



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 10:25 PM UTC

PDB ID : 1T8W / pdb_00001t8w
Title : Crystal Structure of E. coli AMP Nucleosidase
Authors : Zhang, Y.; Cottet, S.E.; Ealick, S.E.
Deposited on : 2004-05-13
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

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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

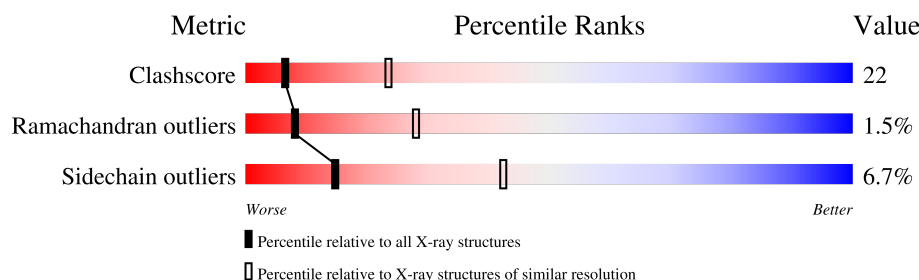
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	484	 58% 33% . . 5%
1	B	484	 57% 34% . 5%
1	C	484	 58% 33% . 5%
1	D	484	 56% 34% . 5%
1	E	484	 56% 34% 5% 5%
1	F	484	 57% 34% . . 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22064 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 AMP nucleosidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	Se	0	0	0
			3648	2317	641	681	5	4			
1	B	461	Total	C	N	O	S	Se	0	0	0
			3648	2317	641	681	5	4			
1	C	461	Total	C	N	O	S	Se	0	0	0
			3648	2317	641	681	5	4			
1	D	461	Total	C	N	O	S	Se	0	0	0
			3648	2317	641	681	5	4			
1	E	461	Total	C	N	O	S	Se	0	0	0
			3648	2317	641	681	5	4			
1	F	461	Total	C	N	O	S	Se	0	0	0
			3648	2317	641	681	5	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	MSE	MET	modified residue	UNP P15272
A	260	MSE	MET	modified residue	UNP P15272
A	302	MSE	MET	modified residue	UNP P15272
A	404	MSE	MET	modified residue	UNP P15272
B	138	MSE	MET	modified residue	UNP P15272
B	260	MSE	MET	modified residue	UNP P15272
B	302	MSE	MET	modified residue	UNP P15272
B	404	MSE	MET	modified residue	UNP P15272
C	138	MSE	MET	modified residue	UNP P15272
C	260	MSE	MET	modified residue	UNP P15272
C	302	MSE	MET	modified residue	UNP P15272
C	404	MSE	MET	modified residue	UNP P15272
D	138	MSE	MET	modified residue	UNP P15272
D	260	MSE	MET	modified residue	UNP P15272
D	302	MSE	MET	modified residue	UNP P15272
D	404	MSE	MET	modified residue	UNP P15272
E	138	MSE	MET	modified residue	UNP P15272

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Chain	Residue	Modelled	Actual	Comment	Reference
E	260	MSE	MET	modified residue	UNP P15272
E	302	MSE	MET	modified residue	UNP P15272
E	404	MSE	MET	modified residue	UNP P15272
F	138	MSE	MET	modified residue	UNP P15272
F	260	MSE	MET	modified residue	UNP P15272
F	302	MSE	MET	modified residue	UNP P15272
F	404	MSE	MET	modified residue	UNP P15272

