



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 12:06 PM UTC

PDB ID : 2AAF / pdb\_00002aaf  
Title : Structure of H278A arginine deiminase with L-arginine forming a S-alkylthiuronium reaction intermediate  
Authors : Galkin, A.; Lu, X.; Dunaway-Mariano, D.; Herzberg, O.  
Deposited on : 2005-07-13  
Resolution : 2.30 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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

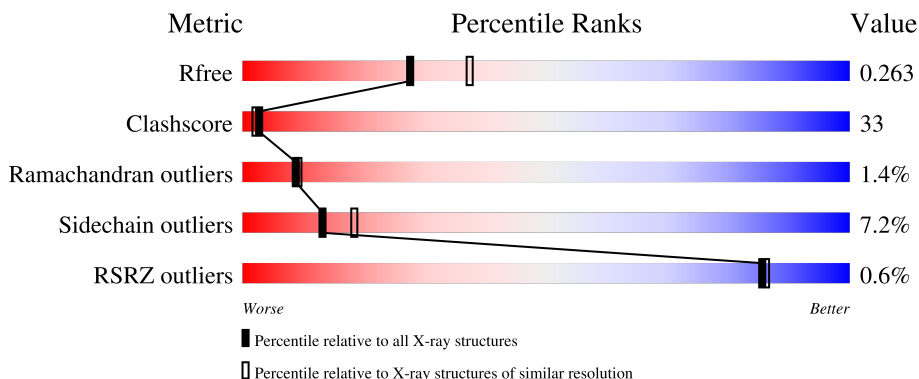
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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  $\geq 3$ , 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	418	 46% 41% 8% ..
1	B	418	 56% 34% 7% ..
1	C	418	 50% 39% 8% ..
1	D	418	 2% 46% 42% 8% ..

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 13542 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 Arginine deiminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	405	3170	2004	553	596	17	0	0	0
1	B	409	3202	2024	557	604	17	0	0	0
1	C	406	3185	2014	554	600	17	0	0	0
1	D	406	3183	2013	554	599	17	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	278	ALA	HIS	engineered mutation	UNP P13981
A	406	CYR	CYS	modified residue	UNP P13981
B	278	ALA	HIS	engineered mutation	UNP P13981
B	406	CYR	CYS	modified residue	UNP P13981
C	278	ALA	HIS	engineered mutation	UNP P13981
C	406	CYR	CYS	modified residue	UNP P13981
D	278	ALA	HIS	engineered mutation	UNP P13981
D	406	CYR	CYS	modified residue	UNP P13981

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	227	Total 227	O 227	0	0
2	B	209	Total 209	O 209	0	0
2	C	187	Total 187	O 187	0	0
2	D	179	Total 179	O 179	0	0





L397	G398	R399	G400	R401	G402	G403	G404	H405	C406	H407	T408	G409	P410	F411	V412	R413	D414	R415	L416	D417	Y418
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.80Å 121.20Å 151.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.30) 98.6 (20.00-2.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.30Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.200 , 0.264 0.200 , 0.263	Depositor DCC
$R_{free}$ test set	3759 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.2	Xtrriage
Anisotropy	0.290	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 56.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13542	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.50 % 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 4.6062e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.90	2/3218 (0.1%)	1.41	54/4363 (1.2%)
1	B	0.96	1/3251 (0.0%)	1.33	38/4407 (0.9%)
1	C	0.86	0/3234	1.36	39/4383 (0.9%)
1	D	0.89	2/3232 (0.1%)	1.44	42/4381 (1.0%)
All	All	0.91	5/12935 (0.0%)	1.38	173/17534 (1.0%)

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	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	389	VAL	CA-CB	6.88	1.62	1.53
1	D	214	PRO	CA-C	-5.79	1.43	1.52
1	A	415	PRO	N-CD	5.18	1.55	1.47
1	A	284	SER	N-CA	5.12	1.52	1.45
1	D	390	ILE	CA-CB	5.08	1.61	1.54

The worst 5 of 173 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	277	MET	CA-C-N	22.12	152.68	121.05
1	D	277	MET	C-N-CA	22.12	152.68	121.05
1	C	166	ASP	N-CA-C	10.25	122.14	110.97
1	D	199	HIS	CA-C-N	10.01	129.65	119.24

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	199	HIS	C-N-CA	10.01	129.65	119.24

