

# Full wwPDB X-ray Structure Validation Report (i)

#### Aug 10, 2020 – 12:21 PM BST

PDB ID : 5R9Z

> Title : PanDDA analysis group deposition Form1 MAP kinase p38-alpha – Fragment

> > N13502a in complex with MAP kinase p38-alpha

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Deposited on 2020-03-04

1.66 Å(reported) Resolution

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

> 1.8.5 (274361), CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13 EDS 2.13.1

Percentile statistics 20191225.v01 (using entries in the PDB archive December 25th 2019)

> Refmac 5.8.0158

7.0.044 (Gargrove) CCP4 Engh & Huber (2001)

Ideal geometry (proteins) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

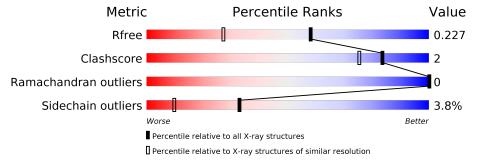
Validation Pipeline (wwPDB-VP) 2.13.1

# 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 1.66 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{resolution range}( ext{Å}))$
$R_{free}$	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)

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%

Mol	Chain	Length	Quality of chain	
1	A	360	91%	



## 2 Entry composition (i)

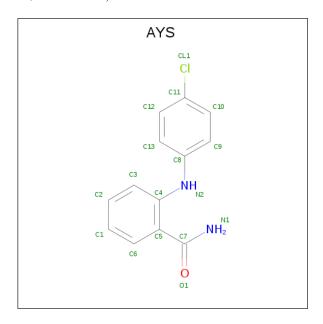
There are 7 unique types of molecules in this entry. The entry contains 3058 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	348	Total	С	N	О	S	0	4	0
1	A	340	2781	1781	469	516	15	0	4	U

• Molecule 2 is 2-[(4-chlorophenyl)amino]benzamide (three-letter code: AYS) (formula:  $C_{13}H_{11}ClN_2O$ ).



Mol	Chain	Residues		Ato	oms		ZeroOcc	AltConf
2	A	1	Total 17		Cl 1	O 1	0	0

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

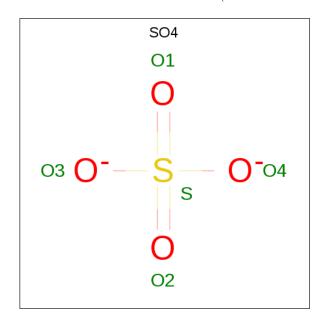
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total Cl 5 5	0	0



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

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

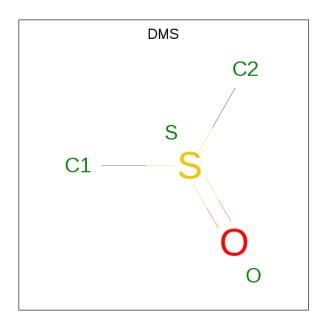
 $\bullet$  Molecule 5 is SULFATE ION (three-letter code: SO4) (formula:  $\mathrm{O_4S}).$ 



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0

 $\bullet$  Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $\mathrm{C_2H_6OS}).$ 





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 4	C 2	O 1	S 1	0	0

• Molecule 7 is water.

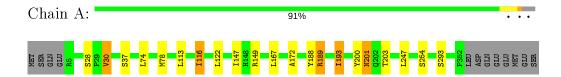
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	240	Total O 240 240	0	0



# 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. 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. 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	45.81Å 86.51Å 127.03Å	Danagitan
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	29.83 - 1.66	Depositor
Resolution (A)	29.81 - 1.66	EDS
% Data completeness	98.7 (29.83-1.66)	Depositor
(in resolution range)	98.7 (29.81-1.66)	EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.35 (at 1.66Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
D D.	0.178 , 0.197	Depositor
$R, R_{free}$	0.227 , $0.227$	DCC
$R_{free}$ test set	2987 reflections $(4.99\%)$	wwPDB-VP
Wilson B-factor $(\mathring{A}^2)$	24.2	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.31, 52.5	EDS
L-test for twinning <sup>2</sup>	$ < L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3058	wwPDB-VP
Average B, all atoms $(Å^2)$	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.65% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $< L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities 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, SO4, AYS, 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	Chain	Bond	lengths	Bond angles		
MIOI		RMSZ	# Z >5	RMSZ	# Z  > 5	
1	A	0.89	0/2847	0.84	$1/3873 \ (0.0\%)$	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	188	TYR	CB-CG-CD2	6.14	124.69	121.00

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	A	2781	0	2702	13	0
2	A	17	0	0	0	0
3	A	5	0	0	0	0
4	A	1	0	0	0	0
5	A	10	0	0	0	0
6	A	4	0	6	0	0
7	A	240	0	0	0	0
All	All	3058	0	2708	13	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 2.

All (13) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{c}  ext{Interatomic} \  ext{distance } ( ext{Å}) \end{array}$	Clash overlap (Å)
1:A:193:ILE:HD12	1:A:200:TYR:CE2	2.33	0.63
1:A:189:ARG:HD3	1:A:193:ILE:HD11	1.82	0.62
1:A:201:ASN:HD22	1:A:201:ASN:C	2.06	0.58
1:A:30:VAL:CG1	1:A:30:VAL:O	2.52	0.57
1:A:116:ILE:CD1	1:A:122:LEU:HD21	2.41	0.51
1:A:149[B]:ARG:HG2	1:A:200:TYR:CD2	2.46	0.50
1:A:201:ASN:ND2	1:A:203:THR:OG1	2.44	0.48
1:A:149[B]:ARG:NH2	1:A:172:ALA:HA	2.29	0.46
1:A:30:VAL:HG13	1:A:30:VAL:O	2.15	0.46
1:A:149[A]:ARG:O	1:A:189:ARG:NH2	2.50	0.44
1:A:147:ILE:HG22	1:A:149[B]:ARG:HG3	2.02	0.41
1:A:203:THR:OG1	1:A:293:SER:HB2	2.20	0.41
1:A:74:LEU:HD11	1:A:78[B]:MET:HE3	2.04	0.40

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	A	350/360 (97%)	345 (99%)	5 (1%)	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	A	$295/319 \ (92\%)$	284 (96%)	11 (4%)	34 10	

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	30	VAL
1	A	37	SER
1	A	113	LEU
1	A	116	ILE
1	A	167	LEU
1	A	189	ARG
1	A	193	ILE
1	A	201	ASN
1	A	247	LEU
1	A	254	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	77	HIS
1	A	115	ASN
1	A	128	GLN
1	A	174	HIS
1	A	201	ASN
1	A	202	GLN
1	A	272	ASN
1	A	310	GLN

#### 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 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	Tuno	Chain	Res	Link	Bond lengths			Bond angles		
MIOI	Type	Chain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	AYS	A	401	_	18,18,18	1.43	4 (22%)	24,24,24	0.86	0
5	SO4	A	409	-	4,4,4	0.39	0	6,6,6	0.07	0
5	SO4	A	408	_	4,4,4	0.33	0	6,6,6	0.28	0
6	DMS	A	410	-	3,3,3	0.22	0	3,3,3	0.09	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
2	AYS	A	401	_	-	0/8/8/8	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	${f Observed(\AA)}$	$\operatorname{Ideal}( ext{\AA})$
2	A	401	AYS	C7-N1	3.34	1.39	1.33
2	A	401	AYS	C3-C4	2.91	1.44	1.39
2	A	401	AYS	C9-C8	2.14	1.42	1.39
2	A	401	AYS	C13-C8	2.03	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)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

