



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2026 – 07:07 PM UTC

PDB ID : 2BLL / pdb\_00002bll  
Title : Apo-structure of the C-terminal decarboxylase domain of ArnA  
Authors : Williams, G.J.; Breazeale, S.D.; Raetz, C.R.H.; Naismith, J.H.  
Deposited on : 2005-03-07  
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

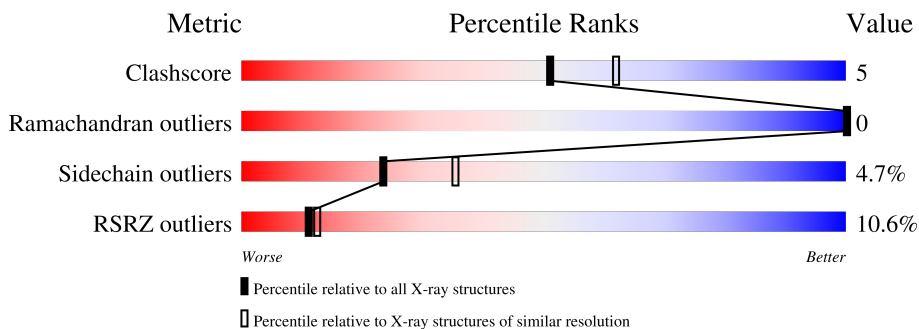
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

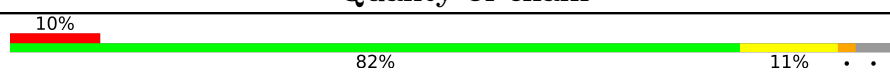
The reported resolution of this entry is 2.30 Å.

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))
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	345	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2827 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 PROTEIN YFBG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	330	2733	1748	481	493	11	0	6	0

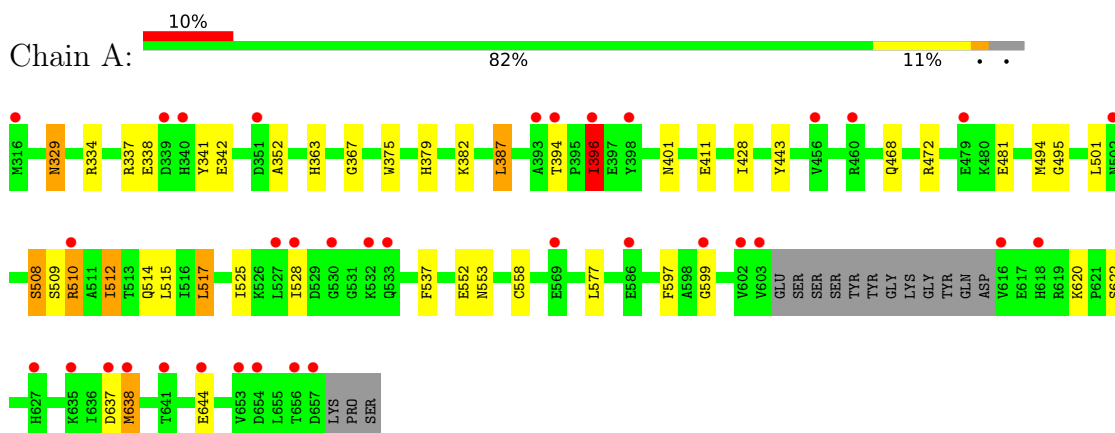
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	94	Total	O	0	0
			94	94		

### 3 Residue-property plots [i](#)

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.

- Molecule 1: PROTEIN YFBG



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.44Å 149.44Å 149.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.70 – 2.30 87.70 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.8 (87.70-2.30) 96.8 (87.70-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.48 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.2.0007	Depositor
R, $R_{free}$	0.186 , 0.230 0.196 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.4	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 39.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2827	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

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	1.12	2/2826 (0.1%)	1.07	8/3824 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	622	SER	C-N	-10.19	1.20	1.33
1	A	382	LYS	C-O	-5.61	1.17	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	622	SER	O-C-N	-15.17	104.28	122.93
1	A	396	ILE	CB-CA-C	-6.36	103.71	112.04
1	A	411	GLU	N-CA-C	5.71	117.18	111.07
1	A	622	SER	CA-C-N	5.49	133.13	122.69
1	A	622	SER	C-N-CA	5.49	133.13	122.69
1	A	495	GLY	CA-C-N	5.18	125.11	119.78
1	A	495	GLY	C-N-CA	5.18	125.11	119.78
1	A	367	GLY	N-CA-C	5.12	118.06	110.63

There are no chirality outliers.

There are no planarity outliers.

### 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	2733	0	2692	28	0
2	A	94	0	0	1	0
All	All	2827	0	2692	28	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 5.

