



# Full wwPDB X-ray Structure Validation Report

Mar 31, 2014 – 03:28 PM BST

PDB ID : 4CLS  
Title : Crystal structure of human soluble Adenylyl Cyclase with Pyrophosphate  
Authors : Kleinboelting, S.; Weyand, M.; Steegborn, C.  
Deposited on : 2014-01-15  
Resolution : 1.85 Å(reported)

This is a full wwPDB validation 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/ValidationPDFNotes.html>

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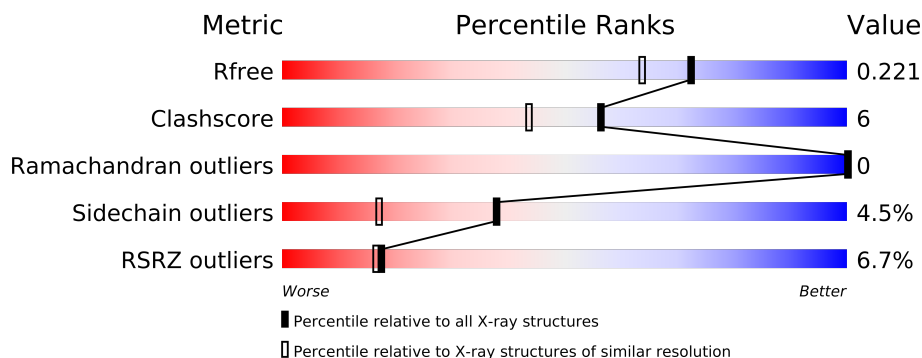
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable23004  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23004

# 1 Overall quality at a glance

The reported resolution of this entry is 1.85 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))
$R_{free}$	66092	1269 (1.86-1.86)
Clashscore	79885	1470 (1.86-1.86)
Ramachandran outliers	78287	1451 (1.86-1.86)
Sidechain outliers	78261	1451 (1.86-1.86)
RSRZ outliers	66119	1269 (1.86-1.86)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	475	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	GOL	A	1471	-	X
7	EDO	A	1473	-	X
7	EDO	A	1474	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3856 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ADENYLATE CYCLASE TYPE 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	0	6	0
			3665	2378	593	659	35			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	470	HIS	-	EXPRESSION TAG	UNP Q96PN6
A	471	HIS	-	EXPRESSION TAG	UNP Q96PN6
A	472	HIS	-	EXPRESSION TAG	UNP Q96PN6
A	473	HIS	-	EXPRESSION TAG	UNP Q96PN6
A	474	HIS	-	EXPRESSION TAG	UNP Q96PN6
A	475	HIS	-	EXPRESSION TAG	UNP Q96PN6

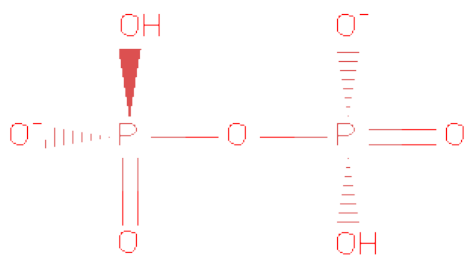
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: H<sub>2</sub>O<sub>7</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			9	7	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



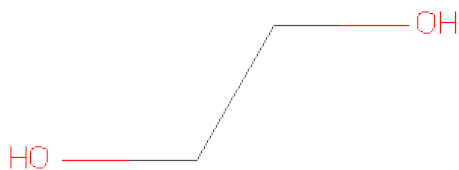
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	162	Total 162	O 162	0	0

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• Molecule 1: ADENYLATE CYCLASE TYPE 10

Figure 1: A schematic diagram of the human genome showing the distribution of 1000 Genomes Project samples across chromosomes 1-22, X, and Y. The diagram is organized into two main sections: the top section shows the distribution of samples by population (European, African, Asian, Admixed American, and Unlabeled), and the bottom section shows the distribution of samples by sex (Male and Female). Each chromosome is represented by a colored bar, and the number of samples for each population/sex is indicated by the length of the bar. The total number of samples is 1000.

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.09Å 100.09Å 97.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	86.68 – 1.85 48.88 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (86.68-1.85) 99.9 (48.88-1.85)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.174 , 0.214 0.186 , 0.221	Depositor DCC
$R_{free}$ test set	2371 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.1	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 38.8	EDS
Estimated twinning fraction	0.054 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 47385 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3856	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, CL, CME, EDO, POP, ACT

