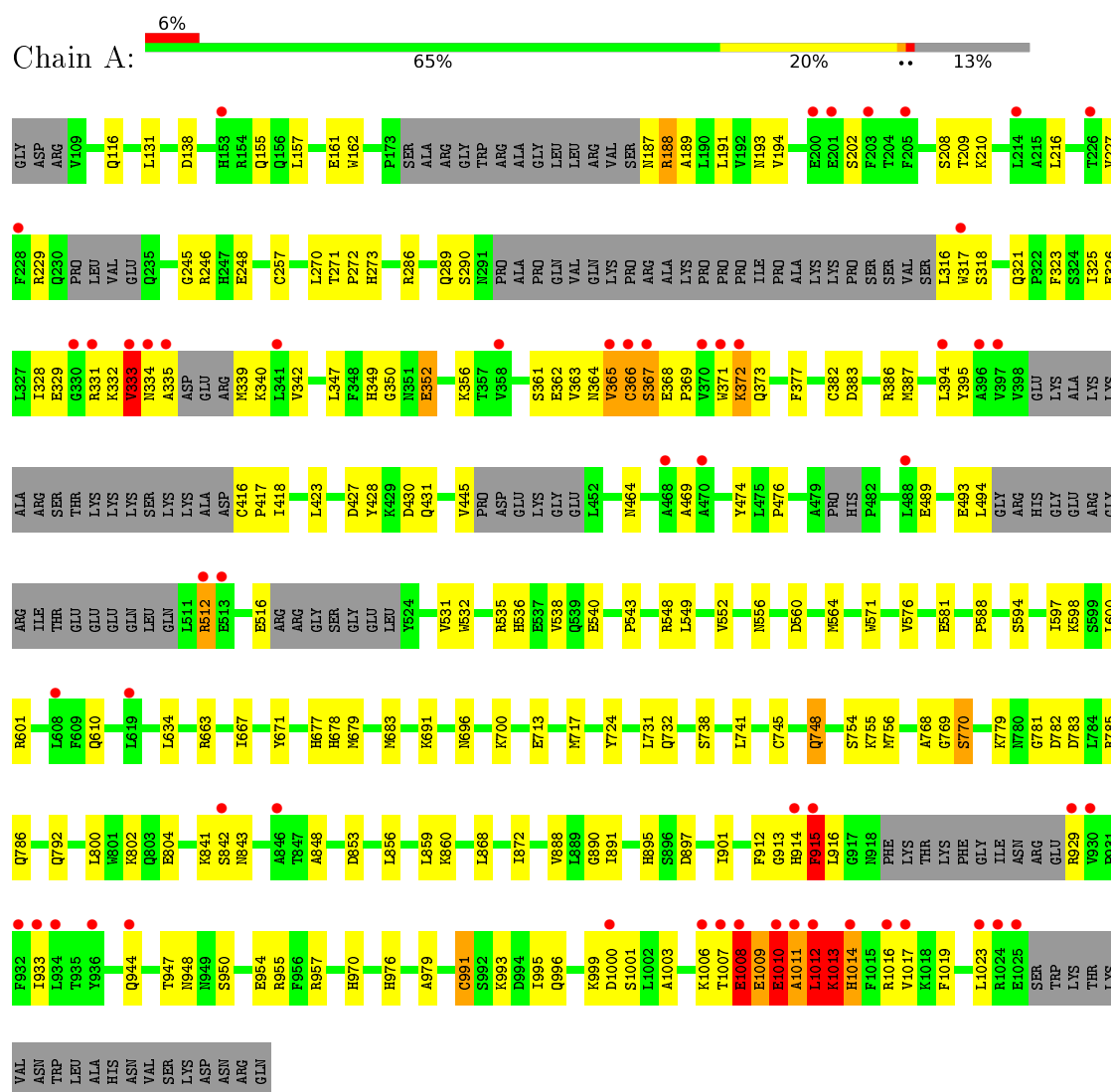
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			31	21	1	8	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	84	Total	O	0	0
			84	84		



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.27Å 143.48Å 221.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.89 – 2.37 45.89 – 2.37	Depositor EDS
% Data completeness (in resolution range)	93.4 (45.89-2.37) 89.1 (45.89-2.37)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 2.37Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.222 , 0.290 0.222 , 0.286	Depositor DCC
$R_{free}$ test set	1917 reflections (5.14%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.9	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 43.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6681	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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: 67T

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	0.48	0/6706	0.63	4/9047 (0.0%)

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	1012	LEU	CA-CB-CG	8.47	134.79	115.30
1	A	1023	LEU	CA-CB-CG	6.13	129.40	115.30
1	A	1009	GLU	N-CA-C	-5.16	97.08	111.00
1	A	1014	HIS	N-CA-CB	5.03	119.65	110.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1008	GLU	Peptide
1	A	1010	GLU	Peptide
1	A	1012	LEU	Peptide
1	A	333	VAL	Peptide

## 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	6566	0	6557	153	0
2	A	31	0	0	0	0
3	A	84	0	0	4	0
All	All	6681	0	6557	153	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 12.

The worst 5 of 153 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:331:ARG:HD3	1:A:368:GLU:HG3	1.48	0.93
1:A:745:CYS:HB3	1:A:748:GLN:HE21	1.34	0.91
1:A:367:SER:OG	1:A:368:GLU:OE2	1.90	0.88
1:A:512:ARG:HH21	1:A:538:VAL:HG22	1.39	0.86
1:A:331:ARG:HA	1:A:368:GLU:HA	1.57	0.86

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	793/939 (84%)	734 (93%)	45 (6%)	14 (2%)	<b>11</b> <b>12</b>

5 of 14 Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	365	VAL
1	A	372	LYS
1	A	770	SER
1	A	913	GLY
1	A	915	PHE

### 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	721/827 (87%)	700 (97%)	21 (3%)	50 69

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	560	ASP
1	A	748	GLN
1	A	1010	GLU
1	A	512	ARG
1	A	1013	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	ASN
1	A	247	HIS
1	A	273	HIS
1	A	334	ASN
1	A	748	GLN

### 5.3.3 RNA ⓘ

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	67T	A	1101	-	34,34,34	1.74	5 (14%)	31,49,49	1.18	3 (9%)

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	67T	A	1101	-	-	0/10/14/14	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	67T	C18-C17	-3.18	1.38	1.42
2	A	1101	67T	C18-C19	-2.77	1.39	1.42
2	A	1101	67T	C11-N09	-2.00	1.43	1.46
2	A	1101	67T	C10-N09	2.63	1.42	1.37
2	A	1101	67T	C10-C05	5.92	1.51	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	1101	67T	C19-C18-C30	2.05	121.50	118.07
2	A	1101	67T	C15-C14-N16	2.31	112.60	109.08
2	A	1101	67T	C25-C11-N09	2.58	122.46	119.25

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, 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	815/939 (86%)	0.50	56 (6%) 20 22	32, 54, 82, 254	0

The worst 5 of 56 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	335	ALA	7.6
1	A	934	LEU	5.2
1	A	333	VAL	5.2
1	A	331	ARG	4.6
1	A	1008	GLU	4.6

### 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(Å <sup>2</sup> )	Q<0.9
2	67T	A	1101	31/31	0.93	0.16	0.47	32,40,47,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.