



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 20, 2016 – 02:07 PM EST

PDB ID : 5FBR
Title : PI4KB in complex with Rab11 and the MI359 Inhibitor
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Deposited on : 2015-12-14
Resolution : 3.28 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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-20028442

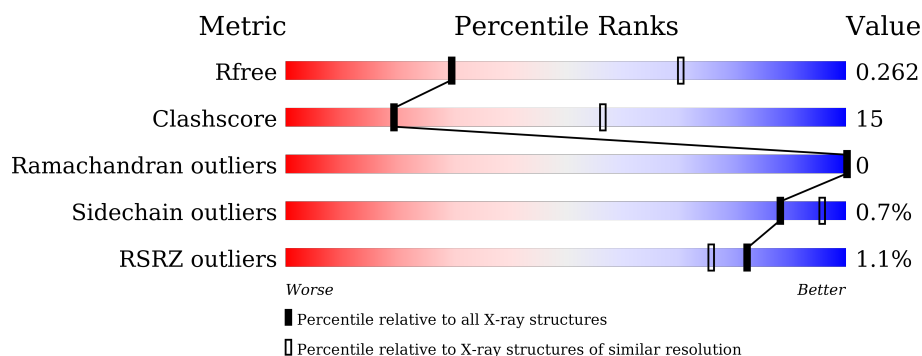
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.28 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}	91344	1756 (3.36-3.20)
Clashscore	102246	1941 (3.36-3.20)
Ramachandran outliers	100387	1905 (3.36-3.20)
Sidechain outliers	100360	1903 (3.36-3.20)
RSRZ outliers	91569	1764 (3.36-3.20)

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. 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	572	<div> <div></div> <div>60%</div> <div>21%</div> <div>19%</div> </div>
2	B	221	<div> <div></div> <div>54%</div> <div>21%</div> <div>•</div> <div>24%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5095 atoms, of which 14 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-kinase beta, Phosphatidylinositol 4-kinase beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	0
			3752	2410	648	670	24			

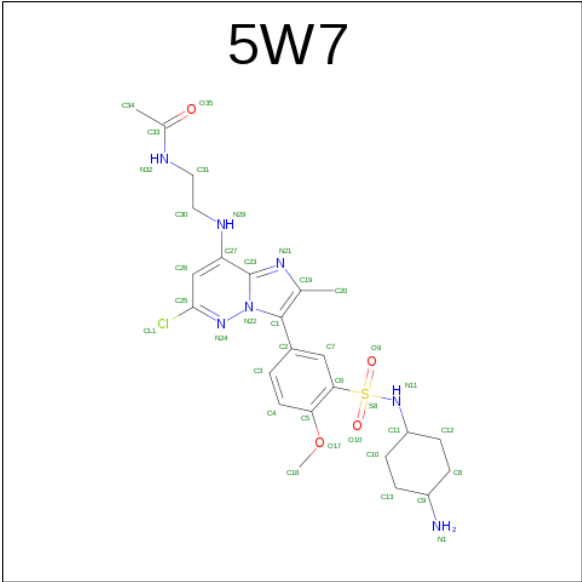
- Molecule 2 is a protein called Ras-related protein Rab-11A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	167	Total	C	N	O	S	0	0	0
			1260	797	214	248	1			

There are 6 discrepancies between the modelled and reference sequences:

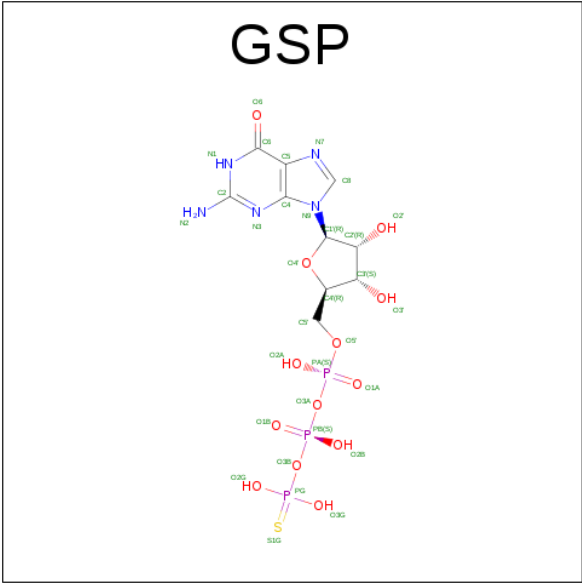
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP P62491
B	-3	ALA	-	expression tag	UNP P62491
B	-2	MET	-	expression tag	UNP P62491
B	-1	GLY	-	expression tag	UNP P62491
B	0	SER	-	expression tag	UNP P62491
B	70	LEU	GLN	engineered mutation	UNP P62491

