



# Full wwPDB X-ray Structure Validation Report

Sep 26, 2014 – 12:10 AM EDT

PDB ID : 4U43  
Title : MAP4K4 in complex with inhibitor (compound 6)  
Authors : Harris, S.F.; Wu, P.; Coons, M.  
Deposited on : 2014-07-23  
Resolution : 2.18 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>

---

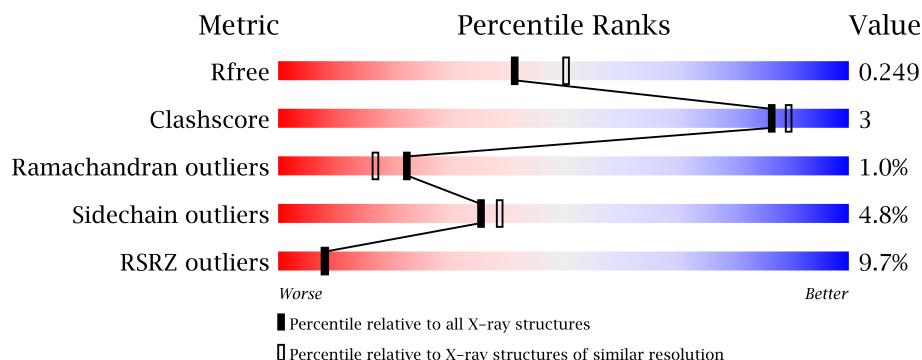
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23828  
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) : stable23828

# 1 Overall quality at a glance

The reported resolution of this entry is 2.18 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	3841 (2.20-2.16)
Clashscore	79885	4835 (2.20-2.16)
Ramachandran outliers	78287	4740 (2.20-2.16)
Sidechain outliers	78261	4741 (2.20-2.16)
RSRZ outliers	66119	3842 (2.20-2.16)

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	332	
1	B	332	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	3D8	A	401	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4999 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.

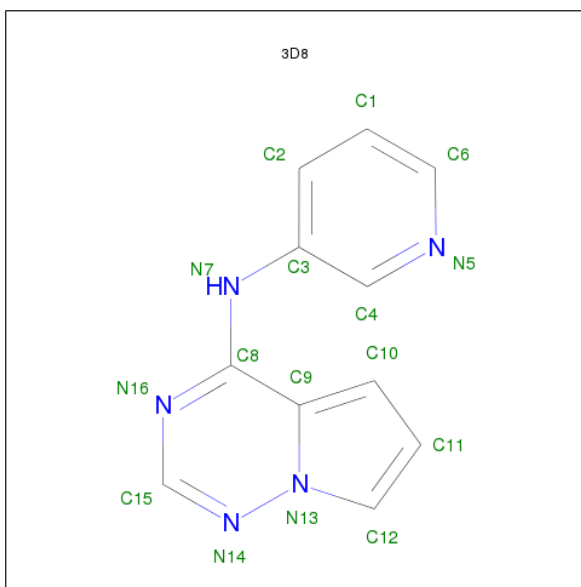
- Molecule 1 is a protein called Mitogen-activated protein kinase kinase kinase kinase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	1	0
			2329	1484	411	421	13			
1	B	302	Total	C	N	O	S	0	1	0
			2446	1555	435	443	13			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP O95819
A	1	SER	-	expression tag	UNP O95819
A	329	GLY	-	expression tag	UNP O95819
A	330	ASN	-	expression tag	UNP O95819
A	331	SER	-	expression tag	UNP O95819
B	0	GLY	-	expression tag	UNP O95819
B	1	SER	-	expression tag	UNP O95819
B	329	GLY	-	expression tag	UNP O95819
B	330	ASN	-	expression tag	UNP O95819
B	331	SER	-	expression tag	UNP O95819

- Molecule 2 is N-(pyridin-3-yl)pyrrolo[2,1-f][1,2,4]triazin-4-amine (three-letter code: 3D8) (formula: C<sub>11</sub>H<sub>9</sub>N<sub>5</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C N	0	0
			16	11 5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	87	Total	O	0	0
			87	87		
3	B	121	Total	O	0	0
			121	121		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.49Å 80.64Å 102.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.08 – 2.18 28.43 – 2.18	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.08-2.18) 99.9 (28.43-2.18)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.99 (at 2.18Å)	Xtriage
Refinement program	BUSTER 2.9.1	Depositor
R, $R_{free}$	0.196 , 0.242 0.202 , 0.249	Depositor DCC
$R_{free}$ test set	1703 reflections (5.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.7	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 50.6	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 33223 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4999	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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: 3D8

