



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 6, 2025 – 12:17 pm GMT

PDB ID : 8RLX  
Title : Erk2 MAP kinase T188A mutant  
Authors : Livnah, O.; Gutman, D.  
Deposited on : 2024-01-04  
Resolution : 1.60 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](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4.02b-467  
Xtrriage (Phenix) : 1.13  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

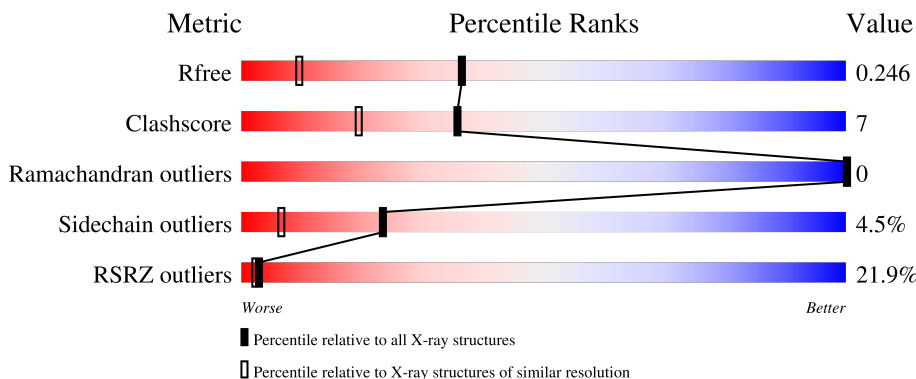
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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))
$R_{free}$	164625	4274 (1.60-1.60)
Clashscore	180529	4682 (1.60-1.60)
Ramachandran outliers	177936	4583 (1.60-1.60)
Sidechain outliers	177891	4582 (1.60-1.60)
RSRZ outliers	164620	4272 (1.60-1.60)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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
1	A	365	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2968 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	347	2829	1818	484	513	14	0	2	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ALA	-	expression tag	UNP P63086
A	-5	HIS	-	expression tag	UNP P63086
A	-4	HIS	-	expression tag	UNP P63086
A	-3	HIS	-	expression tag	UNP P63086
A	-2	HIS	-	expression tag	UNP P63086
A	-1	HIS	-	expression tag	UNP P63086
A	0	HIS	-	expression tag	UNP P63086
A	188	ALA	THR	engineered mutation	UNP P63086

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	139	Total	O	0	0
			139	139		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.57Å 69.51Å 59.42Å 90.00° 109.17° 90.00°	Depositor
Resolution (Å)	43.67 – 1.60 43.67 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (43.67-1.60) 99.2 (43.67-1.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.03	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 1.60Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.210 , 0.241 0.218 , 0.246	Depositor DCC
$R_{free}$ test set	2493 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.8	Xtrriage
Anisotropy	0.029	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 33.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2968	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.79% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.70	0/2903	0.98	6/3934 (0.2%)

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	A	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	89	ARG	NE-CZ-NH1	18.74	129.67	120.30
1	A	89	ARG	NE-CZ-NH2	-15.62	112.49	120.30
1	A	89	ARG	CD-NE-CZ	7.32	133.85	123.60
1	A	89	ARG	CG-CD-NE	-5.57	100.09	111.80
1	A	56	PRO	N-CA-CB	-5.51	96.54	102.60
1	A	255	ASN	CB-CA-C	5.27	120.94	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	PRO	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	A	2829	0	2835	41	0
2	A	139	0	0	7	1
All	All	2968	0	2835	41	1

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 7.

All (41) 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:60:GLN:HE22	1:A:64:GLN:HE21	1.25	0.81
1:A:78:HIS:HD2	1:A:80:ASN:H	1.28	0.79
1:A:89:ARG:HD3	1:A:349:THR:OG1	1.87	0.75
1:A:78:HIS:CD2	1:A:80:ASN:H	2.09	0.71
1:A:237:HIS:HD2	2:A:465:HOH:O	1.76	0.68
1:A:236:ASN:ND2	2:A:401:HOH:O	2.27	0.68
1:A:9:PRO:O	1:A:15:GLN:HA	1.95	0.66
1:A:68:ARG:HD3	1:A:169:ALA:O	1.98	0.64
1:A:178:HIS:NE2	2:A:402:HOH:O	2.29	0.64
1:A:272:PRO:HB2	1:A:274:ASN:ND2	2.17	0.59
1:A:259[A]:ARG:NH1	2:A:404:HOH:O	2.34	0.58
1:A:78:HIS:HE1	2:A:466:HOH:O	1.86	0.56
1:A:279:ASN:HD22	1:A:279:ASN:N	2.05	0.54
1:A:339:GLU:O	1:A:343:GLU:HG3	2.08	0.53
1:A:184:GLU:HA	1:A:184:GLU:OE1	2.09	0.53
1:A:279:ASN:N	1:A:279:ASN:ND2	2.58	0.52
1:A:315:TYR:CZ	1:A:317:PRO:HG3	2.44	0.52
1:A:54:ILE:HG22	1:A:56:PRO:HD3	1.90	0.51
1:A:60:GLN:NE2	1:A:64:GLN:HE21	2.02	0.51
1:A:88:ILE:HB	1:A:100:TYR:HB2	1.92	0.50
1:A:190:TRP:CD1	1:A:227:PRO:HA	2.47	0.49
1:A:254:ILE:HD12	1:A:255:ASN:N	2.28	0.49
1:A:230:HIS:CE1	1:A:233:ASP:HB2	2.48	0.48
1:A:34:TYR:OH	1:A:65:ARG:HD2	2.14	0.47
1:A:35:GLY:HA3	1:A:53:LYS:O	2.16	0.45
1:A:63:CYS:HB3	1:A:341:LEU:HB3	1.97	0.45
1:A:255:ASN:C	1:A:255:ASN:HD22	2.20	0.45
1:A:34:TYR:CZ	1:A:62:TYR:HA	2.52	0.45
1:A:44:LEU:HD13	1:A:44:LEU:C	2.38	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ASN:ND2	2:A:414:HOH:O	2.51	0.43
1:A:114:LEU:HD13	1:A:218:GLU:HG2	2.00	0.43
1:A:202:GLY:HA2	1:A:207:ILE:HG21	2.01	0.43
1:A:42:ASP:OD1	1:A:42:ASP:C	2.58	0.42
1:A:87:ILE:HD13	1:A:349:THR:HG22	2.01	0.42
1:A:239:LEU:HD22	1:A:245:PRO:HD3	2.01	0.42
1:A:225:ILE:HD11	1:A:273:TRP:HZ3	1.85	0.41
1:A:255:ASN:ND2	2:A:415:HOH:O	2.51	0.41
1:A:57:PHE:HA	1:A:63:CYS:SG	2.60	0.41
1:A:23:TYR:CE2	1:A:88:ILE:HD11	2.55	0.41
1:A:333:LEU:HA	1:A:336:LEU:HD12	2.02	0.40
1:A:34:TYR:CE1	1:A:62:TYR:CG	3.09	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:468:HOH:O	2:A:538:HOH:O[2_656]	2.19	0.01

