



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 9, 2017 – 10:58 am GMT

PDB ID : 5M6U  
Title : HUMAN PI3KDELTA IN COMPLEX WITH LASW1579  
Authors : Segarra, V.; Hernandez, B.; Lozoya, E.; Blaesse, M.; Hoeppner, S.; Jestel, A.  
Deposited on : 2016-10-26  
Resolution : 2.85 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : recalc28906  
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) : recalc28906

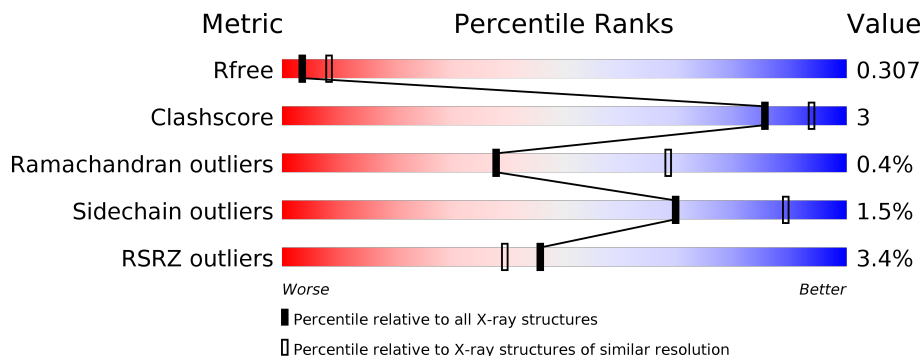
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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	2469 (2.90-2.82)
Clashscore	112137	2749 (2.90-2.82)
Ramachandran outliers	110173	2687 (2.90-2.82)
Sidechain outliers	110143	2690 (2.90-2.82)
RSRZ outliers	101464	2487 (2.90-2.82)

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	1011	<div> <div>3%</div> <div>85%</div> <div>6%</div> <div>9%</div> </div>
2	B	724	<div> <div>21%</div> <div>77%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7700 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	916	Total	C	N	O	S	0	0	0
			6419	4072	1123	1179	45			

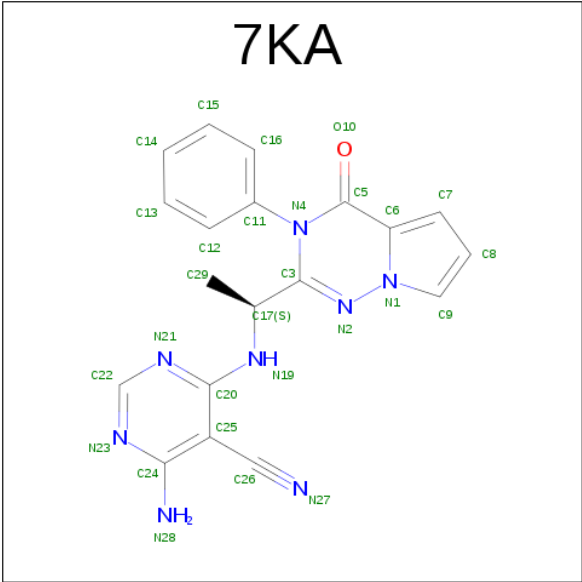
- Molecule 2 is a protein called Phosphatidylinositol 3-kinase regulatory subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	164	Total	C	N	O	S	0	0	0
			1253	795	210	244	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	469	ASP	GLU	conflict	UNP P27986
B	519	THR	LYS	conflict	UNP P27986
B	529	GLU	ASP	conflict	UNP P27986
B	539	VAL	ILE	conflict	UNP P27986

- Molecule 3 is 4-azanyl-6-[[1 {S}]-1-(4-oxidanylidene-3-phenyl-pyrrolo[2,1-f][1,2,4]triazin-2-yl)ethyl]amino]pyrimidine-5-carbonitrile (three-letter code: 7KA) (formula: C<sub>19</sub>H<sub>16</sub>N<sub>8</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	19	8	1		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.49Å 113.21Å 144.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.08 – 2.85 48.28 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (89.08-2.85) 100.0 (48.28-2.85)	Depositor EDS
$R_{merge}$	4.00	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 2.86Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.256 , 0.309 0.250 , 0.307	Depositor DCC
$R_{free}$ test set	997 reflections (2.84%)	DCC
Wilson B-factor (Å <sup>2</sup> )	99.4	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 91.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7700	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: 7KA

