Full wwPDB X-ray Structure Validation Report (i)

May 29, 2024 – 12:56 PM EDT

PDB ID	:	2CPK
Title	:	CRYSTAL STRUCTURE OF THE CATALYTIC SUBUNIT OF CYCLIC ADENOSINE MONOPHOSPHATE-DEPENDENT PROTEIN KINASE
Authors	:	Knighton, D.R.; Zheng, J.; Teneyck, L.F.; Ashford, V.A.; Xuong, N.-H.; Taylor, S.S.; Sowadski, J.M.
Deposited on	:	1992-10-21
Resolution	:	2.70 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 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:

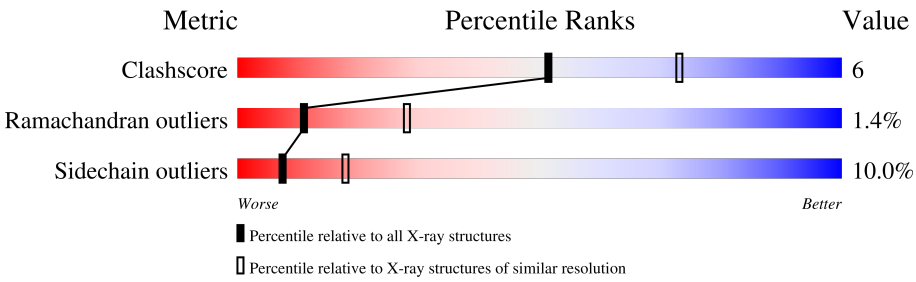
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.70 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	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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	E	350	69% 23% . . .
2	I	20	70% 30%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2822 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	336	2665	1732	439	483	3	8	0	0	0

- Molecule 2 is a protein called PEPTIDE INHIBITOR 20-MER.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	I	20	157	94	32	31	0	0	0

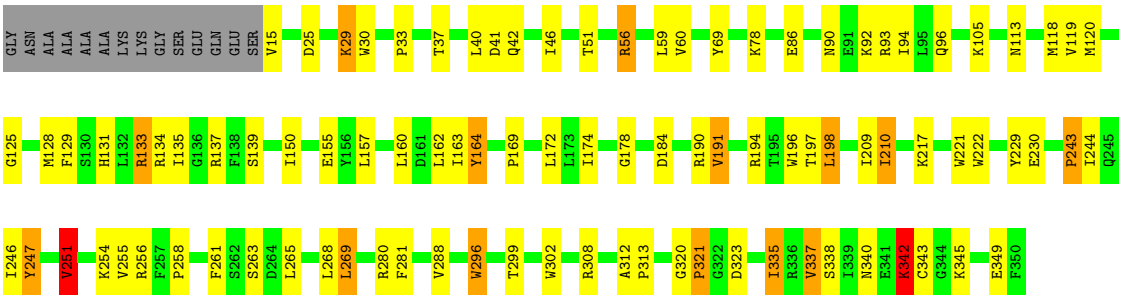
3 Residue-property plots (i)

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.

Note EDS was not executed.

• Molecule 1: cAMP-DEPENDENT PROTEIN KINASE, CATALYTIC SUBUNIT

Chain E: 69% 23% • • •



• Molecule 2: PEPTIDE INHIBITOR 20-MER

Chain I: 70% 30%

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.62Å 76.52Å 80.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2822	wwPDB-VP
Average B, all atoms ($Å^2$)	19.0	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: SEP, TPO

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	1.05	5/2702 (0.2%)	1.79	55/3662 (1.5%)
2	I	0.95	0/159	2.06	7/212 (3.3%)
All	All	1.04	5/2861 (0.2%)	1.81	62/3874 (1.6%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	256	ARG	NE-CZ	6.59	1.41	1.33
1	E	256	ARG	CZ-NH2	5.87	1.40	1.33
1	E	194	ARG	CZ-NH2	5.81	1.40	1.33
1	E	196	TRP	CG-CD2	-5.03	1.35	1.43
1	E	256	ARG	CZ-NH1	5.00	1.39	1.33