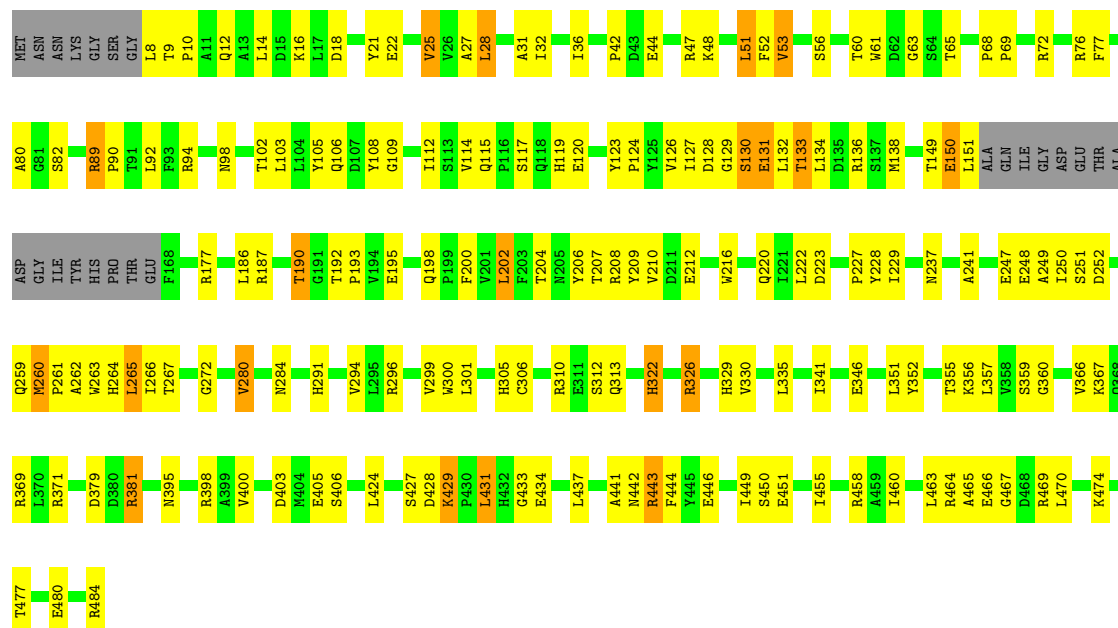
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	22	Total O 22 22	0	0
2	B	37	Total O 37 37	0	0
2	C	33	Total O 33 33	0	0
2	D	30	Total O 30 30	0	0
2	E	24	Total O 24 24	0	0
2	F	30	Total O 30 30	0	0



