



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 09:17 PM GMT

PDB ID : 4E5B  
Title : Structure of p38a MAP kinase without BOG  
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Deposited on : 2012-03-14  
Resolution : 2.00 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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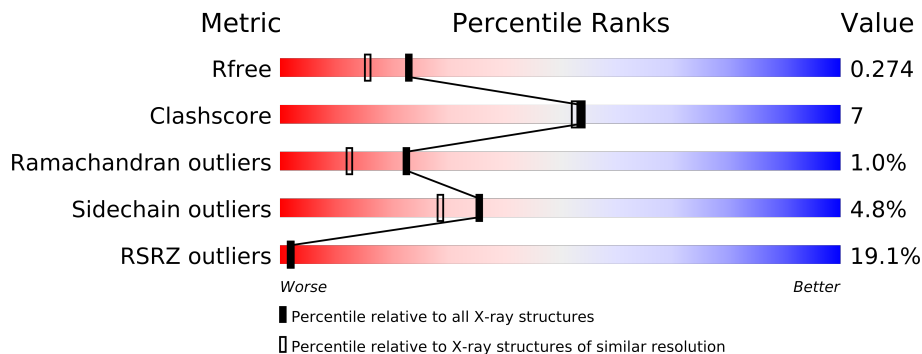
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.00 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	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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	360	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2704 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 Mitogen-activated protein kinase 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2628	1687	449	481	11			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	76	Total	O	0	0
			76	76		

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- Molecule 1: Mitogen-activated protein kinase 14

Protein	Residue	Score	Category
Protein A	1346	0.85	High
	351	0.75	High
	PRO	0.65	High
	LEU	0.55	High
	ASP	0.45	High
	GLN	0.35	High
	GLU	0.25	High
	GLU	0.15	High
	MET	0.05	High
	SER	0.00	High
Protein B	209	0.80	High
	210	0.70	High
	213	0.60	High
	221	0.50	High
	232	0.40	High
	236	0.30	High
	242	0.20	High
	243	0.10	High
	247	0.00	High
	248	0.00	High
Protein C	249	0.80	High
	250	0.70	High
	251	0.60	High
	252	0.50	High
	256	0.40	High
	259	0.30	High
	260	0.20	High
	261	0.10	High
	262	0.00	High
	263	0.00	High
Protein D	264	0.80	High
	265	0.70	High
	266	0.60	High
	267	0.50	High
	268	0.40	High
	269	0.30	High
	284	0.20	High
	288	0.10	High
	298	0.00	High
	301	0.00	High
Protein E	310	0.80	High
	313	0.70	High
	314	0.60	High
	321	0.50	High
	322	0.40	High
	323	0.30	High
	329	0.20	High
	330	0.10	High
	331	0.00	High
	334	0.00	High
Protein F	335	0.80	High
	336	0.70	High
	337	0.60	High
	338	0.50	High
	339	0.40	High
	340	0.30	High
	341	0.20	High
	342	0.10	High
	343	0.00	High
	344	0.00	High
Protein G	345	0.80	High
	346	0.70	High
	347	0.60	High
	348	0.50	High
	349	0.40	High
	350	0.30	High
	351	0.20	High
	352	0.10	High
	353	0.00	High
	354	0.00	High
Protein H	355	0.80	High
	356	0.70	High
	357	0.60	High
	358	0.50	High
	359	0.40	High
	360	0.30	High
	361	0.20	High
	362	0.10	High
	363	0.00	High
	364	0.00	High
Protein I	365	0.80	High
	366	0.70	High
	367	0.60	High
	368	0.50	High
	369	0.40	High
	370	0.30	High
	371	0.20	High
	372	0.10	High
	373	0.00	High
	374	0.00	High
Protein J	375	0.80	High
	376	0.70	High
	377	0.60	High
	378	0.50	High
	379	0.40	High
	380	0.30	High
	381	0.20	High
	382	0.10	High
	383	0.00	High
	384	0.00	High
Protein K	385	0.80	High
	386	0.70	High
	387	0.60	High
	388	0.50	High
	389	0.40	High
	390	0.30	High
	391	0.20	High
	392	0.10	High
	393	0.00	High
	394	0.00	High
Protein L	395	0.80	High
	396	0.70	High
	397	0.60	High
	398	0.50	High
	399	0.40	High
	400	0.30	High
	401	0.20	High
	402	0.10	High
	403	0.00	High
	404	0.00	High
Protein M	405	0.80	High
	406	0.70	High
	407	0.60	High
	408	0.50	High
	409	0.40	High
	410	0.30	High
	411	0.20	High
	412	0.10	High
	413	0.00	High
	414	0.00	High
Protein N	415	0.80	High
	416	0.70	High
	417	0.60	High
	418	0.50	High
	419	0.40	High
	420	0.30	High
	421	0.20	High
	422	0.10	High
	423	0.00	High