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	133	ARG	NE-CZ-NH1	15.51	128.06	120.30
1	E	133	ARG	NE-CZ-NH2	-12.09	114.25	120.30
1	E	247	TYR	CB-CG-CD2	-10.66	114.60	121.00
1	E	93	ARG	NE-CZ-NH1	8.64	124.62	120.30
2	I	7	TYR	CB-CG-CD2	-8.48	115.91	121.00
1	E	256	ARG	NE-CZ-NH2	8.38	124.49	120.30
1	E	164	TYR	CA-C-N	8.10	135.02	117.20
1	E	137	ARG	NE-CZ-NH2	-8.09	116.26	120.30
1	E	308	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	E	93	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	E	221	TRP	CE2-CD2-CG	-7.43	101.36	107.30
1	E	221	TRP	CG-CD2-CE3	7.25	140.42	133.90
2	I	23	HIS	CA-C-N	-7.19	101.37	117.20
1	E	118	MET	CG-SD-CE	-7.15	88.76	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	296	TRP	CE2-CD2-CG	-6.95	101.74	107.30
1	E	56	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	E	221	TRP	CD1-CG-CD2	6.76	111.71	106.30
2	I	18	ARG	NE-CZ-NH1	6.73	123.66	120.30
1	E	302	TRP	CD1-CG-CD2	6.69	111.65	106.30
1	E	337	VAL	CG1-CB-CG2	-6.57	100.39	110.90
1	E	196	TRP	CE2-CD2-CG	-6.54	102.07	107.30
1	E	190	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	E	296	TRP	CD1-CG-CD2	6.47	111.48	106.30
1	E	30	TRP	CE2-CD2-CG	-6.39	102.19	107.30
1	E	302	TRP	CE2-CD2-CG	-6.37	102.20	107.30
1	E	221	TRP	CB-CG-CD1	-6.32	118.78	127.00
1	E	191	VAL	CB-CA-C	-6.28	99.47	111.40
2	I	23	HIS	O-C-N	6.28	132.74	122.70
1	E	134	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	E	196	TRP	CD1-CG-CD2	6.15	111.22	106.30
1	E	30	TRP	CD1-CG-CD2	6.13	111.21	106.30
1	E	254	LYS	N-CA-C	-6.10	94.52	111.00
1	E	191	VAL	CG1-CB-CG2	-6.08	101.17	110.90
1	E	343	CYS	CA-CB-SG	-5.97	103.25	114.00
1	E	247	TYR	CB-CG-CD1	5.96	124.58	121.00
1	E	296	TRP	CG-CD2-CE3	5.96	139.26	133.90
1	E	198	LEU	CA-CB-CG	5.89	128.86	115.30
1	E	30	TRP	CG-CD2-CE3	5.89	139.20	133.90
1	E	137	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	E	86	GLU	O-C-N	-5.72	113.55	122.70
1	E	280	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	E	46	ILE	CA-C-N	5.70	129.74	117.20
1	E	280	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	E	222	TRP	CE2-CD2-CG	-5.67	102.76	107.30
1	E	164	TYR	O-C-N	-5.66	113.65	122.70
1	E	342	LYS	CA-C-N	5.55	129.42	117.20
1	E	229	TYR	CB-CG-CD2	-5.52	117.69	121.00
2	I	19	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	E	46	ILE	O-C-N	-5.44	114.00	122.70
1	E	256	ARG	NH1-CZ-NH2	-5.35	113.52	119.40
2	I	7	TYR	CG-CD1-CE1	-5.28	117.07	121.30
1	E	229	TYR	CG-CD2-CE2	-5.28	117.08	121.30
2	I	8	ALA	CB-CA-C	-5.28	102.18	110.10
1	E	342	LYS	O-C-N	-5.28	114.26	122.70
1	E	251	VAL	N-CA-CB	-5.25	99.95	111.50
1	E	222	TRP	CD1-CG-CD2	5.17	110.43	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	296	TRP	CB-CG-CD1	-5.16	120.29	127.00
1	E	92	LYS	CA-CB-CG	-5.15	102.06	113.40
1	E	86	GLU	CA-C-N	5.11	128.44	117.20
1	E	78	LYS	CA-CB-CG	5.08	124.58	113.40
1	E	198	LEU	CB-CG-CD1	-5.03	102.45	111.00
1	E	335	ILE	N-CA-C	-5.01	97.47	111.00

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	E	2665	0	2532	31	0
2	I	157	0	146	0	0
All	All	2822	0	2678	31	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 6.

