W O R L D W I D E

wwPDB

P R O T E I N D A T A B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 01:12 PM GMT

PDB ID	:	3T8L
Title	:	Crystal Structure of adenine deaminase with Mn/Fe
Authors	:	Bagaria, A.; Kumaran, D.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2011-08-01
Resolution	:	2.80 Å(reported)

The following versions of software and data (see references (1)) were used in the production of this report:

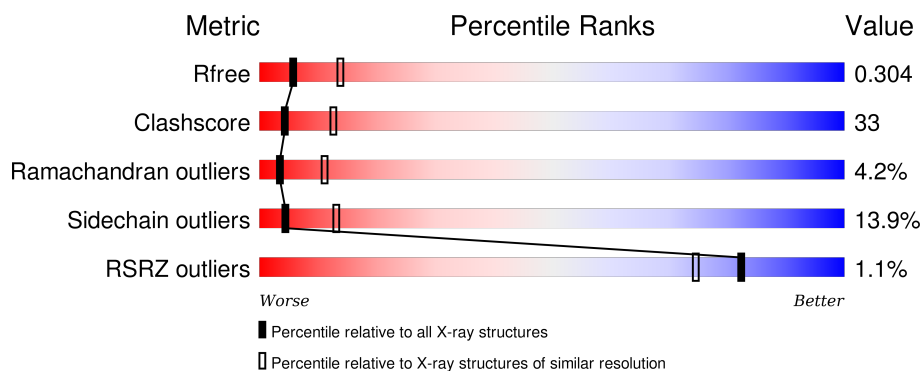|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
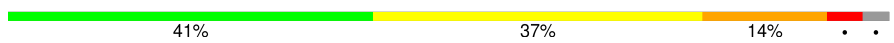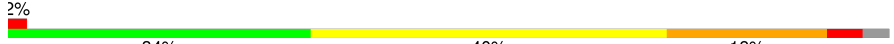*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	Percentile Ranks	Value
Rfree		0.304
Clashscore		33
Ramachandran outliers		4.2%
Sidechain outliers		13.9%
RSRZ outliers		1.1%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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. 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 <=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	608	41% 37% 14% · ·
1	B	608	2% 34% 40% 18% · ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UNX	A	606	-	-	-	X
2	UNX	A	608	-	-	-	X
2	UNX	B	608	-	-	-	X

2   Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8761 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 Adenine deaminase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	587	Total	C	N	O	S	Se	0	0	0
			4337	2723	775	817	6	16			
1	B	587	Total	C	N	O	S	Se	0	0	0
			4335	2721	775	817	6	16			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MSE	-	EXPRESSION TAG	UNP Q7CUX4
A	-1	SER	-	EXPRESSION TAG	UNP Q7CUX4
A	0	LEU	-	EXPRESSION TAG	UNP Q7CUX4
A	598	GLU	-	EXPRESSION TAG	UNP Q7CUX4
A	599	GLY	-	EXPRESSION TAG	UNP Q7CUX4
A	600	HIS	-	EXPRESSION TAG	UNP Q7CUX4
A	601	HIS	-	EXPRESSION TAG	UNP Q7CUX4
A	602	HIS	-	EXPRESSION TAG	UNP Q7CUX4
A	603	HIS	-	EXPRESSION TAG	UNP Q7CUX4
A	604	HIS	-	EXPRESSION TAG	UNP Q7CUX4
A	605	HIS	-	EXPRESSION TAG	UNP Q7CUX4
B	-2	MSE	-	EXPRESSION TAG	UNP Q7CUX4
B	-1	SER	-	EXPRESSION TAG	UNP Q7CUX4
B	0	LEU	-	EXPRESSION TAG	UNP Q7CUX4
B	598	GLU	-	EXPRESSION TAG	UNP Q7CUX4
B	599	GLY	-	EXPRESSION TAG	UNP Q7CUX4
B	600	HIS	-	EXPRESSION TAG	UNP Q7CUX4
B	601	HIS	-	EXPRESSION TAG	UNP Q7CUX4
B	602	HIS	-	EXPRESSION TAG	UNP Q7CUX4
B	603	HIS	-	EXPRESSION TAG	UNP Q7CUX4
B	604	HIS	-	EXPRESSION TAG	UNP Q7CUX4
B	605	HIS	-	EXPRESSION TAG	UNP Q7CUX4

- Molecule 2 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

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

- Molecule 3 is water.

