



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 27, 2016 – 11:14 AM EDT

PDB ID : 5IDM  
Title : Bifunctional histidine kinase CckA (domain, CA) in complex with c-di-GMP and AMPPNP/Mg2+  
Authors : Dubey, B.N.; Schirmer, T.  
Deposited on : 2016-02-24  
Resolution : 1.90 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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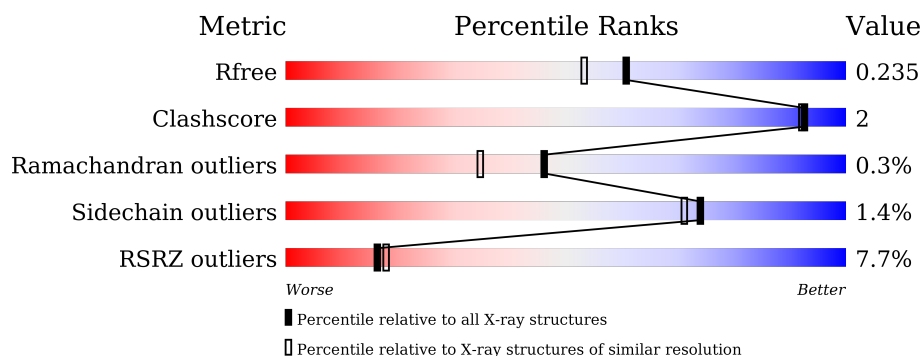
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

i

## X-RAY DIFFRACTION

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.



<b>Metric</b>	<b>Whole archive (#Entries)</b>	<b>Similar resolution (#Entries, resolution range(Å))</b>
$R_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	179	<div> <div>6%</div> <div>93%</div> <div>• •</div> </div>
1	B	179	<div> <div>9%</div> <div>88%</div> <div>9% •</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3251 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 Cell cycle histidine kinase CckA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	177	Total	C	N	O	S	16	0	0
			1365	863	246	254	2			
1	B	177	Total	C	N	O	S	32	0	0
			1370	865	249	254	2			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	548	ALA	-	expression tag	UNP Q9X688
A	549	LEU	-	expression tag	UNP Q9X688
A	550	GLU	-	expression tag	UNP Q9X688
A	551	HIS	-	expression tag	UNP Q9X688
A	552	HIS	-	expression tag	UNP Q9X688
A	553	HIS	-	expression tag	UNP Q9X688
A	554	HIS	-	expression tag	UNP Q9X688
A	555	HIS	-	expression tag	UNP Q9X688
A	556	HIS	-	expression tag	UNP Q9X688
B	548	ALA	-	expression tag	UNP Q9X688
B	549	LEU	-	expression tag	UNP Q9X688
B	550	GLU	-	expression tag	UNP Q9X688
B	551	HIS	-	expression tag	UNP Q9X688
B	552	HIS	-	expression tag	UNP Q9X688
B	553	HIS	-	expression tag	UNP Q9X688
B	554	HIS	-	expression tag	UNP Q9X688
B	555	HIS	-	expression tag	UNP Q9X688
B	556	HIS	-	expression tag	UNP Q9X688

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).

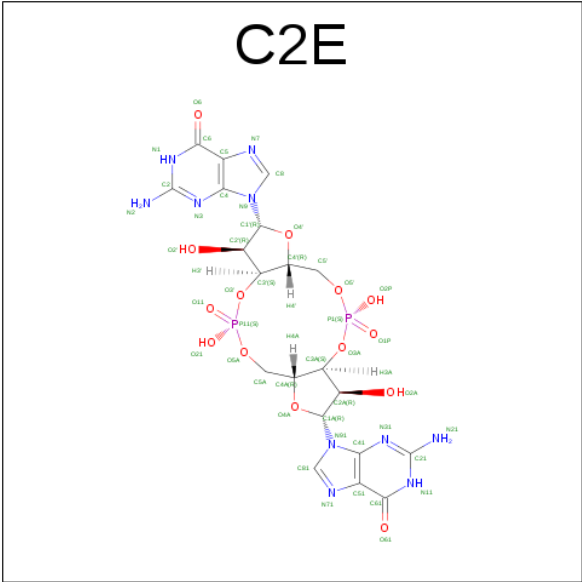


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	B	1	Total 31	C 10	N 6	O 12	P 3	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydroxy-5,12-dioxidoctahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclododecine-2,9-diyl]bis(2-amino-1,9-dihydro-6H-purin-6-one) (three-letter code: C2E) (formula: C<sub>20</sub>H<sub>24</sub>N<sub>10</sub>O<sub>14</sub>P<sub>2</sub>).



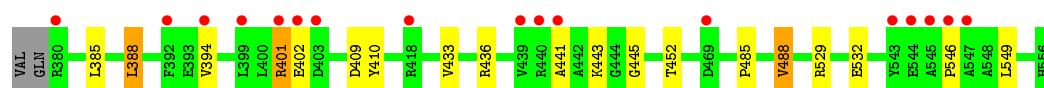
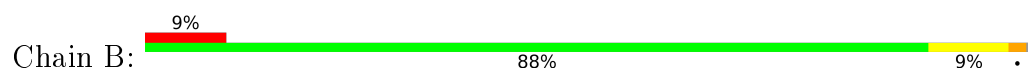
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Cell cycle histidine kinase CckA



