



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 30, 2021 – 10:00 PM EST

PDB ID : 3T81
Title : Crystal Structure of diiron adenine deaminase
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Deposited on : 2011-08-01
Resolution : 2.63 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

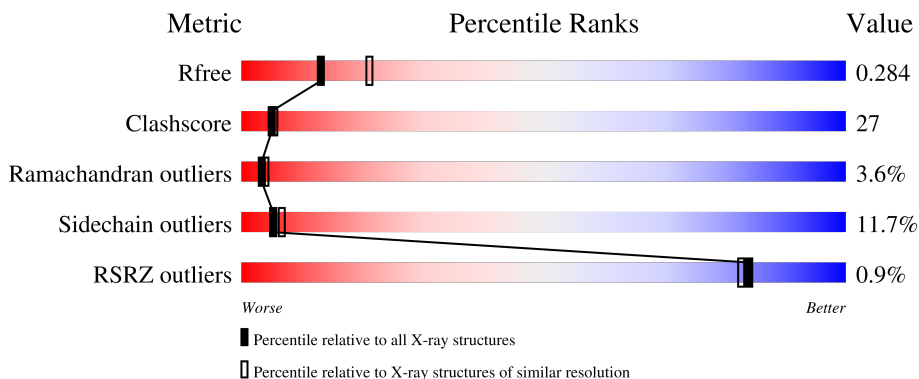
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.63 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}	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. 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	
1	B	608	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8674 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	579	Total	C	N	O	S	Se	0	0	0
			4277	2685	763	807	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 FE (III) ION (three-letter code: FE) (formula: Fe).

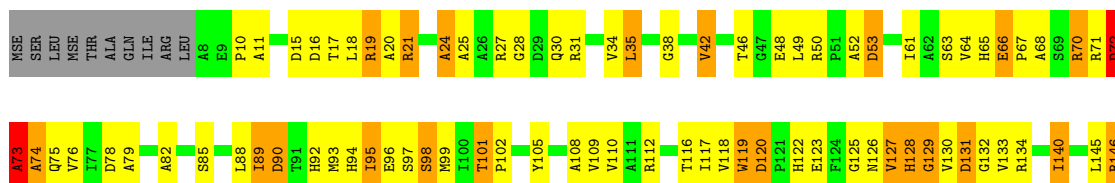
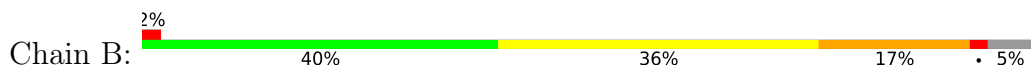
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total 3	Fe 3	0	0
2	A	3	Total 3	Fe 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	23	Total 23	O 23	0	0
3	B	31	Total 31	O 31	0	0

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

Chain A: 47% 37% 12% . .



I593	E594	VAL	GLY	GLY	GLY	HIS	HIS	HIS	HIS	HIS	D528	M451	A452	E453	T456	K457	L461	T462	G463	L464	G465	R466	M467	N468	G469	A470	F471	A472	T473	T474	V475	S476	H477	D478	S479	H480	N481	K482	T483	V484	F485	N488	A489	M492	A493	L494	A495	A496	A497	N497	G505	M506	A507	V508	A509	S510	E511	I517	L520	S523	G524	S527
C381	V385	L386	K387	M390	F391	L392	P393	L394	R395	M396	A397	N398	D399	V402	Q405	GLY	ALA	LYS	VAL	ARG	LEU	ALA	T413	I414	R416	D415	P417	R418	F419	T420	Q421	V422	G423	GLU	T425	E426	A427	D428	V429	K430	D431	V434	V435	A436	P437	E438	T441	N442	I443	T446	H447	R448										
G299	G300	G301	L302	D303	D304	V305	V306	R307	R308	L309	V310	R311	Y312	G313	E317	W318	A319	L320	R321	L331	S334	D335	L336	A341	R344	A345	D346	T347	E351	D352	S357	A358	R359	A363	S364	G365	R366	A367	V368	A369	E370	G371	G372	R373	M374	L375	V376	D377	I378	T380												
R220	G221	L222	K223	N224	A225	D226	L227	N228	A229	F230	M231	G234	V235	S236	S237	D238	H239	E240	L241	E245	D246	L247	M248	A249	L250	L251	R252	L255	T256	I257	E258	L259	S262	H263	D264	F270	V271	L277	T285	L286	C287	T288	D289	D290	V291	F292	P293	D294	D295	L296	L297	Q298										
A147	I148	L149	L150	A151	P152	S153	C154	V155	P156	G160	L161	E162	R163	F168	D169	L173	A174	D175	L176	L177	S178	W179	P180	E181	L182	I185	A186	E187	I188	M189	N190	M191	R192	I195	E196	R197	D198	P199	R200	M201	S202	G203	I204	V205	Q206	L209	A210	V215	G216	G217	H218	A219										

