



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 11:31 am GMT

PDB ID : 5T2D  
Title : mPI3Kd IN COMPLEX WITH 7j  
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Deposited on : 2016-08-23  
Resolution : 2.90 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

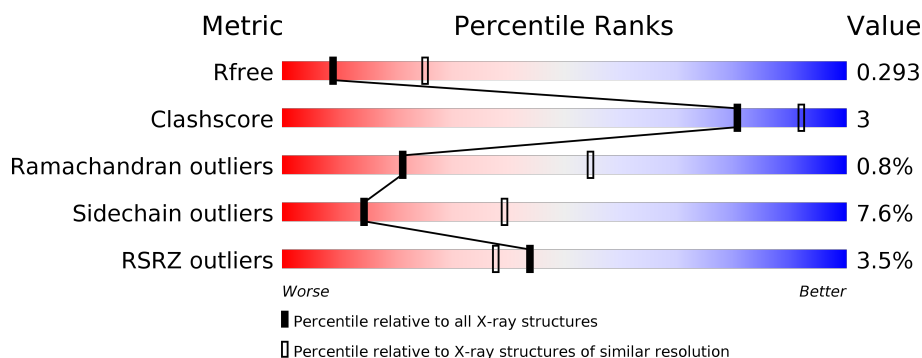
# 1 Overall quality at a glance

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))
$R_{free}$	111664	1716 (2.90-2.90)
Clashscore	122126	1924 (2.90-2.90)
Ramachandran outliers	120053	1884 (2.90-2.90)
Sidechain outliers	120020	1886 (2.90-2.90)
RSRZ outliers	108989	1669 (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	939	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>11%</div> <div>13%</div> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6657 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.

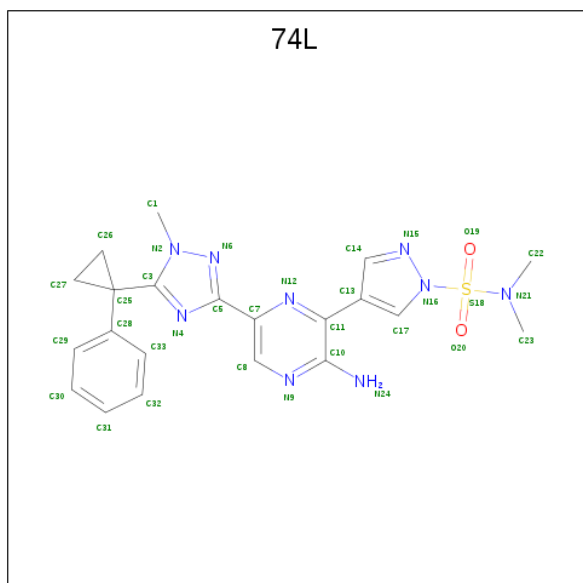
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit delta isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	820	Total	C	N	O	S	0	0	0
			6618	4246	1124	1194	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 4-[3-azanyl-6-[1-methyl-5-(1-phenylcyclopropyl)-1,2,4-triazol-3-yl]pyrazin-2-yl]-{N}, {N}-dimethyl-pyrazole-1-sulfonamide (three-letter code: 74L) (formula: C<sub>21</sub>H<sub>23</sub>N<sub>9</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			33	21	9	2	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.92Å 142.42Å 220.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.38 – 2.90 56.38 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (56.38-2.90) 99.9 (56.38-2.90)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, $R_{free}$	0.223 , 0.287 0.229 , 0.293	Depositor DCC
$R_{free}$ test set	1100 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.6	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 56.0	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	0.91	EDS
Total number of atoms	6657	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 74L

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	0.44	0/6760	0.64	0/9118

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	6618	0	6604	38	0
2	A	33	0	0	0	0
3	A	6	0	0	0	0
All	All	6657	0	6604	38	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 (38) 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:194:VAL:HG21	1:A:216:LEU:HD21	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:THR:HB	1:A:257:CYS:HB3	1.74	0.68
1:A:608:LEU:HD23	1:A:643:ILE:HD13	1.81	0.61
1:A:702:SER:HB3	1:A:711:THR:HG23	1.83	0.60
1:A:549:LEU:HG	1:A:564:MET:CE	2.33	0.57
1:A:549:LEU:HG	1:A:564:MET:HE1	1.88	0.54
1:A:895:HIS:H	1:A:898:ASN:HD21	1.57	0.53
1:A:810:MET:O	1:A:812:PRO:HD3	2.11	0.51
1:A:390:LEU:HB2	1:A:425:LEU:HD21	1.93	0.51
1:A:342:VAL:HG22	1:A:362:GLU:HG2	1.94	0.49
1:A:289:GLN:HG2	1:A:677:HIS:CG	2.48	0.49
1:A:162:TRP:CE3	1:A:286:ARG:HG3	2.48	0.48
1:A:886:THR:HA	1:A:891:ILE:HD12	1.95	0.47
1:A:720:ARG:HH22	1:A:747:GLU:HG2	1.79	0.47
1:A:328:ILE:HG23	1:A:372:LYS:HD3	1.97	0.46
1:A:784:LEU:HD12	1:A:823:GLY:HA3	1.96	0.46
1:A:695:LEU:HD11	1:A:715:MET:HG2	1.97	0.46
1:A:328:ILE:HB	1:A:472:VAL:HG23	1.97	0.46
1:A:135:GLU:HG3	1:A:428:TYR:CG	2.51	0.46
1:A:883:CYS:HB3	1:A:932:PHE:CZ	2.51	0.45
1:A:583:LEU:HD11	1:A:600:LEU:HD11	1.99	0.45
1:A:834:ILE:HG12	1:A:899:ILE:O	2.18	0.44
1:A:329:GLU:H	1:A:472:VAL:HG23	1.82	0.43
1:A:971:GLY:HA3	1:A:1004:LEU:HD21	2.01	0.43
1:A:777:ILE:HB	1:A:825:ILE:HB	2.01	0.42
1:A:247:HIS:HB2	1:A:738:SER:HA	2.00	0.42
1:A:549:LEU:HG	1:A:564:MET:HE2	2.00	0.42
1:A:194:VAL:CG2	1:A:216:LEU:HD21	2.46	0.42
1:A:600:LEU:HD22	1:A:603:LEU:HD11	2.02	0.42
1:A:637:ALA:HB1	1:A:644:GLY:HA2	2.02	0.41
1:A:564:MET:HA	1:A:567:LEU:HD12	2.03	0.41
1:A:597:ILE:O	1:A:601:ARG:HG3	2.20	0.41
1:A:332:LYS:HB2	1:A:333:VAL:H	1.77	0.41
1:A:895:HIS:CE1	1:A:897:ASP:HB2	2.55	0.41
1:A:192:VAL:HG11	1:A:216:LEU:HD11	2.03	0.41
1:A:213:PRO:HD3	1:A:254:TYR:O	2.21	0.40
1:A:343:VAL:HG22	1:A:394:LEU:HD12	2.02	0.40
1:A:439:LEU:HD11	1:A:473:ILE:HG12	2.04	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	796/939 (85%)	751 (94%)	39 (5%)	6 (1%)	21	54

