wwPDB X-ray Structure Validation Summary Report (i)

May 16, 2020 – 01:33 pm BST

PDB ID	:	1CMK
Title	:	CRYSTAL STRUCTURES OF THE MYRISTYLATED CATALYTIC SUBUNIT OF CAMP-DEPENDENT PROTEIN KINASE REVEAL OPEN AND CLOSED CONFORMATIONS
Authors	:	Zheng, J.; Knighton, D.R.; Xuong, N.-H.; Taylor, S.S.; Sowadski, J.M.; Ten Eyck, L.F.
Deposited on	:	1993-11-18
Resolution	:	2.90 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 following versions of software and data (see references (i)) were used in the production of this report:

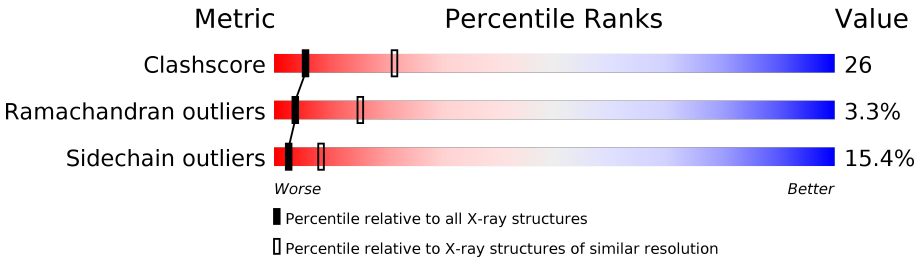
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.90 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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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 on 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	E	350	49% 35% 13% .
2	I	22	36% 27% 18% 9% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MYR	E	0	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3048 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 cAMP-DEPENDENT PROTEIN KINASE CATALYTIC SUBUNIT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	E	350	2874	1857	484	523	2	8	0	0	0

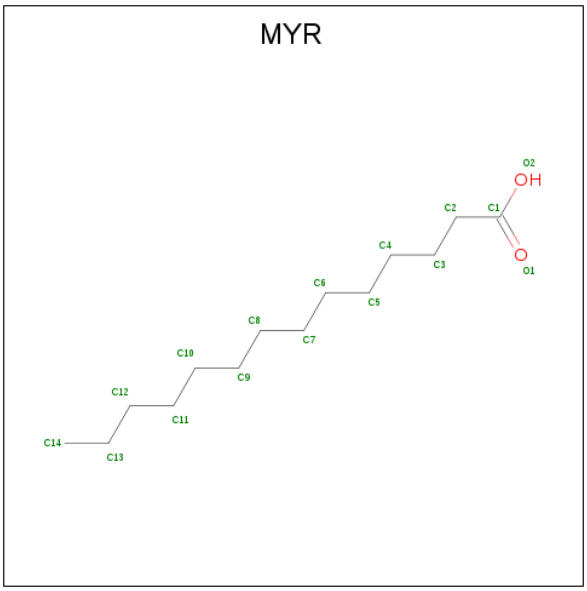
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	63	LYS	MET	CONFLICT	UNP P00517
E	69	PHE	TYR	CONFLICT	UNP P00517
E	108	TYR	PHE	CONFLICT	UNP P00517
E	286	ASP	ASN	CONFLICT	UNP P00517

- Molecule 2 is a protein called cAMP-dependent protein kinase inhibitor, alpha form.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	I	20	157	94	33	30	0	1	0

- Molecule 3 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C O 15 14 1	0	0

- Molecule 4 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	2	Total I 2 2	0	0

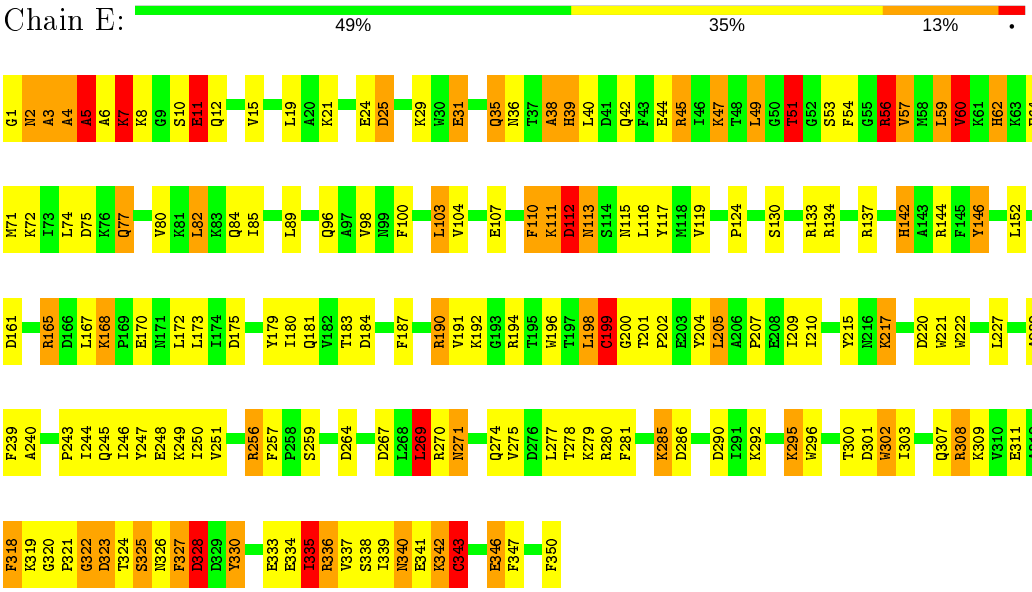
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

