wwPDB X-ray Structure Validation Summary Report (i)

Nov 16, 2023 – 05:15 AM JST

PDB ID	:	6KV3
Title	:	Crystal Structure of NAD+ Synthetase from Staphylococcus aureus
Authors	:	Nasrin, S.K.; Sandeep, S.K.
Deposited on	:	2019-09-03
Resolution	:	2.30 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 (1)) were used in the production of this report:

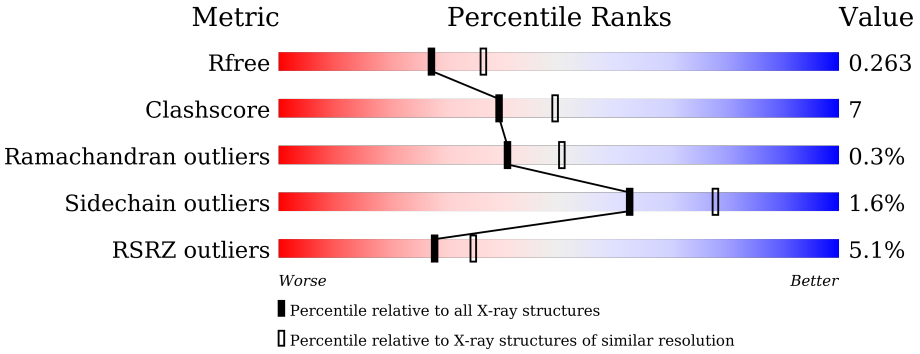
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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% 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	281	4% 80% 9% 11%
1	B	281	4% 75% 14% • 10%
1	C	281	5% 76% 12% 12%
1	D	281	5% 69% 16% • 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8486 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 NH(3)-dependent NAD(+) synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	249	1960	1238	335	382	5	0	0	0
			Total	C	N	O	S			
1	C	248	1927	1219	328	375	5	0	0	0
			Total	C	N	O	S			
1	B	252	1984	1252	341	386	5	0	0	0
			Total	C	N	O	S			
1	D	243	1900	1202	326	367	5	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	274	LEU	-	expression tag	UNP Q5HEK9
A	275	GLU	-	expression tag	UNP Q5HEK9
A	276	HIS	-	expression tag	UNP Q5HEK9
A	277	HIS	-	expression tag	UNP Q5HEK9
A	278	HIS	-	expression tag	UNP Q5HEK9
A	279	HIS	-	expression tag	UNP Q5HEK9
A	280	HIS	-	expression tag	UNP Q5HEK9
A	281	HIS	-	expression tag	UNP Q5HEK9
C	274	LEU	-	expression tag	UNP Q5HEK9
C	275	GLU	-	expression tag	UNP Q5HEK9
C	276	HIS	-	expression tag	UNP Q5HEK9
C	277	HIS	-	expression tag	UNP Q5HEK9
C	278	HIS	-	expression tag	UNP Q5HEK9
C	279	HIS	-	expression tag	UNP Q5HEK9
C	280	HIS	-	expression tag	UNP Q5HEK9
C	281	HIS	-	expression tag	UNP Q5HEK9
B	274	LEU	-	expression tag	UNP Q5HEK9
B	275	GLU	-	expression tag	UNP Q5HEK9
B	276	HIS	-	expression tag	UNP Q5HEK9
B	277	HIS	-	expression tag	UNP Q5HEK9
B	278	HIS	-	expression tag	UNP Q5HEK9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	279	HIS	-	expression tag	UNP Q5HEK9
B	280	HIS	-	expression tag	UNP Q5HEK9
B	281	HIS	-	expression tag	UNP Q5HEK9
D	274	LEU	-	expression tag	UNP Q5HEK9
D	275	GLU	-	expression tag	UNP Q5HEK9
D	276	HIS	-	expression tag	UNP Q5HEK9
D	277	HIS	-	expression tag	UNP Q5HEK9
D	278	HIS	-	expression tag	UNP Q5HEK9
D	279	HIS	-	expression tag	UNP Q5HEK9
D	280	HIS	-	expression tag	UNP Q5HEK9
D	281	HIS	-	expression tag	UNP Q5HEK9

- Molecule 2 is water.

