



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 15, 2018 – 02:50 PM EST

PDB ID : 2X6F
Title : THE CRYSTAL STRUCTURE OF THE DROSOPHILA CLASS III PI3-KINASE VPS34 IN COMPLEX WITH 3-METHYLADENINE
Authors : Miller, S.; Tavshanjian, B.; Oleksy, A.; Perisic, O.; Houseman, B.T.; Shokat, K.M.; Williams, R.L.
Deposited on : 2010-02-17
Resolution : 3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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-20030736
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-20030736

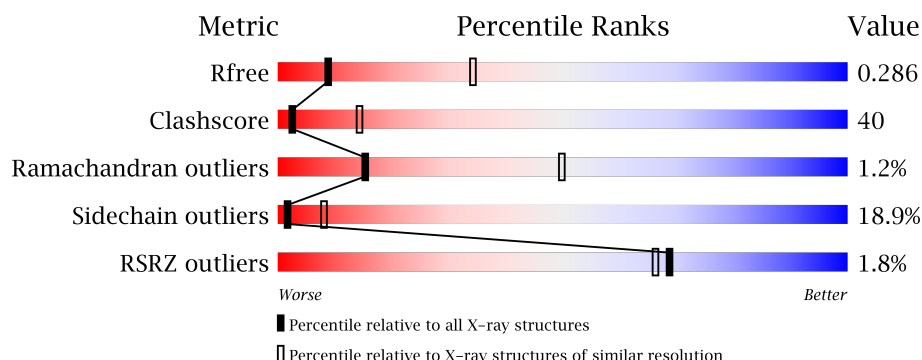
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1034 (3.36-3.24)
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)

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	696	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -5px; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 1%, orange 1%, yellow 34%, green 33%, orange 11%, grey 22%);"></div> <div style="position: absolute; bottom: 5px; left: 0; width: 100%; text-align: center;"> </div> </div> </div>
1	B	696	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -5px; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 2%, orange 2%, yellow 36%, green 32%, orange 9%, grey 22%);"></div> <div style="position: absolute; bottom: 5px; left: 0; width: 100%; text-align: center;"> </div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8897 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.

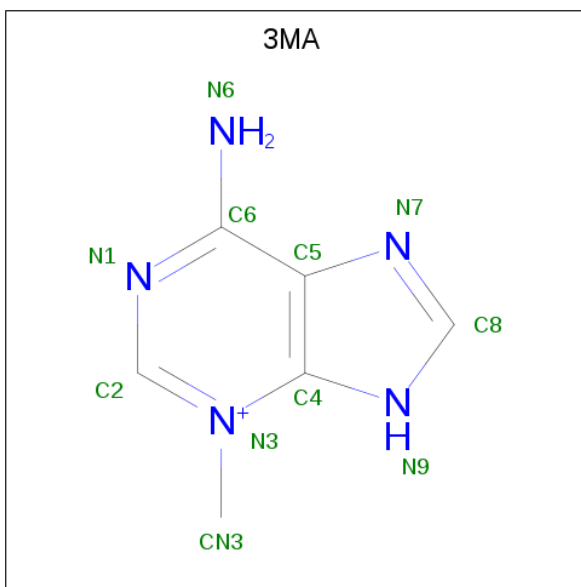
- Molecule 1 is a protein called PHOSPHOTIDYLINOSITOL 3 KINASE 59F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	543	Total	C	N	O	S	0	0	0
			4443	2873	754	789	27			
1	B	542	Total	C	N	O	S	0	0	0
			4432	2867	754	784	27			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	254	GLY	-	expression tag	UNP Q9W1M7
A	255	SER	-	expression tag	UNP Q9W1M7
A	256	HIS	-	expression tag	UNP Q9W1M7
A	257	MET	-	expression tag	UNP Q9W1M7
A	455	ALA	GLY	engineered mutation	UNP Q9W1M7
B	254	GLY	-	expression tag	UNP Q9W1M7
B	255	SER	-	expression tag	UNP Q9W1M7
B	256	HIS	-	expression tag	UNP Q9W1M7
B	257	MET	-	expression tag	UNP Q9W1M7
B	455	ALA	GLY	engineered mutation	UNP Q9W1M7

- Molecule 2 is 6-AMINO-3-METHYLPURINE (three-letter code: 3MA) (formula: C₆H₈N₅).

