



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:01 PM GMT

PDB ID : 1DOF  
Title : THE CRYSTAL STRUCTURE OF ADENYLOSUCCINATE LYASE FROM  
PYROBACULUM AEROPHILUM: INSIGHTS INTO THERMAL STABIL-  
ITY AND HUMAN PATHOLOGY  
Authors : Toth, E.A.; Yeates, T.O.; Goedken, E.; Dixon, J.E.; Marqusee, S.  
Deposited on : 1999-12-20  
Resolution : 2.10 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (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

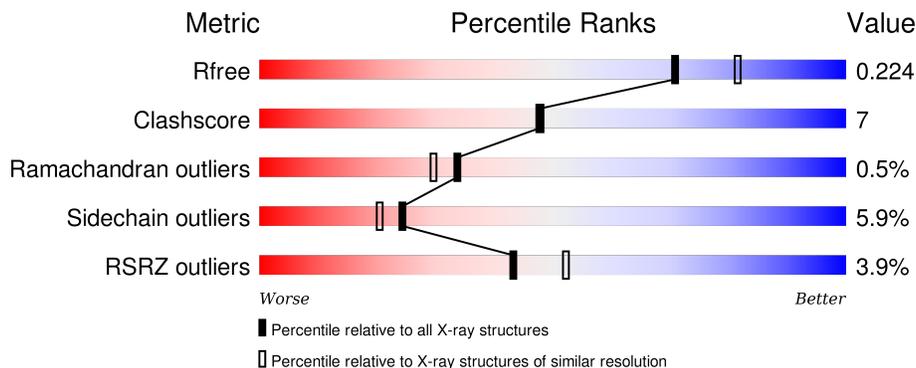
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	403	 3% 77% 14% • •
1	B	403	 4% 70% 19% 5% •
1	C	403	 5% 72% 20% • • •
1	D	403	 2% 73% 18% • • •

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12664 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 ADENYLOSUCCINATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	385	2977	1900	522	543	12	0	0	0
1	B	385	2961	1890	520	539	12	0	0	0
1	C	385	2963	1892	518	541	12	0	0	0
1	D	385	2971	1896	520	543	12	0	0	0

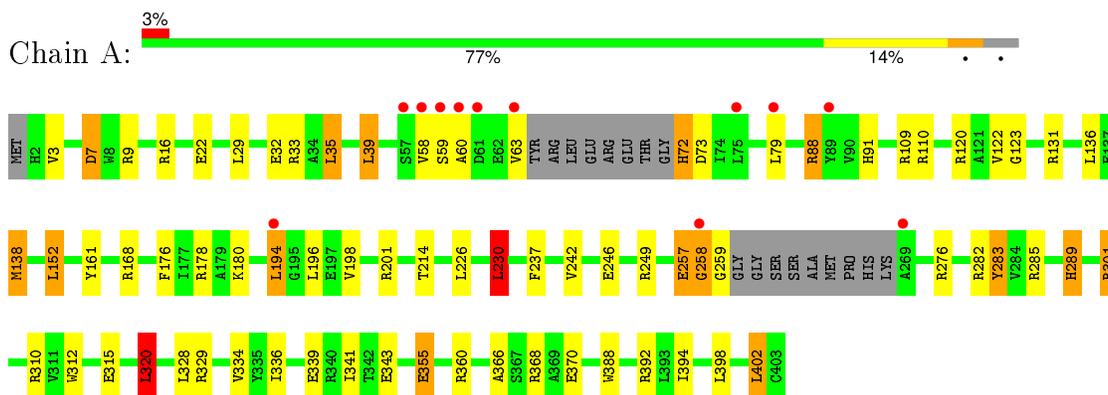
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	197	Total 197	O 197	0	0
2	B	198	Total 198	O 198	0	0
2	C	202	Total 202	O 202	0	0
2	D	195	Total 195	O 195	0	0