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	TYR	Sidechain

## 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	3170	0	3160	233	0
1	B	3202	0	3185	192	0
1	C	3185	0	3168	216	0
1	D	3183	0	3169	234	0
2	A	227	0	0	82	0
2	B	209	0	0	54	0
2	C	187	0	0	79	0
2	D	179	0	0	74	0
All	All	13542	0	12682	847	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 847 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:C:364:LEU:HG	2:C:604:HOH:O	1.29	1.27
1:A:364:LEU:HB3	2:A:634:HOH:O	1.30	1.27
1:B:187:GLN:HG2	2:B:423:HOH:O	1.33	1.26
1:A:192:THR:HB	2:A:623:HOH:O	1.26	1.24
1:A:74:ASN:HB3	2:A:620:HOH:O	1.36	1.22

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	400/418 (96%)	363 (91%)	32 (8%)	5 (1%)	9	10
1	B	404/418 (97%)	374 (93%)	26 (6%)	4 (1%)	12	15
1	C	401/418 (96%)	371 (92%)	28 (7%)	2 (0%)	24	31
1	D	401/418 (96%)	349 (87%)	41 (10%)	11 (3%)	4	3
All	All	1606/1672 (96%)	1457 (91%)	127 (8%)	22 (1%)	9	9

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	275	ALA
1	D	277	MET
1	B	399	ARG
1	D	40	LEU
1	D	273	SER

### 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	343/353 (97%)	315 (92%)	28 (8%)	10	14
1	B	345/353 (98%)	317 (92%)	28 (8%)	11	14
1	C	344/353 (98%)	322 (94%)	22 (6%)	16	23
1	D	344/353 (98%)	323 (94%)	21 (6%)	17	24
All	All	1376/1412 (98%)	1277 (93%)	99 (7%)	13	18

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	33	THR
1	C	264	ARG
1	C	59	VAL
1	C	155	LEU
1	C	351	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	160	ASN
1	C	187	GLN
1	D	199	HIS
1	D	29	HIS
1	D	160	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](#)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	CYR	D	406	1	14,16,17	3.03	4 (28%)	11,19,21	2.68	2 (18%)
1	CYR	B	406	1	14,16,17	2.99	3 (21%)	11,19,21	2.42	4 (36%)
1	CYR	A	406	1	14,16,17	3.09	4 (28%)	11,19,21	2.78	4 (36%)
1	CYR	C	406	1	14,16,17	3.01	4 (28%)	11,19,21	2.99	3 (27%)

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
1	CYR	D	406	1	-	2/15/18/20	-
1	CYR	B	406	1	-	3/15/18/20	-
1	CYR	A	406	1	-	3/15/18/20	-
1	CYR	C	406	1	-	3/15/18/20	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	406	CYR	C7-SG	7.53	1.83	1.76
1	D	406	CYR	C7-SG	7.47	1.83	1.76
1	C	406	CYR	C7-SG	7.30	1.83	1.76
1	B	406	CYR	C7-SG	7.26	1.83	1.76
1	D	406	CYR	C7-N6	6.44	1.47	1.35

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	406	CYR	C5-N6-C7	-9.01	107.44	123.55
1	D	406	CYR	C5-N6-C7	-8.06	109.14	123.55
1	A	406	CYR	C5-N6-C7	-7.43	110.26	123.55
1	B	406	CYR	C5-N6-C7	-6.49	111.94	123.55
1	A	406	CYR	N6-C7-N7	-3.79	109.51	120.61

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	406	CYR	SG-C7-N6-C5
1	A	406	CYR	N7-C7-SG-CB
1	B	406	CYR	N7-C7-SG-CB
1	C	406	CYR	SG-C7-N6-C5
1	C	406	CYR	N7-C7-SG-CB

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	406	CYR	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	406	CYR	3	0
1	A	406	CYR	1	0
1	C	406	CYR	4	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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, 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	404/418 (96%)	-0.55	1 (0%) 91 91	14, 31, 57, 74	0
1	B	408/418 (97%)	-0.64	1 (0%) 91 91	12, 26, 55, 77	0
1	C	405/418 (96%)	-0.54	1 (0%) 91 91	13, 34, 59, 76	0
1	D	405/418 (96%)	-0.45	7 (1%) 69 70	16, 34, 63, 79	0
All	All	1622/1672 (97%)	-0.54	10 (0%) 85 86	12, 31, 59, 79	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	277	MET	4.0
1	D	184	ALA	3.5
1	D	275	ALA	3.3
1	D	400	GLY	3.2
1	D	314	TYR	3.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	CYR	C	406	17/18	0.93	0.10	18,51,67,68	0
1	CYR	B	406	17/18	0.95	0.08	18,34,61,63	0
1	CYR	A	406	17/18	0.95	0.09	15,37,68,68	0
1	CYR	D	406	17/18	0.96	0.07	20,36,65,68	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.