



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2017 – 06:06 PM EDT

PDB ID : 3FYJ
Title : Crystal structure of an optimzied benzothiophene inhibitor bound to MAP-KAP Kinase-2 (MK-2)
Authors : Kurumbail, R.G.; Caspers, N.
Deposited on : unknown
Resolution : 3.80 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-20030345
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-20030345

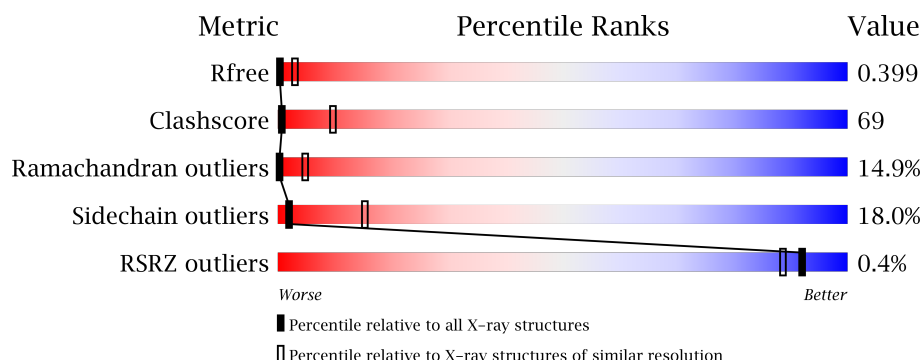
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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))
R_{free}	100719	1019 (4.08-3.52)
Clashscore	112137	1030 (4.04-3.56)
Ramachandran outliers	110173	1011 (4.06-3.54)
Sidechain outliers	110143	1005 (4.06-3.54)
RSRZ outliers	101464	1032 (4.08-3.52)

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	X	327	<div> <div style="width: 16%; background-color: green;"></div> <div style="width: 50%; background-color: yellow;"></div> <div style="width: 20%; background-color: orange;"></div> <div style="width: 14%; background-color: grey;"></div> </div> <div>16% 50% 20% 14%</div>

2 Entry composition [i](#)

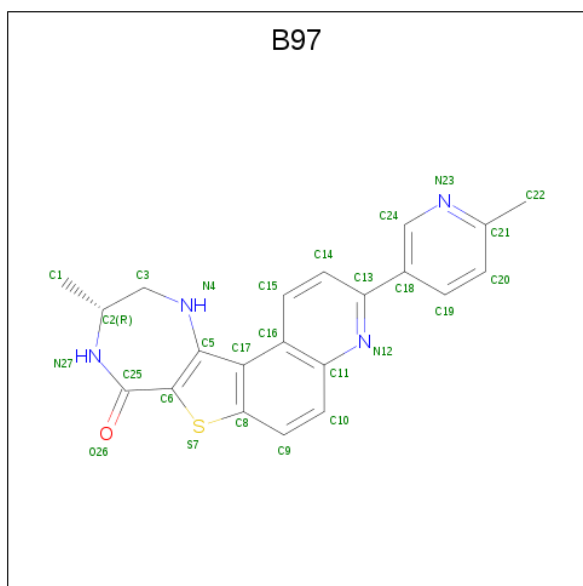
There are 2 unique types of molecules in this entry. The entry contains 2325 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MAP kinase-activated protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	282	Total	C	N	O	S	0	0	0
			2298	1462	396	423	17			

- Molecule 2 is (10R)-10-methyl-3-(6-methylpyridin-3-yl)-9,10,11,12-tetrahydro-8H-[1,4]diazepino[5',6':4,5]thieno[3,2-f]quinolin-8-one (three-letter code: B97) (formula: C₂₁H₁₈N₄OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	X	1	Total	C	N	O	S	0	0
			27	21	4	1	1		

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.

