



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 09:46 AM GMT

PDB ID : 2JDO  
Title : STRUCTURE OF PKB-BETA (AKT2) COMPLEXED WITH ISOQUINOLINE-5-SULFONICACID (2-(2-(4-CHLOROBENZYLOXY)ETHYLAMINO)ETHYL) AMIDE  
Authors : Davies, T.G.; Verdonk, M.L.; Graham, B.; Saalau-Bethell, S.; Hamlett, C.C.F.; Mchardy, T.; Collins, I.; Garrett, M.D.; Workman, P.; Woodhead, S.J.; Jhoti, H.; Barford, D.  
Deposited on : 2007-01-11  
Resolution : 1.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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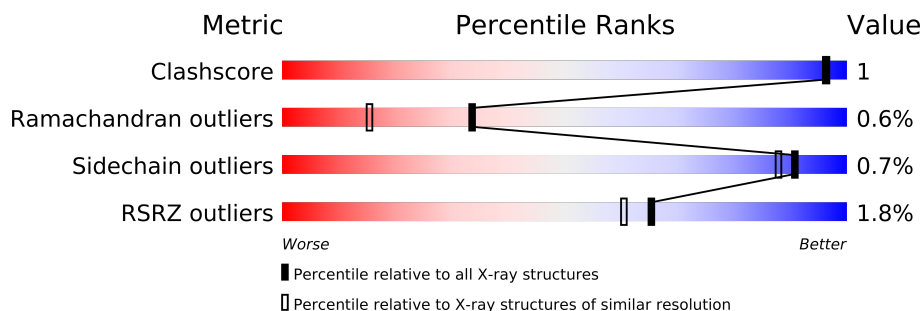
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.80 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))
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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  $\geq 3$ , 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	342	
2	C	10	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	EDO	A	1481	-	X

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 3021 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.

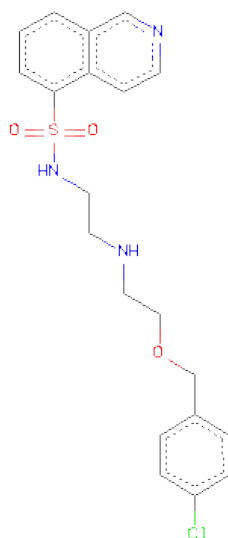
- Molecule 1 is a protein called RAC-BETA SERINE/THREONINE-PROTEINKINASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	315	2587	1662	432	477	1	15	0	0	0

- Molecule 2 is a protein called GLYCOGEN SYNTHASE KINASE-3 BETA.

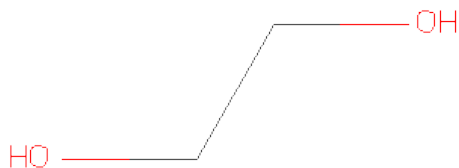
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	10	79	47	16	16	0	0	0

- Molecule 3 is ISOQUINOLINE-5-SULFONICACID (2-(2-(4-CHLOROBENZYLOXY)ETHYLAMINO)ETHYL)AMIDE (three-letter code: I5S) (formula: C<sub>20</sub>H<sub>22</sub>ClN<sub>3</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	N	O	S		
3	A	1	28	20	1	3	3	1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	310	Total	O	0	0
			310	310		
5	C	13	Total	O	0	0
			13	13		

i

- Molecule 1: RAC-BETA SERINE/THREONINE-PROTEINKINASE

GLY				K146		R208	H209	P210	F211		N233		K285		K290		N325		Q353	S447	I448	T449	ILE	THR	PRO	PRO	ASP	ASP	ARG	ASP	TYP	TSP	ASP	SER	LEU	GLY	LEU	LEU	LEU	GLU	GLU	ASP	GLN	ARG	GLU	GLU	GLN	GLU	M469	F470	E471		W479
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Chain C:

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.26Å 60.70Å 132.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.19 – 1.80 55.19 – 1.80	Depositor EDS
% Data completeness (in resolution range)	94.6 (55.19-1.80) 94.6 (55.19-1.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.87 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.175 , 0.210 0.188 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	20.1	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 41.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 32821 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3021	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: TPO, I5S, EDO

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	0.39	0/2635	0.57	0/3548
2	C	0.45	0/80	0.71	0/105
All	All	0.39	0/2715	0.58	0/3653

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2587	0	2547	4	0
2	C	79	0	74	1	0
3	A	28	0	22	1	0
4	A	4	0	6	0	0
5	A	310	0	0	1	0
5	C	13	0	0	0	0
All	All	3021	0	2649	6	0

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 1.

All (6) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:3:GLY:O	2:C:4:ARG:O	2.17	0.62
1:A:290:LYS:NZ	5:A:2148:HOH:O	2.34	0.60
1:A:209:HIS:HD2	1:A:211:PHE:H	1.58	0.50
1:A:209:HIS:CD2	1:A:211:PHE:H	2.31	0.49
1:A:233:ASN:OD1	1:A:285:LYS:HA	2.19	0.43
3:A:1480:I5S:O17	3:A:1480:I5S:H27	2.21	0.41

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	310/342 (91%)	302 (97%)	7 (2%)	1 (0%)	50	31
2	C	8/10 (80%)	7 (88%)	0	1 (12%)	1	0
All	All	318/352 (90%)	309 (97%)	7 (2%)	2 (1%)	33	15

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	4	ARG
1	A	325	ASN

### 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	276/300 (92%)	274 (99%)	2 (1%)	91	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	8/8 (100%)	8 (100%)	0	100	100
All	All	284/308 (92%)	282 (99%)	2 (1%)	91	88

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	ARG
1	A	353	GLN

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	209	HIS
1	A	419	GLN
1	A	446	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue 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
1	TPO	A	309	1	10,10,11	6.14	4 (40%)	12,14,16	1.47	2 (16%)

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
1	TPO	A	309	1	-	0/9/11/13	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	309	TPO	O-C	18.91	1.24	1.11
1	A	309	TPO	P-O1P	2.18	1.58	1.51
1	A	309	TPO	CA-C	2.15	1.52	1.48
1	A	309	TPO	OG1-CB	-2.14	1.41	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	TPO	OG1-CB-CG2	-3.35	104.53	110.13
1	A	309	TPO	CG2-CB-CA	-2.48	108.12	113.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	I5S	A	1480	-	30,30,30	0.83	1 (3%)	40,40,40	0.69	2 (5%)
4	EDO	A	1481	-	3,3,3	0.52	0	2,2,2	0.25	0

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	I5S	A	1480	-	-	0/18/18/18	0/1/3/3
4	EDO	A	1481	-	-	0/1/1/1	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1480	I5S	S16-N15	2.40	1.64	1.61

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1480	I5S	C20-C19-C28	-2.28	118.91	121.00
3	A	1480	I5S	C19-C28-C23	2.08	119.48	117.47

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	315/342 (92%)	-0.15	5 (1%) 68 64	11, 22, 40, 59	0
2	C	10/10 (100%)	0.44	1 (10%) 8 5	23, 28, 46, 46	0
All	All	325/352 (92%)	-0.13	6 (1%) 65 60	11, 22, 41, 59	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	3	GLY	5.0
1	A	448	ILE	4.3
1	A	447	SER	4.2
1	A	471	GLU	4.0
1	A	469	MET	2.9
1	A	449	THR	2.1

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

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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
1	TPO	A	309	11/12	0.10	-0.18	16,19,27,30	0

### 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
4	EDO	A	1481	4/4	0.16	5.38	26,30,30,31	0
3	I5S	A	1480	28/28	0.11	0.61	19,27,31,37	0

## 6.5 Other polymers

There are no such residues in this entry.