All (31) 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:155:GLU:HG3	1:E:288:VAL:HG11	1.60	0.84
1:E:243:PRO:HA	1:E:246:ILE:HD12	1.67	0.76
1:E:198:LEU:HD23	1:E:209:ILE:HG22	1.75	0.69
1:E:210:ILE:HD13	1:E:247:TYR:HB3	1.72	0.68
1:E:125:GLY:HA3	1:E:174:ILE:O	2.04	0.57
1:E:131:HIS:HB3	1:E:135:ILE:HD12	1.89	0.54
1:E:105:LYS:O	1:E:120:MET:HB2	2.11	0.50
1:E:128:MET:HE3	1:E:172:LEU:HB2	1.93	0.49
1:E:258:PRO:HG2	1:E:261:PHE:CE1	2.48	0.49
1:E:244:ILE:H	1:E:244:ILE:HD12	1.78	0.48
1:E:33:PRO:HA	1:E:96:GLN:OE1	2.14	0.48
1:E:69:TYR:HB3	1:E:119:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:ASP:O	1:E:29:LYS:HG2	2.14	0.47
1:E:191:VAL:HG23	1:E:191:VAL:O	2.15	0.47
1:E:210:ILE:HD11	1:E:251:VAL:HG21	1.97	0.46
1:E:342:LYS:HD3	1:E:342:LYS:HA	1.71	0.46
1:E:163:ILE:HD13	1:E:163:ILE:HG21	1.61	0.44
1:E:56:ARG:HG2	1:E:56:ARG:NH1	2.33	0.43
1:E:56:ARG:HG2	1:E:56:ARG:HH11	1.83	0.43
1:E:243:PRO:O	1:E:246:ILE:HB	2.19	0.42
1:E:265:LEU:HG	1:E:269:LEU:HD22	2.02	0.42
1:E:90:ASN:O	1:E:94:ILE:HD12	2.19	0.42
1:E:340:ASN:HB2	1:E:342:LYS:NZ	2.35	0.42
1:E:320:GLY:O	1:E:323:ASP:HB2	2.20	0.42
1:E:29:LYS:HG2	1:E:29:LYS:H	1.69	0.41
1:E:157:LEU:HD13	1:E:164:TYR:HB2	2.02	0.41
1:E:150:ILE:HD11	1:E:172:LEU:HD22	2.01	0.41
1:E:129:PHE:CE1	1:E:133:ARG:NH1	2.89	0.40
1:E:312:ALA:HA	1:E:313:PRO:HD3	1.92	0.40
1:E:133:ARG:NH2	1:E:230:GLU:OE2	2.55	0.40
1:E:178:GLY:HA3	1:E:312:ALA:HB1	2.02	0.40

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	331/350 (95%)	312 (94%)	14 (4%)	5 (2%)	10 26
2	I	18/20 (90%)	18 (100%)	0	0	100 100
All	All	349/370 (94%)	330 (95%)	14 (4%)	5 (1%)	11 28

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	184	ASP
1	E	217	LYS
1	E	321	PRO
1	E	41	ASP
1	E	342	LYS

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	264/302 (87%)	237 (90%)	27 (10%)	7 17
2	I	15/15 (100%)	14 (93%)	1 (7%)	16 37
All	All	279/317 (88%)	251 (90%)	28 (10%)	7 18

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	15	VAL
1	E	29	LYS
1	E	37	THR
1	E	40	LEU
1	E	42	GLN
1	E	51	THR
1	E	59	LEU
1	E	60	VAL
1	E	113	ASN
1	E	160	LEU
1	E	162	LEU
1	E	169	PRO
1	E	210	ILE
1	E	243	PRO
1	E	251	VAL
1	E	255	VAL
1	E	263	SER
1	E	268	LEU
1	E	269	LEU

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Mol	Chain	Res	Type
1	E	281	PHE
1	E	296	TRP
1	E	299	THR
1	E	321	PRO
1	E	335	ILE
1	E	337	VAL
1	E	345	LYS
1	E	349	GLU
2	I	22	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	62	HIS
1	E	158	HIS
1	E	242	GLN
1	E	245	GLN
1	E	307	GLN
2	I	20	ASN
2	I	23	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)

3 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	139	1	8,9,10	0.92	0	8,12,14	2.50	3 (37%)
1	TPO	E	197	1	8,10,11	1.59	2 (25%)	10,14,16	1.58	2 (20%)

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	0.85	0	8,12,14	3.09	3 (37%)

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	139	1	-	0/5/8/10	-
1	TPO	E	197	1	-	1/9/11/13	-
1	SEP	E	338	1	-	2/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	197	TPO	P-OG1	-2.95	1.53	1.59
1	E	197	TPO	P-O2P	-2.23	1.46	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	338	SEP	OG-CB-CA	7.65	115.59	108.14
1	E	139	SEP	OG-CB-CA	5.46	113.46	108.14
1	E	197	TPO	O-C-CA	-3.05	116.79	124.78
1	E	338	SEP	O3P-P-OG	-2.79	99.30	106.73
1	E	139	SEP	O2P-P-OG	-2.65	99.67	106.73
1	E	139	SEP	O3P-P-O2P	2.25	116.25	107.64
1	E	338	SEP	O3P-P-O2P	2.13	115.77	107.64
1	E	197	TPO	OG1-P-O1P	-2.03	101.56	109.39

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	197	TPO	O-C-CA-CB
1	E	338	SEP	N-CA-CB-OG
1	E	338	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides 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 (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.