



Full wwPDB X-ray Structure Validation Report

Sep 25, 2014 – 06:21 PM EDT

PDB ID : 4U45
Title : MAP4K4 in complex with inhibitor (compound 25)
Authors : Harris, S.F.; Wu, P.; Coons, M.
Deposited on : 2014-07-23
Resolution : 2.58 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

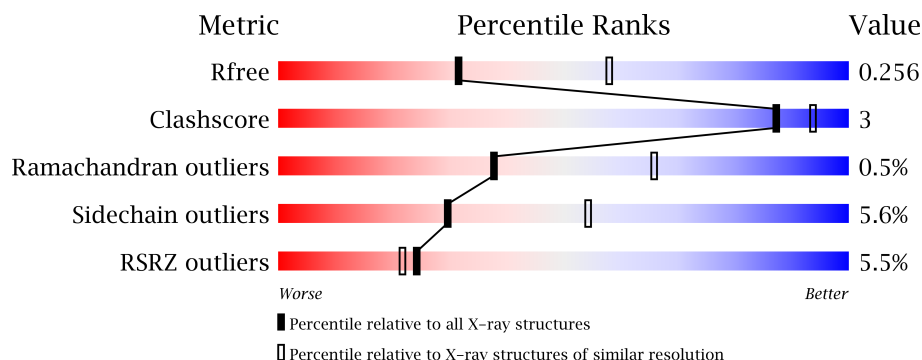
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.58 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	1891 (2.60-2.56)
Clashscore	79885	2358 (2.60-2.56)
Ramachandran outliers	78287	2316 (2.60-2.56)
Sidechain outliers	78261	2316 (2.60-2.56)
RSRZ outliers	66119	1891 (2.60-2.56)

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. 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	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4961 atoms, of which 1 is 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	289	Total	C	N	O	S	0	0	0
			2331	1486	407	425	13			
1	B	295	Total	C	N	O	S	0	1	0
			2388	1518	425	431	14			

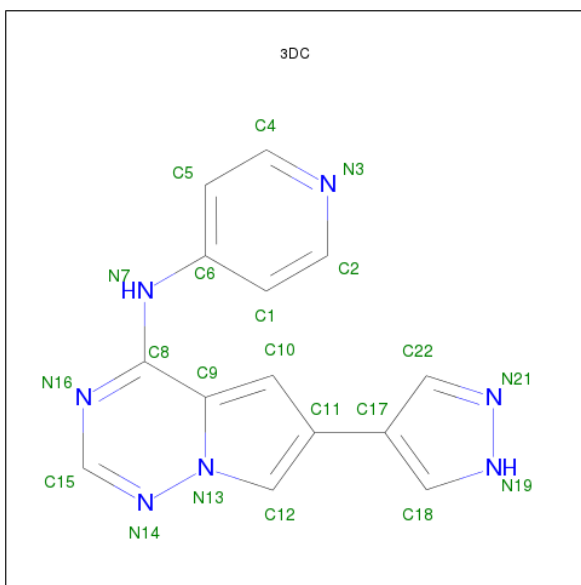
There are 10 discrepancies between the modelled and reference sequences:

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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

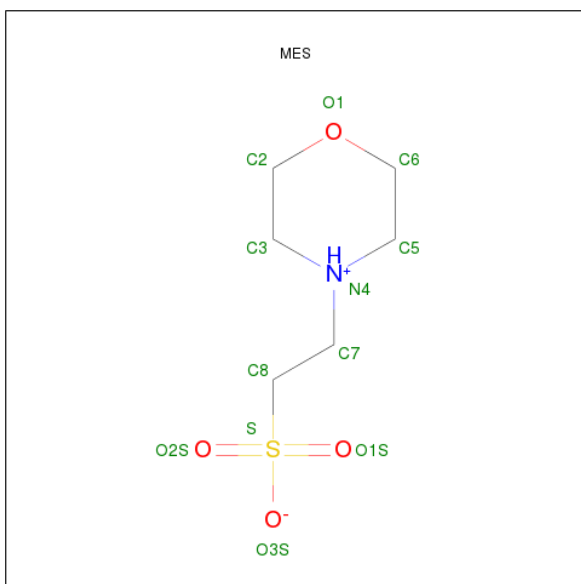
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is 6-(1H-pyrazol-4-yl)-N-(pyridin-4-yl)pyrrolo[2,1-f][1,2,4]triazin-4-amine (three-letter code: 3DC) (formula: C₁₄H₁₁N₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	N	0	0
			22	14	1	7		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONICACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is water.

