

Full wwPDB X-ray Structure Validation Report (i)

Sep 16, 2021 – 02:03 pm BST

PDB ID : 7ATV

Title: Structure of protein kinase ck2 catalytic subunit (csnk2a2 gene product) in

complex with the bivalent inhibitor KN2

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Deposited on : 2020-10-31

Resolution : 0.98 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

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

Xtriage (Phenix) : NOT EXECUTED

EDS : NOT EXECUTED

buster-report : 1.1.7 (2018)

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

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

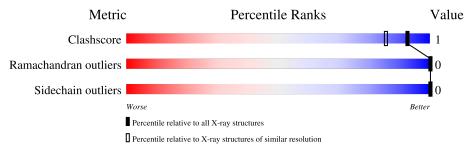
Validation Pipeline (wwPDB-VP) : 2.23.1

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 0.98 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	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{resolution range}(ext{Å}))$		
Clashscore	141614	1241 (1.06-0.90)		
Ramachandran outliers	138981	1159 (1.06-0.90)		
Sidechain outliers	138945	1161 (1.06-0.90)		

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain						
1	A	364	87%	•	10%				



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6633 atoms, of which 3083 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 Casein kinase II subunit alpha'.

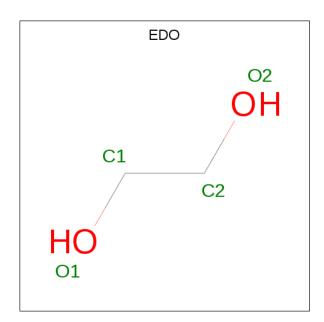
Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace	
1	Λ	328	Total	С	Η	N	О	S	0	60	0
1	А	320	6114	1947	3055	552	550	10			U

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP P19784
A	-12	GLY	-	expression tag	UNP P19784
A	-11	SER	-	expression tag	UNP P19784
A	-10	SER	-	expression tag	UNP P19784
A	-9	HIS	-	expression tag	UNP P19784
A	-8	HIS	-	expression tag	UNP P19784
A	-7	HIS	-	expression tag	UNP P19784
A	-6	HIS	-	expression tag	UNP P19784
A	-5	HIS	-	expression tag	UNP P19784
A	-4	HIS	-	expression tag	UNP P19784
A	-3	SER	-	expression tag	UNP P19784
A	-2	GLN	-	expression tag	UNP P19784
A	-1	ASP	=	expression tag	UNP P19784
A	0	PRO	=	expression tag	UNP P19784
A	336	SER	CYS	conflict	UNP P19784

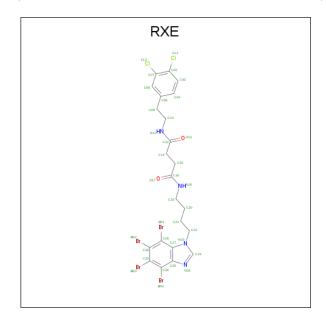
• Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	С	Н	0	0	0
			10	2	О	2		

• Molecule 3 is $\{N\}$ '-[2-(3,4-dichlorophenyl)ethyl]- $\{N\}$ -[4-[4,5,6,7-tetrakis(bromanyl)benzi midazol-1-yl]butyl]butanediamide (three-letter code: RXE) (formula: $C_{23}H_{22}Br_4Cl_2N_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues			Ato	oms				ZeroOcc	AltConf
2	Λ	1	Total	Br	С	Cl	Η	N	О	0	0
) 	A	1	57	4	23	2	22	4	2		U

• Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).



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

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	444	Total O 451 451	0	24

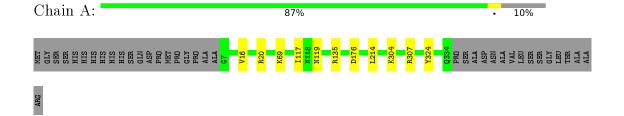


3 Residue-property plots (i)

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.

Note EDS was not executed.