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	ILE
1	A	742	GLU
1	A	755	LYS
1	A	362	GLU
1	A	364	ASN
1	A	911	ASP

### 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	726/827 (88%)	671 (92%)	55 (8%)	14	39

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	LYS
1	A	115	SER
1	A	119	LEU
1	A	154	ARG
1	A	166	SER

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Mol	Chain	Res	Type
1	A	200	GLU
1	A	206	GLN
1	A	247	HIS
1	A	270	LEU
1	A	316	LEU
1	A	317	TRP
1	A	319	LEU
1	A	329	GLU
1	A	332	LYS
1	A	352	GLU
1	A	356	LYS
1	A	360	SER
1	A	365	VAL
1	A	374	ARG
1	A	398	VAL
1	A	415	ASP
1	A	423	LEU
1	A	472	VAL
1	A	475	LEU
1	A	483	VAL
1	A	511	LEU
1	A	512	ARG
1	A	514	ILE
1	A	516	GLU
1	A	517	ARG
1	A	530	LEU
1	A	553	THR
1	A	560	ASP
1	A	586	SER
1	A	590	CYS
1	A	634	LEU
1	A	679	MET
1	A	702	SER
1	A	710	GLN
1	A	731	LEU
1	A	738	SER
1	A	756	MET
1	A	787	ASP
1	A	834	ILE
1	A	841	LYS
1	A	855	LEU
1	A	898	ASN

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Mol	Chain	Res	Type
1	A	915	PHE
1	A	919	PHE
1	A	937	ASP
1	A	947	THR
1	A	999	LYS
1	A	1004	LEU
1	A	1009	GLU
1	A	1027	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	273	HIS
1	A	278	HIS
1	A	291	ASN
1	A	617	GLN
1	A	780	ASN
1	A	898	ASN
1	A	914	HIS

### 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	74L	A	1101	-	33,37,37	1.07	2 (6%)	37,57,57	2.65	6 (16%)

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	74L	A	1101	-	-	0/16/36/36	0/4/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	74L	C3-N4	-2.29	1.31	1.34
2	A	1101	74L	S18-N21	3.60	1.66	1.60

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	74L	N6-C5-N4	-11.12	107.82	114.53
2	A	1101	74L	N4-C3-N2	-2.84	107.30	113.51
2	A	1101	74L	C8-N9-C10	2.46	121.31	118.75
2	A	1101	74L	C5-N6-N2	2.53	107.47	103.15
2	A	1101	74L	C11-C10-N24	2.62	123.24	121.08
2	A	1101	74L	C5-N4-C3	8.76	111.03	101.21

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 ⓘ

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	820/939 (87%)	0.11	29 (3%) 44 38	24, 55, 98, 171	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	187	ASN	4.6
1	A	1005	GLY	4.2
1	A	846	ALA	4.2
1	A	330	GLY	4.0
1	A	843	ASN	3.9
1	A	341	LEU	3.2
1	A	932	PHE	3.1
1	A	317	TRP	3.0
1	A	1006	LYS	3.0
1	A	206	GLN	3.0
1	A	1002	LEU	2.9
1	A	190	LEU	2.8
1	A	517	ARG	2.7
1	A	347	LEU	2.7
1	A	394	LEU	2.6
1	A	934	LEU	2.5
1	A	842	SER	2.5
1	A	945	GLY	2.4
1	A	515	LEU	2.3
1	A	929	ARG	2.3
1	A	845	ALA	2.3
1	A	223	LYS	2.2
1	A	470	ALA	2.2
1	A	153	HIS	2.2
1	A	377	PHE	2.1
1	A	549	LEU	2.0
1	A	332	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	418	ILE	2.0
1	A	1027	TRP	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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	74L	A	1101	33/33	0.96	0.19	26,35,49,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.