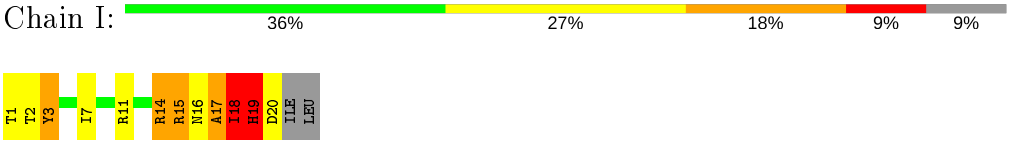
- Molecule 1: cAMP-DEPENDENT PROTEIN KINASE CATALYTIC SUBUNIT

Chain E:



- Molecule 2: cAMP-dependent protein kinase inhibitor, alpha form

Chain I:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, α, β, γ	171.52Å 171.52Å 171.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 2.0	Depositor
R, R_{free}	0.233 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3048	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, MYR, IOD, SEP

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	E	1.11	3/2924 (0.1%)	1.90	83/3936 (2.1%)
2	I	1.72	2/169 (1.2%)	3.32	18/227 (7.9%)
All	All	1.15	5/3093 (0.2%)	2.01	101/4163 (2.4%)

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	E	0	9
2	I	0	2
All	All	0	11

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	112	ASP	C-N	-12.94	1.04	1.34
2	I	19[A]	HIS	C-N	12.12	1.61	1.34
2	I	19[B]	HIS	C-N	12.12	1.61	1.34
1	E	292	LYS	C-N	5.75	1.47	1.34
1	E	5	ALA	C-N	5.36	1.46	1.34

The worst 5 of 101 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	19[A]	HIS	CA-C-N	-17.90	77.82	117.20
2	I	19[B]	HIS	CA-C-N	-17.90	77.82	117.20
2	I	18	ILE	O-C-N	-16.93	95.61	122.70
1	E	137	ARG	NE-CZ-NH2	-15.28	112.66	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	194	ARG	NE-CZ-NH1	14.32	127.46	120.30

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	110	PHE	Mainchain
1	E	112	ASP	Mainchain
1	E	31	GLU	Mainchain
1	E	39	HIS	Mainchain
1	E	5	ALA	Mainchain

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	E	2874	0	2851	151	0
2	I	157	0	146	12	0
3	E	15	0	27	15	0
4	I	2	0	0	0	0
All	All	3048	0	3024	156	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 26.

The worst 5 of 156 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:E:2:ASN:HB3	1:E:301:ASP:HA	1.10	1.09
1:E:303:ILE:HD12	3:E:0:MYR:C5	1.80	1.09
1:E:318:PHE:CD2	1:E:324:THR:CG2	2.39	1.05
1:E:303:ILE:CG2	3:E:0:MYR:H52	1.86	1.03
1:E:318:PHE:CD2	1:E:324:THR:HG23	1.93	1.03

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	E	346/350 (99%)	318 (92%)	19 (6%)	9 (3%)	5 20
2	I	19/22 (86%)	14 (74%)	1 (5%)	4 (21%)	0 0
All	All	365/372 (98%)	332 (91%)	20 (6%)	13 (4%)	4 14

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	4	ALA
1	E	328	ASP
1	E	330	TYR
1	E	343	CYS
2	I	18	ILE

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	E	303/303 (100%)	256 (84%)	47 (16%)	2 8
2	I	16/17 (94%)	14 (88%)	2 (12%)	4 14
All	All	319/320 (100%)	270 (85%)	49 (15%)	2 8

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	130	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	191	VAL
1	E	342	LYS
1	E	165	ARG
1	E	198	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	113	ASN
1	E	181	GLN
1	E	142	HIS
1	E	62	HIS
1	E	158	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	SEP	E	338	1	8,9,10	1.29	1 (12%)	8,12,14	1.94	3 (37%)
1	TPO	E	197	1	8,10,11	1.10	1 (12%)	10,14,16	1.31	1 (10%)

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
1	SEP	E	338	1	-	4/5/8/10	-
1	TPO	E	197	1	-	2/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	338	SEP	P-O3P	3.15	1.67	1.54
1	E	197	TPO	P-O2P	-2.49	1.45	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	197	TPO	O2P-P-O1P	3.08	122.76	110.68
1	E	338	SEP	O2P-P-O1P	2.93	122.16	110.68
1	E	338	SEP	OG-CB-CA	-2.75	105.47	108.14
1	E	338	SEP	P-OG-CB	2.69	125.72	118.30

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	338	SEP	CB-OG-P-O2P
1	E	338	SEP	CB-OG-P-O3P
1	E	338	SEP	N-CA-CB-OG
1	E	338	SEP	CB-OG-P-O1P
1	E	197	TPO	CB-OG1-P-O3P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	338	SEP	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are 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	$\#\|Z\| > 2$
3	MYR	E	0	1	14,14,15	0.81	1 (7%)	13,13,15	1.72	2 (15%)

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	MYR	E	0	1	-	8/11/12/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	0	MYR	O1-C1	-2.63	1.04	1.19

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	0	MYR	O1-C1-C2	-4.84	95.13	126.89
3	E	0	MYR	C5-C4-C3	-2.13	103.62	114.42

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	0	MYR	C1-C2-C3-C4
3	E	0	MYR	C5-C6-C7-C8
3	E	0	MYR	C2-C3-C4-C5
3	E	0	MYR	C4-C5-C6-C7
3	E	0	MYR	C11-C10-C9-C8

There are no ring outliers.

1 monomer is involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	0	MYR	15	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	I	1
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	19:HIS	C	20:ASP	N	1.61
1	E	112:ASP	C	113:ASN	N	1.04

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.