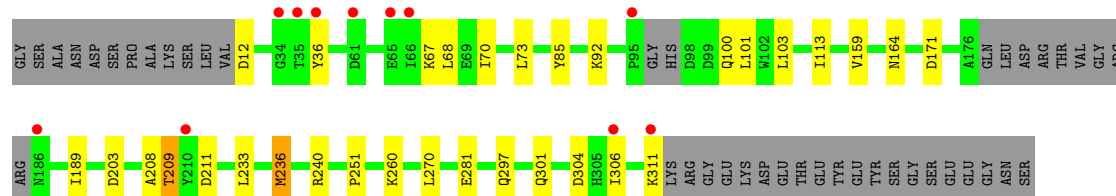
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	111	Total 111	O 111	0	0
5	B	95	Total 95	O 95	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

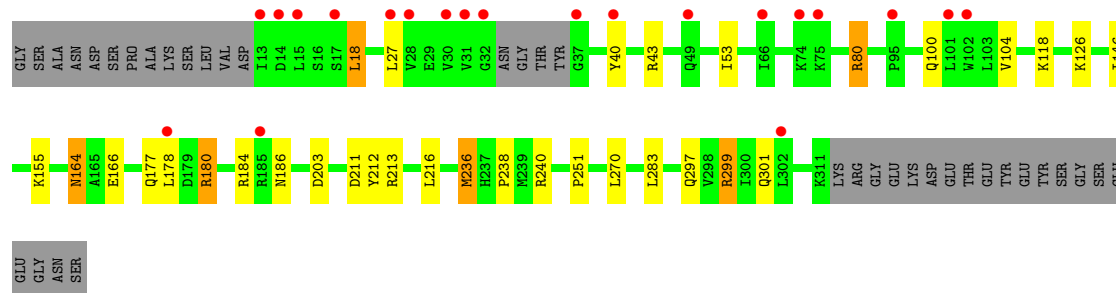
- Molecule 1: Mitogen-activated protein kinase kinase kinase 4

Chain A: 



- Molecule 1: Mitogen-activated protein kinase kinase kinase 4

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.92Å 89.02Å 91.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.77 – 2.58 63.77 – 2.58	Depositor EDS
% Data completeness (in resolution range)	99.9 (63.77-2.58) 99.8 (63.77-2.58)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.27 (at 2.58Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.195 , 0.244 0.205 , 0.256	Depositor DCC
R_{free} test set	1077 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	52.5	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 46.3	EDS
Estimated twinning fraction	0.019 for -h,l,k	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 21109 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4961	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: MG, MES, 3DC

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	0.48	0/2385	0.69	0/3224
1	B	0.46	0/2443	0.64	0/3301
All	All	0.47	0/4828	0.66	0/6525

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	2331	0	2327	10	0
1	B	2388	0	2394	15	0
2	A	2	0	0	0	0
3	A	21	1	0	0	0
4	B	12	0	13	0	0
5	A	111	0	0	0	0
5	B	95	0	0	2	0
All	All	4960	1	4734	24	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 (24) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:189:ILE:HG13	1:B:238:PRO:HB2	1.76	0.68
1:A:73:LEU:HG	1:A:85:TYR:HB2	1.77	0.64
1:B:211:ASP:OD1	1:B:213:ARG:HD3	2.04	0.58
1:B:212:TYR:CE2	1:B:213:ARG:HD2	2.43	0.53
1:B:166:GLU:HG2	1:B:299:ARG:HH12	1.76	0.51
1:B:155:LYS:HD2	5:B:595:HOH:O	2.11	0.50
1:B:53:ILE:HG12	1:B:104:VAL:HG13	1.94	0.50
1:A:251:PRO:HD2	1:A:270:LEU:HD13	1.94	0.49
1:B:177:GLN:NE2	1:B:180:ARG:HD3	2.29	0.48
1:A:236:MET:HG3	1:A:240:ARG:HG2	1.96	0.48
1:B:236:MET:HG3	1:B:240:ARG:HG2	1.95	0.48
1:B:27:LEU:HD22	1:B:40:TYR:HB2	1.97	0.47
1:A:67:LYS:HA	1:A:70:ILE:HD12	1.98	0.46
1:A:208:ALA:O	1:A:209:THR:HG23	2.16	0.45
1:B:251:PRO:HD2	1:B:270:LEU:HD13	1.98	0.45
1:A:70:ILE:HG12	1:A:103:LEU:HD13	1.99	0.44
1:A:113:ILE:HG12	1:A:159:VAL:HB	1.99	0.44
1:B:216:LEU:HD22	1:B:283:LEU:HD12	2.00	0.44
1:B:164:ASN:HD22	1:B:166:GLU:HG3	1.81	0.44
1:B:18:LEU:HD12	1:B:18:LEU:HA	1.90	0.44
1:B:80:ARG:HG2	5:B:560:HOH:O	2.18	0.42
1:B:297:GLN:HG3	1:B:301:GLN:HE21	1.85	0.42
1:A:297:GLN:HG3	1:A:301:GLN:HE21	1.85	0.41
1:A:233:LEU:O	1:A:236:MET:HB2	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	283/332 (85%)	266 (94%)	15 (5%)	2 (1%)	30 56

