wwPDB X-ray Structure Validation Summary Report (i)

Jan 30, 2024 – 08:21 PM EST

PDB ID	:	1KAM
Title	:	Structure of Bacillus subtilis Nicotinic Acid Mononucleotide Adenylyl Transferase
Authors	:	Olland, A.M.; Underwood, K.W.; Czerwinski, R.M.; Lo, M.C.; Aulabaugh, A.; Bard, J.; Stahl, M.L.; Somers, W.S.; Sullivan, F.X.; Chopra, R.
Deposited on	:	2001-11-02
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

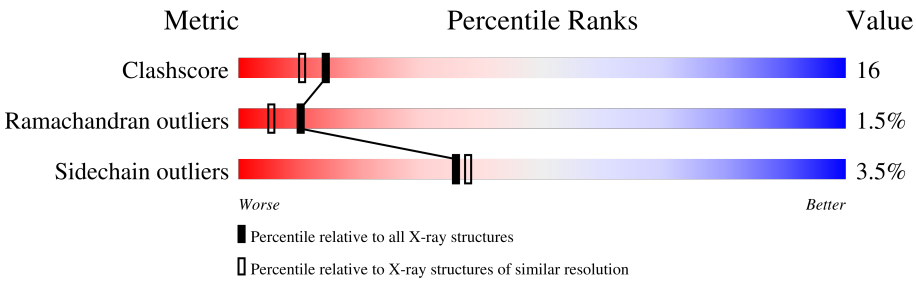
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	194	61% 27% • 7%
1	B	194	63% 25% • 10%
1	C	194	66% 23% • 8%
1	D	194	62% 25% • • 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5984 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 NICOTINATE-NUCLEOTIDE ADENYLYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	180	1485	973	235	271	6	0	0	0
1	B	175	1445	948	231	260	6	0	0	0
1	C	179	1478	970	234	268	6	0	0	0
1	D	174	1437	944	228	259	6	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	expression tag	UNP P54455
A	-3	MET	-	expression tag	UNP P54455
A	-2	PRO	-	expression tag	UNP P54455
A	-1	GLY	-	expression tag	UNP P54455
A	0	GLY	-	expression tag	UNP P54455
A	1	SER	MET	cloning artifact	UNP P54455
B	-4	HIS	-	expression tag	UNP P54455
B	-3	MET	-	expression tag	UNP P54455
B	-2	PRO	-	expression tag	UNP P54455
B	-1	GLY	-	expression tag	UNP P54455
B	0	GLY	-	expression tag	UNP P54455
B	1	SER	MET	cloning artifact	UNP P54455
C	-4	HIS	-	expression tag	UNP P54455
C	-3	MET	-	expression tag	UNP P54455
C	-2	PRO	-	expression tag	UNP P54455
C	-1	GLY	-	expression tag	UNP P54455
C	0	GLY	-	expression tag	UNP P54455
C	1	SER	MET	cloning artifact	UNP P54455
D	-4	HIS	-	expression tag	UNP P54455
D	-3	MET	-	expression tag	UNP P54455
D	-2	PRO	-	expression tag	UNP P54455

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP P54455
D	0	GLY	-	expression tag	UNP P54455
D	1	SER	MET	cloning artifact	UNP P54455

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	33	33	33	0	0
			Total	O		
2	B	27	27	27	0	0
			Total	O		
2	C	45	45	45	0	0
			Total	O		
2	D	34	34	34	0	0

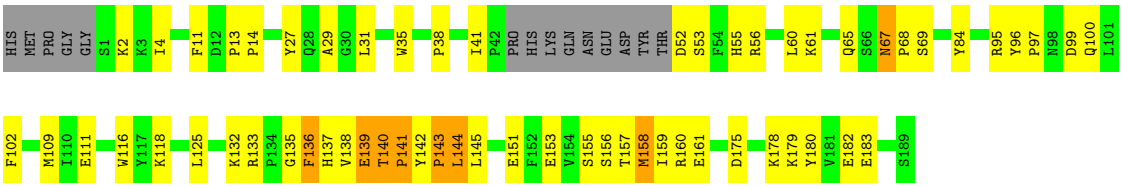
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

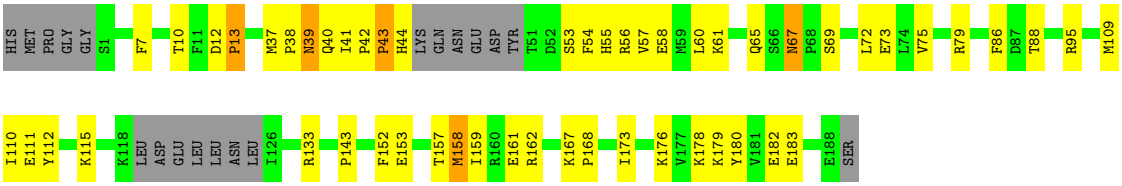
• Molecule 1: NICOTINATE-NUCLEOTIDE ADENYLYLTRANSFERASE