- Molecule 1: Cell cycle histidine kinase CckA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.28 Å 62.11 Å 103.89 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 29.75 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-1.90) 99.0 (29.75-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.09 (at 1.91 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.194 , 0.229 0.200 , 0.235	Depositor DCC
$R_{free}$ test set	1492 reflections (5.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.9	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 43.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3251	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.08 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.1691e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP, C2E

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	0.72	2/1392 (0.1%)	0.85	6/1888 (0.3%)
1	B	1.00	4/1399 (0.3%)	0.90	6/1896 (0.3%)
All	All	0.87	6/2791 (0.2%)	0.88	12/3784 (0.3%)

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	A	0	2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	529	ARG	CB-CG	-23.19	0.90	1.52
1	B	441	ALA	C-N	-20.26	0.87	1.34
1	A	532	GLU	CB-CG	-18.68	1.16	1.52
1	B	532	GLU	CB-CG	-10.76	1.31	1.52
1	A	553	HIS	C-O	7.36	1.37	1.23

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	529	ARG	CA-CB-CG	13.11	142.25	113.40
1	B	441	ALA	O-C-N	-10.11	106.53	122.70
1	A	532	GLU	CA-CB-CG	9.92	135.22	113.40
1	B	441	ALA	CA-C-N	7.33	133.33	117.20
1	B	546	PRO	N-CA-CB	6.08	110.59	103.30



There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	553	HIS	Mainchain,Peptide

## 5.2 Too-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 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	1365	0	1357	7	4
1	B	1370	0	1352	7	4
2	A	31	0	13	0	0
2	B	31	0	13	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	46	0	22	0	0
5	A	223	0	0	2	0
5	B	183	0	0	1	0
All	All	3251	0	2757	11	4

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 2.

The worst 5 of 11 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:552:HIS:CD2	1:A:554:HIS:C	2.67	0.68
1:A:386:GLY:HA2	5:A:719:HOH:O	2.03	0.57
1:A:552:HIS:NE2	1:A:554:HIS:C	2.63	0.53
1:B:394:VAL:HG23	5:B:747:HOH:O	2.12	0.50
1:A:457:ARG:NH1	5:A:704:HOH:O	2.49	0.46

All (4) 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:529:ARG:NH2	1:B:402:GLU:CG[2_545]	1.70	0.50
1:A:529:ARG:NH2	1:B:401:ARG:O[2_545]	1.75	0.45
1:A:529:ARG:CZ	1:B:402:GLU:CG[2_545]	2.04	0.16
1:A:529:ARG:NE	1:B:402:GLU:CD[2_545]	2.05	0.15

## 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	175/179 (98%)	171 (98%)	4 (2%)	0	100	100
1	B	175/179 (98%)	169 (97%)	5 (3%)	1 (1%)	30	17
All	All	350/358 (98%)	340 (97%)	9 (3%)	1 (0%)	46	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	443	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	A	141/144 (98%)	140 (99%)	1 (1%)	88	88
1	B	141/144 (98%)	138 (98%)	3 (2%)	61	55
All	All	282/288 (98%)	278 (99%)	4 (1%)	74	71

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	532	GLU
1	B	388	LEU
1	B	401	ARG
1	B	488	VAL

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

Mol	Chain	Res	Type
1	A	551	HIS
1	B	525	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	ANP	A	601	3	29,33,33	2.01	9 (31%)	26,52,52	2.29	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	C2E	A	603	-	44,52,52	1.17	5 (11%)	50,82,82	2.14	14 (28%)
2	ANP	B	600	3	29,33,33	1.82	6 (20%)	26,52,52	2.01	4 (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
2	ANP	A	601	3	-	0/13/38/38	0/3/3/3
4	C2E	A	603	-	-	0/22/62/62	0/6/7/7
2	ANP	B	600	3	-	0/13/38/38	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	ANP	PG-O3G	-3.23	1.48	1.56
2	A	601	ANP	PB-O2B	-2.39	1.50	1.56
2	B	600	ANP	PG-O3G	-2.14	1.51	1.56
4	A	603	C2E	O4'-C1'	2.17	1.44	1.41
2	A	601	ANP	C2-N3	2.35	1.36	1.32

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	ANP	N3-C2-N1	-9.05	121.76	128.87
2	B	600	ANP	N3-C2-N1	-7.69	122.83	128.87
4	A	603	C2E	C51-C61-N11	-4.24	117.98	123.52
4	A	603	C2E	N3-C2-N1	-4.03	122.07	127.56
4	A	603	C2E	C5-C6-N1	-3.94	118.37	123.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	441:ALA	C	442:ALA	N	0.87

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	177/179 (98%)	0.45	10 (5%)	28 31	6, 14, 26, 49	3 (1%)
1	B	173/179 (96%)	0.56	17 (9%)	10 11	7, 14, 36, 52	2 (1%)
All	All	350/358 (97%)	0.51	27 (7%)	16 18	6, 14, 34, 52	5 (1%)

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	378	VAL	7.9
1	B	547	ALA	6.8
1	B	403	ASP	5.2
1	B	546	PRO	4.9
1	A	554	HIS	4.7

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ANP	B	600	31/31	0.98	0.07	-1.17	7,8,12,12	0
4	C2E	A	603	46/46	0.98	0.07	-1.20	6,7,7,8	0
2	ANP	A	601	31/31	0.98	0.08	-1.66	6,7,11,11	0
3	MG	A	602	1/1	0.98	0.06	-3.64	8,8,8,8	0
3	MG	B	601	1/1	0.99	0.04	-	12,12,12,12	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.