



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 11:03 pm GMT

PDB ID : 1B04  
Title : STRUCTURE OF THE ADENYLATION DOMAIN OF AN NAD<sup>+</sup> DEPENDENT LIGASE  
Authors : Singleton, M.R.; Hakansson, K.; Timson, D.J.; Wigley, D.B.  
Deposited on : 1998-11-16  
Resolution : 2.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

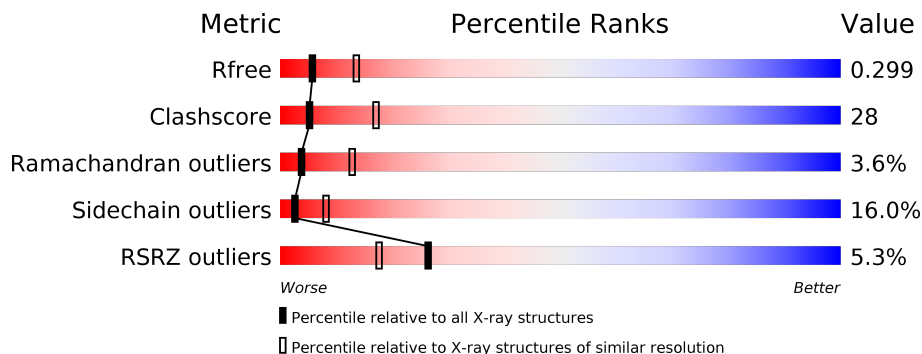
# 1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	2792 (2.80-2.80)
Clashscore	122126	3209 (2.80-2.80)
Ramachandran outliers	120053	3158 (2.80-2.80)
Sidechain outliers	120020	3160 (2.80-2.80)
RSRZ outliers	108989	2726 (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  $\geq 3$ , 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  $\leq 5\%$ . 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	318	
1	B	318	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5126 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 (DNA LIGASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2464	1547	444	467	6			
1	B	311	Total	C	N	O	S	0	0	0
			2472	1552	445	468	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	114	ALA	LYS	ENGINEERED	UNP O87703
B	114	ALA	LYS	ENGINEERED	UNP O87703

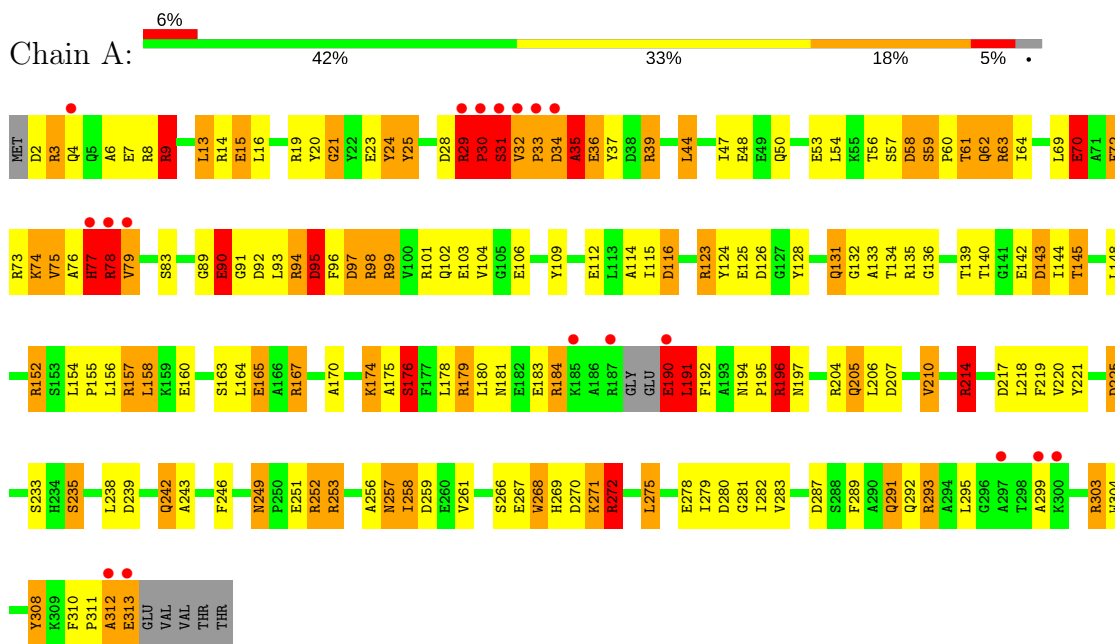
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	78	Total	O	0	0
			78	78		
2	B	112	Total	O	0	0
			112	112		