Chain A:



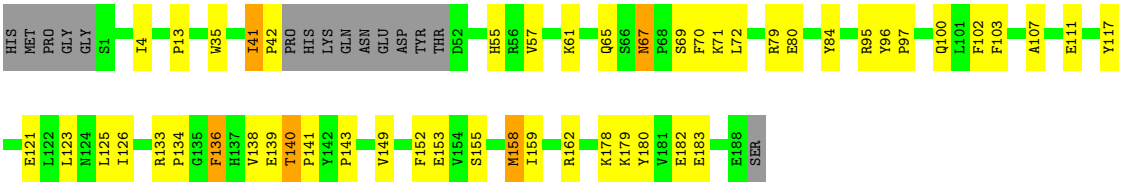
• Molecule 1: NICOTINATE-NUCLEOTIDE ADENYLYLTRANSFERASE

Chain B:



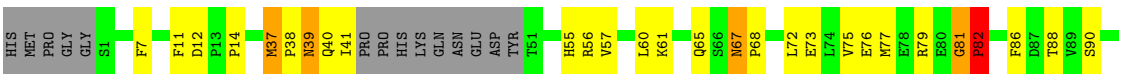
• Molecule 1: NICOTINATE-NUCLEOTIDE ADENYLYLTRANSFERASE

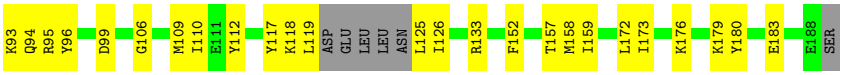
Chain C:



• Molecule 1: NICOTINATE-NUCLEOTIDE ADENYLYLTRANSFERASE

Chain D:




K93
Q94
R95
Y96
D99
G106
M109
I110
E111
Y112
Y117
K118
L119
ASP
GLU
LEU
LEU
ASN
L125
I126
R133
F152
T157
M158
I159
L172
I173
K176
K179
Y180
E183
E188
SER

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	43.98Å 126.10Å 70.58Å 90.00° 92.73° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	96.9 (20.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5984	wwPDB-VP
Average B, all atoms (Å^2)	27.0	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	0.42	0/1527	0.63	2/2064 (0.1%)
1	B	0.38	0/1488	0.61	1/2012 (0.0%)
1	C	0.40	0/1520	0.61	0/2056
1	D	0.38	0/1477	0.67	1/1995 (0.1%)
All	All	0.40	0/6012	0.63	4/8127 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	81	GLY	C-N-CD	-6.98	105.25	120.60
1	A	145	LEU	N-CA-C	-5.26	96.80	111.00
1	B	143	PRO	N-CA-C	-5.21	98.55	112.10
1	A	139	GLU	N-CA-C	-5.16	97.07	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	1485	0	1474	54	0
1	B	1445	0	1429	57	0
1	C	1478	0	1469	43	0
1	D	1437	0	1430	51	0
2	A	33	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	27	0	0	0	0
2	C	45	0	0	1	0
2	D	34	0	0	1	0
All	All	5984	0	5802	181	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 16.

The worst 5 of 181 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:37:MET:HE1	1:B:75:VAL:HG22	1.48	0.95
1:D:37:MET:HE1	1:D:75:VAL:HG22	1.54	0.90
1:C:117:TYR:O	1:C:121:GLU:HG2	1.73	0.89
1:B:37:MET:CE	1:B:75:VAL:HG22	2.10	0.81
1:D:37:MET:CE	1:D:75:VAL:HG22	2.12	0.79

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	176/194 (91%)	168 (96%)	3 (2%)	5 (3%)	5 1
1	B	169/194 (87%)	163 (96%)	5 (3%)	1 (1%)	25 21
1	C	175/194 (90%)	169 (97%)	3 (2%)	3 (2%)	9 4
1	D	168/194 (87%)	164 (98%)	3 (2%)	1 (1%)	25 21
All	All	688/776 (89%)	664 (96%)	14 (2%)	10 (2%)	10 5

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	PHE
1	A	140	THR
1	A	141	PRO
1	A	143	PRO
1	A	144	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	165/177 (93%)	160 (97%)	5 (3%)	41	44
1	B	160/177 (90%)	154 (96%)	6 (4%)	33	34
1	C	164/177 (93%)	158 (96%)	6 (4%)	34	35
1	D	159/177 (90%)	153 (96%)	6 (4%)	33	34
All	All	648/708 (92%)	625 (96%)	23 (4%)	36	38

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	125	LEU
1	D	7	PHE
1	C	158	MET
1	D	37	MET
1	B	13	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	23	ASN
1	D	55	HIS
1	D	67	ASN
1	D	65	GLN
1	B	55	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 monosaccharides 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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.