



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 02:31 PM GMT

PDB ID : 2X6F
Title : THE CRYSTAL STRUCTURE OF THE DROSOPHILA CLASS III PI3-KINASE VPS34 IN COMPLEX WITH 3-METHYLADENINE
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Deposited on : 2010-02-17
Resolution : 3.30 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

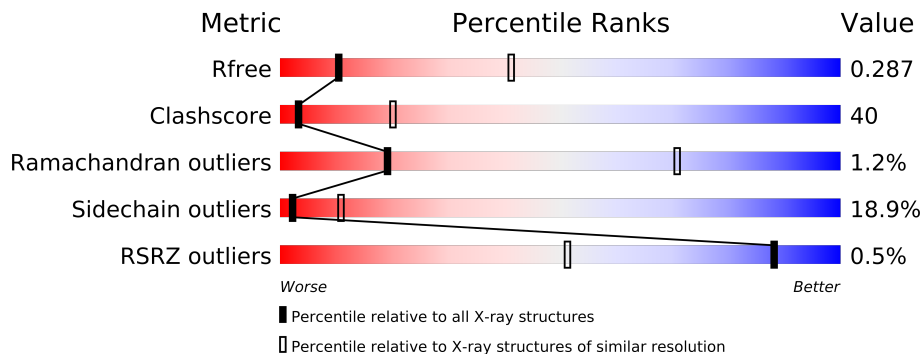
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	696	
1	B	696	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8897 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

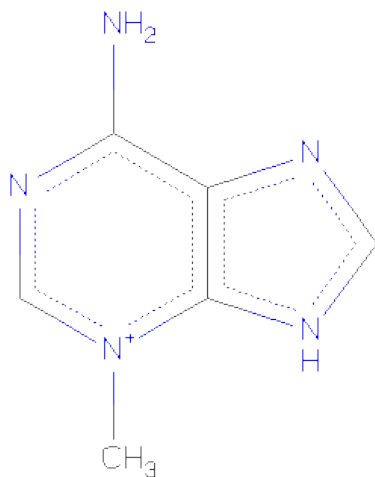
- Molecule 1 is a protein called PHOSPHOTIDYLINOSITOL 3 KINASE 59F.

