



# Full wwPDB X-ray Structure Validation Report

Sep 24, 2014 – 12:06 PM EDT

PDB ID : 4NU0  
Title : Crystal structure of Adenylate kinase from Streptococcus pneumoniae with Ap5A  
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Deposited on : 2013-12-03  
Resolution : 1.49 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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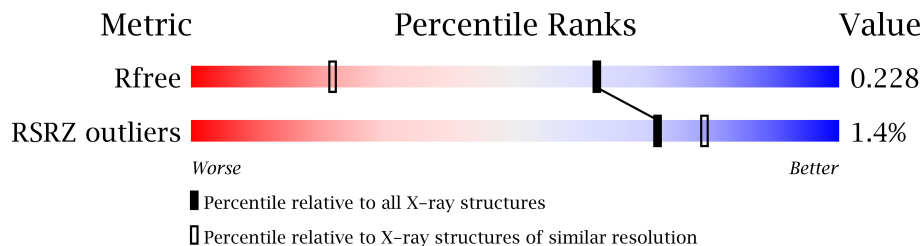
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : **FAILED**  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23489  
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) : stable23489

# 1 Overall quality at a glance

The reported resolution of this entry is 1.49 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	2222 (1.50-1.46)
RSRZ outliers	66119	2223 (1.50-1.46)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7376 atoms, of which 3340 are hydrogens 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 kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	212	Total	C	H	N	O	S	0	0	0
			3338	1048	1670	288	327	5			
1	B	212	Total	C	H	N	O	S	0	0	0
			3338	1048	1670	288	327	5			

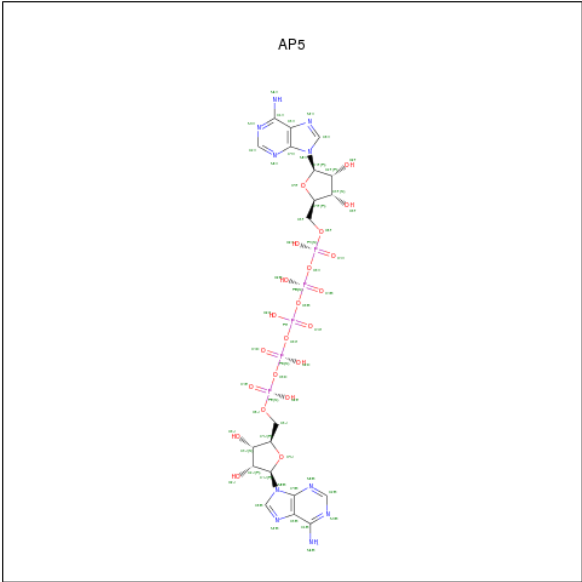
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	EXPRESSION TAG	UNP Q04ML5
A	-3	ALA	-	EXPRESSION TAG	UNP Q04ML5
A	-2	MET	-	EXPRESSION TAG	UNP Q04ML5
A	-1	GLY	-	EXPRESSION TAG	UNP Q04ML5
A	0	SER	-	EXPRESSION TAG	UNP Q04ML5
B	-4	GLY	-	EXPRESSION TAG	UNP Q04ML5
B	-3	ALA	-	EXPRESSION TAG	UNP Q04ML5
B	-2	MET	-	EXPRESSION TAG	UNP Q04ML5
B	-1	GLY	-	EXPRESSION TAG	UNP Q04ML5
B	0	SER	-	EXPRESSION TAG	UNP Q04ML5

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

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

- Molecule 3 is BIS(ADENOSINE)-5'-PENTAPHOSPHATE (three-letter code: AP5) (formula: C<sub>20</sub>H<sub>29</sub>N<sub>10</sub>O<sub>22</sub>P<sub>5</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			57	20	10	22	5		
3	B	1	Total	C	N	O	P	0	0
			57	20	10	22	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	311	Total	O	0	0
			311	311		
4	B	273	Total	O	0	0
			273	273		

### 3 Residue-property plots

MolProbity failed to run properly - this section will therefore be empty.

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	39.20Å 48.34Å 52.57Å 75.30° 72.95° 88.77°	Depositor
Resolution (Å)	37.42 – 1.49 37.42 – 1.49	Depositor EDS
% Data completeness (in resolution range)	93.0 (37.42-1.49) 90.0 (37.42-1.49)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.80 (at 1.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1555)	Depositor
R, $R_{free}$	0.193 , 0.230 0.192 , 0.228	Depositor DCC
$R_{free}$ test set	1936 reflections (3.66%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.1	Xtriage
Anisotropy	0.545	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.49 , 55.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 54770 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7376	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	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 59.25 % 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 1.8157e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

## 5 Model quality

### 5.1 Standard geometry

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### 5.2 Close contacts

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### 5.3 Torsion angles

#### 5.3.1 Protein backbone

MolProbity failed to run properly - this section will therefore be empty.

#### 5.3.2 Protein sidechains

MolProbity failed to run properly - this section will therefore be empty.

#### 5.3.3 RNA

MolProbity failed to run properly - this section will therefore be empty.

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

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

### 5.5 Carbohydrates

There are no carbohydrates in this entry.