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	0.46	0/2385	0.68	0/3224
1	B	0.47	0/2504	0.69	0/3387
All	All	0.47	0/4889	0.68	0/6611

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	2329	0	2325	12	0
1	B	2446	0	2446	17	0
2	A	16	0	0	0	0
3	A	87	0	0	0	0
3	B	121	0	0	0	0
All	All	4999	0	4771	25	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 3.

All (25) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:189:ILE:O	1:B:189:ILE:O	2.11	0.69
1:A:38:GLN:HG3	1:B:36:TYR:HB3	1.79	0.65
1:B:75:LYS:HE3	1:B:76:TYR:H	1.66	0.61
1:B:62:GLU:O	1:B:66:ILE:HG12	2.04	0.57
1:B:173:GLY:HA3	1:B:178:LEU:HD12	1.91	0.53
1:B:132:TYR:HA	1:B:292:GLN:HE22	1.74	0.52
1:A:132:TYR:HA	1:A:292:GLN:HE22	1.76	0.51
1:A:77:SER:HB3	1:A:84:THR:HA	1.91	0.51
1:A:35:THR:HA	1:A:36:TYR:C	2.32	0.50
1:B:184:ARG:HH21	1:B:186:ASN:HD21	1.62	0.48
1:A:243:PHE:O	1:A:247[B]:ARG:HD2	2.14	0.47
1:A:189:ILE:HG13	1:B:238:PRO:HB2	1.96	0.47
1:A:192:PRO:HB3	1:A:242:LEU:HD13	1.97	0.47
1:A:295:GLU:HA	1:A:298:VAL:HG22	1.96	0.46
1:B:251:PRO:HD2	1:B:270:LEU:HD13	1.98	0.45
1:A:251:PRO:HD2	1:A:270:LEU:HD13	1.98	0.45
1:B:78[A]:HIS:CD2	1:B:84:THR:OG1	2.70	0.45
1:A:189:ILE:HD13	1:B:242:LEU:HD22	2.00	0.44
1:B:75:LYS:HA	1:B:75:LYS:HD2	1.64	0.44
1:B:18:LEU:HD11	1:B:90:ILE:HG12	1.99	0.44
1:A:151:HIS:CD2	1:A:172:PHE:HB3	2.53	0.43
1:B:192:PRO:HB3	1:B:242:LEU:HD13	2.00	0.43
1:B:78[A]:HIS:CG	1:B:79:HIS:N	2.85	0.42

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	284/332 (86%)	274 (96%)	7 (2%)	3 (1%)	21	15
1	B	301/332 (91%)	282 (94%)	16 (5%)	3 (1%)	22	17

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	585/664 (88%)	556 (95%)	23 (4%)	6 (1%)	22	17

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	GLU
1	B	208	ALA
1	A	35	THR
1	A	62	GLU
1	B	177	GLN
1	B	182	VAL

### 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	254/290 (88%)	240 (94%)	14 (6%)	30	32
1	B	267/290 (92%)	256 (96%)	11 (4%)	41	47
All	All	521/580 (90%)	496 (95%)	25 (5%)	35	39

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	36	TYR
1	A	49	GLN
1	A	63	GLU
1	A	66	ILE
1	A	105	MET
1	A	157	GLN
1	A	163	GLU
1	A	207	ASP
1	A	213	ARG
1	A	235	ASP
1	A	236	MET
1	A	260	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	295	GLU
1	B	33	ASN
1	B	38	GLN
1	B	56	MET
1	B	60	GLU
1	B	75	LYS
1	B	80	ARG
1	B	118	LYS
1	B	146	ILE
1	B	184	ARG
1	B	295	GLU
1	B	308	ARG

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	81	ASN
1	A	186	ASN
1	A	292	GLN
1	A	301	GLN
1	B	81	ASN
1	B	186	ASN
1	B	237	HIS
1	B	292	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 ⓘ