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

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		

L317	A389	ALA	SER	D574	N645	T730	L800	F882
K320	P390	THR	LEU	H575	N648	F731	L801	M885
F321	SER	SER	PRO	Y576	F649	Y732	G802	V886
E392	GLY	GLY	CYS	A577	M578	K733	V803	D887
L325	ASP	LEU	ASP	M579	I652	V734	R806	T889
S326	SER	HIS	ASN	L580	P653	L735	H807	
S327	ALA	ALA	ASN	K581	F654	A736	N810	E896
H328	L395	ALA	SER	M582	F655	T737	L811	P897
L329	L396	VAL	ASN	K585	L656	S739	L812	D898
L398	Y397	ILE	ALA	L585	D657	K740	L813	K899
L330	L399	PRO	MTT	M586	P658	H741		
K331	Q400	ALA	LEU	L587	Y661	G742	K818	K902
L332	L401	ASN	ALA	E588	P662	F743	L819	
T333	V402	GLN	GLY	M589	T663	L744	F820	E906
K334	Q403	ARG	ILE	O590	K664	Q745	H821	N907
F335	A404	ALA	ILE	N591	I665	Y746	I822	L908
L336	L405	ALA	SER	F592	V666	V747	D823	
	K406	SER	PHE	K595		D748	F824	L912
T339	Y407	VAL	GLY	F598	L672	S749	G825	T913
K342	E408	LEU	SER	Y599	M677	C750	Y826	D914
L343	D409	ALA	VAL	N609	P678	T751	I827	E915
E344	P410	ALA	PRO	L601	M679	V752	L828	E916
T348	H411	ILE	ALA	K602	P679	A753	G829	A917
L351	I413	SER	N532	K603	V685	E754	R830	V913
L354	I414	ASP	L533		T686	V755	D831	Q919
	H417	LYS	F536		S687	A757	P832	
W357	H418	SER	R540		D608	R758	M835	S923
M360	G419	PRO	N544		E610	E759	P836	L924
D361	I420	GLY	A545		L611	T761	P837	L925
V362	F421	SER	T546		V612	V762	P839	D926
E363	PRD	GLU	L547		K613	H763	M839	V927
D364	GLY	ALA	A548		L614	N764	K840	A931
A365	ARG	GLY	N549		V615	F765	L841	V932
L366	ASP	SER	Y550		V618	F766	S842	
E367	VAL	GLY	F551		L703	R767	V846	V937
L368	VAL	SER	Y552		R704	K768	E947	T940
L369	ARG	GLY	W553		Q705	H769	A848	H941
S370	GLY	GLY	Y554		D706			R942
P371	ILE	GLN	L555		Q707	Y777	I852	F943
ASP	GLY	GLY	S556		L708	G778	S853	T944
ASP	LEU	SER	I557		L709	T779	S854	
ASN	ASP	VAL	E558		L710	S780	K862	R948
F373	ALA	ALA	V559		M712	A781		K949
T374	LEU	LEU	E560		T713	E782	Y865	
H375	GLY	PRO	GLU		L714	V783	T866	
P376	ASN	ASN	VAL		L715		A867	
Q377	LEU	PRO	GLU		M716	T786	L871	
V378	LEU	SER	GLU		D717	Y787	N876	
R379	GLN	ALA	VAL		K718	I788	M878	
K380	PRO	PRO	ARG		L719	K789	L879	
Y381	SER	ALA	LYS		L720	S790	N877	
A382	LEU	THR	Q568		Y639	Y794	M879	
V383	SER	PRO	R571		D640	C795	N880	
S384	ASP	GLY	A572		K643	T798	L881	
L385	LEU	SER	H573		V644	Y799		

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 0.239 , 0.287	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 , 42.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 31662 reflections	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.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 40.

The worst 5 of 721 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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%)	14	62
1	B	536/696 (77%)	504 (94%)	28 (5%)	4 (1%)	30	81
All	All	1073/1392 (77%)	1012 (94%)	48 (4%)	13 (1%)	19	71

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%)	2	10
1	B	487/612 (80%)	397 (82%)	90 (18%)	2	11
All	All	976/1224 (80%)	792 (81%)	184 (19%)	2	11

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

Mol	Chain	Res	Type
1	A	819	LEU
1	B	330	LYS
1	B	846	VAL
1	A	831	ASP

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Mol	Chain	Res	Type
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 chains 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	-	12,12,12	1.43	1 (8%)	17,17,17	5.70	2 (11%)
2	3MA	B	1950	-	12,12,12	1.38	2 (16%)	17,17,17	5.53	2 (11%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1949	3MA	C5-C4	3.63	1.48	1.40
2	B	1950	3MA	C5-C4	3.12	1.47	1.40
2	B	1950	3MA	C4-N3	-2.33	1.33	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1949	3MA	N9-C4-N3	23.23	135.05	127.55
2	B	1950	3MA	N9-C4-N3	22.43	134.79	127.55
2	B	1950	3MA	C5-C4-N3	-2.56	118.68	125.05
2	A	1949	3MA	C5-C4-N3	-2.37	119.16	125.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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%)	0.03	3 (0%)	86 46	34, 77, 136, 142	0
1	B	542/696 (77%)	0.03	2 (0%)	90 57	66, 93, 143, 156	0
All	All	1085/1392 (77%)	0.03	5 (0%)	88 51	34, 85, 138, 156	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	322	ARG	3.0
1	A	323	PHE	2.6
1	B	322	ARG	2.5
1	A	346	GLU	2.1
1	B	636	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	3MA	A	1949	11/11	0.29	0.41	84,85,87,87	0
2	3MA	B	1950	11/11	0.27	-0.35	93,93,94,94	0

6.5 Other polymers ⓘ

There are no such residues in this entry.