



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 6OTS / pdb_00006ots
Title : Rat ERK2 E320K
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Deposited on : 2019-05-03
Resolution : 2.10 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 ⓘ 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

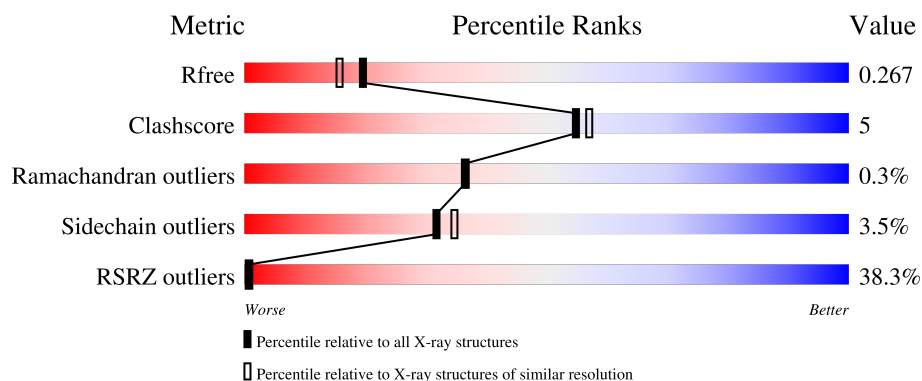
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 ≥ 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	358	35% 79% 11% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5367 atoms, of which 2629 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
1	A	324	Total	C	H	N	O	S	0	2	0
			5262	1694	2629	448	476	15			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	320	LYS	GLU	engineered mutation	UNP P63086

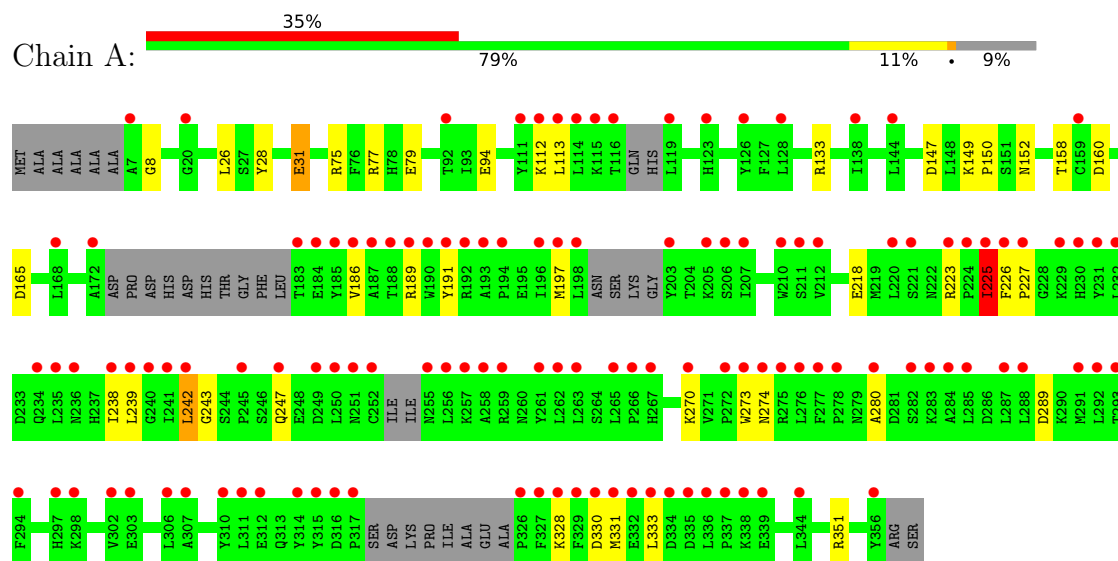
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	105	Total	O	0	0
			105	105		

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 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	182.31Å 41.95Å 50.34Å 90.00° 105.86° 90.00°	Depositor
Resolution (Å)	43.84 – 2.10 43.84 – 2.10	Depositor EDS
% Data completeness (in resolution range)	78.4 (43.84-2.10) 78.4 (43.84-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.231 , 0.264 0.232 , 0.267	Depositor DCC
R_{free} test set	1005 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 79.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5367	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

5 Model quality

5.1 Standard geometry

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	0.15	0/2695	0.36	1/3646 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	ASP	N-CA-C	7.54	119.73	110.91

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	2633	2629	2622	25	2
2	A	105	0	0	7	0
All	All	2738	2629	2622	25	2

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 5.

All (25) 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:160:ASP:OD1	2:A:401:HOH:O	2.01	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:LEU:O	1:A:242:LEU:HD22	1.87	0.74
1:A:79:GLU:OE2	1:A:133:ARG:NH1	2.35	0.59
1:A:242:LEU:C	1:A:242:LEU:HD13	2.29	0.58
1:A:77:ARG:NH1	2:A:405:HOH:O	2.38	0.57
1:A:351:ARG:NH1	2:A:408:HOH:O	2.43	0.50
1:A:242:LEU:HA	1:A:270:LYS:HG3	1.94	0.50
1:A:158:THR:O	2:A:401:HOH:O	2.20	0.49
1:A:147:ASP:O	1:A:152:ASN:ND2	2.46	0.48
1:A:28:TYR:OH	1:A:31:GLU:OE1	2.32	0.48
1:A:239:LEU:O	1:A:243:GLY:HA2	2.14	0.47
1:A:273:TRP:NE1	1:A:289:ASP:OD1	2.44	0.46
1:A:226:PHE:CE1	1:A:238:ILE:HA	2.51	0.46
1:A:225:ILE:O	1:A:226:PHE:CD1	2.69	0.46
1:A:328:LYS:N	2:A:417:HOH:O	2.49	0.45
1:A:112:LYS:NZ	2:A:416:HOH:O	2.49	0.44
1:A:189:ARG:NH1	2:A:420:HOH:O	2.50	0.44
1:A:191:TYR:OH	1:A:218:GLU:OE1	2.26	0.43
1:A:226:PHE:N	1:A:227:PRO:HD3	2.34	0.42
1:A:223:ARG:NH1	1:A:225:ILE:HG22	2.34	0.42
1:A:242:LEU:H	1:A:242:LEU:HD12	1.86	0.41
1:A:238:ILE:HG22	1:A:242:LEU:HD11	2.02	0.41
1:A:330:ASP:O	1:A:331:MET:HB2	2.20	0.41
1:A:149:LYS:HB2	1:A:150:PRO:HD2	2.02	0.41