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	0.93	1/3760 (0.0%)	0.94	5/5088 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	405	THR	CB-CG2	-5.03	1.35	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	ASP	CB-CG-OD2	-9.77	109.50	118.30
1	A	290	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	A	418	MET	CG-SD-CE	-6.14	90.38	100.20
1	A	123	SER	CB-CA-C	5.33	120.23	110.10
1	A	303	ASP	CB-CG-OD1	5.04	122.84	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3665	0	0	22	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	9	0	0	2	0
5	A	6	0	8	1	0
6	A	4	0	3	0	0
7	A	8	0	12	3	0
8	A	162	0	0	7	0
All	All	3856	0	23	24	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (24) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:328:PHE:CD2	1:A:365[B]:CYS:SG	2.35	1.20
1:A:328:PHE:CG	1:A:365[B]:CYS:SG	2.38	1.17
1:A:328:PHE:CB	1:A:365[B]:CYS:SG	2.45	1.04
1:A:9:GLN:CB	8:A:2007:HOH:O	2.34	0.76
1:A:28:HIS:CE1	8:A:2023:HOH:O	2.59	0.55
1:A:300:MET:CE	8:A:2123:HOH:O	2.59	0.51
1:A:9:GLN:N	8:A:2007:HOH:O	2.45	0.49
7:A:1474:EDO:H21	8:A:2073:HOH:O	2.13	0.48
1:A:239:TYR:N	5:A:1471:GOL:HO2	2.13	0.47
1:A:402:HIS:CD2	8:A:2140:HOH:O	2.68	0.47
1:A:27:GLY:O	1:A:28:HIS:C	2.51	0.46
1:A:47:ASP:OD2	4:A:1470:POP:O3	2.32	0.45
7:A:1474:EDO:H12	8:A:2075:HOH:O	2.17	0.45
1:A:142:ARG:CD	1:A:142:ARG:N	2.80	0.45
1:A:288:GLU:OE2	1:A:351:PRO:CG	2.65	0.45
1:A:335:VAL:N	7:A:1474:EDO:HO1	2.15	0.44
1:A:290:ARG:NE	1:A:349:GLY:O	2.50	0.44
1:A:99:ASP:OD2	4:A:1470:POP:O6	2.37	0.43
1:A:302:GLU:OE1	1:A:302:GLU:N	2.52	0.43
1:A:30:SER:OG	1:A:32:GLU:CG	2.67	0.43
1:A:173:ASP:OD2	1:A:305:ASP:OD1	2.38	0.41
1:A:183:GLN:O	1:A:184:MET:C	2.57	0.41
1:A:320:HIS:NE2	1:A:368:ASP:OD1	2.54	0.41
1:A:210:GLN:CA	1:A:210:GLN:NE2	2.84	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	460/475 (97%)	447 (97%)	13 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	403/418 (96%)	385 (96%)	18 (4%)	38	17

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	51	PHE
1	A	142	ARG
1	A	154	MET
1	A	183	GLN
1	A	217	PHE
1	A	222	PRO
1	A	223	ASN
1	A	296	PHE
1	A	329	GLN
1	A	338	PHE
1	A	350	PHE
1	A	354	LYS
1	A	402	HIS
1	A	429	SER
1	A	447	LYS

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Mol	Chain	Res	Type
1	A	453	VAL
1	A	467	GLU

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

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	CME	A	253	1	9,9,10	4.60	2 (22%)	7,9,11	1.17	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
1	CME	A	253	1	-	0/6/8/10	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	CME	O-C	13.47	1.20	1.11
1	A	253	CME	CA-C	2.22	1.52	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\# Z  > 2$
4	POP	A	1470	2	8,8,8	0.88	0	13,13,13	1.37	2 (15%)
5	GOL	A	1471	-	5,5,5	1.08	0	5,5,5	1.20	1 (20%)
6	ACT	A	1472	-	1,3,3	1.40	0	0,3,3	0.00	-
7	EDO	A	1473	-	3,3,3	1.24	0	2,2,2	1.14	0
7	EDO	A	1474	-	3,3,3	1.09	0	2,2,2	0.81	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
4	POP	A	1470	2	-	0/6/6/6	0/0/0/0
5	GOL	A	1471	-	-	0/4/4/4	0/0/0/0
6	ACT	A	1472	-	-	0/0/0/0	0/0/0/0
7	EDO	A	1473	-	-	0/1/1/1	0/0/0/0
7	EDO	A	1474	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	A	1470	POP	O6-P2-O	-2.65	98.47	106.65
4	A	1470	POP	P2-O-P1	-2.62	123.86	131.74
5	A	1471	GOL	O2-C2-C3	2.04	117.53	108.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	459/475 (96%)	0.02	31 (6%) 17 16	15, 31, 68, 87	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	PHE	5.3
1	A	351	PRO	5.3
1	A	454	ALA	4.9
1	A	356	PRO	4.0
1	A	453	VAL	3.9
1	A	377	HIS	3.6
1	A	449	VAL	3.5
1	A	339	ASP	3.5
1	A	352	GLY	3.3
1	A	209	ASP	3.2
1	A	211	ARG	3.2
1	A	350	PHE	3.1
1	A	208	PRO	3.1
1	A	132	THR	3.0
1	A	451	LYS	2.9
1	A	328	PHE	2.9
1	A	338	PHE	2.9
1	A	303	ASP	2.8
1	A	329	GLN	2.7
1	A	130	PHE	2.7
1	A	142	ARG	2.7
1	A	5	LYS	2.5
1	A	141	ILE	2.5
1	A	51	PHE	2.3
1	A	185	ASN	2.3
1	A	436	ASN	2.2
1	A	340	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	223	ASN	2.2
1	A	302	GLU	2.1
1	A	7	GLU	2.0
1	A	466	THR	2.0

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

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	CME	A	253	10/11	0.06	-0.80	20,23,29,29	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	EDO	A	1474	4/4	0.21	6.46	34,37,47,51	0
7	EDO	A	1473	4/4	0.15	5.16	36,38,43,48	0
5	GOL	A	1471	6/6	0.14	3.37	30,34,40,45	0
4	POP	A	1470	9/9	0.20	1.92	66,75,85,94	0
6	ACT	A	1472	4/4	0.12	1.17	53,57,59,69	0
2	MG	A	1468	1/1	0.07	-1.23	55,55,55,55	0
3	CL	A	1469	1/1	0.08	-2.71	30,30,30,30	0



## 6.5 Other polymers ⓘ

There are no such residues in this entry.