



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 10, 2017 – 02:58 PM EDT

PDB ID : 5T2B
Title : mPI3Kd IN COMPLEX WITH 5e
Authors : Petersen, J.; Terstige, I.; Perry, M.; Svensson, T.; Tyrchan, C.; Lindmark, H.; Oster, L.
Deposited on : 2016-08-23
Resolution : 2.30 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
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-20029077

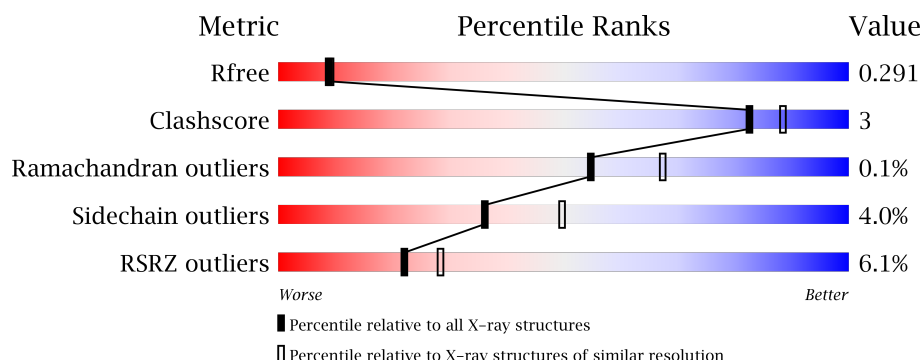
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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>5%</div> <div>78%</div> <div>9%</div> <div>13%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6693 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.

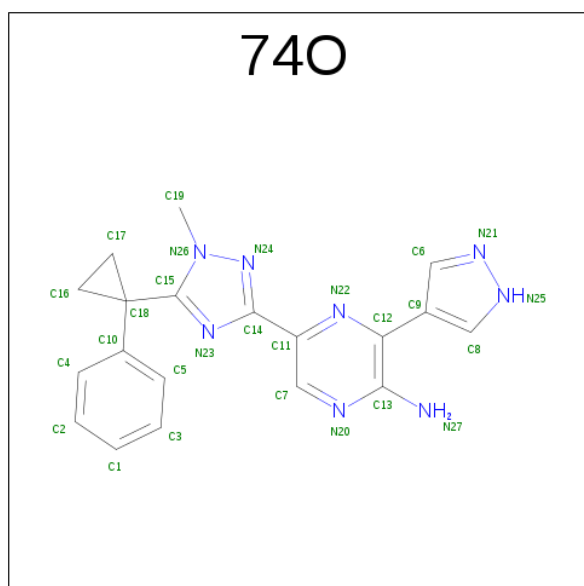
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit delta isoform.

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

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 5-[1-methyl-5-(1-phenylcyclopropyl)-1,2,4-triazol-3-yl]-3-(1 {H}-pyrazol-4-yl)pyrazin-2-amine (three-letter code: 74O) (formula: C₁₉H₁₈N₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			27	19	8		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total	O	0	0
			45	45		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.79Å 64.50Å 115.98Å 90.00° 103.36° 90.00°	Depositor
Resolution (Å)	49.93 – 2.30 49.93 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.8 (49.93-2.30) 97.8 (49.93-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.222 , 0.271 0.236 , 0.291	Depositor DCC
R_{free} test set	2243 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6693	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.94% 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

5.1 Standard geometry

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

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	0.45	0/6763	0.64	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

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	38	0
2	A	27	0	0	0	0
3	A	45	0	0	0	0
All	All	6693	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:245:GLY:HA3	1:A:768:ALA:HB2	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:VAL:H	1:A:360:SER:HB3	1.67	0.60
1:A:1002:LEU:HB3	1:A:1004:LEU:HD23	1.84	0.58
1:A:553:THR:HG21	1:A:564:MET:HG2	1.85	0.57
1:A:549:LEU:HG	1:A:564:MET:CE	2.35	0.57
1:A:549:LEU:HG	1:A:564:MET:HE3	1.88	0.55
1:A:894:ARG:HA	1:A:898:ASN:HD21	1.72	0.54
1:A:421:ALA:HB2	1:A:441:MET:HG2	1.91	0.53
1:A:583:LEU:HD11	1:A:600:LEU:HD11	1.91	0.53
1:A:324:SER:HB3	1:A:376:GLU:HG3	1.91	0.53
1:A:712:LYS:HE3	1:A:750:THR:HB	1.92	0.52
1:A:784:LEU:HD12	1:A:823:GLY:HA3	1.93	0.51
1:A:326:GLU:HB3	1:A:474:TYR:HB3	1.91	0.51
1:A:247:HIS:HB2	1:A:738:SER:HA	1.92	0.51
1:A:344:GLN:HB2	1:A:395:TYR:HE1	1.76	0.51
1:A:271:THR:O	1:A:273:HIS:HD2	1.97	0.47
1:A:929:ARG:HH22	1:A:1001:SER:HA	1.79	0.47
1:A:213:PRO:O	1:A:217:MET:HG3	2.16	0.46
1:A:806:LEU:HB2	1:A:962:ARG:HH21	1.80	0.46
1:A:118:SER:HB3	1:A:124:GLY:HA2	1.98	0.46
1:A:383:ASP:HB3	1:A:556:ASN:O	2.16	0.46
1:A:808:LEU:HD11	1:A:963:ALA:HB2	1.99	0.45
1:A:777:ILE:HB	1:A:825:ILE:HB	1.99	0.45
1:A:390:LEU:HB3	1:A:423:LEU:HD12	1.98	0.45
1:A:328:ILE:HD11	1:A:474:TYR:HB2	1.99	0.45
1:A:637:ALA:HB1	1:A:644:GLY:HA2	1.99	0.44
1:A:419:ALA:HB1	1:A:441:MET:HB3	2.00	0.43
1:A:194:VAL:HG21	1:A:216:LEU:HD21	2.01	0.42
1:A:172:GLU:HG3	1:A:263:CYS:SG	2.60	0.42
1:A:331:ARG:HG3	1:A:470:ALA:HB3	2.01	0.42
1:A:247:HIS:CD2	1:A:740:LEU:HD21	2.55	0.42
1:A:328:ILE:HB	1:A:472:VAL:HG23	2.02	0.41
1:A:332:LYS:HB3	1:A:469:ALA:HB1	2.01	0.41
1:A:587:PHE:HB3	1:A:592:VAL:HG11	2.02	0.41
1:A:761:ILE:HB	1:A:776:ILE:HG13	2.02	0.41
1:A:332:LYS:HG2	1:A:394:LEU:HD21	2.02	0.41
1:A:349:HIS:HB2	1:A:354:LEU:HD21	2.01	0.41
1:A:855:LEU:HD22	1:A:941:VAL:HG21	2.02	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	796/939 (85%)	774 (97%)	21 (3%)	1 (0%)	55 67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	726/827 (88%)	697 (96%)	29 (4%)	36 50