• Molecule 1: Casein kinase II subunit alpha'





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source	
Space group	P 1	Depositor	
Cell constants	46.78Å 47.56Å 51.00Å	Depositor	
a, b, c, α , β , γ	66.80° 88.96° 88.75°	Depositor	
Resolution (Å)	33.28 - 0.98	Depositor	
% Data completeness	81.8 (33.28-0.98)	Depositor	
(in resolution range)	01.0 (99.20 0.90)	1	
R_{merge}	0.05	Depositor	
R_{sym}	0.05	Depositor	
Refinement program	PHENIX 1.18.2_3874	Depositor	
R, R_{free}	0.127 , 0.141	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	6633	wwPDB-VP	
Average B, all atoms (Å ²)	17.0	wwPDB-VP	



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: EDO, CL, RXE

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	Boı	nd lengths	Bond angles		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5	
1	Α	0.56	$1/3368 \ (0.0\%)$	0.73	1/4536 (0.0%)	

All (1) bond length outliers are listed below:

\mathbf{Mol}	Chain	Res	Type	Atoms	\mathbf{Z}	${ m Observed}({ m \AA})$	$\operatorname{Ideal}(ext{\AA})$
1	A	16	VAL	CB-CG1	-5.13	1.42	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
1	A	20	ARG	NE-CZ-NH1	5.29	122.94	120.30

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	3059	3055	2797	9	0
2	A	4	6	5	3	0
3	A	35	22	0	1	0
4	A	1	0	0	0	0
5	A	451	0	0	2	0
All	All	3550	3083	2802	9	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 1.

All (9) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{l} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{array}$	$egin{array}{c} { m Clash} \ { m overlap} \ ({ m \AA}) \end{array}$
1:A:176:ASP:HA	2:A:401:EDO:H21	1.63	0.78
1:A:214:LEU:CD1	5:A:700:HOH:O	2.56	0.53
1:A:304:LYS:HA	1:A:307[B]:ARG:HE	1.74	0.53
1:A:135:ARG:HG2	1:A:324:TYR:CZ	2.51	0.45
1:A:214:LEU:HD11	5:A:700:HOH:O	2.15	0.45
1:A:176:ASP:CA	2:A:401:EDO:H21	2.43	0.44
1:A:69:LYS:HD2	2:A:401:EDO:H22	1.99	0.43
1:A:117:ILE:O	3:A:402:RXE:BR2	2.92	0.43

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	$386/364 \ (106\%)$	377 (98%)	9 (2%)	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	$oxed{ Analysed} oxed{ Rotameric} oxed{ Outlie}$		Perce	${f ntiles}$
1	A	353/327 (108%)	353 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	Bo	ond leng	ths	В	ond ang	les
IV	101	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
	3	RXE	A	402	-	33,37,37	0.97	1 (3%)	40,51,51	1.15	4 (10%)
	2	EDO	A	401	_	3,3,3	1.28	1 (33%)	2,2,2	1.31	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
3	RXE	A	402	-	-	4/19/19/19	0/3/3/3
2	EDO	A	401	_	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	${ m Observed}({ m \AA})$	$\operatorname{Ideal}(ext{\AA})$
3	A	402	RXE	C16-N18	2.90	1.40	1.33
2	A	401	EDO	O2-C2	-2.02	1.31	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	${f Atoms}$	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
3	A	402	RXE	C30-C28-C27	-3.61	117.53	121.33
3	A	402	RXE	C15-C14-C12	3.58	118.83	112.56
3	A	402	RXE	C14-C15-C16	-2.62	107.96	112.56
3	A	402	RXE	BR2-C30-C28	-2.14	117.35	120.60

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	RXE	N18-C19-C20-C21
3	A	402	RXE	C20-C21-C22-N23
3	A	402	RXE	N11-C12-C14-C15
3	A	402	RXE	O13-C12-C14-C15
2	A	401	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	RXE	1	0
2	A	401	EDO	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the



average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

