



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 01:25 pm GMT

PDB ID : 5T2M
Title : mPI3Kd IN COMPLEX WITH 7m
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Deposited on : 2016-08-23
Resolution : 2.80 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

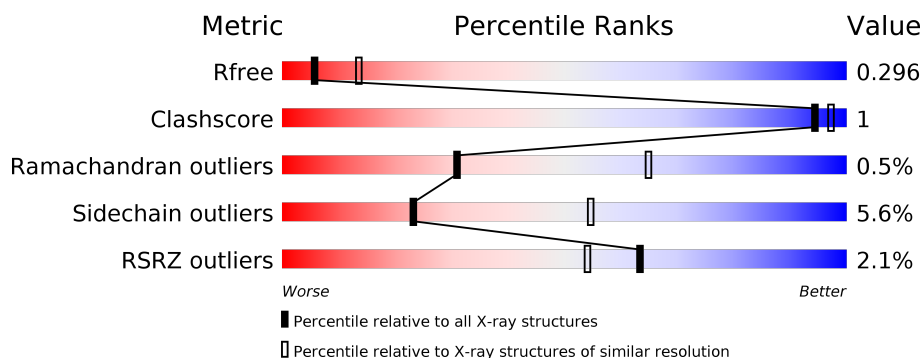
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2792 (2.80-2.80)
Clashscore	122126	3209 (2.80-2.80)
Ramachandran outliers	120053	3158 (2.80-2.80)
Sidechain outliers	120020	3160 (2.80-2.80)
RSRZ outliers	108989	2726 (2.80-2.80)

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 ≥ 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>2%</div> <div> <div></div> <div>79%</div> <div>8%</div> <div>13%</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6653 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.

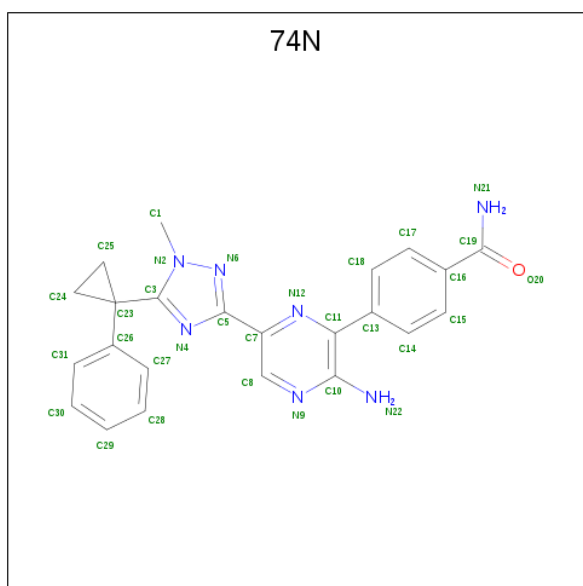
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit delta isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	820	6621	4248	1124	1196	53	0	0	0

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]benzamide (three-letter code: 74N) (formula: C₂₃H₂₁N₇O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	31	23	7	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	63.58Å 141.78Å 219.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.52 – 2.80 58.01 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (59.52-2.80) 99.0 (58.01-2.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.228 , 0.270 0.252 , 0.296	Depositor DCC
R_{free} test set	1190 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	57.6	Xtriage
Anisotropy	0.580	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6653	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 74N

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	0.40	0/6763	0.59	0/9123

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 [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	6621	0	6604	19	0
2	A	31	0	0	0	0
3	A	1	0	0	0	0
All	All	6653	0	6604	19	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 1.

