



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 03:04 PM GMT

PDB ID : 1DOF
Title : THE CRYSTAL STRUCTURE OF ADENYLOSUCCINATE LYASE FROM
PYROBACULUM AEROPHILUM: INSIGHTS INTO THERMAL STABIL-
ITY AND HUMAN PATHOLOGY
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Deposited on : 1999-12-20
Resolution : 2.10 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

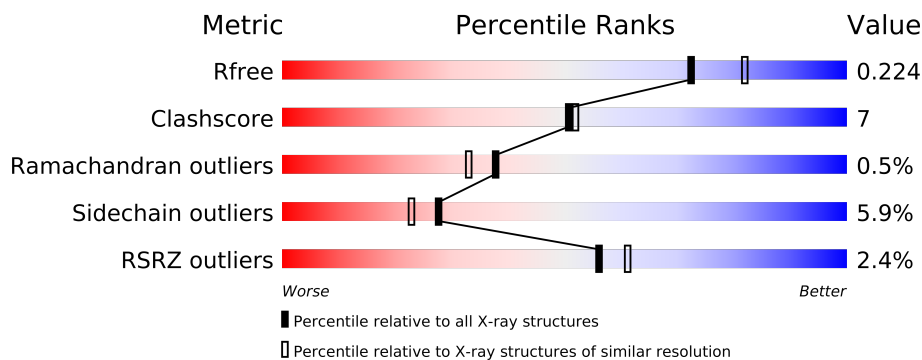
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	403	
1	B	403	
1	C	403	
1	D	403	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12664 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	385	Total	C	N	O	S	0	0	0
			2977	1900	522	543	12			
1	B	385	Total	C	N	O	S	0	0	0
			2961	1890	520	539	12			
1	C	385	Total	C	N	O	S	0	0	0
			2963	1892	518	541	12			
1	D	385	Total	C	N	O	S	0	0	0
			2971	1896	520	543	12			

- Molecule 2 is water.

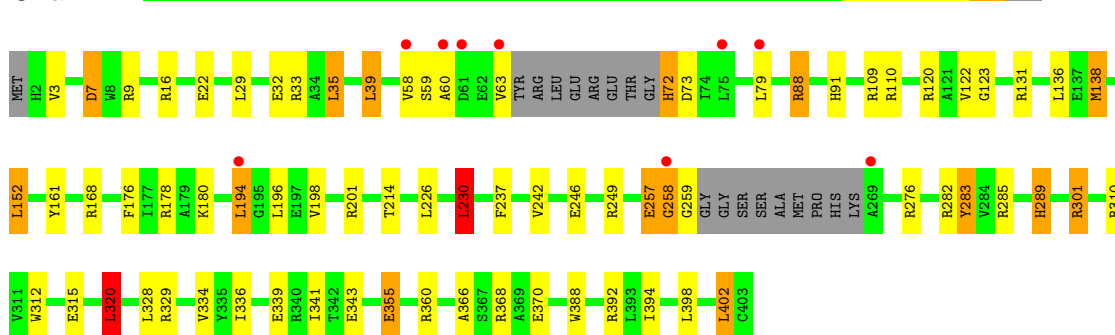
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	197	Total	O	0	0
			197	197		
2	B	198	Total	O	0	0
			198	198		
2	C	202	Total	O	0	0
			202	202		
2	D	195	Total	O	0	0
			195	195		

3 Residue-property plots

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.

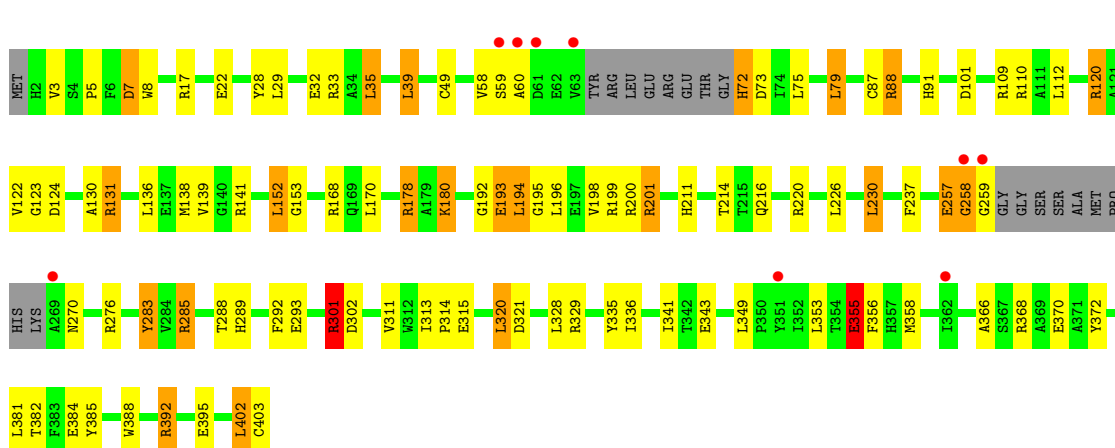
• Molecule 1: ADENYLOSUCCINATE LYASE

Chain A:



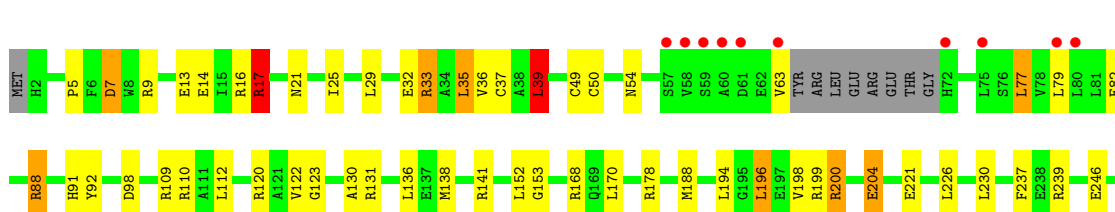
• Molecule 1: ADENYLOSUCCINATE LYASE

Chain B:



• Molecule 1: ADENYLOSUCCINATE LYASE

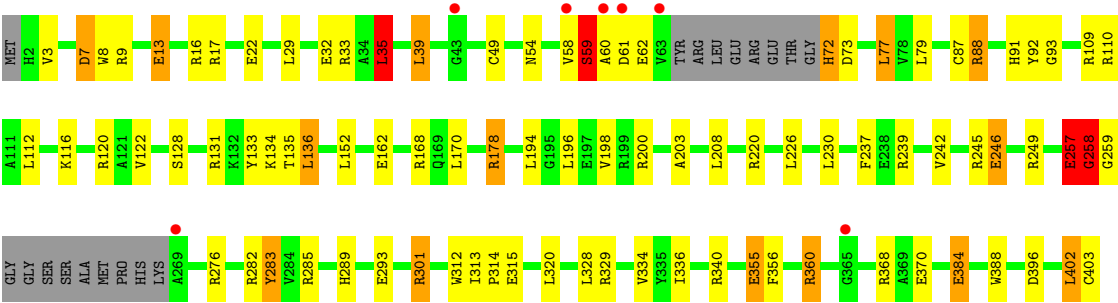
Chain C:





● Molecule 1: ADENYLOSUCCINATE LYASE

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	6.41 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.203 , 0.245 0.187 , 0.224	Depositor DCC
R_{free} test set	5017 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.623	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.59$, $\langle L^2 \rangle = 0.45$	Xtriage
Outliers	7 of 100464 reflections (0.007%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12664	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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	0.78	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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

The worst 5 of 164 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(Å)
1:A:360:ARG:NH1	2:B:563:HOH:O[2_454]	0.60	1.60
1:A:360:ARG:CZ	2:B:563:HOH:O[2_454]	1.01	1.19

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

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	379/403 (94%)	368 (97%)	10 (3%)	1 (0%)	50	49
1	B	379/403 (94%)	368 (97%)	9 (2%)	2 (0%)	38	33
1	C	379/403 (94%)	366 (97%)	12 (3%)	1 (0%)	50	49
1	D	379/403 (94%)	363 (96%)	13 (3%)	3 (1%)	27	20
All	All	1516/1612 (94%)	1465 (97%)	44 (3%)	7 (0%)	38	33

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 ⓘ

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%)	31	27
1	B	292/329 (89%)	275 (94%)	17 (6%)	28	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	291/329 (88%)	274 (94%)	17 (6%)	28	23
1	D	293/329 (89%)	274 (94%)	19 (6%)	24	20
All	All	1170/1316 (89%)	1101 (94%)	69 (6%)	28	23

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 ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	385/403 (95%)	-0.26	9 (2%) 57 62	10, 19, 47, 84	0
1	B	385/403 (95%)	-0.22	9 (2%) 57 62	9, 19, 48, 84	0
1	C	385/403 (95%)	-0.23	12 (3%) 47 52	10, 18, 50, 78	0
1	D	385/403 (95%)	-0.30	7 (1%) 65 69	10, 19, 42, 87	0
All	All	1540/1612 (95%)	-0.25	37 (2%) 56 61	9, 19, 47, 87	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	61	ASP	5.5
1	C	259	GLY	5.1
1	B	60	ALA	3.9
1	C	58	VAL	3.7
1	B	59	SER	3.6

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.