## 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	345/365 (94%)	323 (94%)	22 (6%)	0	<b>100</b> <b>100</b>

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	311/323 (96%)	297 (96%)	14 (4%)	23 6

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

Mol	Chain	Res	Type
1	A	15	GLN
1	A	22	ARG
1	A	31	GLU
1	A	56	PRO
1	A	60	GLN
1	A	75	ARG
1	A	89	ARG
1	A	204	THR
1	A	232	LEU
1	A	255	ASN
1	A	274	ASN
1	A	279	ASN
1	A	331	MET
1	A	344	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	25	ASN
1	A	45	ASN
1	A	60	GLN
1	A	78	HIS
1	A	85	ASN
1	A	121	ASN
1	A	152	ASN
1	A	236	ASN
1	A	237	HIS
1	A	251	ASN
1	A	255	ASN
1	A	260	ASN
1	A	274	ASN
1	A	279	ASN

### 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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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

### 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	347/365 (95%)	1.01	76 (21%) <b>3</b> <b>2</b>	12, 25, 60, 81	2 (0%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	PRO	8.0
1	A	44	LEU	6.4
1	A	34	TYR	5.9
1	A	21	PRO	5.8
1	A	20	GLY	5.6
1	A	7	ALA	5.2
1	A	26	LEU	5.2
1	A	28	TYR	5.1
1	A	33	ALA	4.9
1	A	355	GLY	4.9
1	A	8	GLY	4.8
1	A	4	ALA	4.6
1	A	178	HIS	4.6
1	A	38	CYS	4.5
1	A	335	ASP	4.5
1	A	29	ILE	4.5
1	A	37	VAL	4.4
1	A	333	LEU	4.3
1	A	329	PHE	4.2
1	A	43	ASN	4.1
1	A	47	VAL	4.1
1	A	41	TYR	4.0
1	A	35	GLY	4.0
1	A	338	LYS	4.0
1	A	36	MET	4.0
1	A	5	ALA	4.0
1	A	332	GLU	4.0

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	186	VAL	3.9
1	A	24	THR	3.8
1	A	32	GLY	3.8
1	A	15	GLN	3.7
1	A	354	PRO	3.6
1	A	61	THR	3.5
1	A	59	HIS	3.5
1	A	6	ALA	3.5
1	A	16	VAL	3.5
1	A	49	VAL	3.4
1	A	331	MET	3.4
1	A	40	ALA	3.4
1	A	27	SER	3.3
1	A	30	GLY	3.1
1	A	23	TYR	3.0
1	A	279	ASN	3.0
1	A	223	ARG	2.9
1	A	340	LYS	2.9
1	A	45	ASN	2.8
1	A	275	ARG	2.8
1	A	39	SER	2.8
1	A	58	GLU	2.7
1	A	185	TYR	2.7
1	A	328	LYS	2.7
1	A	230	HIS	2.6
1	A	22	ARG	2.6
1	A	46	LYS	2.6
1	A	31	GLU	2.6
1	A	62	TYR	2.6
1	A	42	ASP	2.6
1	A	334	ASP	2.6
1	A	231	TYR	2.5
1	A	184	GLU	2.4
1	A	251	ASN	2.3
1	A	17	PHE	2.3
1	A	48	ARG	2.3
1	A	254	ILE	2.3
1	A	229	LYS	2.2
1	A	351	ARG	2.2
1	A	336	LEU	2.2
1	A	60	GLN	2.2
1	A	271	VAL	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	25	ASN	2.1
1	A	337	PRO	2.1
1	A	327	PHE	2.1
1	A	343	GLU	2.1
1	A	182	LEU	2.1
1	A	341	LEU	2.1
1	A	252	CYS	2.0

## 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.