



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:28 PM GMT

PDB ID : 5AE9  
Title : Crystal structure of mouse PI3 kinase delta in complex with GSK2292767  
Authors : Down, K.D.; Amour, A.; Baldwin, I.R.; Cooper, A.W.J.; Deakin, A.M.; Felton, L.M.; Guntrip, S.B.; Hardy, C.; Harrison, Z.A.; Jones, K.L.; Jones, P.; Keeling, S.E.; Le, J.; Livia, S.; Lucas, F.; Lunniss, C.J.; Parr, N.J.; Robinson, E.; Rowland, P.; Smith, S.; Thomas, D.A.; Vitulli, G.; Washio, Y.; Hamblin, N.  
Deposited on : 2015-08-26  
Resolution : 2.44 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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-20026982  
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-20026982



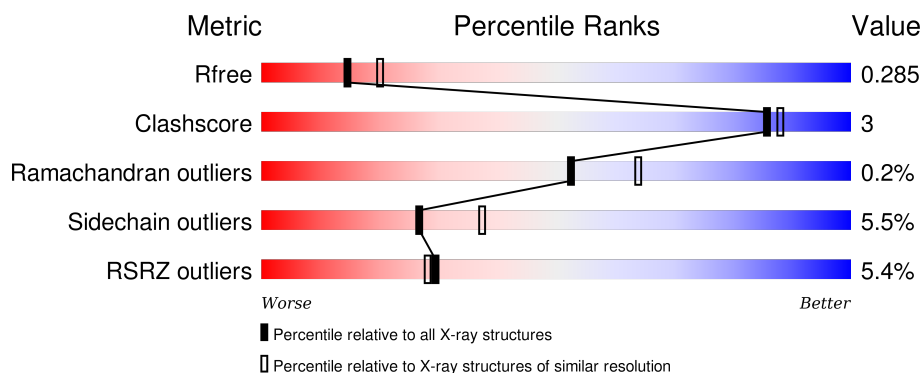
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.44 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	1003 (2.46-2.42)
Clashscore	102246	1071 (2.46-2.42)
Ramachandran outliers	100387	1065 (2.46-2.42)
Sidechain outliers	100360	1065 (2.46-2.42)
RSRZ outliers	91569	1005 (2.46-2.42)

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	940	



## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7494 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.

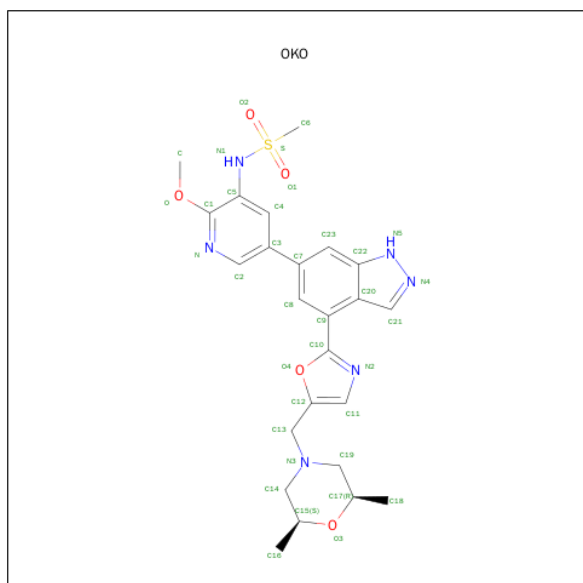
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL 4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT DELTA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	858	Total	C	N	O	S	0	0	0
			6925	4424	1189	1258	54			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	GLY	-	EXPRESSION TAG	UNP Q3UDT3

- Molecule 2 is N-[5-[4-(5-{[(2R,6S)-2,6-DIMETHYL-4-MORPHOLINYLMETHYL]-1,3-OXAZOL-2-YL)-1H-INDAZOL-6-YL]-2-(METHYLOXY)-3-PYRIDINYLMETHANESULFO



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			36	24	6	5	1		



- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	533	Total	O	0	0
			533	533		