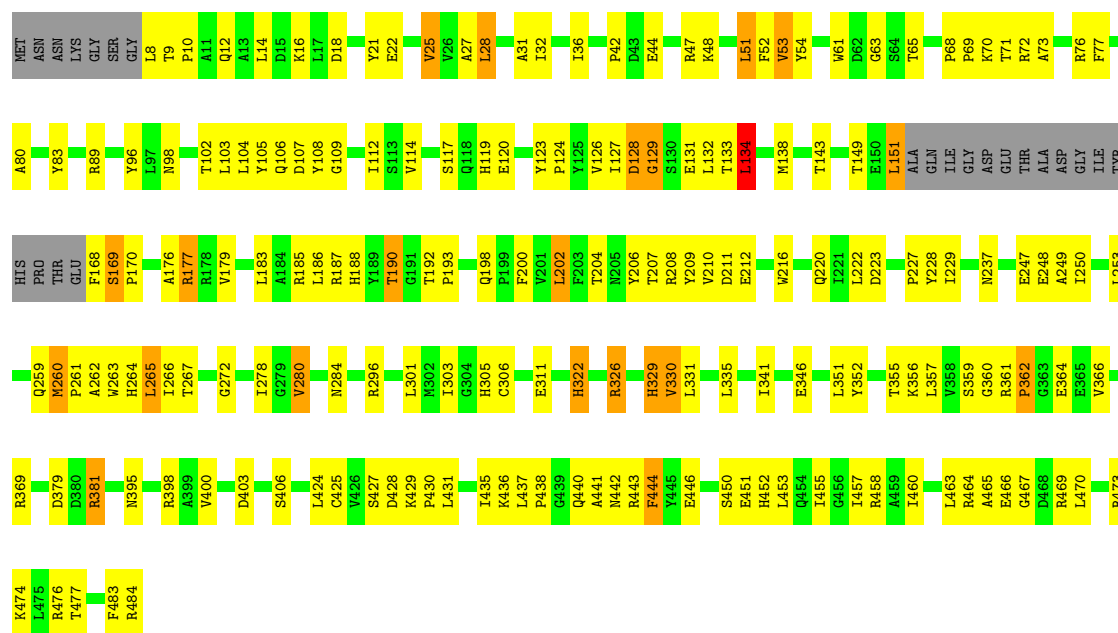
• Molecule 1: AMP nucleosidase

Chain C: 58% 33% 5%



• Molecule 1: AMP nucleosidase

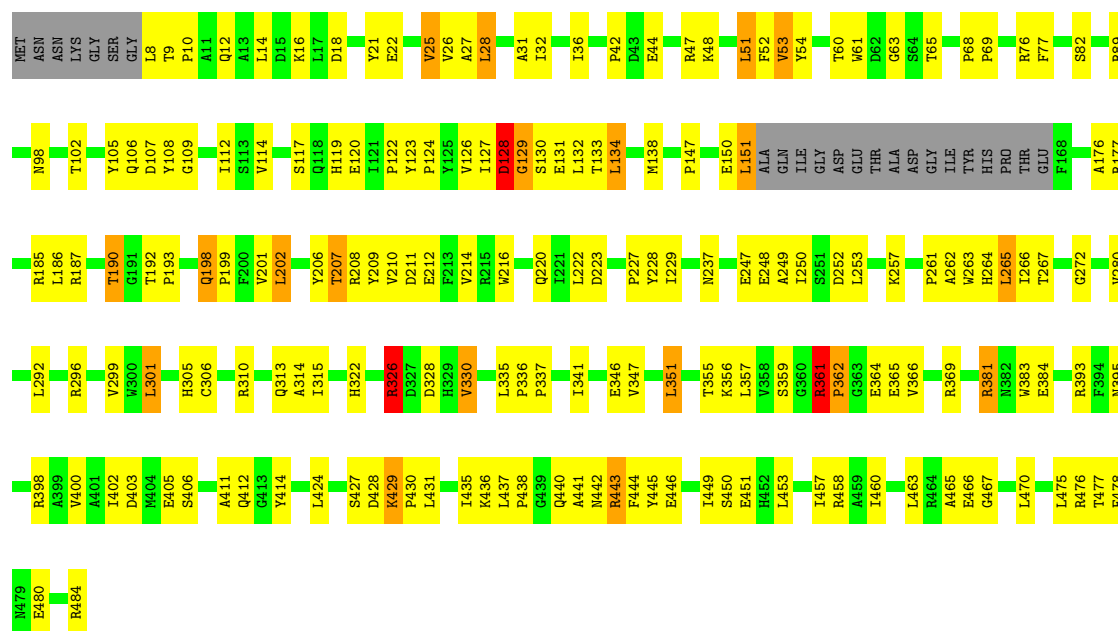
Chain D: 56% 34% 5%



• Molecule 1: AMP nucleosidase

G467	G363	E248	THR	G75	MT
G476	G364	A249	ALA	R76	ASN
L470	E366	I250	GLY	F77	ASN
K474	V366	L253	ILE	A80	LVS
L475	Q368	L253	TYR	Y83	GLY
R476	R371	Q259	HRP	Y83	SER
T477	R371	M260	PRO	I87	L8
F478	R381	P261	THR	T88	T9
N479	R381	A262	GLU	T88	P10
E480	S390	V263	F168	R89	A11
P481	S390	H264	S169	P90	Q12
P482	F394	L265	P170	A13	Q12
F483	N395	L266	H173	N98	L14
R484	N395	T267	F174	L101	L14
	R398	A268	D175	T102	K16
	A399	G272	A176	L103	L17
	V400	G272	R177	L104	D18
	D403	L278	L186	Y105	
	S406	V280	R187	Y108	Y21
	A411	R296	T180	G109	E22
	Q412	P297	G191	I112	V25
	G413	L301	T192	S113	V26
	Y414	L301	P193	V114	A27
	L424	R305	Q198	Q115	L28
		C306	P199	P116	R29
	S427	R310	V201	S117	N30
	D428	Q313	H119	Q118	A31
	K429		L202	E120	I36
	P430				
	L431				G39
	E434				
	I435				P42
	A441	R322	Y206	Y123	D43
	M442		T207	P124	E44
	R443	R326	R208	Y125	
	F444		Y209	V126	
	Y445		V210	I127	
	E446		D211	D128	R47
			E212	G129	K48
			F213		
			V214	L132	L51
			W216	T133	F52
				L134	V53
				D135	
				R136	S56
				S137	L57
				M138	
					W61
				F146	D62
				P147	G63
					S64
				L151	T65
				ALA	
				G1N	P68
				I1E	P69
				GLY	
				ASP	R72
				CTD	

