wwPDB X-ray Structure Validation Summary Report (i)

Jun 18, 2024 – 10:58 AM EDT

PDB ID	:	4M8T
Title	:	RSK2 T493M C-Terminal Kinase Domain in complex with 3-(3-(1H-pyrazol-4-yl)phenyl)-2-cyanoacrylamide
Authors	:	Miller, R.M.; Taunton, J.
Deposited on	:	2013-08-13
Resolution	:	3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

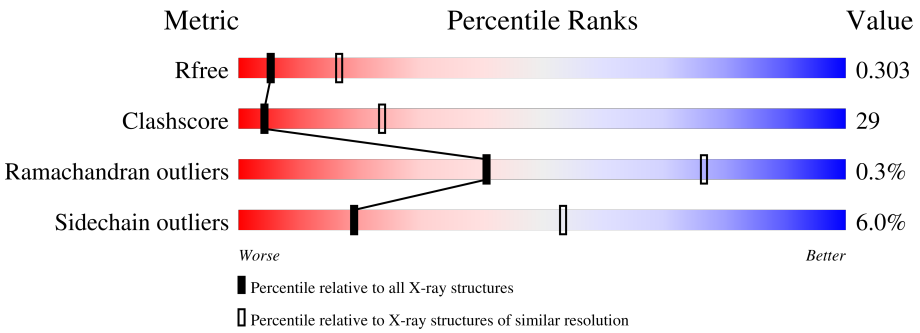
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	355	47% 35% • 15%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4717 atoms, of which 2328 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.

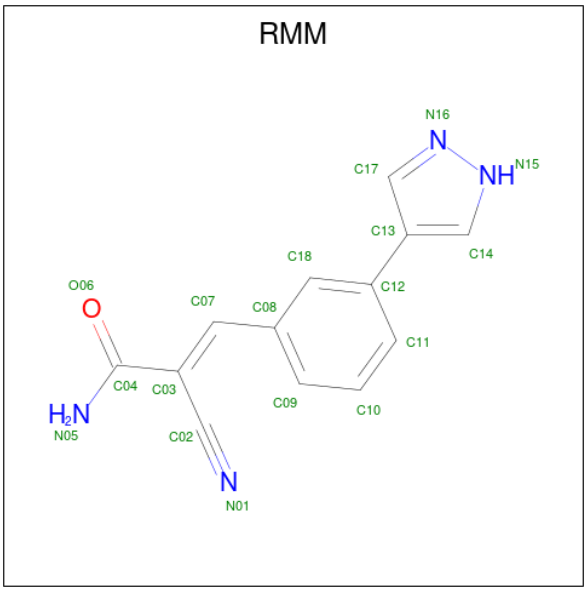
- Molecule 1 is a protein called Ribosomal protein S6 kinase alpha-3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	303	4688	1510	2318	403	445	12	0	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	386	ALA	-	EXPRESSION TAG	UNP P18654
A	387	HIS	-	EXPRESSION TAG	UNP P18654
A	388	HIS	-	EXPRESSION TAG	UNP P18654
A	389	HIS	-	EXPRESSION TAG	UNP P18654
A	390	HIS	-	EXPRESSION TAG	UNP P18654
A	391	HIS	-	EXPRESSION TAG	UNP P18654
A	392	HIS	-	EXPRESSION TAG	UNP P18654
A	393	VAL	-	EXPRESSION TAG	UNP P18654
A	394	ASP	-	EXPRESSION TAG	UNP P18654
A	395	ASP	-	EXPRESSION TAG	UNP P18654
A	396	ASP	-	EXPRESSION TAG	UNP P18654
A	397	ASP	-	EXPRESSION TAG	UNP P18654
A	398	LYS	-	EXPRESSION TAG	UNP P18654
A	493	MET	THR	ENGINEERED MUTATION	UNP P18654
A	591	GLU	LYS	CONFLICT	UNP P18654

- Molecule 2 is (2E)-2-cyano-3-[3-(1H-pyrazol-4-yl)phenyl]prop-2-enamide (three-letter code: RMM) (formula: $C_{13}H_{10}N_4O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
2	A	1	28	13	10	4	1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