All (28) 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:494:MET:CE	1:A:512:ILE:HG21	2.03	0.88
1:A:468:GLN:HE21	1:A:472:ARG:HE	1.32	0.77
1:A:494:MET:HE1	1:A:512:ILE:HG21	1.66	0.76
1:A:443:TYR:CE1	1:A:620:LYS:HD3	2.25	0.72
1:A:494:MET:HE2	1:A:512:ILE:HG21	1.70	0.71
1:A:334:ARG:NH1	1:A:338:GLU:OE2	2.33	0.61
1:A:342:GLU:OE1	1:A:363:HIS:HE1	1.86	0.58
1:A:443:TYR:CZ	1:A:620:LYS:HD3	2.40	0.57
1:A:341:TYR:OH	1:A:552:GLU:OE2	2.24	0.54
1:A:509:SER:HB3	1:A:512:ILE:HD12	1.91	0.53
1:A:515:LEU:HD22	1:A:525:ILE:HG23	1.92	0.52
1:A:329:ASN:ND2	1:A:352:ALA:O	2.42	0.52
1:A:638:MET:HA	1:A:638:MET:HE2	1.93	0.51
1:A:468:GLN:NE2	1:A:472:ARG:HH21	2.08	0.51
1:A:501:LEU:HD22	1:A:517:LEU:HD23	1.94	0.49
1:A:508:SER:O	1:A:510:ARG:HD3	2.11	0.49
1:A:379:HIS:HE1	2:A:2018:HOH:O	1.95	0.48
1:A:468:GLN:HE21	1:A:472:ARG:NE	2.05	0.48
1:A:468:GLN:NE2	1:A:472:ARG:HE	2.07	0.47
1:A:501:LEU:HD21	1:A:514:GLN:NE2	2.30	0.47
1:A:597:PHE:CE2	1:A:599:GLY:HA2	2.49	0.46
1:A:553:ASN:ND2	1:A:558:CYS:H	2.14	0.46
1:A:494:MET:HE3	1:A:537:PHE:HB3	2.01	0.43
1:A:494:MET:HE2	1:A:512:ILE:CG2	2.46	0.42
1:A:375:TRP:O	1:A:379:HIS:HD2	2.03	0.42
1:A:387:LEU:HD13	1:A:428:ILE:O	2.21	0.41
1:A:394:THR:HG22	1:A:396:ILE:HG13	2.02	0.41

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	332/345 (96%)	319 (96%)	13 (4%)	0	100 100

There are no Ramachandran outliers to report.

### 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	302/309 (98%)	288 (95%)	14 (5%)	24 36

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	329	ASN
1	A	337	ARG
1	A	387	LEU
1	A	396	ILE
1	A	401	ASN
1	A	481	GLU
1	A	508	SER
1	A	510	ARG
1	A	512	ILE
1	A	517	LEU
1	A	528	ILE
1	A	577	LEU
1	A	638	MET

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Mol	Chain	Res	Type
1	A	644	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	363	HIS
1	A	372	HIS
1	A	379	HIS
1	A	468	GLN
1	A	514	GLN
1	A	553	ASN
1	A	570	ASN
1	A	618	HIS
1	A	627	HIS
1	A	639	GLN

### 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 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	622:SER	C	623:ILE	N	1.20

## 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	330/345 (95%)	0.86	35 (10%) <b>11</b> <b>12</b>	26, 40, 57, 67	10 (3%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	532	LYS	7.7
1	A	603	VAL	5.9
1	A	340[A]	HIS	3.8
1	A	528	ILE	3.5
1	A	635	LYS	3.5
1	A	616	VAL	3.1
1	A	339	ASP	2.9
1	A	393	ALA	2.9
1	A	316	MET	2.9
1	A	638	MET	2.9
1	A	460	ARG	2.8
1	A	479	GLU	2.8
1	A	396	ILE	2.8
1	A	656	THR	2.8
1	A	657	ASP	2.8
1	A	586	GLU	2.7
1	A	502	ASN	2.7
1	A	653	VAL	2.7
1	A	602	VAL	2.7
1	A	654	ASP	2.7
1	A	530	GLY	2.6
1	A	510	ARG	2.5
1	A	637[A]	ASP	2.5
1	A	599	GLY	2.4
1	A	394	THR	2.4
1	A	527	LEU	2.4
1	A	398	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	569	GLU	2.2
1	A	351	ASP	2.2
1	A	641	THR	2.2
1	A	456	VAL	2.1
1	A	618	HIS	2.1
1	A	627	HIS	2.1
1	A	533	GLN	2.0
1	A	644	GLU	2.0

## 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 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.