- Chain X: 16% 50% 20% 14%

T362	V294	GLU	A173	Q45
M363	S295	VAL	I174	F46
R364	E296	LEU	Q175	H47
VAL	E297	GLY	Y176	V48
ASP	V298	PRO	L177	K49
TYR	K299	GLU	H178	L52
GLU	M300	K299	S179	Q53
GLN	L301	Y240	I180	I118
ILE	R302	D241	N181	I120
LYS	I303	K242	I182	V121
	N304	S243	A183	
	L305		H184	A58
	L306	M246	R185	L59
	K307	W247	D186	I60
	T308	S248	V187	D61
	E309	L249	K188	L127
	P310	G250	P189	V63
	T311	V251	E190	K64
	R312	L252	N191	V65
	R313	M253	L192	T66
	M314	Y254	L193	
	T315	L255	Y194	V69
	L316	L256	T195	L70
	T317	L257	S196	G71
	E318	G258	K197	
	F319	G259	R198	L74
	M320	Y260	P199	
		P261	N200	K77
	E323	P262	A201	V78
	W324	F263	L202	L79
	I325	Y264	K203	Q80
	M326	S265	L204	L81
	Q327	ASN	L205	F82
	S328	HIS	T206	N83
	T329	GLY	D207	K84
	K330	LEU	F208	R85
	V331	ALA	G209	T86
	Q332	ILE	F210	Q87
	Q333	SER	A211	E88
		PRO	K212	K89
	H337	GLY	E213	F90
	T338	MET	T214	A91
		LYS	T215	L92
	V341	THR	S216	K93
	E344	ARG	HIS	
		ILE	ASN	Q96
	W349	ARG	SER	D97
	E350	MET	LEU	C98
	D351	G252	THR	P99
	V352	Y284	PRO	K100
	K353	E285	CYS	A101
	E354	F286	TVR	R102
	E355	P287	THR	L103
	M356	M288	PRO	E104
	T357	P289	TVR	V105
	S358	E290	TVR	E106
	A359	W291	ALA	L107
	L360	S292	ALA	H108
	I361	E293	PRO	W109
				R110
				L111

4 Data and refinement statistics

Property	Value	Source
Space group	F 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	255.55Å 255.55Å 255.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.51 – 3.80 29.51 – 3.80	Depositor EDS
% Data completeness (in resolution range)	85.1 (29.51-3.80) 85.5 (29.51-3.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.12 (at 3.75Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.328 , 0.388 0.327 , 0.399	Depositor DCC
R_{free} test set	294 reflections (4.83%)	DCC
Wilson B-factor (Å ²)	129.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	2325	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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: B97

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	X	0.56	0/2344	0.72	1/3157 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	X	134	LEU	CA-CB-CG	-5.21	103.31	115.30

There are no chirality outliers.

There are no planarity outliers.

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	X	2298	0	2315	321	0
2	X	27	0	18	6	0
All	All	2325	0	2333	322	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 69.

The worst 5 of 322 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:X:108:HIS:CE1	1:X:208:PHE:CD1	2.37	1.11
1:X:196:SER:OG	1:X:198:ARG:HG2	1.60	1.01
1:X:188:LYS:HB3	1:X:190:GLU:OE2	1.60	0.99
1:X:184:HIS:HD2	1:X:205:LEU:HD21	1.25	0.99
1:X:288:ASN:HB2	1:X:289:PRO:HD3	1.43	0.97

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	X	276/327 (84%)	156 (56%)	79 (29%)	41 (15%)	0 5

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	74	ILE
1	X	146	LEU
1	X	187	VAL
1	X	262	PRO
1	X	263	PHE

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	X	256/296 (86%)	210 (82%)	46 (18%)	2 15

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	151	GLN
1	X	206	THR
1	X	354	GLU
1	X	155	ASP
1	X	182	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	X	96	GLN
1	X	327	GLN
1	X	126	ASN
1	X	57	ASN
1	X	304	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	B97	X	372	-	26,31,31	1.56	5 (19%)	29,46,46	1.26	4 (13%)

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	B97	X	372	-	-	0/4/17/17	0/4/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	372	B97	C10-C11	-2.80	1.36	1.41
2	X	372	B97	C9-C8	-2.12	1.37	1.40
2	X	372	B97	C18-C13	-2.05	1.45	1.48
2	X	372	B97	C5-C17	2.12	1.44	1.41
2	X	372	B97	C25-N27	4.71	1.37	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	372	B97	C14-C13-C18	-2.05	117.88	121.94
2	X	372	B97	C15-C16-C17	-2.04	120.02	123.18
2	X	372	B97	C18-C13-N12	2.24	120.52	117.15
2	X	372	B97	C17-C16-C11	3.90	123.04	118.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	X	372	B97	6	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	X	282/327 (86%)	-0.23	1 (0%) 92 88	80, 80, 80, 80	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	239	LYS	2.6

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(Å ²)	Q<0.9
2	B97	X	372	27/27	0.83	0.31	0.36	80,80,80,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.