



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 8JBD / pdb_00008jbd
Title : Crystal structure of Adenylosuccinate lyase from *Thermus thermophilus* HB8, TtPurB
Authors : Nemoto, N.; Kawai, G.; Sampei, G.
Deposited on : 2023-05-08
Resolution : 2.38 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

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
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

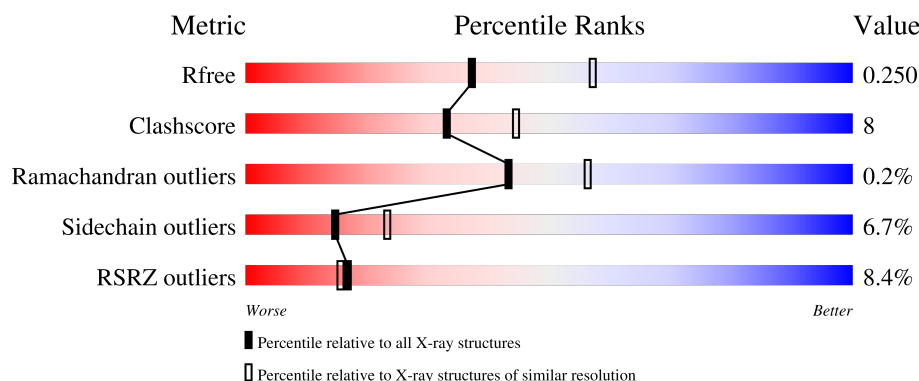
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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 ≥ 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	457	6% 58% 10% • 31%
1	B	457	5% 54% 10% •• 33%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5111 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
1	A	316	Total	C	N	O	S	0	0	0
			2482	1581	446	450	5			
1	B	304	Total	C	N	O	S	0	0	0
			2378	1518	427	428	5			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP Q5SI61
A	-19	GLY	-	expression tag	UNP Q5SI61
A	-18	SER	-	expression tag	UNP Q5SI61
A	-17	SER	-	expression tag	UNP Q5SI61
A	-16	HIS	-	expression tag	UNP Q5SI61
A	-15	HIS	-	expression tag	UNP Q5SI61
A	-14	HIS	-	expression tag	UNP Q5SI61
A	-13	HIS	-	expression tag	UNP Q5SI61
A	-12	HIS	-	expression tag	UNP Q5SI61
A	-11	HIS	-	expression tag	UNP Q5SI61
A	-10	SER	-	expression tag	UNP Q5SI61
A	-9	SER	-	expression tag	UNP Q5SI61
A	-8	GLY	-	expression tag	UNP Q5SI61
A	-7	GLU	-	expression tag	UNP Q5SI61
A	-6	ASN	-	expression tag	UNP Q5SI61
A	-5	LEU	-	expression tag	UNP Q5SI61
A	-4	TYR	-	expression tag	UNP Q5SI61
A	-3	PHE	-	expression tag	UNP Q5SI61
A	-2	GLN	-	expression tag	UNP Q5SI61
A	-1	GLY	-	expression tag	UNP Q5SI61
A	0	HIS	-	expression tag	UNP Q5SI61
B	-20	MET	-	initiating methionine	UNP Q5SI61
B	-19	GLY	-	expression tag	UNP Q5SI61
B	-18	SER	-	expression tag	UNP Q5SI61
B	-17	SER	-	expression tag	UNP Q5SI61

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP Q5SI61
B	-15	HIS	-	expression tag	UNP Q5SI61
B	-14	HIS	-	expression tag	UNP Q5SI61
B	-13	HIS	-	expression tag	UNP Q5SI61
B	-12	HIS	-	expression tag	UNP Q5SI61
B	-11	HIS	-	expression tag	UNP Q5SI61
B	-10	SER	-	expression tag	UNP Q5SI61
B	-9	SER	-	expression tag	UNP Q5SI61
B	-8	GLY	-	expression tag	UNP Q5SI61
B	-7	GLU	-	expression tag	UNP Q5SI61
B	-6	ASN	-	expression tag	UNP Q5SI61
B	-5	LEU	-	expression tag	UNP Q5SI61
B	-4	TYR	-	expression tag	UNP Q5SI61
B	-3	PHE	-	expression tag	UNP Q5SI61
B	-2	GLN	-	expression tag	UNP Q5SI61
B	-1	GLY	-	expression tag	UNP Q5SI61
B	0	HIS	-	expression tag	UNP Q5SI61