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	SER
1	A	188	ARG
1	A	190	LEU
1	A	203	PHE
1	A	263	CYS
1	A	264	SER
1	A	270	LEU
1	A	291	ASN
1	A	316	LEU
1	A	317	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	332	LYS
1	A	340	LYS
1	A	356	LYS
1	A	368	GLU
1	A	511	LEU
1	A	514	ILE
1	A	517	ARG
1	A	530	LEU
1	A	553	THR
1	A	560	ASP
1	A	634	LEU
1	A	743	GLU
1	A	841	LYS
1	A	855	LEU
1	A	898	ASN
1	A	915	PHE
1	A	937	ASP
1	A	998	LEU
1	A	1004	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	HIS
1	A	278	HIS
1	A	291	ASN
1	A	351	ASN
1	A	851	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 [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	74O	A	1101	-	29,31,31	1.69	6 (20%)	31,46,46	1.33	6 (19%)

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	74O	A	1101	-	-	0/10/24/24	0/4/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	74O	C12-C13	-4.96	1.38	1.45
2	A	1101	74O	C9-C12	-3.48	1.45	1.49
2	A	1101	74O	C18-C10	-3.26	1.49	1.54
2	A	1101	74O	N24-N26	-2.95	1.34	1.37
2	A	1101	74O	C11-C14	-2.45	1.44	1.49
2	A	1101	74O	C13-N27	2.28	1.40	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	74O	C17-C18-C15	-2.56	113.58	118.55
2	A	1101	74O	C8-C9-C12	-2.39	123.45	127.74
2	A	1101	74O	C7-N20-C13	-2.18	116.41	118.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	74O	N23-C15-N26	-2.08	108.97	113.51
2	A	1101	74O	C14-N23-C15	2.03	103.49	101.21
2	A	1101	74O	C6-C9-C12	2.61	132.43	127.74

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 [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, 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%)	0.54	50 (6%)	22 28	24, 47, 79, 149	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	515	LEU	5.9
1	A	341	LEU	5.4
1	A	317	TRP	5.4
1	A	936	TYR	5.2
1	A	517	ARG	4.8
1	A	483	VAL	4.8
1	A	1017	VAL	4.8
1	A	530	LEU	4.6
1	A	514	ILE	4.5
1	A	334	ASN	4.2
1	A	396	ALA	3.8
1	A	377	PHE	3.8
1	A	531	VAL	3.7
1	A	1024	ARG	3.7
1	A	109	VAL	3.4
1	A	1023	LEU	3.4
1	A	196	PHE	3.2
1	A	478	VAL	3.2
1	A	316	LEU	3.1
1	A	866	GLU	3.1
1	A	136	VAL	3.0
1	A	471	LEU	2.9
1	A	512	ARG	2.9
1	A	526	HIS	2.9
1	A	342	VAL	2.8
1	A	474	TYR	2.8
1	A	371	TRP	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	226	THR	2.7
1	A	329	GLU	2.7
1	A	488	LEU	2.7
1	A	319	LEU	2.6
1	A	270	LEU	2.6
1	A	416	CYS	2.6
1	A	529	ASP	2.6
1	A	466	GLU	2.4
1	A	533	LYS	2.4
1	A	228	PHE	2.4
1	A	395	TYR	2.3
1	A	227	VAL	2.2
1	A	330	GLY	2.2
1	A	111	LYS	2.1
1	A	537	GLU	2.1
1	A	995	ILE	2.1
1	A	919	PHE	2.1
1	A	320	GLU	2.0
1	A	133	ASP	2.0
1	A	323	PHE	2.0
1	A	125	LEU	2.0
1	A	523	LEU	2.0
1	A	945	GLY	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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	74O	A	1101	27/27	0.96	0.15	-0.74	24,29,35,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.