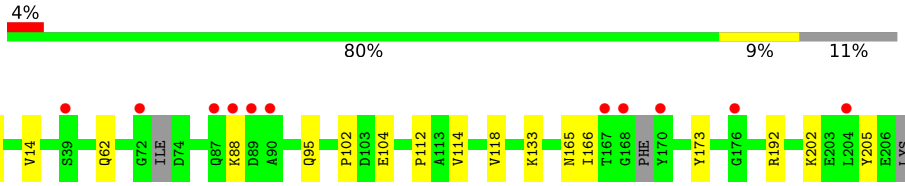
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	201	201	201	0	0
			Total	O		
2	C	157	157	157	0	0
			Total	O		
2	B	197	197	197	0	0
			Total	O		
2	D	160	160	160	0	0

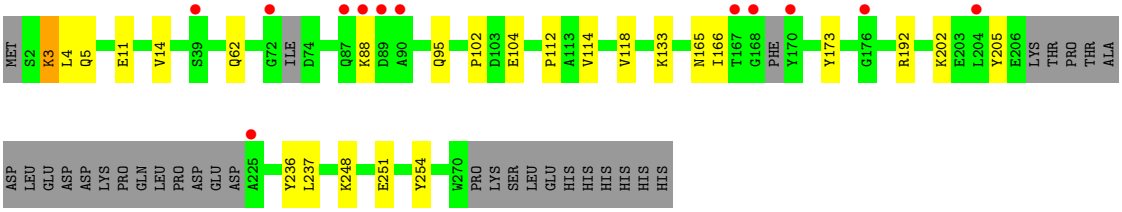
3 Residue-property plots (i)

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 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: NH(3)-dependent NAD(+) synthetase

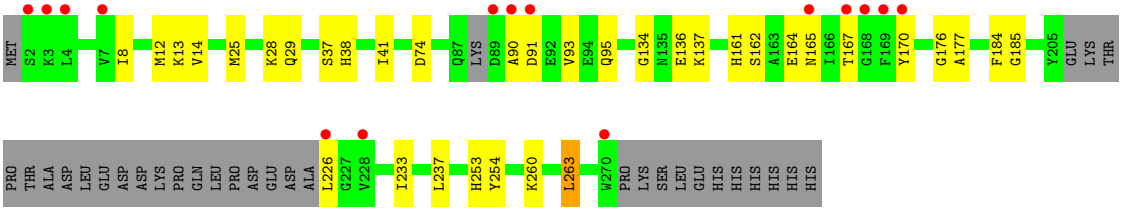
Chain A:





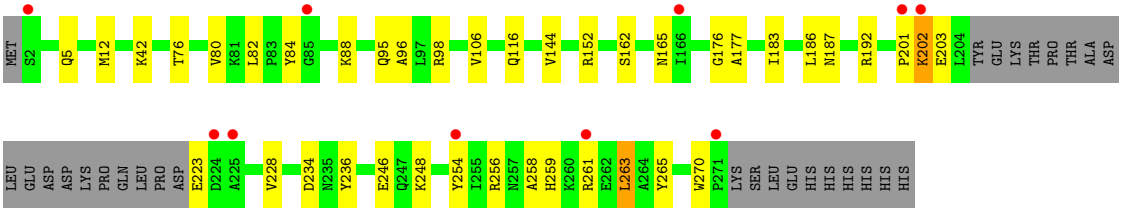
• Molecule 1: NH(3)-dependent NAD(+) synthetase

Chain C:



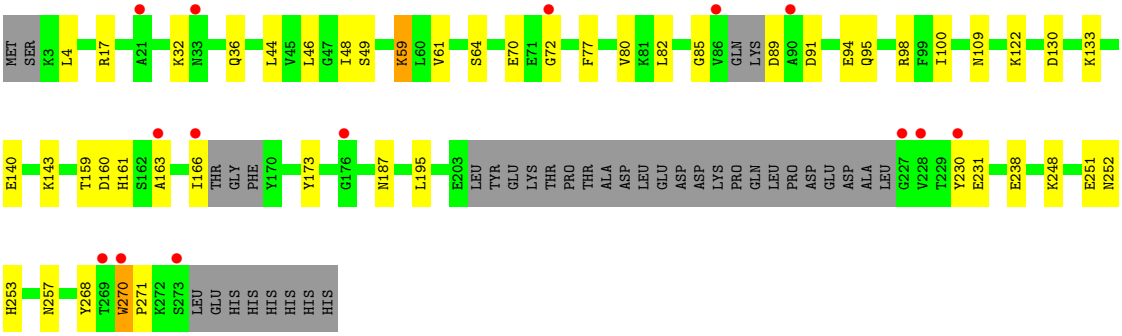
• Molecule 1: NH(3)-dependent NAD(+) synthetase

Chain B:



• Molecule 1: NH(3)-dependent NAD(+) synthetase

Chain D:


MET
SER
K3
L4
R17
A21
K32
N33
Q36
L44
V45
L46
G47
I48
S49
K59
L60
V61
S64
E70
E71
G72
F77
V80
K81
L82
G85
V86
GLN
LYS
D89
A90
D91
E94
Q95
R98
F99
I100
N109
K122
D130
K133
E140
K143
T159
D160
H161
S162
A163
I166
THR
GLY
PHE
Y170
Y173
G176
N187
L195
E203
LEU
TYR
GLU
LYS
THR
PRO
THR
ALA
ASP
LEU
GLU
ASP
ASP
LYS
PRO
GLN
LEU
PRO
ASP
GLU
ASP
ALA
LEU
G227
V228
T229
Y230
E231
E238
K248
E251
N252
H253
N257
Y268
T269
W270
P271
K272
S273
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	50.98Å 107.71Å 93.99Å 90.00° 96.72° 90.00°	Depositor
Resolution (Å)	46.67 – 2.30 53.86 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (46.67-2.30) 97.5 (53.86-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.96 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.211 , 0.267 0.213 , 0.263	Depositor DCC
R_{free} test set	1991 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å^2)	23.8	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 59.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	8486	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.44	0/1985	0.58	0/2670
1	B	0.42	0/2012	0.56	0/2712
1	C	0.43	0/1955	0.57	0/2637
1	D	0.44	0/1927	0.60	0/2597
All	All	0.43	0/7879	0.58	0/10616

There are no bond length outliers.

There are no bond angle outliers.

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	1960	0	1953	19	0
1	B	1984	0	1988	29	0
1	C	1927	0	1910	34	0
1	D	1900	0	1898	38	1
2	A	201	0	0	5	2
2	B	197	0	0	9	3
2	C	157	0	0	3	1
2	D	160	0	0	8	1
All	All	8486	0	7749	115	5

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 7.

The worst 5 of 115 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:C:167:THR:HB	1:C:226:LEU:CD1	1.74	1.18
1:D:91:ASP:O	1:D:95:GLN:HG3	1.55	1.04
1:C:167:THR:HB	1:C:226:LEU:HD13	1.39	1.02
1:C:167:THR:HA	1:C:226:LEU:HD21	1.51	0.93
2:A:314:HOH:O	1:D:17:ARG:HD3	1.71	0.91

All (5) 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)
2:B:492:HOH:O	2:B:494:HOH:O[1_655]	1.20	1.00
1:D:36:GLN:OE1	1:D:122:LYS:NZ[1_655]	1.43	0.77
2:A:459:HOH:O	2:C:426:HOH:O[1_654]	1.90	0.30
2:A:474:HOH:O	2:B:486:HOH:O[2_545]	1.98	0.22
2:B:443:HOH:O	2:D:367:HOH:O[2_556]	2.18	0.02

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	241/281 (86%)	232 (96%)	8 (3%)	1 (0%)	34	42
1	B	248/281 (88%)	239 (96%)	8 (3%)	1 (0%)	34	42
1	C	242/281 (86%)	238 (98%)	4 (2%)	0	100	100
1	D	235/281 (84%)	229 (97%)	5 (2%)	1 (0%)	34	42
All	All	966/1124 (86%)	938 (97%)	25 (3%)	3 (0%)	41	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	201	PRO
1	D	270	TRP
1	A	165	ASN

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	210/244 (86%)	207 (99%)	3 (1%)	67	81
1	B	214/244 (88%)	210 (98%)	4 (2%)	57	73
1	C	205/244 (84%)	201 (98%)	4 (2%)	55	72
1	D	204/244 (84%)	202 (99%)	2 (1%)	76	87
All	All	833/976 (85%)	820 (98%)	13 (2%)	62	78

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	202	LYS
1	B	223	GLU
1	D	230	TYR
1	B	263	LEU
1	D	59	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	252	ASN

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)

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	249/281 (88%)	0.50	12 (4%)	30	37	17, 24, 47, 58	0
1	B	252/281 (89%)	0.55	10 (3%)	38	45	17, 26, 45, 58	0
1	C	248/281 (88%)	0.52	15 (6%)	21	28	15, 25, 51, 77	0
1	D	243/281 (86%)	0.56	14 (5%)	23	29	15, 26, 49, 64	0
All	All	992/1124 (88%)	0.53	51 (5%)	28	35	15, 25, 48, 77	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	90	ALA	7.6
1	B	2	SER	5.9
1	A	168	GLY	5.3
1	C	167	THR	5.0
1	D	72	GLY	4.8

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 monosaccharides 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.