



Full wwPDB X-ray Structure Validation Report

Jun 6, 2014 – 08:23 AM EDT

PDB ID : 4N4S
Title : A Double Mutant Rat Erk2 in Complex With a Pyrazolo[3,4-d]pyrimidine Inhibitor
Authors : Hari, S.B.; Maly, D.J.; Merritt, E.A.
Deposited on : 2013-10-08
Resolution : 2.20 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>

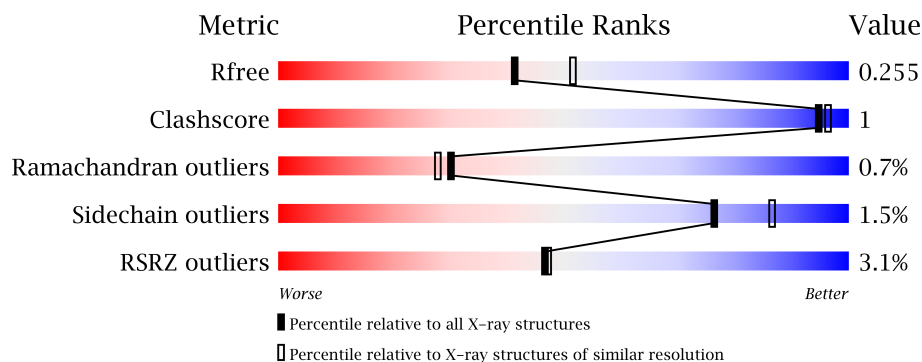
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : **FAILED**
Xtriage (Phenix) : dev-1439
EDS : stable23161
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) : stable23161

1 Overall quality at a glance

The reported resolution of this entry is 2.20 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	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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	359	
1	B	359	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 5659 atoms, of which 0 are 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.

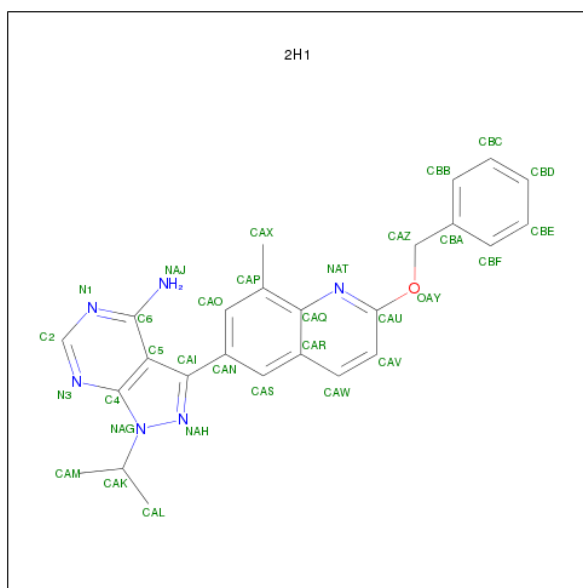
- Molecule 1 is a protein called Mitogen-activated protein kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2778	1789	470	505	14			
1	B	337	Total	C	N	O	S	0	1	0
			2734	1763	466	490	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	ALA	GLN	ENGINEERED MUTATION	UNP P63086
A	164	LEU	CYS	ENGINEERED MUTATION	UNP P63086
B	103	ALA	GLN	ENGINEERED MUTATION	UNP P63086
B	164	LEU	CYS	ENGINEERED MUTATION	UNP P63086

- Molecule 2 is 3-[2-(BENZYLOXY)-8-METHYLQUINOLIN-6-YL]-1-(PROPAN-2-YL)-1H-PYRAZOLO[3,4-D]PYRIMIDIN-4-AMINE (three-letter code: 2H1) (formula: C₂₅H₂₄N₆O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			32	25	6	1		
2	B	1	Total	C	N	O	0	0
			32	25	6	1		

- Molecule 3 is water.

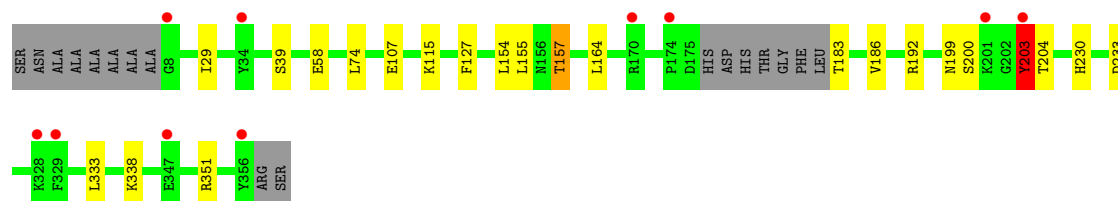
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	48	Total	O	0	0
			48	48		
3	B	35	Total	O	0	0
			35	35		

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.

