



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 06:02 PM GMT

PDB ID : 2AMX
Title : Crystal structure of Plasmodium Yoelii Adenosine deaminase (PY02076)
Authors : Dong, A.; Vedadi, M.; Wasney, G.; Zhao, Y.; Lew, J.; Alam, Z.; Melone, M.; Koeieradzki, I.; Edwards, A.M.; Arrowsmith, C.H.; Weigelt, J.; Sundstrom, M.; Bochkarev, A.; Hui, R.; Amani, M.; Structural Genomics Consortium (SGC)
Deposited on : 2005-08-10
Resolution : 2.02 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>

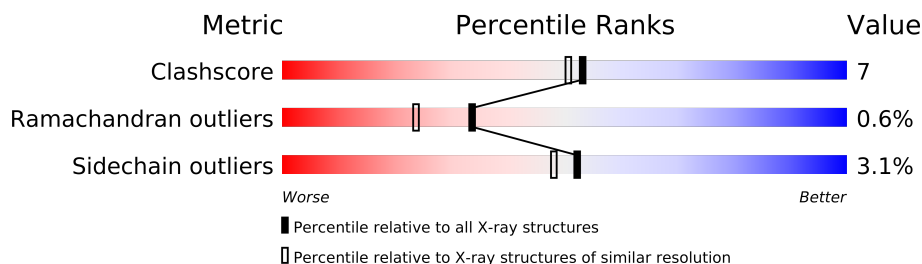
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : **FAILED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.02 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	79885	7467 (2.04-2.00)
Ramachandran outliers	78287	7370 (2.04-2.00)
Sidechain outliers	78261	7368 (2.04-2.00)

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 ≥ 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.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	376	
1	B	376	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6372 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 adenosine deaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	0	0
			2958	1900	499	549	10			
1	B	356	Total	C	N	O	S	0	0	0
			2908	1870	489	539	10			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	CLONING ARTIFACT	UNP Q7RMV2
A	2	GLY	-	CLONING ARTIFACT	UNP Q7RMV2
A	3	SER	-	CLONING ARTIFACT	UNP Q7RMV2
A	4	SER	-	CLONING ARTIFACT	UNP Q7RMV2
A	5	HIS	-	EXPRESSION TAG	UNP Q7RMV2
A	6	HIS	-	EXPRESSION TAG	UNP Q7RMV2
A	7	HIS	-	EXPRESSION TAG	UNP Q7RMV2
A	8	HIS	-	EXPRESSION TAG	UNP Q7RMV2
A	9	HIS	-	EXPRESSION TAG	UNP Q7RMV2
A	10	HIS	-	EXPRESSION TAG	UNP Q7RMV2
A	11	SER	-	CLONING ARTIFACT	UNP Q7RMV2
A	12	SER	-	CLONING ARTIFACT	UNP Q7RMV2
A	13	GLY	-	CLONING ARTIFACT	UNP Q7RMV2
A	14	LEU	-	CLONING ARTIFACT	UNP Q7RMV2
A	15	VAL	-	CLONING ARTIFACT	UNP Q7RMV2
A	16	PRO	-	CLONING ARTIFACT	UNP Q7RMV2
A	17	ARG	-	CLONING ARTIFACT	UNP Q7RMV2
A	18	GLY	-	CLONING ARTIFACT	UNP Q7RMV2
A	19	SER	-	CLONING ARTIFACT	UNP Q7RMV2
B	1	MET	-	CLONING ARTIFACT	UNP Q7RMV2
B	2	GLY	-	CLONING ARTIFACT	UNP Q7RMV2
B	3	SER	-	CLONING ARTIFACT	UNP Q7RMV2
B	4	SER	-	CLONING ARTIFACT	UNP Q7RMV2
B	5	HIS	-	EXPRESSION TAG	UNP Q7RMV2
B	6	HIS	-	EXPRESSION TAG	UNP Q7RMV2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	7	HIS	-	EXPRESSION TAG	UNP Q7RMV2
B	8	HIS	-	EXPRESSION TAG	UNP Q7RMV2
B	9	HIS	-	EXPRESSION TAG	UNP Q7RMV2
B	10	HIS	-	EXPRESSION TAG	UNP Q7RMV2
B	11	SER	-	CLONING ARTIFACT	UNP Q7RMV2
B	12	SER	-	CLONING ARTIFACT	UNP Q7RMV2
B	13	GLY	-	CLONING ARTIFACT	UNP Q7RMV2
B	14	LEU	-	CLONING ARTIFACT	UNP Q7RMV2
B	15	VAL	-	CLONING ARTIFACT	UNP Q7RMV2
B	16	PRO	-	CLONING ARTIFACT	UNP Q7RMV2
B	17	ARG	-	CLONING ARTIFACT	UNP Q7RMV2
B	18	GLY	-	CLONING ARTIFACT	UNP Q7RMV2
B	19	SER	-	CLONING ARTIFACT	UNP Q7RMV2