All (19) 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:752:MET:HB2	1:A:758:PRO:HD2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:886:THR:HA	1:A:891:ILE:HD12	1.81	0.61
1:A:494:LEU:HD21	1:A:559:GLU:HG2	1.89	0.55
1:A:620:LYS:HE2	1:A:660:VAL:HG11	1.89	0.54
1:A:340:LYS:HG2	1:A:362:GLU:HB3	1.89	0.53
1:A:247:HIS:HB2	1:A:738:SER:HA	1.91	0.52
1:A:756:MET:HG2	1:A:781:GLY:HA3	1.92	0.51
1:A:574:LEU:HD12	1:A:582:LEU:HD11	1.96	0.48
1:A:617:GLN:HE21	1:A:984:ALA:HA	1.79	0.46
1:A:209:THR:HB	1:A:257:CYS:HB3	1.98	0.46
1:A:971:GLY:HA3	1:A:1004:LEU:HD21	1.99	0.43
1:A:317:TRP:HA	1:A:382:CYS:HB2	2.01	0.43
1:A:883:CYS:HB3	1:A:932:PHE:CZ	2.53	0.43
1:A:263:CYS:HA	1:A:266:LEU:HD12	2.01	0.42
1:A:189:ALA:HA	1:A:208:SER:HA	2.02	0.41
1:A:289:GLN:HG2	1:A:677:HIS:CG	2.55	0.41
1:A:355:CYS:SG	1:A:377:PHE:HB3	2.61	0.41
1:A:574:LEU:HA	1:A:574:LEU:HD23	1.94	0.40
1:A:271:THR:HA	1:A:272:PRO:HD3	2.01	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%)	759 (95%)	33 (4%)	4 (0%)	31 65

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	ILE
1	A	742	GLU
1	A	865	GLY

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Mol	Chain	Res	Type
1	A	435	GLY

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%)	685 (94%)	41 (6%)	23 54

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	LEU
1	A	200	GLU
1	A	228	PHE
1	A	247	HIS
1	A	263	CYS
1	A	270	LEU
1	A	316	LEU
1	A	317	TRP
1	A	321	GLN
1	A	332	LYS
1	A	340	LYS
1	A	344	GLN
1	A	352	GLU
1	A	356	LYS
1	A	394	LEU
1	A	415	ASP
1	A	423	LEU
1	A	437	ARG
1	A	471	LEU
1	A	483	VAL
1	A	511	LEU
1	A	516	GLU
1	A	517	ARG
1	A	523	LEU
1	A	530	LEU

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Mol	Chain	Res	Type
1	A	553	THR
1	A	560	ASP
1	A	634	LEU
1	A	731	LEU
1	A	756	MET
1	A	779	LYS
1	A	787	ASP
1	A	795	GLN
1	A	841	LYS
1	A	898	ASN
1	A	915	PHE
1	A	919	PHE
1	A	962	ARG
1	A	986	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	278	HIS
1	A	291	ASN
1	A	539	GLN
1	A	610	GLN
1	A	617	GLN
1	A	696	ASN
1	A	780	ASN
1	A	898	ASN

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
2	74N	A	1101	-	33,35,35	1.00	1 (3%)	42,52,52	2.56	9 (21%)

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	74N	A	1101	-	-	0/18/28/28	0/4/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	74N	C3-N4	-2.31	1.31	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	74N	N6-C5-N4	-11.08	107.85	114.53
2	A	1101	74N	O20-C19-N21	-3.33	117.76	122.60
2	A	1101	74N	N4-C3-N2	-2.78	107.42	113.51
2	A	1101	74N	C5-C7-N12	2.08	119.96	117.39
2	A	1101	74N	C5-N6-N2	2.43	107.29	103.15
2	A	1101	74N	C8-N9-C10	2.73	121.59	118.75
2	A	1101	74N	C16-C19-N21	2.80	121.01	117.76
2	A	1101	74N	C13-C11-N12	3.03	119.22	115.13
2	A	1101	74N	C5-N4-C3	8.67	110.93	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 [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, 95th 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 ²)	Q<0.9
1	A	820/939 (87%)	0.02	17 (2%) 63 54	22, 58, 102, 161	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	206	GLN	5.3
1	A	846	ALA	4.1
1	A	1005	GLY	3.3
1	A	317	TRP	3.0
1	A	517	ARG	2.9
1	A	1004	LEU	2.9
1	A	266	LEU	2.7
1	A	394	LEU	2.4
1	A	1027	TRP	2.4
1	A	222	ARG	2.3
1	A	397	VAL	2.3
1	A	187	ASN	2.3
1	A	347	LEU	2.3
1	A	515	LEU	2.2
1	A	226	THR	2.2
1	A	845	ALA	2.2
1	A	256	LEU	2.1

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, 95th 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(\AA^2)	Q<0.9
2	74N	A	1101	31/31	0.96	0.20	28,33,43,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.