

Full wwPDB X-ray Structure Validation Report (i)

Aug 9, 2020 – 11:30 PM BST

PDB ID	:	5R9V
Title	:	PanDDA analysis group deposition Form1 MAP kinase p38-alpha – Fragment
		N13596a in complex with MAP kinase p38-alpha
Authors	:	De Nicola, G.F.; Nichols, C.E.
Deposited on		
$\operatorname{Resolution}$:	1.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

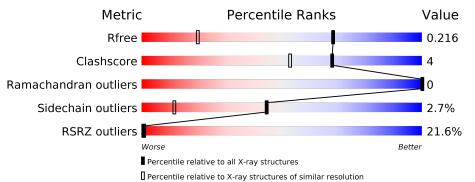
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
\mathbf{X} triage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
$\operatorname{CCP4}$:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	$egin{array}{llllllllllllllllllllllllllllllllllll$	${f Similar\ resolution}\ (\#{ m Entries}, { m resolution\ range}({ m \AA}))$
R_{free}	130704	1156 (1.46-1.46)
Clashscore	141614	1202(1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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 respectively. 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 <=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	
			21%	
1	А	360	88%	7% • •



2 Entry composition (i)

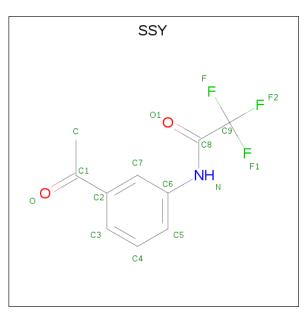
There are 7 unique types of molecules in this entry. The entry contains 3061 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Mitogen-activated protein kinase 14.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Λ	348	Total	С	Ν	Ο	S	0	4	0
	А	040	2781	1781	469	516	15		±	0

• Molecule 2 is $\{N\}$ -(3-ethanoylphenyl)-2,2,2-tris(fluoranyl)ethanamide (three-letter code: SSY) (formula: $C_{10}H_8F_3NO_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
2	А	1	Total 16	C 10	F 3	N 1	0 2	0	0

• Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

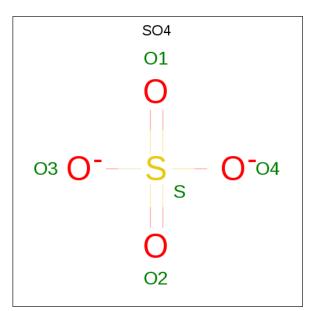
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	5	TotalCl55	0	0



• Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

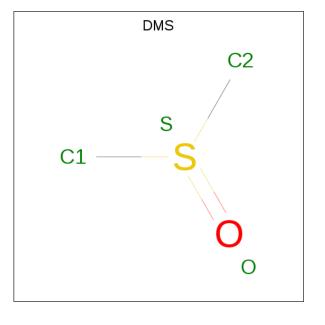
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Mg 1 1	0	0

 $\bullet\,$ Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: ${\rm O_4S}).$



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	А	1	Total 5	0 4	${ m S}$ 1	0	0

• Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	А	1	Total 4	$\begin{array}{c} \mathrm{C} \\ \mathrm{2} \end{array}$	0 1	S 1	0	0

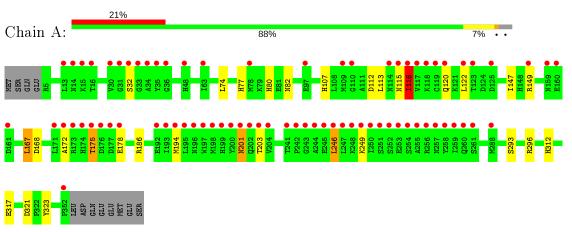
• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	249	Total O 249 249	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.