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.30Å 64.62Å 116.37Å 90.00° 103.32° 90.00°	Depositor
Resolution (Å)	47.44 – 2.44 58.56 – 2.44	Depositor EDS
% Data completeness (in resolution range)	98.0 (47.44-2.44) 98.1 (58.56-2.44)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 2.45Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, $R_{free}$	0.186 , 0.263 0.198 , 0.285	Depositor DCC
$R_{free}$ test set	1889 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.7	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 80.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 37808 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7494	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.91% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OKO

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	0.51	0/7075	0.68	0/9549

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-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 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	6925	0	6910	39	0
2	A	36	0	28	1	0
3	A	533	0	0	3	0
All	All	7494	0	6938	39	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 3.

All (39) 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:374:ARG:HH12	1:A:476:PRO:HG3	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:LEU:HB3	1:A:262:ILE:HG21	1.88	0.55
1:A:187:ASN:HB2	1:A:210:LYS:HD3	1.88	0.55
1:A:971:GLY:HA3	1:A:1004:LEU:HD11	1.88	0.54
1:A:329:GLU:H	1:A:472:VAL:HG23	1.78	0.49
1:A:194:VAL:HG21	1:A:216:LEU:HD21	1.95	0.49
1:A:244:ASN:ND2	1:A:273:HIS:HB3	2.30	0.47
1:A:695:LEU:HD23	1:A:759:LEU:HD13	1.97	0.47
1:A:975:LEU:HD11	1:A:999:LYS:HG2	1.97	0.47
1:A:859:LEU:HD21	1:A:905:GLY:HA2	1.97	0.46
1:A:812:PRO:HA	3:A:2397:HOH:O	2.15	0.46
1:A:991:CYS:SG	1:A:993:LYS:HB2	2.56	0.45
1:A:316:LEU:HA	1:A:319:LEU:HD12	1.99	0.45
1:A:609:PHE:HE1	1:A:646:PHE:CD2	2.35	0.45
1:A:600:LEU:HD22	1:A:603:LEU:HD11	1.98	0.44
1:A:637:ALA:HB1	1:A:644:GLY:HA2	2.00	0.44
1:A:159:TRP:CE2	1:A:279:SER:HB3	2.52	0.44
1:A:579:ALA:HA	1:A:582:LEU:HD12	2.00	0.44
1:A:208:SER:OG	1:A:210:LYS:HG2	2.18	0.44
1:A:327:LEU:HD11	1:A:471:LEU:HD22	1.98	0.44
1:A:621:TYR:CZ	1:A:983:ALA:HB2	2.53	0.43
1:A:779:LYS:NZ	2:A:4000:OKO:H1	2.16	0.43
1:A:976:HIS:O	1:A:980:LEU:HG	2.18	0.43
1:A:784:LEU:HD12	1:A:823:GLY:HA3	2.00	0.43
1:A:759:LEU:O	1:A:777:ILE:HA	2.19	0.42
1:A:317:TRP:HA	1:A:382:CYS:HB2	2.01	0.42
1:A:345:ALA:HA	1:A:391:CYS:O	2.20	0.42
1:A:386:ARG:HG3	1:A:387:MET:HE2	2.01	0.42
1:A:246:ARG:NH1	1:A:248:GLU:OE1	2.53	0.41
1:A:154:ARG:HD2	1:A:165:TYR:CZ	2.55	0.41
1:A:209:THR:HB	1:A:257:CYS:HB3	2.01	0.41
1:A:205:PHE:CZ	1:A:220:ALA:HA	2.55	0.41
1:A:213:PRO:HD3	1:A:254:TYR:O	2.21	0.41
1:A:194:VAL:CG2	1:A:216:LEU:HD21	2.51	0.41
1:A:390:LEU:HG	1:A:392:PHE:CE2	2.56	0.41
1:A:497:HIS:HA	3:A:2221:HOH:O	2.21	0.41
1:A:192:VAL:HG22	1:A:272:PRO:HG2	2.03	0.40
1:A:336:ASP:HA	3:A:2132:HOH:O	2.22	0.40
1:A:126:HIS:CE1	1:A:127:GLU:HG3	2.56	0.40

