



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:24 PM GMT

PDB ID : 1K4K
Title : Crystal structure of E. coli Nicotinic acid mononucleotide adenylyltransferase
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Deposited on : 2001-10-08
Resolution : 2.00 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
<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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

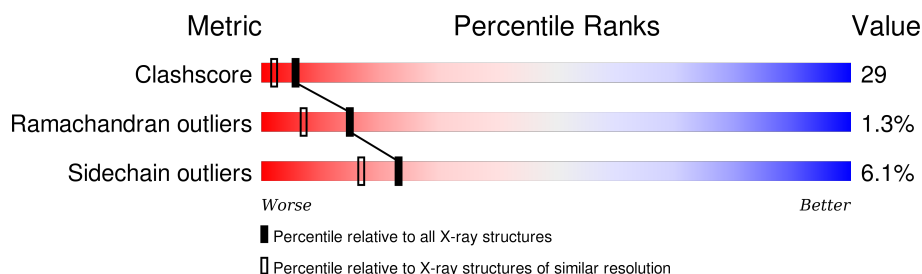
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	213	
1	B	213	
1	C	213	
1	D	213	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	XE	A	631	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7426 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 Nicotinic acid mononucleotide adenylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1734	1111	298	320	5			
1	B	204	Total	C	N	O	S	0	0	0
			1647	1049	288	305	5			
1	C	213	Total	C	N	O	S	0	0	0
			1734	1111	298	320	5			
1	D	212	Total	C	N	O	S	0	0	0
			1722	1105	294	318	5			

- Molecule 2 is XENON (three-letter code: XE) (formula: Xe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Xe	0	0
			1	1		
2	A	2	Total	Xe	0	0
			2	2		
2	C	1	Total	Xe	0	0
			1	1		

- Molecule 3 is water.

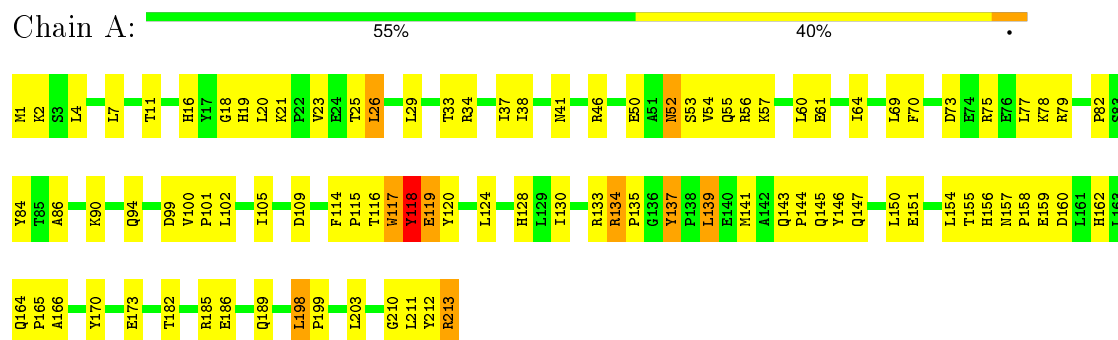
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	146	Total	O	0	0
			146	146		
3	B	118	Total	O	0	0
			118	118		
3	C	154	Total	O	0	0
			154	154		
3	D	167	Total	O	0	0
			167	167		

3 Residue-property plots

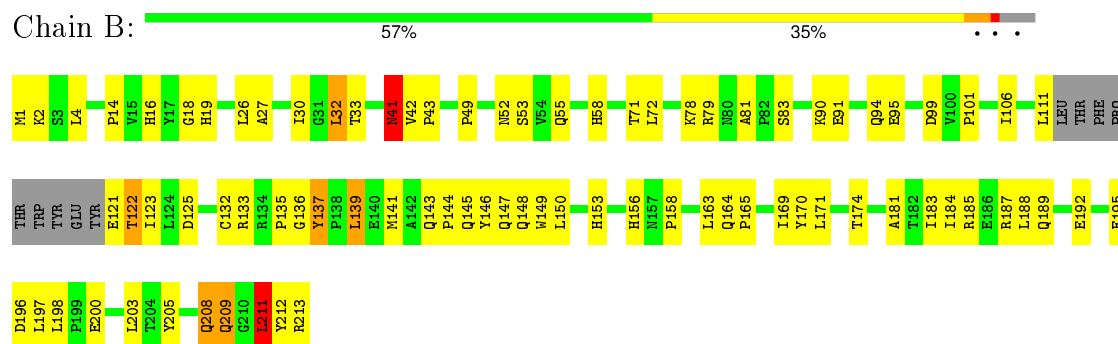
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