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	3D8	A	401	-	18,18,18	3.92	12 (66%)	22,24,24	4.24	12 (54%)

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	3D8	A	401	-	-	0/4/4/4	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	3D8	C8-N16	7.67	1.45	1.34
2	A	401	3D8	C2-C3	7.46	1.51	1.39
2	A	401	3D8	C15-N16	5.20	1.44	1.33
2	A	401	3D8	N14-N13	4.97	1.43	1.36
2	A	401	3D8	C8-N7	4.19	1.44	1.36
2	A	401	3D8	C12-N13	-4.11	1.31	1.37
2	A	401	3D8	C4-N5	4.00	1.43	1.34
2	A	401	3D8	C12-C11	3.48	1.42	1.37
2	A	401	3D8	C6-N5	3.27	1.43	1.33
2	A	401	3D8	C4-C3	3.18	1.45	1.39
2	A	401	3D8	C1-C2	2.98	1.45	1.38
2	A	401	3D8	C9-N13	2.47	1.43	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	3D8	C15-N16-C8	10.70	124.72	116.50
2	A	401	3D8	C11-C12-N13	9.25	112.17	106.77

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	3D8	C12-N13-N14	7.67	129.38	125.61
2	A	401	3D8	N14-C15-N16	-6.39	117.79	128.64
2	A	401	3D8	C6-N5-C4	4.85	125.59	116.86
2	A	401	3D8	C9-C8-N7	3.88	123.08	119.62
2	A	401	3D8	C3-C4-N5	-3.21	116.66	123.30
2	A	401	3D8	N7-C8-N16	3.07	121.96	118.96
2	A	401	3D8	C1-C2-C3	2.43	122.84	119.72
2	A	401	3D8	C10-C9-N13	-2.42	106.31	117.30
2	A	401	3D8	C2-C3-N7	2.10	127.40	120.67
2	A	401	3D8	C3-N7-C8	-2.03	124.68	128.65

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	287/332 (86%)	0.54	34 (11%) 5 5	31, 58, 103, 132	0
1	B	302/332 (90%)	0.25	23 (7%) 14 14	30, 50, 90, 124	0
All	All	589/664 (88%)	0.39	57 (9%) 8 8	30, 53, 98, 132	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	LEU	7.9
1	A	174	VAL	6.4
1	A	15	LEU	5.8
1	A	36	TYR	5.5
1	B	94	PRO	5.3
1	A	66	ILE	5.1
1	B	186	ASN	4.8
1	A	14	ASP	4.7
1	A	35	THR	4.5
1	A	306	ILE	4.1
1	A	16	SER	4.1
1	A	60	GLU	4.1
1	B	185	ARG	3.8
1	A	59	THR	3.8
1	B	11	VAL	3.7
1	B	310	ARG	3.6
1	A	61	ASP	3.5
1	B	95	PRO	3.5
1	A	63	GLU	3.4
1	B	308	ARG	3.3
1	B	182	VAL	3.3
1	B	204	GLU	3.3
1	A	23	GLY	3.3
1	A	188	PHE	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	64	GLU	3.2
1	A	310	ARG	3.1
1	B	296	ARG	3.1
1	A	58	VAL	3.0
1	B	97	HIS	3.0
1	A	67	LYS	2.7
1	B	180	ARG	2.6
1	B	33	ASN	2.6
1	A	207	ASP	2.5
1	B	188	PHE	2.4
1	A	34	GLY	2.4
1	B	181	THR	2.4
1	B	159	VAL	2.4
1	A	62	GLU	2.4
1	A	72	MET	2.4
1	B	184	ARG	2.3
1	A	293	PRO	2.3
1	B	96	GLY	2.3
1	A	65	GLU	2.3
1	B	207	ASP	2.3
1	B	167	VAL	2.2
1	A	172	PHE	2.2
1	A	82	ILE	2.2
1	A	296	ARG	2.2
1	B	93	SER	2.2
1	A	17	SER	2.2
1	B	133	ILE	2.1
1	A	186	ASN	2.1
1	A	311	LYS	2.1
1	B	113	ILE	2.1
1	A	105	MET	2.0
1	A	294	ASN	2.0
1	A	95	PRO	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, 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
2	3D8	A	401	16/16	0.12	-0.26	42,46,50,50	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.