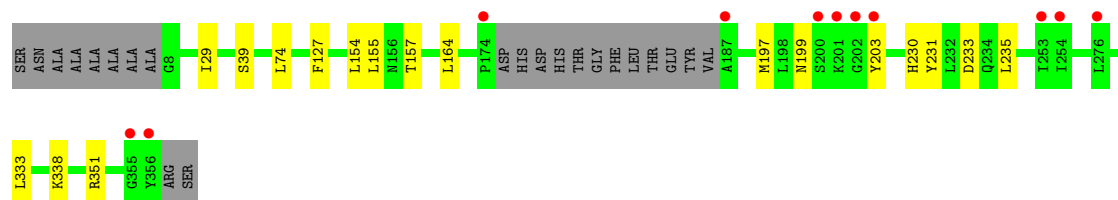
- Molecule 1: Mitogen-activated protein kinase 1

Chain A: 



- Molecule 1: Mitogen-activated protein kinase 1

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	46.09Å 57.63Å 68.00Å 86.57° 88.98° 81.05°	Depositor
Resolution (Å)	56.90 – 2.20 45.53 – 2.20	Depositor EDS
% Data completeness (in resolution range)	79.8 (56.90-2.20) 79.8 (45.53-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.221 , 0.253 0.227 , 0.255	Depositor DCC
R_{free} test set	1400 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 27933 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5659	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.77% 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: 2H1

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	0.34	0/2844	0.54	0/3856
1	B	0.33	0/2802	0.53	0/3797
All	All	0.33	0/5646	0.53	0/7653

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	2778	0	2779	9	0
1	B	2734	0	2752	7	0
2	A	32	0	0	0	0
2	B	32	0	0	0	0
3	A	48	0	0	1	0
3	B	35	0	0	0	0
All	All	5659	0	5531	16	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 1.

All (16) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:74:LEU:HD22	1:B:351:ARG:NH1	2.26	0.51
1:A:74:LEU:HD22	1:A:351:ARG:NH1	2.26	0.50
1:A:186:VAL:HG21	1:A:192:ARG:NH2	2.28	0.49
1:A:29:ILE:HD11	1:A:39:SER:HB3	1.94	0.49
1:B:197:MET:CE	1:B:235:LEU:HG	2.44	0.48
1:B:29:ILE:HD11	1:B:39:SER:HB3	1.96	0.47
1:A:115:LYS:HE2	3:A:511:HOH:O	2.15	0.46
1:B:127:PHE:CE1	1:B:155:LEU:HD22	2.52	0.45
1:B:197:MET:O	1:B:231:TYR:OH	2.35	0.44
1:A:127:PHE:CE1	1:A:155:LEU:HD22	2.53	0.43
1:A:107:GLU:HG3	1:A:157:THR:HG23	2.00	0.43
1:B:230:HIS:CE1	1:B:233:ASP:HB2	2.54	0.42
1:A:154:LEU:HG	1:A:164:LEU:HD11	2.01	0.42
1:A:203:TYR:HB3	1:A:204:THR:HG23	2.01	0.42
1:A:230:HIS:CE1	1:A:233:ASP:HB2	2.54	0.42
1:B:154:LEU:HG	1:B:164:LEU:HD11	2.01	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	338/359 (94%)	326 (96%)	9 (3%)	3 (1%)	25	21
1	B	334/359 (93%)	323 (97%)	9 (3%)	2 (1%)	33	32
All	All	672/718 (94%)	649 (97%)	18 (3%)	5 (1%)	30	28

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	TYR
1	A	338	LYS
1	B	338	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	199	ASN
1	B	199	ASN

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	305/318 (96%)	299 (98%)	6 (2%)	68	79
1	B	300/318 (94%)	297 (99%)	3 (1%)	85	93
All	All	605/636 (95%)	596 (98%)	9 (2%)	76	86

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	GLU
1	A	157	THR
1	A	183	THR
1	A	200	SER
1	A	203	TYR
1	A	333	LEU
1	B	157	THR
1	B	203	TYR
1	B	333	LEU

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

Mol	Chain	Res	Type
1	A	45	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

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	342/359 (95%)	-0.01	10 (2%) 49 50	23, 38, 83, 141	0
1	B	337/359 (93%)	0.12	11 (3%) 44 45	26, 44, 73, 102	0
All	All	679/718 (94%)	0.05	21 (3%) 47 47	23, 42, 76, 141	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	201	LYS	11.0
1	B	356	TYR	7.3
1	A	201	LYS	4.4
1	A	203	TYR	4.0
1	B	200	SER	3.6
1	B	174	PRO	3.6
1	A	174	PRO	3.2
1	B	203	TYR	3.0
1	A	34	TYR	3.0
1	B	355	GLY	2.8
1	B	253	ILE	2.8
1	A	8	GLY	2.7
1	A	170	ARG	2.6
1	B	187	ALA	2.5
1	A	347	GLU	2.4
1	B	202	GLY	2.4
1	B	276	LEU	2.4
1	A	329	PHE	2.2
1	A	356	TYR	2.2
1	A	328	LYS	2.1
1	B	254	ILE	2.1

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
2	2H1	A	401	32/32	0.12	-0.24	26,31,45,45	0
2	2H1	B	401	32/32	0.12	-0.38	32,34,39,40	0

6.5 Other polymers

There are no such residues in this entry.