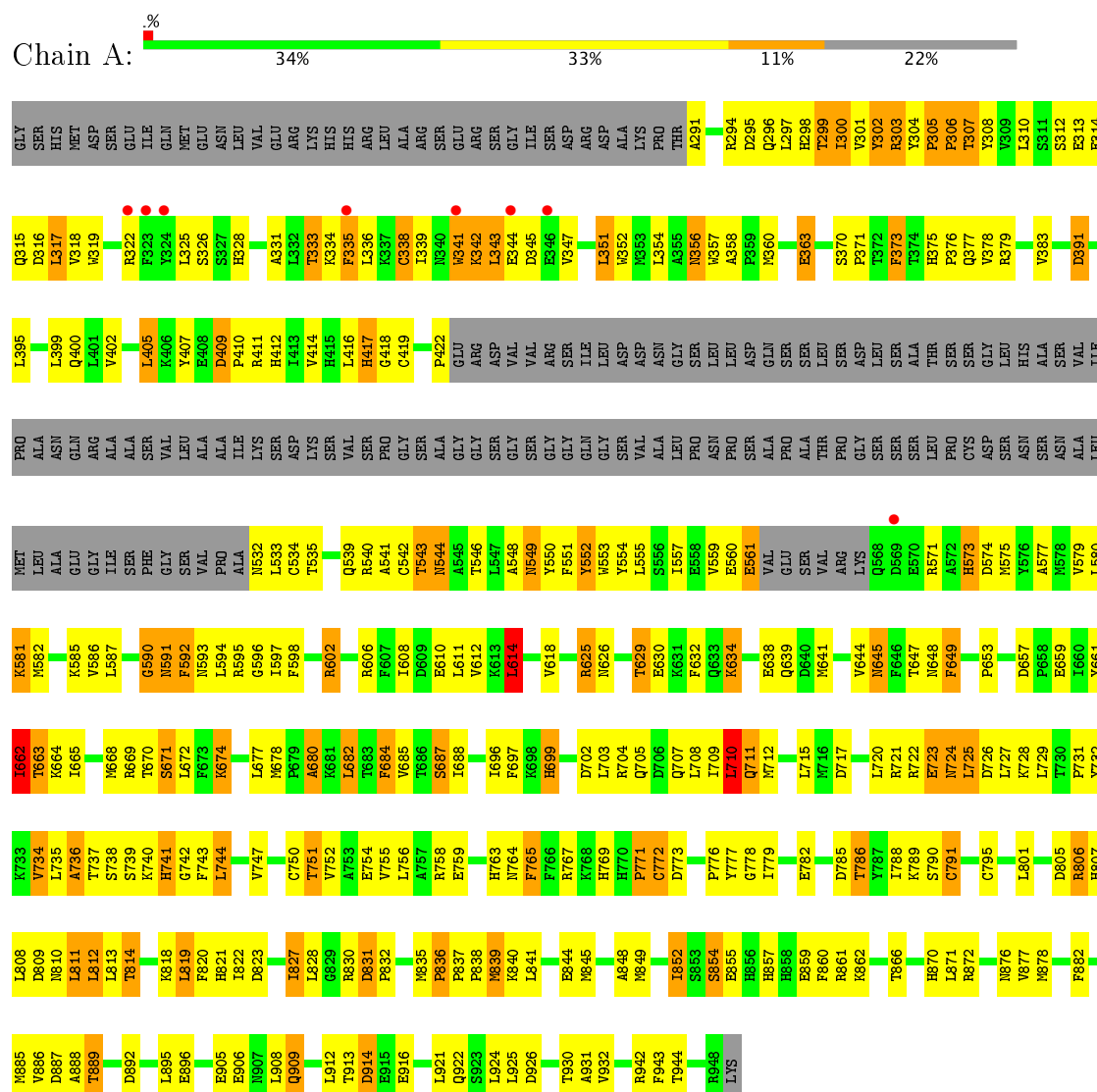


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			11	6	5		
2	B	1	Total	C	N	0	0
			11	6	5		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: PHOSPHOTIDYLINOSITOL 3 KINASE 59F



• Molecule 1: PHOSPHOTIDYLINOSITOL 3 KINASE 59F





4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	112.07Å 155.14Å 244.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.13 – 3.30 61.13 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.5 (61.13-3.30) 97.5 (61.13-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.242 , 0.293 0.237 , 0.286	Depositor DCC
R_{free} test set	1564 reflections (5.20%)	DCC
Wilson B-factor (Å ²)	114.7	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 77.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8897	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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: 3MA