All (2) 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)
1:A:274:ASN:ND2	1:A:280:ALA:O[2_556]	2.09	0.11
1:A:8:GLY:O	1:A:77:ARG:HH22[4_445]	1.59	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	314/358 (88%)	285 (91%)	28 (9%)	1 (0%)	36	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	ILE

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	288/318 (91%)	278 (96%)	10 (4%)	32	35

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
1	A	75	ARG
1	A	94	GLU
1	A	113	LEU
1	A	186	VAL
1	A	197	MET
1	A	225	ILE
1	A	242	LEU
1	A	247	GLN
1	A	333	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	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, 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	324/358 (90%)	1.70	124 (38%) 1 1	7, 77, 169, 199	1 (0%)

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	225	ILE	6.3
1	A	188	THR	6.1
1	A	239	LEU	5.8
1	A	187	ALA	5.8
1	A	250	LEU	5.6
1	A	198	LEU	5.5
1	A	185	TYR	5.4
1	A	326	PRO	5.3
1	A	191	TYR	5.2
1	A	194	PRO	5.2
1	A	331	MET	5.1
1	A	335	ASP	5.0
1	A	336	LEU	4.9
1	A	329	PHE	4.9
1	A	317	PRO	4.8
1	A	333	LEU	4.8
1	A	238	ILE	4.7
1	A	190	TRP	4.7
1	A	186	VAL	4.7
1	A	276	LEU	4.6
1	A	207	ILE	4.6
1	A	337	PRO	4.5
1	A	231	TYR	4.2
1	A	245	PRO	4.2
1	A	230	HIS	4.1
1	A	235	LEU	4.1
1	A	292	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	119	LEU	4.0
1	A	232	LEU	4.0
1	A	263	LEU	4.0
1	A	334	ASP	4.0
1	A	280	ALA	3.9
1	A	256	LEU	3.9
1	A	262	LEU	3.9
1	A	241	ILE	3.9
1	A	192	ARG	3.8
1	A	302	VAL	3.7
1	A	278	PRO	3.7
1	A	114	LEU	3.6
1	A	189	ARG	3.6
1	A	330	ASP	3.6
1	A	112	LYS	3.6
1	A	255	ASN	3.6
1	A	258	ALA	3.5
1	A	272	PRO	3.4
1	A	236	ASN	3.4
1	A	251	ASN	3.4
1	A	193	ALA	3.4
1	A	203	TYR	3.4
1	A	242	LEU	3.4
1	A	294	PHE	3.4
1	A	287	LEU	3.3
1	A	111	TYR	3.2
1	A	306	LEU	3.2
1	A	277	PHE	3.2
1	A	315	TYR	3.1
1	A	205	LYS	3.1
1	A	247	GLN	3.1
1	A	210	TRP	3.1
1	A	252	CYS	3.0
1	A	168	LEU	3.0
1	A	297	HIS	3.0
1	A	293	THR	3.0
1	A	291	MET	2.9
1	A	259	ARG	2.9
1	A	285	LEU	2.9
1	A	311	LEU	2.9
1	A	283	LYS	2.9
1	A	226	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	113	LEU	2.8
1	A	332	GLU	2.8
1	A	327	PHE	2.8
1	A	196	ILE	2.8
1	A	270	LYS	2.8
1	A	220	LEU	2.8
1	A	240	GLY	2.7
1	A	265	LEU	2.7
1	A	261	TYR	2.7
1	A	144	LEU	2.7
1	A	197	MET	2.7
1	A	20	GLY	2.7
1	A	275	ARG	2.7
1	A	183	THR	2.6
1	A	128	LEU	2.6
1	A	338	LYS	2.6
1	A	316	ASP	2.6
1	A	267	HIS	2.5
1	A	184	GLU	2.5
1	A	303	GLU	2.5
1	A	339	GLU	2.5
1	A	159	CYS	2.5
1	A	227	PRO	2.5
1	A	274	ASN	2.5
1	A	249	ASP	2.4
1	A	284	ALA	2.4
1	A	115	LYS	2.4
1	A	273	TRP	2.4
1	A	206	SER	2.3
1	A	126	TYR	2.3
1	A	123	HIS	2.3
1	A	138	ILE	2.3
1	A	224	PRO	2.3
1	A	307	ALA	2.3
1	A	288	LEU	2.3
1	A	223	ARG	2.2
1	A	282	SER	2.2
1	A	92	THR	2.2
1	A	211	SER	2.2
1	A	234	GLN	2.2
1	A	356	TYR	2.2
1	A	229	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	314	TYR	2.1
1	A	257	LYS	2.1
1	A	266	PRO	2.1
1	A	312	GLU	2.1
1	A	116	THR	2.1
1	A	310	TYR	2.1
1	A	328	LYS	2.1
1	A	212	VAL	2.1
1	A	344	LEU	2.0
1	A	221	SER	2.0
1	A	7	ALA	2.0
1	A	172	ALA	2.0
1	A	298	LYS	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 oligosaccharides 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.