



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 20, 2017 – 02:15 PM EDT

PDB ID : 5NGB  
Title : X-Ray Diffraction Crystal Structure of the murine PI3K p110delta in complex with a pan inhibitor  
Authors : Berndt, A.; Williams, R.L.  
Deposited on : unknown  
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

<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 : rb-20029824  
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) : rb-20029824

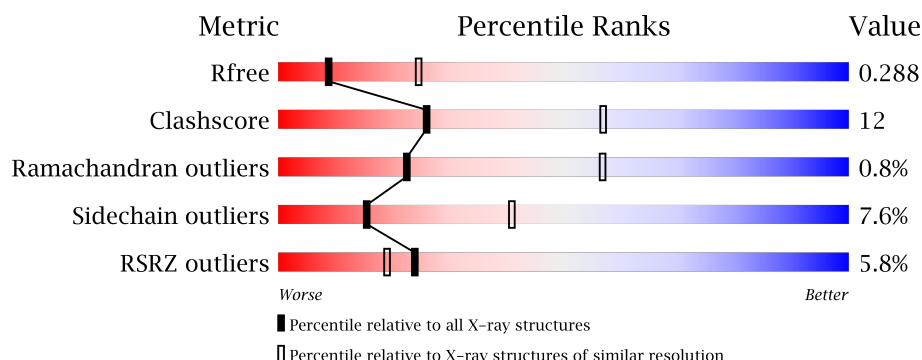
# 1 Overall quality at a glance

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))
$R_{free}$	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (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	1079	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6625 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	816	Total	C	N	O	S	0	0	0
			6593	4228	1120	1192	53			

There are 35 discrepancies between the modelled and reference sequences:

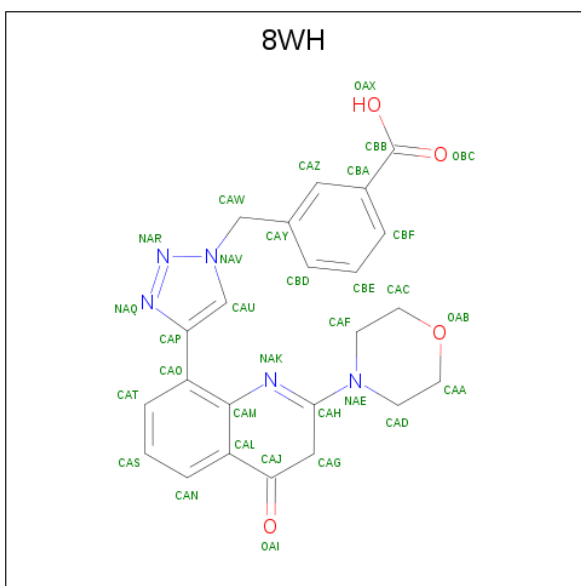
Chain	Residue	Modelled	Actual	Comment	Reference
A	-34	MET	-	initiating methionine	UNP Q3UDT3
A	-33	SER	-	expression tag	UNP Q3UDT3
A	-32	TYR	-	expression tag	UNP Q3UDT3
A	-31	TYR	-	expression tag	UNP Q3UDT3
A	-30	HIS	-	expression tag	UNP Q3UDT3
A	-29	HIS	-	expression tag	UNP Q3UDT3
A	-28	HIS	-	expression tag	UNP Q3UDT3
A	-27	HIS	-	expression tag	UNP Q3UDT3
A	-26	HIS	-	expression tag	UNP Q3UDT3
A	-25	HIS	-	expression tag	UNP Q3UDT3
A	-24	ASP	-	expression tag	UNP Q3UDT3
A	-23	TYR	-	expression tag	UNP Q3UDT3
A	-22	ASP	-	expression tag	UNP Q3UDT3
A	-21	ILE	-	expression tag	UNP Q3UDT3
A	-20	PRO	-	expression tag	UNP Q3UDT3
A	-19	THR	-	expression tag	UNP Q3UDT3
A	-18	THR	-	expression tag	UNP Q3UDT3
A	-17	GLU	-	expression tag	UNP Q3UDT3
A	-16	ASN	-	expression tag	UNP Q3UDT3
A	-15	LEU	-	expression tag	UNP Q3UDT3
A	-14	TYR	-	expression tag	UNP Q3UDT3
A	-13	PHE	-	expression tag	UNP Q3UDT3
A	-12	GLN	-	expression tag	UNP Q3UDT3
A	-11	GLY	-	expression tag	UNP Q3UDT3
A	-10	ALA	-	expression tag	UNP Q3UDT3
A	-9	MET	-	expression tag	UNP Q3UDT3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ASP	-	expression tag	UNP Q3UDT3
A	-7	LEU	-	expression tag	UNP Q3UDT3
A	99	GLU	-	insertion	UNP Q3UDT3
A	100	ASN	-	insertion	UNP Q3UDT3
A	101	LEU	-	insertion	UNP Q3UDT3
A	102	TYR	-	insertion	UNP Q3UDT3
A	103	PHE	-	insertion	UNP Q3UDT3
A	104	GLN	-	insertion	UNP Q3UDT3
A	105	GLY	-	insertion	UNP Q3UDT3