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	0.57	1/4552 (0.0%)	0.84	4/6165 (0.1%)
1	B	0.46	0/4540	0.68	4/6147 (0.1%)
All	All	0.52	1/9092 (0.0%)	0.76	8/12312 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	590	GLY	C-O	5.43	1.32	1.23

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	710	LEU	CA-CB-CG	-6.57	100.18	115.30
1	B	398	LEU	CA-CB-CG	6.05	129.22	115.30
1	B	351	LEU	CA-CB-CG	5.64	128.27	115.30
1	B	677	LEU	CA-CB-CG	5.61	128.20	115.30
1	B	344	GLU	N-CA-C	5.42	125.64	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	590	GLY	Mainchain
1	A	591	ASN	Mainchain
1	A	680	ALA	Peptide
1	A	734	VAL	Peptide
1	A	736	ALA	Peptide

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	4443	0	4472	350	1
1	B	4432	0	4468	383	0
2	A	11	0	8	1	0
2	B	11	0	8	2	0
All	All	8897	0	8956	721	1

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 40.

The worst 5 of 721 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:B:300:ILE:HG12	1:B:304:TYR:CE2	1.58	1.38
1:B:360:MET:HB3	1:B:364:ASP:OD2	1.28	1.27
1:B:305:PRO:HG3	1:B:308:TYR:CD1	1.71	1.25
1:B:299:THR:HA	1:B:302:TYR:CE2	1.82	1.14
1:B:811:LEU:HD22	1:B:821:HIS:CD2	1.86	1.10

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ASP:OD2	1:A:724:ASN:ND2[6_555]	2.15	0.05

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	537/696 (77%)	508 (95%)	20 (4%)	9 (2%)	11	42
1	B	536/696 (77%)	504 (94%)	28 (5%)	4 (1%)	25	60
All	All	1073/1392 (77%)	1012 (94%)	48 (4%)	13 (1%)	15	50

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	663	THR
1	A	724	ASN
1	B	836	PRO
1	A	836	PRO
1	B	592	PHE

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	489/612 (80%)	395 (81%)	94 (19%)	1	7
1	B	487/612 (80%)	397 (82%)	90 (18%)	2	8
All	All	976/1224 (80%)	792 (81%)	184 (19%)	2	8

5 of 184 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	819	LEU

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Mol	Chain	Res	Type
1	B	330	LYS
1	B	846	VAL
1	A	831	ASP
1	A	930	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	922	GLN
1	B	403	GLN
1	B	876	ASN
1	A	941	HIS
1	B	328	HIS

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 ⓘ

2 ligands are 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	3MA	A	1949	-	7,12,12	1.58	1 (14%)	5,17,17	1.73	2 (40%)
2	3MA	B	1950	-	7,12,12	1.43	1 (14%)	5,17,17	1.77	2 (40%)

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	3MA	A	1949	-	-	0/0/0/0	0/2/2/2
2	3MA	B	1950	-	-	0/0/0/0	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1950	3MA	C5-C4	3.12	1.47	1.40
2	A	1949	3MA	C5-C4	3.63	1.48	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1950	3MA	C4-C5-N7	-2.58	106.91	109.41
2	A	1949	3MA	C5-C4-N9	-2.48	105.79	110.68
2	B	1950	3MA	C5-C4-N9	-2.10	106.53	110.68
2	A	1949	3MA	N6-C6-N1	2.26	123.24	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1949	3MA	1	0
2	B	1950	3MA	2	0

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	543/696 (78%)	-0.04	8 (1%) 74 70	34, 77, 136, 142	0
1	B	542/696 (77%)	0.05	11 (2%) 65 63	66, 93, 143, 156	0
All	All	1085/1392 (77%)	0.00	19 (1%) 69 66	34, 85, 138, 156	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	323	PHE	4.4
1	B	298	HIS	3.9
1	A	322	ARG	3.1
1	B	322	ARG	3.1
1	B	690	HIS	2.9

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	3MA	A	1949	11/11	0.92	0.22	-0.83	84,85,87,87	0
2	3MA	B	1950	11/11	0.95	0.20	-1.70	93,93,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.