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.66Å 131.84Å 69.63Å 90.00° 97.04° 90.00°	Depositor
Resolution (Å)	48.89 – 2.63 48.88 – 2.63	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.89-2.63) 99.6 (48.88-2.63)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.61Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.185 , 0.287 0.185 , 0.284	Depositor DCC
R_{free} test set	1663 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8674	wwPDB-VP
Average B, all atoms (Å ²)	51.0	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.83	79/4402 (1.8%)	1.65	67/5964 (1.1%)
1	B	1.79	73/4340 (1.7%)	1.67	75/5878 (1.3%)
All	All	1.81	152/8742 (1.7%)	1.66	142/11842 (1.2%)

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	5
1	B	0	9
All	All	0	14

The worst 5 of 152 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	451	MSE	SE-CE	10.07	2.54	1.95
1	A	189	MSE	SE-CE	9.45	2.51	1.95
1	B	496	ALA	CA-CB	-8.90	1.33	1.52
1	B	448	ARG	CZ-NH1	8.55	1.44	1.33
1	B	133	VAL	CB-CG2	-8.37	1.35	1.52

The worst 5 of 142 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	ARG	NE-CZ-NH2	-13.26	113.67	120.30
1	A	50	ARG	NE-CZ-NH2	12.07	126.34	120.30
1	B	311	ARG	NE-CZ-NH2	-11.54	114.53	120.30
1	A	241	LEU	CB-CG-CD1	-11.32	91.75	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	536	ARG	NE-CZ-NH2	-11.26	114.67	120.30

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	217	GLY	Peptide
1	A	396	MSE	Peptide
1	A	402	VAL	Peptide
1	A	451	MSE	Peptide
1	A	48	GLU	Peptide

5.2 Too-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 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	198	0
1	B	4277	0	4273	285	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	23	0	0	4	0
3	B	31	0	0	4	0
All	All	8674	0	8617	471	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 27.

The worst 5 of 471 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:B:393:PRO:CB	1:B:393:PRO:CG	1.76	1.45
1:A:231:MSE:SE	1:A:231:MSE:CE	2.15	1.44
1:A:201:MSE:SE	1:A:201:MSE:CG	2.16	1.42
1:B:248:MSE:SE	1:B:248:MSE:CE	2.17	1.42
1:B:588:MSE:CE	1:B:588:MSE:SE	2.18	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%)	516 (88%)	54 (9%)	15 (3%)	5	7
1	B	573/608 (94%)	474 (83%)	72 (13%)	27 (5%)	2	2
All	All	1158/1216 (95%)	990 (86%)	126 (11%)	42 (4%)	3	4

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	ALA
1	A	397	ALA
1	A	430	LYS
1	A	431	ASP
1	A	588	MSE

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%)	401 (90%)	44 (10%)	8	10
1	B	439/444 (99%)	380 (87%)	59 (13%)	4	4
All	All	884/888 (100%)	781 (88%)	103 (12%)	5	7

5 of 103 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	95	ILE
1	B	181	GLU
1	B	555	TYR
1	B	97	SER
1	B	161	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	65	HIS
1	B	126	ASN
1	B	447	HIS
1	A	481	ASN
1	A	488	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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.

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%)	-0.58	0 100 100	28, 46, 68, 80	0
1	B	563/608 (92%)	-0.36	10 (1%) 68 66	31, 50, 89, 100	0
All	All	1134/1216 (93%)	-0.47	10 (0%) 84 83	28, 48, 83, 100	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	435	VAL	3.4
1	B	413	THR	2.9
1	B	414	ILE	2.8
1	B	554	PRO	2.7
1	B	366	ARG	2.7

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 monosaccharides 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. 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	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FE	A	607	1/1	0.97	0.11	45,45,45,45	0
2	FE	B	608	1/1	0.98	0.15	59,59,59,59	0
2	FE	A	606	1/1	0.98	0.07	49,49,49,49	0
2	FE	A	608	1/1	0.98	0.10	50,50,50,50	0
2	FE	B	606	1/1	0.99	0.09	52,52,52,52	0
2	FE	B	607	1/1	0.99	0.11	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.