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	0.43	0/6560	0.57	0/8953
2	B	0.44	0/1272	0.59	1/1719 (0.1%)
All	All	0.43	0/7832	0.57	1/10672 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	542	ARG	NE-CZ-NH1	5.45	123.03	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	6419	0	5292	31	0
2	B	1253	0	1064	6	0
3	A	28	0	0	0	0
All	All	7700	0	6356	36	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 (36) 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:742:ALA:HB3	1:A:765:ASN:HB3	1.72	0.71
1:A:387:MET:HE3	1:A:590:CYS:HB3	1.86	0.58
1:A:25:LEU:HD13	2:B:497:GLN:HG3	1.88	0.56
1:A:971:GLY:HA3	1:A:1004:LEU:HD21	1.92	0.51
1:A:613:LEU:HD13	1:A:788:MET:HE1	1.93	0.50
2:B:449:LEU:HD22	2:B:584:LEU:HD12	1.93	0.50
1:A:800:LEU:HD22	1:A:970:HIS:ND1	2.28	0.49
1:A:534:LEU:O	1:A:538:VAL:HG23	2.12	0.49
1:A:640:ASN:HB3	1:A:643:ILE:HD12	1.96	0.48
1:A:74:ASN:HB3	1:A:76:THR:HG22	1.96	0.48
1:A:773:SER:O	1:A:829:LEU:HD11	2.15	0.47
1:A:618:VAL:HG13	1:A:621:TYR:CZ	2.50	0.47
1:A:564:MET:HE2	1:A:564:MET:HB2	1.92	0.45
2:B:501:GLN:HG2	2:B:528:TYR:CD1	2.52	0.45
1:A:24:PHE:CD1	1:A:49:LEU:HD22	2.53	0.44
1:A:618:VAL:HG13	1:A:621:TYR:CE1	2.51	0.44
1:A:479:ALA:HB1	1:A:480:PRO:HD2	2.00	0.43
1:A:549:LEU:HG	1:A:564:MET:HE3	1.99	0.43
1:A:790:THR:HG21	1:A:912:PHE:CD1	2.53	0.43
1:A:589:ASP:CG	1:A:591:HIS:HD1	2.21	0.42
1:A:886:THR:HG22	1:A:891:ILE:HD12	2.01	0.42
1:A:421:ALA:HB2	1:A:441:MET:HA	2.01	0.42
1:A:424:MET:SD	1:A:459:VAL:HG21	2.59	0.42
2:B:442:ILE:HG23	2:B:589:VAL:HG21	2.02	0.42
2:B:439:GLU:HB2	2:B:445:VAL:HG22	2.01	0.42
1:A:891:ILE:HD13	1:A:912:PHE:CD1	2.55	0.42
1:A:860:LYS:HA	1:A:868:LEU:HD13	2.02	0.41
1:A:385:PRO:HD2	1:A:388:ALA:HB2	2.02	0.41
1:A:504:THR:HG22	1:A:506:GLU:H	1.86	0.41
2:B:481:ARG:NH2	2:B:549:LEU:HD21	2.36	0.41
1:A:1013:LYS:O	1:A:1017:VAL:HG23	2.20	0.41
1:A:696:ASN:HA	1:A:759:LEU:HD11	2.02	0.41
1:A:651:LEU:HD22	1:A:664:PHE:CG	2.55	0.41
1:A:696:ASN:CA	1:A:759:LEU:HD11	2.51	0.40
1:A:74:ASN:CB	1:A:76:THR:HG22	2.50	0.40
1:A:20:VAL:HG23	1:A:38:ARG:HG3	2.03	0.40

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	900/1011 (89%)	850 (94%)	46 (5%)	4 (0%)	38	68
2	B	162/724 (22%)	157 (97%)	5 (3%)	0	100	100
All	All	1062/1735 (61%)	1007 (95%)	51 (5%)	4 (0%)	38	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	518	ARG
1	A	520	SER
1	A	106	GLY
1	A	896	SER

### 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	493/896 (55%)	486 (99%)	7 (1%)	71	90
2	B	98/654 (15%)	96 (98%)	2 (2%)	60	85
All	All	591/1550 (38%)	582 (98%)	9 (2%)	70	89

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	50	TRP

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Mol	Chain	Res	Type
1	A	317	TRP
1	A	511	LEU
1	A	560	ASP
1	A	696	ASN
1	A	915	PHE
2	B	474	SER
2	B	501	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	193	ASN
1	A	539	GLN
1	A	614	GLN
1	A	792	GLN
1	A	918	ASN
1	A	944	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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	$\# Z  > 2$
3	7KA	A	1101	-	28,31,31	1.26	3 (10%)	22,44,44	1.78	5 (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
3	7KA	A	1101	-	-	0/8/14/14	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	7KA	C11-N4	-4.17	1.40	1.46
3	A	1101	7KA	C20-N19	2.58	1.39	1.35
3	A	1101	7KA	C5-C6	2.90	1.46	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	7KA	N21-C22-N23	-4.06	122.05	128.65
3	A	1101	7KA	C25-C20-N21	-2.85	118.02	121.23
3	A	1101	7KA	C29-C17-C3	-2.34	108.09	111.02
3	A	1101	7KA	C20-C25-C26	3.11	123.81	119.32
3	A	1101	7KA	C8-C9-N1	3.91	109.05	106.77

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 ⓘ

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	916/1011 (90%)	0.10	35 (3%) 41 35	64, 108, 177, 227	0
2	B	164/724 (22%)	-0.20	2 (1%) 79 77	71, 91, 120, 143	0
All	All	1080/1735 (62%)	0.06	37 (3%) 46 39	64, 103, 174, 227	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	200	GLU	9.3
1	A	202	SER	8.9
1	A	268	SER	8.7
1	A	201	GLU	6.7
1	A	269	GLY	5.7
1	A	770	SER	4.5
1	A	270	LEU	4.5
1	A	767	GLU	4.2
1	A	892	GLY	3.9
1	A	723	ALA	3.8
1	A	768	ALA	3.8
1	A	199	SER	3.6
1	A	192	VAL	3.5
1	A	191	LEU	3.4
1	A	194	VAL	3.4
1	A	193	ASN	3.2
1	A	208	SER	3.1
1	A	195	LYS	3.0
2	B	486	ALA	2.8
1	A	272	PRO	2.7
1	A	198	GLY	2.6
1	A	769	GLY	2.6
1	A	271	THR	2.6
1	A	854	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	956	PHE	2.5
1	A	838	GLN	2.4
1	A	173	PRO	2.4
1	A	719	MET	2.4
2	B	455	GLN	2.3
1	A	566	TYR	2.3
1	A	209	THR	2.3
1	A	1015	PHE	2.2
1	A	932	PHE	2.2
1	A	273	HIS	2.2
1	A	981	MET	2.1
1	A	666	LEU	2.1
1	A	614	GLN	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( $\text{\AA}^2$ )	Q<0.9
3	7KA	A	1101	28/28	0.94	0.21	0.48	68,98,106,107	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.