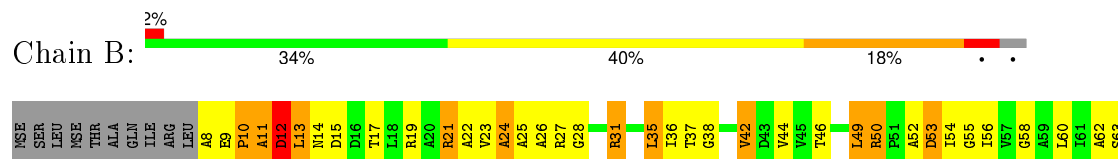| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total 33	O 33	0	0
3	B	50	Total 50	O 50	0	0

3 Residue-property plots ⓘ

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: Adenine deaminase 2

- Molecule 1: Adenine deaminase 2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.54Å 131.17Å 69.28Å 90.00° 97.04° 90.00°	Depositor
Resolution (Å)	48.73 – 2.80 47.46 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.73-2.80) 99.7 (47.46-2.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.29 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.174 , 0.301 0.182 , 0.304	Depositor DCC
R_{free} test set	1362 reflections (5.36%)	DCC
Wilson B-factor (Å^2)	56.2	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 47.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.33$	Xtriage
Outliers	0 of 26789 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8761	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: UNX

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	2.10	137/4402 (3.1%)	1.79	93/5964 (1.6%)
1	B	1.96	105/4400 (2.4%)	1.75	77/5961 (1.3%)
All	All	2.03	242/8802 (2.7%)	1.77	170/11925 (1.4%)

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
1	B	0	6
All	All	0	8

The worst 5 of 242 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	141	GLU	CD-OE2	12.79	1.39	1.25
1	A	451	MSE	SE-CE	12.26	2.67	1.95
1	A	396	MSE	SE-CE	11.74	2.64	1.95
1	A	163	ARG	CZ-NH1	11.57	1.48	1.33
1	B	189	MSE	SE-CE	11.45	2.63	1.95

The worst 5 of 170 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	163	ARG	NE-CZ-NH2	-20.65	109.97	120.30
1	B	197	ARG	NE-CZ-NH1	-18.11	111.25	120.30
1	A	343	ARG	NE-CZ-NH1	17.08	128.84	120.30
1	A	163	ARG	NE-CZ-NH1	15.14	127.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	343	ARG	NE-CZ-NH2	-13.68	113.46	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	396	MSE	Peptide
1	A	430	LYS	Peptide
1	B	152	PRO	Peptide
1	B	412	ALA	Peptide
1	B	417	PRO	Peptide

5.2 Too-close contacts (i)

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	4337	0	4344	222	0
1	B	4335	0	4339	363	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	33	0	0	5	0
3	B	50	0	0	16	0
All	All	8761	0	8683	572	0

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 33.

The worst 5 of 572 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:385:VAL:CB	1:A:385:VAL:CG1	1.76	1.58
1:B:231:MSE:CG	1:B:231:MSE:SE	2.14	1.44
1:A:492:MSE:SE	1:A:492:MSE:CE	2.14	1.44
1:A:393:PRO:CB	1:A:393:PRO:CG	1.79	1.43
1:B:577:MSE:SE	1:B:577:MSE:CE	2.15	1.42

There are no symmetry-related clashes.

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	585/608 (96%)	520 (89%)	49 (8%)	16 (3%)	6	21
1	B	585/608 (96%)	483 (83%)	69 (12%)	33 (6%)	2	6
All	All	1170/1216 (96%)	1003 (86%)	118 (10%)	49 (4%)	3	11

5 of 49 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	ASN
1	A	406	GLY
1	B	72	ASP
1	B	224	ASN
1	B	418	ARG

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	445/444 (100%)	386 (87%)	59 (13%)	5	14
1	B	444/444 (100%)	379 (85%)	65 (15%)	4	11
All	All	889/888 (100%)	765 (86%)	124 (14%)	4	13

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	583	LEU
1	B	126	ASN
1	B	494	LEU
1	A	588	MSE
1	B	17	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	488	ASN
1	B	126	ASN
1	B	488	ASN
1	A	573	HIS
1	B	65	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 6 ligands modelled in this entry, 6 are unknown - 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.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

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, 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	571/608 (93%)	-0.60	1 (0%)	95 94	28, 44, 66, 80	0
1	B	571/608 (93%)	-0.30	12 (2%)	67 56	28, 49, 83, 98	27 (4%)
All	All	1142/1216 (93%)	-0.45	13 (1%)	82 74	28, 46, 75, 98	27 (2%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	594	GLU	4.4
1	B	406	GLY	4.0
1	B	411	LEU	3.7
1	B	412	ALA	3.4
1	B	464	TRP	2.8

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, 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	UNX	A	606	1/1	0.68	0.72	20.86	53,53,53,53	0
2	UNX	B	608	1/1	0.52	0.54	17.57	50,50,50,50	0
2	UNX	A	608	1/1	0.38	0.58	14.59	43,43,43,43	0
2	UNX	B	606	1/1	0.71	0.61	-	51,51,51,51	0
2	UNX	B	607	1/1	0.63	0.58	-	60,60,60,60	0
2	UNX	A	607	1/1	0.62	0.64	-	43,43,43,43	0

6.5   Other polymers (i)

There are no such residues in this entry.