



wwPDB X-ray Structure Validation Summary Report i

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 wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

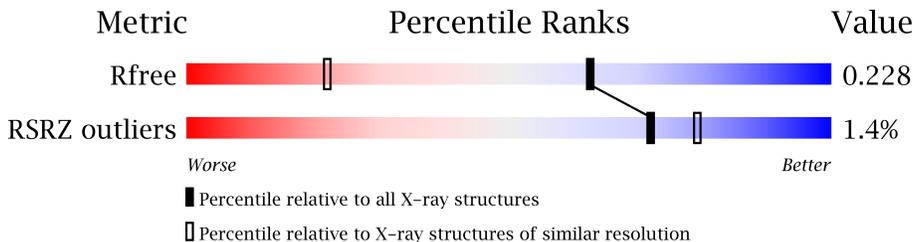
The following versions of software and data (see [references](#)) were used in the production of this report:

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 i

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	
			Total	C	H	N	O				S
1	A	212	3338	1048	1670	288	327	5	0	0	0
1	B	212	3338	1048	1670	288	327	5	0	0	0

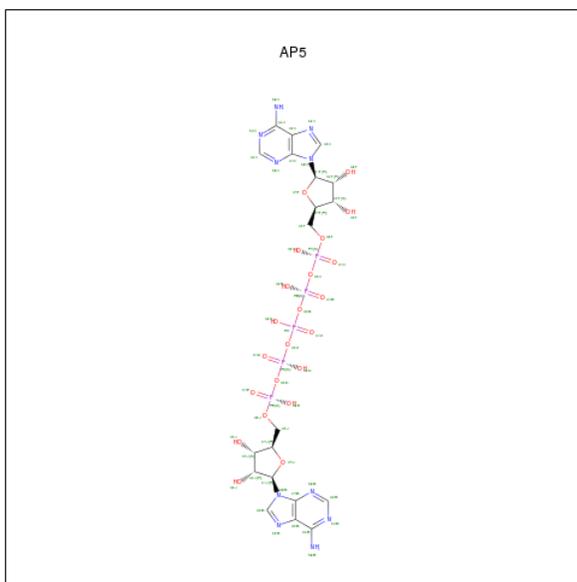
There are 10 discrepancies between the modelled and reference sequences:

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
			Total	Mg		
2	B	1	1	1	0	0
2	A	1	1	1	0	0

- Molecule 3 is BIS(ADENOSINE)-5'-PENTAPHOSPHATE (three-letter code: AP5) (formula: C₂₀H₂₉N₁₀O₂₂P₅).



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

- Molecule 4 is water.

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

3 Residue-property plots

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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	18.1	Xtriage
Anisotropy	0.545	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	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 ²)	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.*

¹Intensities estimated from amplitudes.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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5.2 Close contacts [i](#)

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5.3 Torsion angles

5.3.1 Protein backbone [i](#)

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5.3.2 Protein sidechains [i](#)

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5.3.3 RNA [i](#)

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

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 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

The worst 5 of 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

The worst 5 of 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

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, 95th 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 ²)	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

The worst 5 of 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

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, 95th 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(\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.