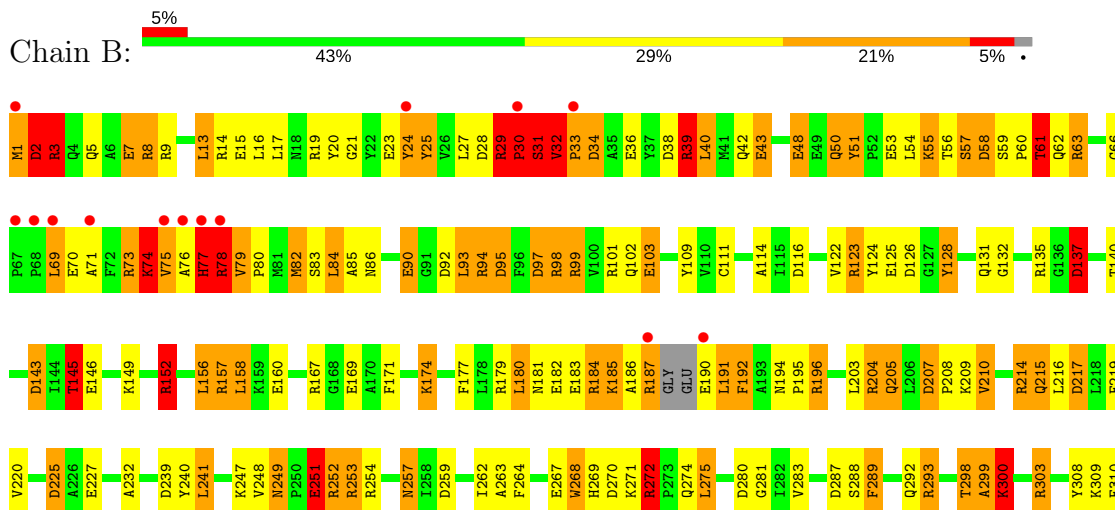
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 (DNA LIGASE)



#### • Molecule 1: PROTEIN (DNA LIGASE)



P311  
A312  
E313  
GLU  
VAL  
VAL  
THR  
THR

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.72Å 95.72Å 225.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.76 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (20.00-2.80) 97.6 (19.76-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.66 (at 2.79Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.230 , 0.310 0.226 , 0.299	Depositor DCC
$R_{free}$ test set	1301 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.7	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 79.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	5126	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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

### 5.1 Standard geometry

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	0.88	4/2511 (0.2%)	2.60	155/3393 (4.6%)
1	B	0.88	1/2519 (0.0%)	2.84	190/3403 (5.6%)
All	All	0.88	5/5030 (0.1%)	2.73	345/6796 (5.1%)

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	2
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	313	GLU	CD-OE1	14.15	1.41	1.25
1	A	313	GLU	CG-CD	10.33	1.67	1.51
1	A	313	GLU	CB-CG	6.76	1.65	1.52
1	B	78	ARG	NE-CZ	5.88	1.40	1.33
1	A	313	GLU	C-O	5.31	1.33	1.23

The worst 5 of 345 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	19	ARG	CD-NE-CZ	33.88	171.03	123.60
1	A	19	ARG	CD-NE-CZ	33.58	170.61	123.60
1	A	179	ARG	CD-NE-CZ	32.97	169.76	123.60
1	B	252	ARG	CD-NE-CZ	27.32	161.85	123.60
1	B	187	ARG	CD-NE-CZ	22.25	154.75	123.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	242	GLN	Mainchain
1	A	29	ARG	Mainchain
1	B	32	VAL	Mainchain
1	B	69	LEU	Mainchain

## 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	2464	0	2425	142	1
1	B	2472	0	2438	148	1
2	A	78	0	0	5	0
2	B	112	0	0	5	0
All	All	5126	0	4863	277	1

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 28.

The worst 5 of 277 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:32:VAL:HB	1:A:33:PRO:HD2	1.36	1.06
1:A:205:GLN:NE2	1:A:207:ASP:H	1.59	1.01
1:A:205:GLN:HE22	1:A:207:ASP:H	1.05	0.95
1:A:58:ASP:HB3	1:A:156:LEU:HB3	1.48	0.95
1:B:77:HIS:O	1:B:78:ARG:HB2	1.67	0.95

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:GLU:N	1:B:31:SER:OG[7_455]	2.05	0.15

## 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	306/318 (96%)	270 (88%)	24 (8%)	12 (4%)	3	11
1	B	307/318 (96%)	282 (92%)	15 (5%)	10 (3%)	4	14
All	All	613/636 (96%)	552 (90%)	39 (6%)	22 (4%)	4	13

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	PRO
1	A	31	SER
1	A	32	VAL
1	A	77	HIS
1	A	78	ARG

### 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	252/259 (97%)	214 (85%)	38 (15%)	3	9
1	B	253/259 (98%)	210 (83%)	43 (17%)	2	7
All	All	505/518 (98%)	424 (84%)	81 (16%)	2	8

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	275	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	39	ARG
1	B	249	ASN
1	A	293	ARG
1	B	13	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	42	GLN
1	B	50	GLN
1	B	215	GLN
1	A	291	GLN
1	B	249	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 carbohydrates 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	310/318 (97%)	-0.10	18 (5%) 23 15	6, 49, 85, 97	0
1	B	311/318 (97%)	-0.24	15 (4%) 30 21	22, 39, 80, 90	0
All	All	621/636 (97%)	-0.17	33 (5%) 26 17	6, 43, 82, 97	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	31	SER	5.9
1	A	312	ALA	4.9
1	A	313	GLU	4.7
1	B	67	PRO	4.3
1	A	32	VAL	3.8

### 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](#)

There are no ligands in this entry.

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

There are no such residues in this entry.