• Molecule 1: Mitogen-activated protein kinase 14



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	45.84Å 86.20 Å 127.63 Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.34 - 1.45	Depositor
Resolution (A)	29.32 - 1.45	EDS
% Data completeness	98.9(29.34-1.45)	Depositor
(in resolution range)	99.0(29.32 - 1.45)	EDS
R _{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.93 ~({\rm at}~ 1.45 {\rm \AA})$	Xtriage
Refinement program	REFMAC $5.8.0238$	Depositor
R, R_{free}	0.180 , 0.190	Depositor
III, IIIfree	0.215 , 0.216	DCC
R_{free} test set	4455 reflections $(4.96%)$	wwPDB-VP
Wilson B-factor (Å ²)	20.6	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , 48.7	EDS
L-test for twinning ²	$ \langle L \rangle = 0.48, \langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3061	wwPDB-VP
Average B, all atoms $(Å^2)$	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.24% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: MG, DMS, SSY, SO4, CL

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).

Mal	Bond lengths		Bond angles		
Mol Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.97	0/2847	0.99	4/3873~(0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	323	TYR	CB-CG-CD1	-7.70	116.38	121.00
1	А	323	TYR	CB-CG-CD2	6.61	124.97	121.00
1	А	116	ILE	O-C-N	-6.07	112.98	122.70
1	А	296	ARG	CG-CD-NE	-5.01	101.28	111.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	116	ILE	Mainchain
1	А	186	ARG	Sidechain
1	А	246	LEU	Peptide



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	А	2781	0	2702	21	0
2	А	16	0	0	0	0
3	А	5	0	0	0	0
4	А	1	0	0	0	0
5	А	5	0	0	0	0
6	А	4	0	6	0	0
7	А	249	0	0	5	0
All	All	3061	0	2708	21	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 4.

All (21) 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:A:249:LYS:HE2	7:A:507:HOH:O	1.71	0.91
1:A:80:HIS:HD2	1:A:82:ASN:H	1.32	0.75
1:A:80:HIS:CD2	1:A:82:ASN:H	2.07	0.73
1:A:246:LEU:HB3	7:A:506:HOH:O	1.90	0.72
1:A:246:LEU:HG	1:A:246:LEU:O	1.89	0.71
1:A:201:ASN:HD22	1:A:201:ASN:C	1.98	0.66
1:A:203:THR:OG1	1:A:293:SER:HB2	2.03	0.58
1:A:312:HIS:HD2	1:A:317:GLU:OE2	1.90	0.55
1:A:249:LYS:CE	7:A:507:HOH:O	2.43	0.55
1:A:107:HIS:HD2	7:A:583:HOH:O	1.91	0.52
1:A:116:ILE:CD1	1:A:122:LEU:HD21	2.41	0.50
1:A:246:LEU:HD23	7:A:707:HOH:O	2.12	0.49
1:A:175:THR:HG22	1:A:178:GLU:CG	2.46	0.46
1:A:149[B]:ARG:NH2	1:A:172:ALA:HA	2.31	0.46
1:A:74:LEU:C	1:A:74:LEU:HD13	2.36	0.45
1:A:175:THR:HG22	1:A:178:GLU:CD	2.37	0.45
1:A:201:ASN:ND2	1:A:201:ASN:C	2.70	0.43
1:A:112:ASP:H	1:A:115:ASN:ND2	2.17	0.43
1:A:77:HIS:HE1	1:A:321:ASP:O	2.01	0.42
1:A:147:ILE:HG22	1:A:149[B]:ARG:HG3	2.01	0.42



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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LEU:HD12	1:A:168:ASP:CG	2.39	0.42

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	А	350/360~(97%)	337~(96%)	13~(4%)	0	100 100

There are no Ramachandran outliers to report.

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	295/319~(92%)	287~(97%)	8 (3%)	44 12

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	32	SER
1	А	113	LEU
1	А	116	ILE
1	А	120	GLN
1	А	167	LEU



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Mol	Chain	Res	Type
1	А	175	THR
1	А	194	MET
1	А	201	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	77	HIS
1	А	80	HIS
1	А	107	HIS
1	А	115	ASN
1	А	128	GLN
1	А	174	HIS
1	А	201	ASN
1	А	272	ASN
1	А	310	GLN
1	А	312	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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



Mol	Type Chain	Res	Tink	Link Bond lengths			Bond angles			
	туре	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
5	SO4	А	408	-	4,4,4	0.43	0	$6,\!6,\!6$	0.34	0
6	DMS	А	409	-	3,3,3	0.20	0	3, 3, 3	0.12	0
2	SSY	А	401	-	16, 16, 16	1.23	2 (12%)	$23,\!23,\!23$	0.85	0

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).