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	128	Total O 128 128	0	0
2	B	123	Total O 123 123	0	0

- Molecule 1: Adenylosuccinate lyase



PRO	GLU	ASN	PRO	LEU	LYS	GLY	LYS	GLU	LEU	ARG	ALA	LEU	PHE	ASP	PRO	LYS	PRO	L423	L424	L425	L436

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	158.66Å 158.66Å 151.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 2.38 19.99 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.99-2.38) 99.7 (19.99-2.38)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	12.17 (at 2.38Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.205 , 0.248 (Not available) , 0.250	Depositor DCC
R_{free} test set	2262 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5111	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	1.19	0/2527	1.50	9/3417 (0.3%)
1	B	1.11	3/2412 (0.1%)	1.53	12/3251 (0.4%)
All	All	1.15	3/4939 (0.1%)	1.52	21/6668 (0.3%)

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	A	0	1
1	B	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	322	PRO	C-O	-5.72	1.16	1.24
1	B	329	HIS	CE1-NE2	5.57	1.38	1.32
1	B	217	LEU	C-O	5.17	1.30	1.23

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	297	PHE	CA-CB-CG	-7.57	106.23	113.80
1	A	434	PHE	CA-CB-CG	-5.78	108.02	113.80
1	A	25	ARG	CG-CD-NE	-5.70	99.45	112.00
1	B	312	SER	CA-C-N	5.61	131.79	121.70
1	B	312	SER	C-N-CA	5.61	131.79	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	304	ALA	Peptide
1	B	310	ASP	Peptide

5.2 Too-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 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	2482	0	2515	36	1
1	B	2378	0	2432	52	0
2	A	128	0	0	3	0
2	B	123	0	0	8	0
All	All	5111	0	4947	76	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 8.

The worst 5 of 76 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:B:55:LYS:O	1:B:86:TRP:HH2	1.13	1.22
1:B:55:LYS:O	1:B:86:TRP:CH2	2.05	1.09
1:B:322:PRO:O	1:B:326:THR:HG23	1.74	0.87
1:A:155:PRO:HD2	2:A:606:HOH:O	1.78	0.84
1:B:35:GLU:HG3	1:B:40:VAL:HG22	1.60	0.82

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:130:GLU:OE1	1:A:130:GLU:OE1[12_564]	1.92	0.28

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	304/457 (66%)	298 (98%)	5 (2%)	1 (0%)	36	48
1	B	284/457 (62%)	274 (96%)	10 (4%)	0	100	100
All	All	588/914 (64%)	572 (97%)	15 (3%)	1 (0%)	43	56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	LEU

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	252/372 (68%)	233 (92%)	19 (8%)	12	19
1	B	241/372 (65%)	227 (94%)	14 (6%)	18	29
All	All	493/744 (66%)	460 (93%)	33 (7%)	15	23

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	311	ILE
1	B	326	THR
1	B	425	ARG
1	A	220	GLN
1	A	198	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	170	GLN
1	B	284	ASN
1	B	313	HIS
1	A	220	GLN
1	A	170	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 [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, 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	316/457 (69%)	0.31	27 (8%) 16 15	24, 40, 85, 114	0
1	B	304/457 (66%)	0.25	25 (8%) 17 16	24, 40, 83, 114	0
All	All	620/914 (67%)	0.28	52 (8%) 17 15	24, 40, 84, 114	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ILE	6.7
1	A	422	PRO	6.5
1	B	311	ILE	6.3
1	B	305	LEU	5.9
1	A	308	GLU	5.8

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 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.