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Co 3 3	0	0
2	A	2	Total Co 2 2	0	0

- Molecule 3 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total X 1 1	0	0
3	A	5	Total X 5 5	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	233	Total O 233 233	0	0
4	B	262	Total O 262 262	0	0

4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.72Å 90.33Å 137.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.90 – 2.02	Depositor
% Data completeness (in resolution range)	99.7 (42.90-2.02)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.196 , 0.246	Depositor
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.152	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 54922 reflections	Xtriage
Total number of atoms	6372	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: UNX, CO

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	0.87	0/3024	0.83	7/4080 (0.2%)
1	B	0.98	5/2972 (0.2%)	1.16	10/4007 (0.2%)
All	All	0.92	5/5996 (0.1%)	1.01	17/8087 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	304	ASP	CB-CG	10.06	1.72	1.51
1	B	304	ASP	CG-OD1	8.67	1.45	1.25
1	B	166	LYS	CE-NZ	6.51	1.65	1.49
1	B	166	LYS	CD-CE	5.52	1.65	1.51
1	B	336	TYR	CE1-CZ	5.16	1.45	1.38

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	304	ASP	CB-CG-OD1	31.60	146.74	118.30
1	B	304	ASP	CB-CG-OD2	-26.41	94.53	118.30
1	B	263	ARG	NE-CZ-NH2	-18.32	111.14	120.30
1	B	263	ARG	NE-CZ-NH1	15.36	127.98	120.30
1	A	263	ARG	NE-CZ-NH2	-13.68	113.46	120.30

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	2958	0	2939	31	2
1	B	2908	0	2891	49	3
2	A	2	0	0	0	0
2	B	3	0	0	0	0
3	A	5	0	0	1	0
3	B	1	0	0	1	0
4	A	233	0	0	6	0
4	B	262	0	0	11	0
All	All	6372	0	5830	82	3

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 7.

The worst 5 of 82 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:B:2005:UNX:UNK	4:B:2019:HOH:O	1.44	0.96
1:A:271:SER:O	1:A:310:LYS:HE2	1.67	0.94
1:B:26:LYS:HA	1:B:351:MET:CE	2.00	0.92
1:A:30:GLN:H	1:A:30:GLN:CD	1.76	0.89
1:B:219:LEU:HD22	1:B:222:HIS:HD2	1.40	0.86

All (3) 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	Distance(Å)	Clash(Å)
1:A:227:HIS:NE2	1:B:304:ASP:OD1[4.555]	1.82	0.38
1:B:17:ARG:NH2	1:B:282:LYS:O[4.445]	1.91	0.29
1:A:231:ASP:OD1	1:B:304:ASP:OD1[4.555]	2.01	0.19

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	362/376 (96%)	352 (97%)	8 (2%)	2 (1%)	33	24
1	B	352/376 (94%)	343 (97%)	7 (2%)	2 (1%)	33	24
All	All	714/752 (95%)	695 (97%)	15 (2%)	4 (1%)	33	24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	LYS
1	A	266	HIS
1	B	217	ILE
1	B	266	HIS

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	327/338 (97%)	319 (98%)	8 (2%)	61	60
1	B	323/338 (96%)	311 (96%)	12 (4%)	45	40
All	All	650/676 (96%)	630 (97%)	20 (3%)	52	48

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	17	ARG
1	B	30	GLN
1	B	217	ILE
1	A	278	GLU
1	B	14	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	ASN
1	B	203	HIS
1	B	75	ASN
1	A	222	HIS

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Mol	Chain	Res	Type
1	A	299	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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 11 ligands modelled in this entry, 6 are unknown and 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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