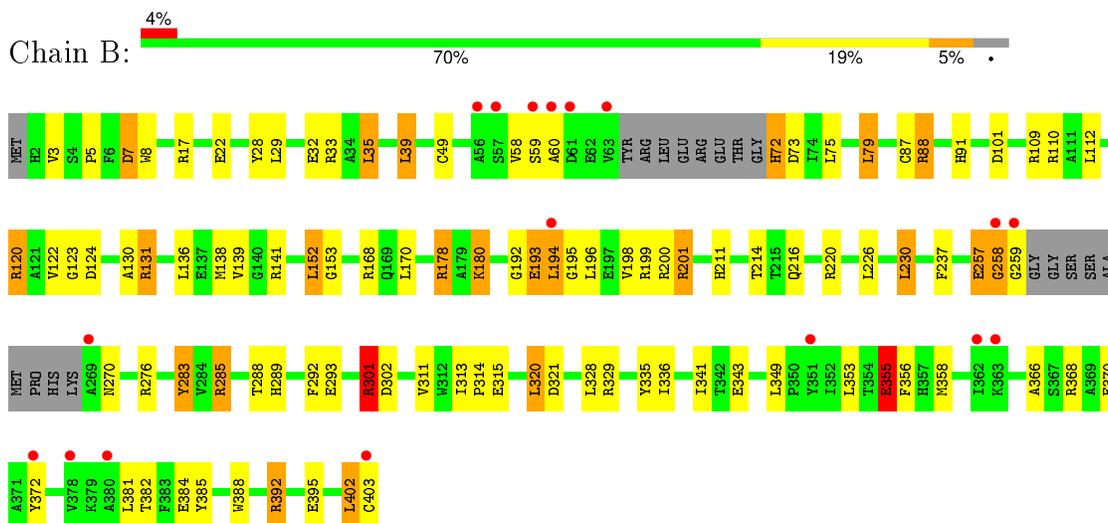
### 3 Residue-property plots [i](#)

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

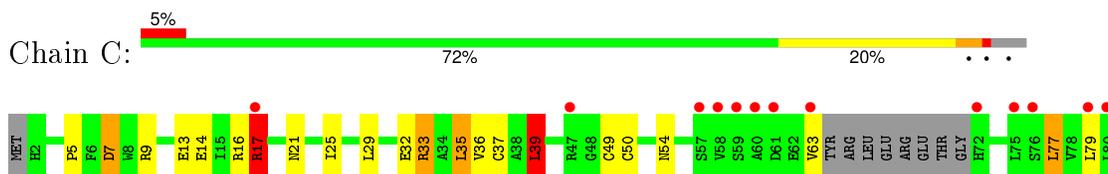
- Molecule 1: ADENYLOSUCCINATE LYASE



- Molecule 1: ADENYLOSUCCINATE LYASE



- Molecule 1: ADENYLOSUCCINATE LYASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.62Å 150.31Å 173.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 48.13 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.10) 99.5 (48.13-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.41 (at 2.10Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.203 , 0.245 0.187 , 0.224	Depositor DCC
$R_{free}$ test set	5014 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.8	Xtrriage
Anisotropy	0.623	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 63.3	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.59$ , $\langle L^2 \rangle = 0.45$	Xtrriage
Outliers	7 of 100464 reflections (0.007%)	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12664	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	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 46.91 % 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 1.0701e-04. 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.78	6/3028 (0.2%)	1.61	46/4109 (1.1%)
1	B	0.94	6/3012 (0.2%)	1.69	58/4090 (1.4%)
1	C	0.90	5/3014 (0.2%)	1.69	51/4093 (1.2%)
1	D	0.84	6/3022 (0.2%)	1.93	54/4102 (1.3%)
All	All	0.87	23/12076 (0.2%)	1.74	209/16394 (1.3%)