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	292/332 (88%)	280 (96%)	11 (4%)	1 (0%)	50	76
All	All	575/664 (87%)	546 (95%)	26 (4%)	3 (0%)	38	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	THR
1	B	18	LEU
1	A	171	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	255/290 (88%)	240 (94%)	15 (6%)	28	51
1	B	261/290 (90%)	247 (95%)	14 (5%)	31	56
All	All	516/580 (89%)	487 (94%)	29 (6%)	30	54

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	A	36	TYR
1	A	68	LEU
1	A	92	LYS
1	A	100	GLN
1	A	101	LEU
1	A	164	ASN
1	A	203	ASP
1	A	211	ASP
1	A	236	MET
1	A	260	LYS
1	A	281	GLU
1	A	304	ASP
1	A	306	ILE
1	A	311	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	43	ARG
1	B	80	ARG
1	B	100	GLN
1	B	118	LYS
1	B	126	LYS
1	B	146	ILE
1	B	164	ASN
1	B	178	LEU
1	B	180	ARG
1	B	184	ARG
1	B	186	ASN
1	B	203	ASP
1	B	236	MET
1	B	299	ARG

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	38	GLN
1	A	157	GLN
1	B	164	ASN

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 ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	3DC	A	403	-	24,24,24	1.01	1 (4%)	31,33,33	1.36	7 (22%)
4	MES	B	401	-	12,12,12	0.17	0	16,16,16	0.40	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	3DC	A	403	-	-	0/8/8/8	0/4/4/4
4	MES	B	401	-	-	0/6/14/14	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	3DC	C9-N13	3.34	1.44	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	3DC	C11-C10-C9	-3.21	107.44	109.35
3	A	403	3DC	C17-C22-N21	-2.94	111.36	112.48
3	A	403	3DC	C15-N16-C8	2.37	118.32	116.50
3	A	403	3DC	C9-C8-N16	2.27	122.27	118.03
3	A	403	3DC	C12-C11-C17	-2.16	123.42	127.49
3	A	403	3DC	C22-N21-N19	2.08	105.18	103.95
3	A	403	3DC	C17-C18-N19	-2.03	107.42	108.15

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, 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	289/332 (87%)	0.14	11 (3%) 38 36	32, 53, 101, 133	0
1	B	295/332 (88%)	0.41	21 (7%) 16 13	34, 65, 113, 125	0
All	All	584/664 (87%)	0.28	32 (5%) 24 22	32, 61, 108, 133	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	30	VAL	7.3
1	A	36	TYR	7.1
1	B	32	GLY	6.4
1	B	31	VAL	5.3
1	A	35	THR	4.9
1	A	61	ASP	4.7
1	B	95	PRO	4.7
1	B	15	LEU	4.4
1	A	186	ASN	4.2
1	B	13	ILE	4.0
1	A	65	GLU	4.0
1	B	185	ARG	3.6
1	A	34	GLY	3.6
1	B	178	LEU	3.6
1	B	37	GLY	3.5
1	B	40	TYR	3.3
1	B	49	GLN	3.3
1	B	28	VAL	3.0
1	A	210	TYR	2.9
1	A	66	ILE	2.9
1	B	75	LYS	2.7
1	B	101	LEU	2.7
1	B	14	ASP	2.5
1	B	102	TRP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	17	SER	2.4
1	B	66	ILE	2.4
1	B	302	LEU	2.4
1	A	95	PRO	2.2
1	B	27	LEU	2.2
1	B	74	LYS	2.2
1	A	311	LYS	2.1
1	A	306	ILE	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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MES	B	401	12/12	0.27	1.87	95,97,107,108	0
3	3DC	A	403	21/21	0.14	-0.32	44,49,52,53	0
2	MG	A	401	1/1	0.10	-1.50	58,58,58,58	0
2	MG	A	402	1/1	0.10	-1.71	60,60,60,60	0

6.5 Other polymers ⓘ

There are no such residues in this entry.