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	844/940 (90%)	815 (97%)	27 (3%)	2 (0%)	52	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	911	ASP
1	A	328	ILE

### 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	760/827 (92%)	718 (94%)	42 (6%)	27	37

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	LEU
1	A	166	SER
1	A	176	ARG
1	A	187	ASN
1	A	190	LEU
1	A	195	LYS
1	A	203	PHE
1	A	223	LYS
1	A	248	GLU

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Mol	Chain	Res	Type
1	A	256	LEU
1	A	263	CYS
1	A	270	LEU
1	A	279	SER
1	A	290	SER
1	A	325	ILE
1	A	329	GLU
1	A	333	VAL
1	A	352	GLU
1	A	423	LEU
1	A	429	LYS
1	A	430	ASP
1	A	444	SER
1	A	445	VAL
1	A	472	VAL
1	A	475	LEU
1	A	503	ILE
1	A	509	LEU
1	A	523	LEU
1	A	530	LEU
1	A	696	ASN
1	A	710	GLN
1	A	766	GLU
1	A	770	SER
1	A	787	ASP
1	A	795	GLN
1	A	866	GLU
1	A	915	PHE
1	A	933	ILE
1	A	950	SER
1	A	992	SER
1	A	1004	LEU
1	A	1017	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	HIS
1	A	137	ASN
1	A	344	GLN
1	A	614	GLN
1	A	617	GLN

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Mol	Chain	Res	Type
1	A	696	ASN
1	A	710	GLN
1	A	780	ASN
1	A	918	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 [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	OKO	A	4000	-	35,40,40	1.09	3 (8%)	36,59,59	0.99	1 (2%)

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	OKO	A	4000	-	-	0/14/31/31	0/4/5/5



All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4000	OKO	C13-C12	-2.11	1.49	1.51
2	A	4000	OKO	C19-C17	3.19	1.57	1.51
2	A	4000	OKO	C14-C15	3.81	1.58	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4000	OKO	C13-C12-C11	4.78	137.78	128.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4000	OKO	1	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 ⓘ

### 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	858/940 (91%)	0.24	46 (5%)	29 28	23, 54, 104, 134	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	501	GLY	7.5
1	A	499	GLU	5.0
1	A	503	ILE	4.3
1	A	381	VAL	4.3
1	A	370	VAL	4.3
1	A	335	ALA	4.1
1	A	495	GLY	4.0
1	A	317	TRP	3.8
1	A	509	LEU	3.8
1	A	371	TRP	3.6
1	A	470	ALA	3.3
1	A	330	GLY	3.2
1	A	205	PHE	3.1
1	A	473	ILE	3.0
1	A	323	PHE	3.0
1	A	226	THR	3.0
1	A	529	ASP	2.9
1	A	482	PRO	2.8
1	A	269	GLY	2.7
1	A	358	VAL	2.6
1	A	270	LEU	2.6
1	A	472	VAL	2.6
1	A	228	PHE	2.6
1	A	341	LEU	2.6
1	A	534	MET	2.5
1	A	342	VAL	2.5
1	A	515	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	319	LEU	2.4
1	A	1031	VAL	2.4
1	A	325	ILE	2.4
1	A	393	ALA	2.4
1	A	365	VAL	2.3
1	A	493	GLU	2.3
1	A	497	HIS	2.3
1	A	537	GLU	2.3
1	A	542	PHE	2.3
1	A	506	GLU	2.2
1	A	512	ARG	2.2
1	A	481	HIS	2.2
1	A	146	PHE	2.1
1	A	192	VAL	2.1
1	A	214	LEU	2.1
1	A	337	GLU	2.1
1	A	551	LEU	2.1
1	A	109	VAL	2.1
1	A	471	LEU	2.0

## 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	OKO	A	4000	36/36	0.97	0.16	1.23	18,32,44,48	0



## 6.5 Other polymers

There are no such residues in this entry.