- Molecule 2 is 3-[[4-(2-morpholin-4-yl-4-oxidanylidene-3 {H}-quinolin-8-yl)-1,2,3-triazol-1-yl]methyl]benzoic acid (three-letter code: 8WH) (formula: C<sub>23</sub>H<sub>21</sub>N<sub>5</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			32	23	5	4		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.44Å 143.59Å 220.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.63 – 2.90 45.52 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.63-2.90) 99.8 (45.52-2.89)	Depositor EDS
$R_{merge}$	0.25	Depositor
$R_{sym}$	0.25	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.242 , 0.290 0.243 , 0.288	Depositor DCC
$R_{free}$ test set	1166 reflections (5.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.7	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	6625	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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: 8WH

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	0.57	0/6734	0.78	5/9084 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	957	ARG	NE-CZ-NH2	6.30	123.45	120.30
1	A	927	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	A	821	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	374	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	720	ARG	NE-CZ-NH2	-5.01	117.79	120.30

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	6593	0	6573	155	1
2	A	32	0	0	2	0
All	All	6625	0	6573	156	1

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 156 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:369:PRO:HB2	1:A:371:TRP:CH2	1.61	1.33
1:A:954:GLU:HG2	1:A:957:ARG:NH1	1.60	1.15
1:A:746:VAL:O	1:A:748:GLN:N	1.83	1.12
1:A:341:LEU:HD21	1:A:365:VAL:HG13	1.34	1.08
1:A:224:LYS:HG3	1:A:228:PHE:CE2	1.87	1.08

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:948:ASN:ND2	1:A:948:ASN:ND2[3_655]	2.02	0.18

## 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	792/1079 (73%)	757 (96%)	29 (4%)	6 (1%)	22 57

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	746	VAL
1	A	747	GLU
1	A	917	GLY
1	A	229	ARG
1	A	364	ASN



### 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	724/957 (76%)	669 (92%)	55 (8%)	15	41

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	490	LYS
1	A	537	GLU
1	A	915	PHE
1	A	522	GLU
1	A	530	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	617	GLN
1	A	716	HIS
1	A	906	GLN
1	A	344	GLN
1	A	898	ASN

### 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

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	8WH	A	1101	-	31,36,36	3.37	8 (25%)	40,51,51	1.92	9 (22%)

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	8WH	A	1101	-	-	0/11/36/36	0/4/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	8WH	NAQ-NAR	-12.89	1.16	1.34
2	A	1101	8WH	CAL-CAJ	-6.08	1.39	1.48
2	A	1101	8WH	CAU-CAP	-5.87	1.30	1.37
2	A	1101	8WH	CAO-CAP	-5.13	1.33	1.48
2	A	1101	8WH	NAR-NAV	-4.11	1.26	1.34

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	8WH	CAL-CAM-NAK	-4.52	118.59	122.69
2	A	1101	8WH	OAB-CAC-CAF	-2.86	105.43	111.83
2	A	1101	8WH	OAI-CAJ-CAG	-2.79	116.95	121.19
2	A	1101	8WH	CAO-CAP-NAQ	2.78	125.28	120.96
2	A	1101	8WH	CAG-CAJ-CAL	3.11	121.03	116.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	8WH	2	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	816/1079 (75%)	0.30	47 (5%) 24 19	19, 49, 85, 140	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	341	LEU	7.4
1	A	369	PRO	7.2
1	A	366	CYS	6.9
1	A	317	TRP	6.1
1	A	187	ASN	6.0

### 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(Å <sup>2</sup> )	Q<0.9
2	8WH	A	1101	32/32	0.95	0.17	-0.45	26,37,50,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.