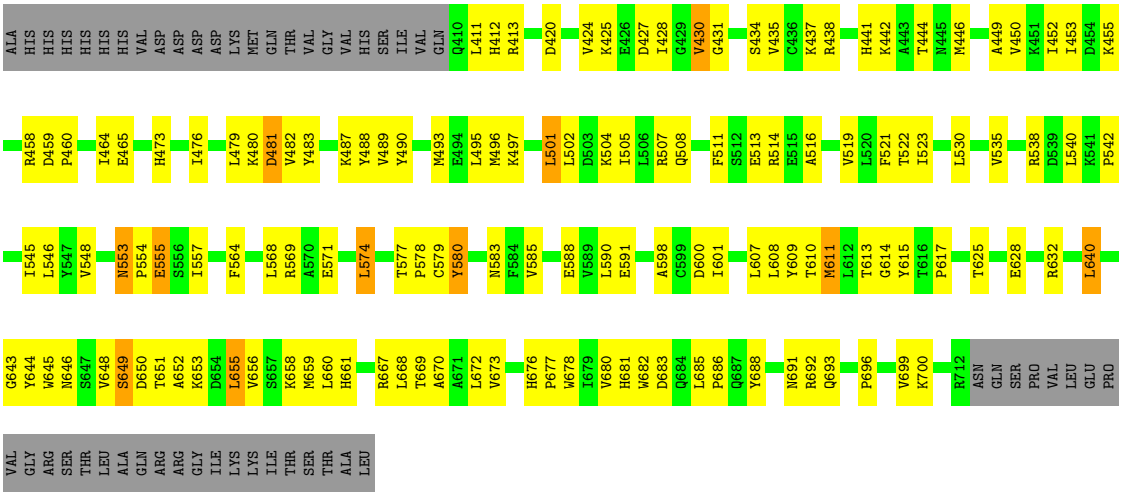
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
3	A	1	1	1	0	0

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: Ribosomal protein S6 kinase alpha-3

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	46.99Å 46.99Å 291.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.39 – 3.00 46.39 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.39-3.00) 79.8 (46.39-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.38 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.252 , 0.311 0.244 , 0.303	Depositor DCC
R_{free} test set	1038 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	-19.1	Xtriage
Anisotropy	-1.366	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 39.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.37	EDS
Total number of atoms	4717	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] 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.

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: RMM, NA

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	0.29	0/2424	0.50	0/3291

There are no bond length outliers.

There are no bond angle outliers.

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	2370	2318	2305	136	3
2	A	18	10	9	3	0
3	A	1	0	0	0	0
All	All	2389	2328	2314	138	3

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 29.

The worst 5 of 138 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:430:VAL:CB	1:A:431:GLY:CA	2.53	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:VAL:CB	1:A:431:GLY:HA2	2.14	0.78
1:A:411:LEU:HA	1:A:412:HIS:HB2	1.70	0.73
1:A:452:ILE:HD12	1:A:490:TYR:CD2	2.25	0.71
1:A:585:VAL:HG11	1:A:590:LEU:HD21	1.74	0.70

All (3) 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:579:CYS:HG	1:A:579:CYS:HG[7_465]	1.08	0.52
1:A:579:CYS:SG	1:A:579:CYS:HG[7_465]	1.20	0.40
1:A:579:CYS:CB	1:A:579:CYS:HG[7_465]	1.48	0.12

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	301/355 (85%)	276 (92%)	24 (8%)	1 (0%)	41 76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	430	VAL

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	251/308 (82%)	236 (94%)	15 (6%)	19 53

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	574	LEU
1	A	655	LEU
1	A	580	TYR
1	A	700	LYS
1	A	649	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	583	ASN
1	A	646	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	RMM	A	801	1	17,19,19	3.91	7 (41%)	21,25,25	3.31	5 (23%)

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	RMM	A	801	1	-	7/13/14/14	0/2/2/2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	RMM	C07-C03	11.15	1.49	1.35
2	A	801	RMM	C10-C09	6.15	1.49	1.38
2	A	801	RMM	C18-C08	5.51	1.49	1.39
2	A	801	RMM	C11-C12	5.12	1.49	1.39
2	A	801	RMM	C04-N05	3.53	1.43	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	RMM	C07-C03-C02	-9.36	110.06	123.59
2	A	801	RMM	C07-C03-C04	-7.36	109.19	118.90
2	A	801	RMM	C02-C03-C04	-5.76	109.22	117.64
2	A	801	RMM	C08-C07-C03	-5.42	123.77	131.46
2	A	801	RMM	C03-C04-N05	3.48	120.03	117.28

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	RMM	C02-C03-C04-N05
2	A	801	RMM	C02-C03-C04-O06
2	A	801	RMM	C07-C03-C04-N05
2	A	801	RMM	C07-C03-C04-O06
2	A	801	RMM	C04-C03-C07-C08

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	RMM	3	0

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.