- Molecule 3 is {N}-[2-[[3-[3-[(4-azanylcyclohexyl)sulfamoyl]-4-methoxy-phenyl]-6-chloranyl-2-methyl-imidazo[1,2-b]pyridazin-8-yl]amino]ethyl]ethanamide (three-letter code: 5W7) (formula: C₂₄H₃₂ClN₇O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
3	A	1	37	24	1	7	4	0	0

- Molecule 4 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: C₁₀H₁₆N₅O₁₃P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
4	B	1	46	10	14	5	13	3	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.27Å 103.94Å 187.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.65 – 3.28 47.65 – 3.28	Depositor EDS
% Data completeness (in resolution range)	96.9 (47.65-3.28) 90.6 (47.65-3.28)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.25Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.225 , 0.264 0.227 , 0.262	Depositor DCC
R_{free} test set	699 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	96.7	Xtrriage
Anisotropy	0.864	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 66.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5095	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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: GSP, 5W7

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	0.25	0/3829	0.47	0/5169
2	B	0.30	0/1278	0.51	0/1737
All	All	0.26	0/5107	0.48	0/6906

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
2	B	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	60	ILE	Mainchain
2	B	9	ASP	Mainchain

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	3752	0	3803	106	0
2	B	1260	0	1214	47	0
3	A	37	0	0	1	0
4	B	32	14	11	8	0
All	All	5081	14	5028	153	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 15.

The worst 5 of 153 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:340:GLU:HA	1:A:343:LEU:HD13	1.44	0.98
1:A:349:PRO:HB3	1:A:364:VAL:HA	1.49	0.94
2:B:76:ILE:H	2:B:76:ILE:HD12	1.39	0.86
2:B:26:ASN:ND2	4:B:301:GSP:O2A	2.10	0.85
1:A:643:THR:HG23	1:A:646:PHE:H	1.44	0.82

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	455/572 (80%)	439 (96%)	16 (4%)	0	100	100
2	B	163/221 (74%)	150 (92%)	13 (8%)	0	100	100
All	All	618/793 (78%)	589 (95%)	29 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	417/517 (81%)	415 (100%)	2 (0%)	92	96
2	B	129/191 (68%)	127 (98%)	2 (2%)	70	89
All	All	546/708 (77%)	542 (99%)	4 (1%)	88	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	343	LEU
1	A	391	CYS
2	B	46	VAL
2	B	78	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	HIS
1	A	577	GLN
1	A	749	GLN

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
3	5W7	A	801	-	36,40,40	2.51	6 (16%)	43,58,58	2.61	9 (20%)
4	GSP	B	301	-	26,34,34	4.84	14 (53%)	24,54,54	3.51	5 (20%)

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
3	5W7	A	801	-	-	0/24/34/34	0/4/4/4
4	GSP	B	301	-	-	0/17/38/38	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	5W7	C6-S8	-11.43	1.60	1.77
4	B	301	GSP	C2'-C3'	-10.77	1.24	1.53
4	B	301	GSP	O4'-C4'	-7.08	1.28	1.45
4	B	301	GSP	C5-C4	-2.02	1.36	1.40
4	B	301	GSP	PG-S1G	2.55	1.95	1.90

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	5W7	O9-S8-O10	-7.99	108.94	119.54
3	A	801	5W7	C11-N11-S8	-7.58	109.85	122.12
3	A	801	5W7	C26-C25-N24	-6.37	120.47	125.05
3	A	801	5W7	C2-C1-N22	-3.97	118.56	123.55
4	B	301	GSP	PB-O3B-PG	-2.83	122.42	132.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	5W7	1	0
4	B	301	GSP	8	0

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 [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	465/572 (81%)	0.19	5 (1%)	82 76	72, 107, 135, 154	0
2	B	167/221 (75%)	0.19	2 (1%)	81 74	95, 122, 154, 171	0
All	All	632/793 (79%)	0.19	7 (1%)	82 76	72, 112, 142, 171	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	708	PHE	3.3
2	B	110	ARG	3.1
1	A	531	VAL	2.7
1	A	630	LEU	2.4
1	A	697	SER	2.4

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
3	5W7	A	801	37/37	0.90	0.30	0.18	91,100,112,141	0
4	GSP	B	301	32/32	0.93	0.19	-0.49	92,103,125,142	0

6.5 Other polymers [i](#)

There are no such residues in this entry.