### 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	AP5	A	302	2	62,62,62	1.94	14 (22%)	98,98,98	2.26	17 (17%)
3	AP5	B	302	2	62,62,62	1.98	15 (24%)	98,98,98	2.29	17 (17%)

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	AP5	A	302	2	-	0/44/76/76	0/6/6/6
3	AP5	B	302	2	-	0/44/76/76	0/6/6/6

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	AP5	C2F-C1F	-5.74	1.45	1.53
3	A	302	AP5	C2F-C1F	-5.62	1.45	1.53
3	A	302	AP5	C2J-C1J	-5.61	1.45	1.53
3	B	302	AP5	C2J-C1J	-5.50	1.45	1.53
3	B	302	AP5	O4J-C1J	5.10	1.47	1.41
3	A	302	AP5	O4J-C1J	4.97	1.47	1.41
3	B	302	AP5	O4F-C1F	4.97	1.47	1.41
3	A	302	AP5	O4F-C1F	4.88	1.47	1.41
3	A	302	AP5	C2F-C3F	-3.86	1.42	1.53
3	B	302	AP5	C2F-C3F	-3.77	1.43	1.53
3	A	302	AP5	C2J-C3J	-3.68	1.43	1.53
3	B	302	AP5	C2J-C3J	-3.66	1.43	1.53
3	B	302	AP5	C2A-N3A	2.89	1.37	1.32
3	A	302	AP5	C2A-N3A	2.87	1.37	1.32
3	A	302	AP5	C6B-N6B	2.85	1.43	1.34
3	B	302	AP5	C6B-N6B	2.81	1.43	1.34
3	A	302	AP5	C3F-C4F	-2.80	1.45	1.53
3	B	302	AP5	C3F-C4F	-2.80	1.45	1.53
3	A	302	AP5	C1J-N9B	-2.77	1.40	1.48
3	B	302	AP5	C1J-N9B	-2.75	1.40	1.48
3	B	302	AP5	PD-O3G	-2.55	1.55	1.59
3	A	302	AP5	C3J-C4J	-2.51	1.46	1.53
3	B	302	AP5	C3J-C4J	-2.49	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	AP5	C6A-N6A	2.42	1.42	1.34
3	A	302	AP5	C6A-N6A	2.41	1.42	1.34
3	B	302	AP5	C2B-N3B	2.25	1.36	1.32
3	B	302	AP5	PG-O3G	-2.25	1.55	1.59
3	A	302	AP5	PD-O3G	-2.22	1.56	1.59
3	A	302	AP5	C2B-N3B	2.12	1.35	1.32

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	AP5	N3B-C2B-N1B	-10.21	119.91	128.89
3	A	302	AP5	N3A-C2A-N1A	-10.09	120.01	128.89
3	B	302	AP5	N3A-C2A-N1A	-10.07	120.03	128.89
3	B	302	AP5	N3B-C2B-N1B	-9.98	120.11	128.89
3	A	302	AP5	C5B-C4B-N3B	-6.76	119.39	125.98
3	B	302	AP5	C5B-C4B-N3B	-6.65	119.50	125.98
3	B	302	AP5	C5A-C4A-N3A	-6.19	119.95	125.98
3	A	302	AP5	C5A-C4A-N3A	-6.18	119.95	125.98
3	A	302	AP5	N3B-C4B-N9B	5.30	134.49	125.39
3	B	302	AP5	N3B-C4B-N9B	5.21	134.33	125.39
3	B	302	AP5	PD-O3G-PG	-5.02	118.02	131.93
3	A	302	AP5	N3A-C4A-N9A	4.83	133.68	125.39
3	B	302	AP5	N3A-C4A-N9A	4.81	133.65	125.39
3	A	302	AP5	C4F-O4F-C1F	-4.53	104.74	109.72
3	B	302	AP5	C4J-O4J-C1J	-4.47	104.81	109.72
3	B	302	AP5	C4F-O4F-C1F	-4.41	104.87	109.72
3	A	302	AP5	C4J-O4J-C1J	-4.27	105.02	109.72
3	B	302	AP5	PE-O3D-PD	-3.57	122.05	131.93
3	A	302	AP5	PD-O3G-PG	-3.45	122.38	131.93
3	A	302	AP5	C2B-N3B-C4B	2.72	121.11	113.27
3	A	302	AP5	PE-O3D-PD	-2.63	124.64	131.93
3	A	302	AP5	C4A-C5A-N7A	-2.62	106.88	109.41
3	B	302	AP5	C2B-N3B-C4B	2.62	120.81	113.27
3	A	302	AP5	C3F-C2F-C1F	2.61	105.02	100.92
3	B	302	AP5	C3F-C2F-C1F	2.53	104.89	100.92
3	A	302	AP5	O3D-PD-O3G	2.51	106.77	101.66
3	B	302	AP5	C4A-C5A-N7A	-2.49	107.00	109.41
3	A	302	AP5	C2A-N3A-C4A	2.48	120.42	113.27
3	B	302	AP5	C2A-N3A-C4A	2.47	120.37	113.27
3	B	302	AP5	C3J-C2J-C1J	2.42	104.71	100.92
3	A	302	AP5	C4B-C5B-N7B	-2.34	107.15	109.41
3	A	302	AP5	C3J-C2J-C1J	2.32	104.56	100.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	AP5	C4B-C5B-N7B	-2.30	107.19	109.41
3	B	302	AP5	O3D-PD-O3G	2.18	106.09	101.66

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	212/217 (97%)	0.04	4 (1%) 64 71	14, 25, 47, 78	0
1	B	212/217 (97%)	0.07	2 (0%) 81 87	15, 27, 47, 60	0
All	All	424/434 (97%)	0.06	6 (1%) 72 79	14, 26, 47, 78	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	147	ASP	3.5
1	A	146	VAL	3.4
1	A	148	TYR	2.8
1	A	149	LYS	2.4
1	B	146	VAL	2.2
1	A	147	ASP	2.1

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

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

### 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( $\text{\AA}^2$ )	Q<0.9
3	AP5	B	302	57/57	0.10	1.08	12,18,39,71	0
3	AP5	A	302	57/57	0.09	0.71	12,18,26,44	0
2	MG	A	301	1/1	0.07	-0.18	21,21,21,21	0
2	MG	B	301	1/1	0.07	-0.58	20,20,20,20	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.