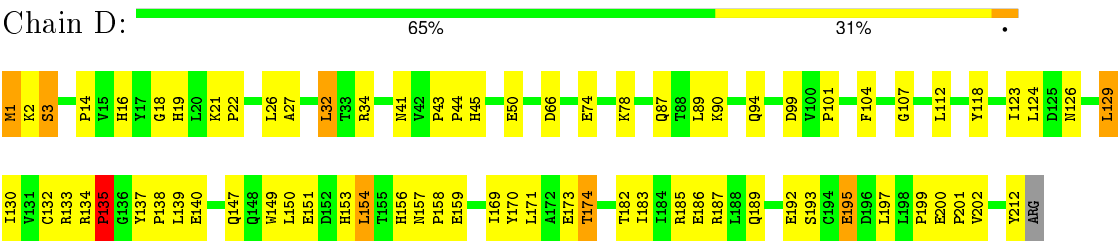
- Molecule 1: Nicotinic acid mononucleotide adenylyltransferase



- Molecule 1: Nicotinic acid mononucleotide adenylyltransferase



● Molecule 1: Nicotinic acid mononucleotide adenylyltransferase



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	58.44Å 66.53Å 72.86Å 72.68° 88.77° 69.55°	Depositor
Resolution (Å)	40.00 – 2.00	Depositor
% Data completeness (in resolution range)	91.5 (40.00-2.00)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.210 , 0.262	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7426	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: XE

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	0.53	0/1784	0.77	1/2437 (0.0%)
1	B	0.51	0/1690	0.74	2/2304 (0.1%)
1	C	0.53	0/1784	0.80	1/2437 (0.0%)
1	D	0.57	0/1772	0.77	1/2423 (0.0%)
All	All	0.54	0/7030	0.77	5/9601 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	41	ASN	N-CA-C	-6.24	94.16	111.00
1	A	118	TYR	N-CA-C	5.64	126.24	111.00
1	C	119	GLU	N-CA-C	-5.35	96.55	111.00
1	B	41	ASN	N-CA-C	-5.13	97.14	111.00
1	B	211	LEU	N-CA-C	5.03	124.58	111.00

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	1734	0	1708	121	0
1	B	1647	0	1632	101	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1734	0	1708	91	0
1	D	1722	0	1695	80	0
2	A	2	0	0	6	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	146	0	0	56	0
3	B	118	0	0	32	0
3	C	154	0	0	32	0
3	D	167	0	0	33	0
All	All	7426	0	6743	393	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 29.

The worst 5 of 393 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:181:ALA:HB2	3:B:742:HOH:O	1.42	1.15
1:A:69:LEU:HA	3:A:753:HOH:O	1.45	1.12
1:A:20:LEU:HD23	2:A:631:XE:XE	2.36	1.03
1:B:133:ARG:CZ	1:B:171:LEU:HD21	1.89	1.02
1:A:189:GLN:HB3	3:A:747:HOH:O	1.58	1.01

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	211/213 (99%)	204 (97%)	5 (2%)	2 (1%)	21 13
1	B	200/213 (94%)	191 (96%)	4 (2%)	5 (2%)	7 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	211/213 (99%)	201 (95%)	8 (4%)	2 (1%)	21	13
1	D	210/213 (99%)	202 (96%)	6 (3%)	2 (1%)	19	11
All	All	832/852 (98%)	798 (96%)	23 (3%)	11 (1%)	15	7

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	TYR
1	A	119	GLU
1	B	211	LEU
1	C	118	TYR
1	D	135	PRO

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	190/190 (100%)	178 (94%)	12 (6%)	22	16
1	B	181/190 (95%)	173 (96%)	8 (4%)	35	30
1	C	190/190 (100%)	176 (93%)	14 (7%)	17	11
1	D	189/190 (100%)	177 (94%)	12 (6%)	22	16
All	All	750/760 (99%)	704 (94%)	46 (6%)	23	17

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	14	PRO
1	C	111	LEU
1	D	150	LEU
1	C	32	LEU
1	C	44	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	148	GLN
1	C	16	HIS
1	D	58	HIS
1	B	164	GLN
1	A	94	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.