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.09Å 74.04Å 74.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.41 – 2.00 33.13 – 1.99	Depositor EDS
% Data completeness (in resolution range)	97.1 (52.41-2.00) 97.0 (33.13-1.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.234 , 0.279 0.233 , 0.274	Depositor DCC
$R_{free}$ test set	1283 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.1	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 54.0	EDS
Estimated twinning fraction	0.027 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 25206 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2704	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.15% 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 ⓘ

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	0.71	0/2686	0.78	1/3640 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	335	ASP	CB-CG-OD1	5.32	123.09	118.30

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	2628	0	2623	36	0
2	A	76	0	0	2	0
All	All	2704	0	2623	36	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 7.

All (36) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:186:ARG:HD2	1:A:186:ARG:C	1.96	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:126:HIS:HE1	1:A:162:CYS:SG	2.06	0.79
1:A:148:HIS:O	1:A:149:ARG:HB2	1.94	0.67
1:A:195:LEU:HD13	1:A:197:TRP:CZ2	2.32	0.64
1:A:256:ARG:O	1:A:260:GLN:HG2	1.98	0.62
1:A:13:LEU:HD22	1:A:29:PRO:HG2	1.81	0.62
1:A:49:ARG:HG2	1:A:108:LEU:HD23	1.83	0.60
1:A:267:LYS:HE3	2:A:473:HOH:O	2.02	0.60
1:A:30:VAL:HG12	1:A:30:VAL:O	2.02	0.59
1:A:232:LEU:HD22	1:A:236:LEU:HG	1.86	0.57
1:A:242:PRO:HG2	1:A:259:ILE:HG21	1.86	0.57
1:A:59:PHE:CD2	1:A:338:LYS:HE2	2.41	0.56
1:A:62:ILE:HG13	1:A:334:ILE:HG13	1.88	0.54
1:A:169:PHE:HD2	1:A:169:PHE:N	2.06	0.54
1:A:61:SER:HA	1:A:334:ILE:HD11	1.91	0.53
1:A:169:PHE:CD2	1:A:169:PHE:N	2.77	0.52
1:A:160:GLU:C	1:A:162:CYS:H	2.13	0.51
1:A:321:ASP:HB3	1:A:322:PRO:HD2	1.92	0.51
1:A:242:PRO:HB2	1:A:247:LEU:HD13	1.92	0.51
1:A:126:HIS:CE1	1:A:162:CYS:SG	2.96	0.51
1:A:195:LEU:HD22	1:A:259:ILE:HD11	1.93	0.49
1:A:187:TRP:CE3	1:A:221:THR:HG21	2.49	0.47
1:A:5:ARG:NH2	1:A:92:PRO:O	2.47	0.47
1:A:201:ASN:HB3	1:A:203:THR:H	1.81	0.46
1:A:186:ARG:HD2	1:A:187:TRP:N	2.29	0.46
1:A:247:LEU:HD12	1:A:250:ILE:HD12	1.99	0.45
1:A:310:GLN:HG2	2:A:441:HOH:O	2.16	0.44
1:A:298:THR:H	1:A:301:GLN:HE21	1.67	0.43
1:A:168:ASP:O	1:A:168:ASP:CG	2.57	0.42
1:A:157:ALA:HB2	1:A:167:LEU:HD11	2.02	0.41
1:A:250:ILE:HG22	1:A:256:ARG:HG3	2.02	0.41
1:A:247:LEU:HD12	1:A:247:LEU:HA	1.95	0.41
1:A:204:VAL:HG23	1:A:205:ASP:N	2.36	0.41
1:A:57:ARG:HD3	1:A:60:GLN:OE1	2.20	0.40
1:A:146:ILE:HD11	1:A:323:TYR:CD2	2.56	0.40
1:A:262:LEU:HA	1:A:262:LEU:HD23	1.84	0.40