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	\mathbf{Res}	Link	Chirals	Torsions	Rings
2	SSY	А	401	-	-	0/14/14/14	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	А	401	SSY	C7-C2	2.50	1.43	1.39
2	А	401	SSY	C7-C6	2.09	1.42	1.39

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	А	348/360~(96%)	1.00	75~(21%) 0 1	13, 22, 47, 80	49 (14%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	246	LEU	14.9
1	А	258	TYR	12.0
1	А	259	ILE	10.8
1	А	204	VAL	10.7
1	А	250	ILE	9.3
1	А	247	LEU	8.9
1	А	193	ILE	8.9
1	А	117	VAL	8.8
1	А	288[A]	MET	8.8
1	А	34	ALA	8.6
1	А	35	TYR	8.6
1	А	197	TRP	8.0
1	А	203	THR	7.9
1	А	78[A]	MET	7.8
1	А	255	ALA	7.6
1	А	241	THR	7.6
1	А	194	MET	7.4
1	А	242	PRO	7.0
1	А	195	LEU	7.0
1	А	122	LEU	6.7
1	А	149[A]	ARG	6.6
1	А	33	GLY	6.6
1	А	200	TYR	6.5
1	А	244	ALA	6.3
1	А	173	ARG	6.1
1	А	119	CYS	6.1
1	А	202	GLN	6.0



Mol	Chain	Res	Type	RSRZ
1	А	261	SER	5.9
1	А	172	ALA	5.7
1	А	174	HIS	5.6
1	А	116	ILE	5.1
1	А	352	PRO	4.9
1	А	254	SER	4.9
1	А	201	ASN	4.8
1	А	251	SER	4.8
1	А	257	ASN	4.7
1	А	63	ILE	4.6
1	А	245	GLU	4.5
1	А	260	GLN	4.5
1	А	31	GLY	4.4
1	А	256	ARG	4.1
1	А	196	ASN	4.0
1	А	253	GLU	3.9
1	А	32	SER	3.9
1	А	48	HIS	3.8
1	А	115	ASN	3.8
1	А	243	GLY	3.8
1	А	114	ASN	3.7
1	А	125[A]	ASP	3.7
1	А	178	GLU	3.7
1	А	36	GLY	3.6
1	А	175	THR	3.6
1	А	123	THR	3.5
1	А	252	SER	3.4
1	А	192	GLU	3.2
1	А	13	LEU	3.2
1	А	15	LYS	3.1
1	А	160	GLU	3.1
1	А	199	HIS	3.1
1	А	171	LEU	3.0
1	А	14	ASN	3.0
1	А	161	ASP	2.9
1	А	198	MET	2.8
1	А	16	THR	2.7
1	А	249	LYS	2.7
1	А	97	GLU	2.5
1	А	110	GLY	2.4
1	А	176	ASP	2.4
1	А	248	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	А	118	LYS	2.3
1	А	120	GLN	2.3
1	А	177	ASP	2.3
1	А	159	ASN	2.1
1	А	109	MET	2.1
1	А	30	VAL	2.0

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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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	SSY	А	401	16/16	0.54	0.33	$23,\!26,\!37,\!38$	16
6	DMS	А	409	4/4	0.75	0.17	$72,\!78,\!82,\!86$	0
5	SO4	А	408	5/5	0.85	0.24	$41,\!42,\!55,\!74$	0
3	CL	А	404	1/1	0.91	0.14	45,45,45,45	0
4	MG	А	407	1/1	0.96	0.24	$26,\!26,\!26,\!26$	0
3	CL	А	406	1/1	0.99	0.09	$29,\!29,\!29,\!29$	0
3	CL	А	403	1/1	0.99	0.07	$35,\!35,\!35,\!35$	0
3	CL	А	405	1/1	0.99	0.13	32,32,32,32	0
3	CL	А	402	1/1	0.99	0.16	$38,\!38,\!38,\!38$	0

6.5 Other polymers (i)

There are no such residues in this entry.