Chain F: 57% 34% . . 5%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	271.80Å 271.80Å 113.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.93 – 2.80	Depositor
% Data completeness (in resolution range)	93.7 (25.93-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.223 , 0.245	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22064	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

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	0.49	0/3738	0.95	11/5088 (0.2%)
1	B	0.54	0/3738	0.94	9/5088 (0.2%)
1	C	0.56	0/3738	0.98	15/5088 (0.3%)
1	D	0.53	0/3738	0.96	11/5088 (0.2%)
1	E	0.50	0/3738	0.98	18/5088 (0.4%)
1	F	0.50	0/3738	0.95	9/5088 (0.2%)
All	All	0.52	0/22428	0.96	73/30528 (0.2%)

There are no bond length outliers.

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	169	SER	CA-C-N	8.48	129.01	119.93
1	E	169	SER	C-N-CA	8.48	129.01	119.93
1	C	429	LYS	CA-C-N	8.33	128.82	119.32
1	C	429	LYS	C-N-CA	8.33	128.82	119.32
1	B	429	LYS	CA-C-N	8.05	128.49	119.32

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	3648	0	3576	175	0
1	B	3648	0	3576	178	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3648	0	3576	159	0
1	D	3648	0	3576	168	0
1	E	3648	0	3576	170	0
1	F	3648	0	3576	175	0
2	A	22	0	0	1	0
2	B	37	0	0	3	0
2	C	33	0	0	3	0
2	D	30	0	0	3	0
2	E	24	0	0	2	0
2	F	30	0	0	2	0
All	All	22064	0	21456	944	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 22.

The worst 5 of 944 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:192:THR:HG21	1:A:264:HIS:NE2	1.74	1.02
1:F:361:ARG:HB2	1:F:365:GLU:HG2	1.42	1.00
1:C:190:THR:CG2	1:C:192:THR:HB	1.91	1.00
1:A:190:THR:CG2	1:A:192:THR:HB	1.93	0.99
1:D:190:THR:CG2	1:D:192:THR:HB	1.92	0.98

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	457/484 (94%)	408 (89%)	43 (9%)	6 (1%)	9	31
1	B	457/484 (94%)	413 (90%)	38 (8%)	6 (1%)	9	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	457/484 (94%)	410 (90%)	43 (9%)	4 (1%)	14	41
1	D	457/484 (94%)	409 (90%)	39 (8%)	9 (2%)	6	21
1	E	457/484 (94%)	414 (91%)	38 (8%)	5 (1%)	11	36
1	F	457/484 (94%)	409 (90%)	37 (8%)	11 (2%)	4	17
All	All	2742/2904 (94%)	2463 (90%)	238 (9%)	41 (2%)	8	28

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	362	PRO
1	C	130	SER
1	D	129	GLY
1	F	129	GLY
1	B	129	GLY

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	390/403 (97%)	363 (93%)	27 (7%)	14	41
1	B	390/403 (97%)	363 (93%)	27 (7%)	14	41
1	C	390/403 (97%)	365 (94%)	25 (6%)	16	44
1	D	390/403 (97%)	363 (93%)	27 (7%)	14	41
1	E	390/403 (97%)	364 (93%)	26 (7%)	15	42
1	F	390/403 (97%)	366 (94%)	24 (6%)	16	45
All	All	2340/2418 (97%)	2184 (93%)	156 (7%)	15	42

5 of 156 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	190	THR
1	F	210	VAL

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Mol	Chain	Res	Type
1	E	222	LEU
1	E	431	LEU
1	F	351	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	329	HIS
1	F	284	ASN
1	D	237	ASN
1	F	237	ASN
1	F	329	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 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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.