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	314/360 (87%)	296 (94%)	15 (5%)	3 (1%)	22 12

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	GLY
1	A	161	ASP
1	A	168	ASP

### 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	289/320 (90%)	275 (95%)	14 (5%)	35 28

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	13	LEU
1	A	49	ARG
1	A	57	ARG
1	A	74	LEU
1	A	115	ASN
1	A	168	ASP
1	A	169	PHE
1	A	186	ARG
1	A	232	LEU
1	A	247	LEU

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Mol	Chain	Res	Type
1	A	251	SER
1	A	259	ILE
1	A	269	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	114	ASN
1	A	126	HIS
1	A	201	ASN
1	A	264	GLN
1	A	269	ASN
1	A	272	ASN
1	A	301	GLN

### 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 ⓘ

There are no ligands in this entry.

### 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	324/360 (90%)	1.11	62 (19%) 2 2	36, 52, 75, 86	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	32	SER	9.0
1	A	261	SER	8.0
1	A	31	GLY	5.2
1	A	266	PRO	4.7
1	A	30	VAL	4.3
1	A	138	LEU	4.3
1	A	263	THR	4.1
1	A	268	MET	4.1
1	A	265	MET	4.0
1	A	13	LEU	3.9
1	A	162	CYS	3.9
1	A	15	LYS	3.9
1	A	206	ILE	3.8
1	A	200	TYR	3.8
1	A	120	GLN	3.7
1	A	160	GLU	3.6
1	A	111	ALA	3.5
1	A	243	GLY	3.4
1	A	199	HIS	3.2
1	A	313	ASP	3.1
1	A	97	GLU	3.1
1	A	260	GLN	3.0
1	A	161	ASP	3.0
1	A	168	ASP	3.0
1	A	95	SER	3.0
1	A	36	GLY	2.9
1	A	262	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	12	GLU	2.8
1	A	267	LYS	2.8
1	A	96	LEU	2.8
1	A	112	ASP	2.8
1	A	166	ILE	2.8
1	A	4	GLU	2.8
1	A	314	PRO	2.7
1	A	135	LEU	2.7
1	A	284	LEU	2.7
1	A	288	MET	2.6
1	A	209	VAL	2.6
1	A	24	TYR	2.6
1	A	131	ILE	2.6
1	A	210	GLY	2.5
1	A	20	VAL	2.5
1	A	329	SER	2.5
1	A	259	ILE	2.5
1	A	75	LEU	2.4
1	A	331	ASP	2.3
1	A	134	ILE	2.3
1	A	5	ARG	2.2
1	A	52	VAL	2.2
1	A	346	ILE	2.2
1	A	252	SER	2.2
1	A	186	ARG	2.2
1	A	113	LEU	2.2
1	A	94	ARG	2.1
1	A	213	MET	2.1
1	A	248	LYS	2.1
1	A	247	LEU	2.1
1	A	204	VAL	2.1
1	A	10	ARG	2.1
1	A	207	TRP	2.1
1	A	264	GLN	2.0
1	A	103	TYR	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 ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.