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	D	0	2

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	259	GLY	N-CA	-24.07	1.09	1.46
1	C	259	GLY	N-CA	-18.49	1.18	1.46
1	C	344	ASN	N-CA	16.08	1.78	1.46
1	C	258	GLY	CA-C	-14.79	1.28	1.51
1	B	258	GLY	CA-C	-14.41	1.28	1.51

The worst 5 of 209 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	178	ARG	CD-NE-CZ	38.88	178.03	123.60
1	D	109	ARG	CD-NE-CZ	28.63	163.68	123.60
1	D	59	SER	O-C-N	25.31	163.20	122.70
1	B	258	GLY	O-C-N	23.65	163.40	123.20
1	D	257	GLU	C-N-CA	-23.41	73.14	122.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	257	GLU	Mainchain
1	D	72	HIS	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	2977	0	2952	33	3
1	B	2961	0	2932	45	0
1	C	2963	0	2926	59	0
1	D	2971	0	2940	51	3
2	A	197	0	0	1	0
2	B	198	0	0	3	3
2	C	202	0	0	2	3
2	D	195	0	0	4	0
All	All	12664	0	11750	164	6

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 7.

The worst 5 of 164 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:344:ASN:N	1:C:344:ASN:CA	1.78	1.42
1:D:13:GLU:HG2	2:D:549:HOH:O	1.13	1.26
1:C:17:ARG:HH11	1:C:17:ARG:HG2	1.21	1.06
1:C:343:GLU:C	1:C:344:ASN:CA	2.35	0.94
1:C:14:GLU:HA	1:C:17:ARG:NH1	1.84	0.92

The worst 5 of 6 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:360:ARG:NH1	2:B:563:HOH:O[2_454]	0.60	1.60

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:ARG:CZ	2:B:563:HOH:O[2_454]	1.01	1.19
1:D:360:ARG:CZ	2:C:565:HOH:O[2_555]	1.14	1.06
1:D:360:ARG:NH1	2:C:565:HOH:O[2_555]	1.19	1.01
1:A:360:ARG:NH2	2:B:563:HOH:O[2_454]	1.73	0.47

## 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	379/403 (94%)	368 (97%)	10 (3%)	1 (0%)	46	45
1	B	379/403 (94%)	368 (97%)	9 (2%)	2 (0%)	34	30
1	C	379/403 (94%)	366 (97%)	12 (3%)	1 (0%)	46	45
1	D	379/403 (94%)	363 (96%)	13 (3%)	3 (1%)	24	17
All	All	1516/1612 (94%)	1465 (97%)	44 (3%)	7 (0%)	34	30

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	301	ARG
1	B	301	ARG
1	C	301	ARG
1	D	301	ARG
1	B	8	TRP

### 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	294/329 (89%)	278 (95%)	16 (5%)	27	24
1	B	292/329 (89%)	275 (94%)	17 (6%)	25	21
1	C	291/329 (88%)	274 (94%)	17 (6%)	25	21
1	D	293/329 (89%)	274 (94%)	19 (6%)	21	17
All	All	1170/1316 (89%)	1101 (94%)	69 (6%)	24	20

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	388	TRP
1	C	136	LEU
1	D	301	ARG
1	B	392	ARG
1	C	39	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	359	ASN
1	C	91	HIS
1	D	91	HIS
1	B	145	GLN
1	B	289	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](#)

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	385/403 (95%)	-0.20	12 (3%) 52 61	10, 19, 47, 84	0
1	B	385/403 (95%)	-0.13	17 (4%) 38 47	9, 19, 48, 84	0
1	C	385/403 (95%)	-0.16	21 (5%) 29 37	10, 18, 50, 78	0
1	D	385/403 (95%)	-0.23	10 (2%) 59 66	10, 19, 42, 87	0
All	All	1540/1612 (95%)	-0.18	60 (3%) 43 52	9, 19, 47, 87	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	61	ASP	6.8
1	C	259	GLY	5.5
1	B	60	ALA	4.5
1	C	79	LEU	4.3
1	B	59	SER	4.2

### 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

There are no such residues in this entry.