



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 11:22 PM UTC

PDB ID : 6KV3 / pdb_00006kv3
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 ⓘ 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

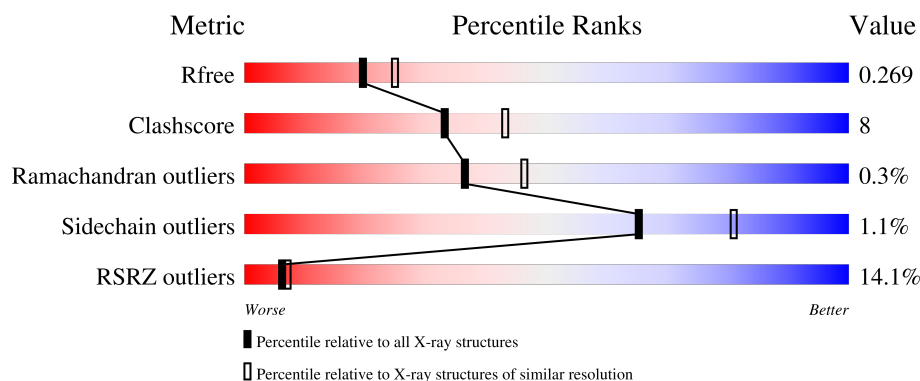
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. 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	281	12% 80% 8% 11%
1	B	281	12% 75% 13% 10%
1	C	281	12% 77% 11% 12%
1	D	281	14% 68% 17% 14%

2 Entry composition

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

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

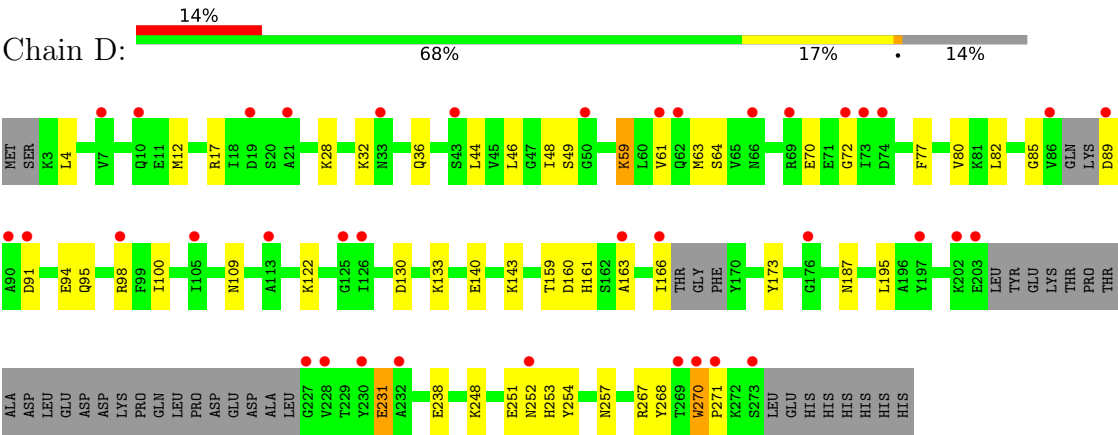
- Molecule 2 is water.

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

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



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



4 Data and refinement statistics

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 46.67 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (46.67-2.30) 97.5 (46.67-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.96 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.211 , 0.267 0.219 , 0.269	Depositor DCC
R_{free} test set	1991 reflections (4.44%)	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)	0.37 , 66.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	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.*

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 [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	0/1985	0.65	0/2670
1	B	0.42	0/2012	0.60	1/2712 (0.0%)
1	C	0.42	0/1955	0.63	0/2637
1	D	0.43	0/1927	0.67	1/2597 (0.0%)
All	All	0.42	0/7879	0.64	2/10616 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	GLU	N-CA-C	-6.10	105.84	113.28
1	D	231	GLU	CA-CB-CG	-5.01	104.07	114.10

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	30	0
1	C	1927	0	1910	37	0
1	D	1900	0	1898	40	1
2	A	201	0	0	5	2
2	B	197	0	0	10	3
2	C	157	0	0	3	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	160	0	0	8	1
All	All	8486	0	7749	121	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 8.

The worst 5 of 121 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%)	30	38
1	B	248/281 (88%)	239 (96%)	8 (3%)	1 (0%)	30	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	242/281 (86%)	238 (98%)	4 (2%)	0	100	100
1	D	235/281 (84%)	229 (97%)	5 (2%)	1 (0%)	30	38
All	All	966/1124 (86%)	938 (97%)	25 (3%)	3 (0%)	36	46

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 ⓘ

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%)	208 (99%)	2 (1%)	68	82
1	B	214/244 (88%)	211 (99%)	3 (1%)	59	76
1	C	205/244 (84%)	203 (99%)	2 (1%)	68	82
1	D	204/244 (84%)	202 (99%)	2 (1%)	68	82
All	All	833/976 (85%)	824 (99%)	9 (1%)	65	81

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	59	LYS
1	D	267	ARG
1	C	263	LEU
1	B	202	LYS
1	B	223	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	153	GLN
1	D	161	HIS
1	D	252	ASN
1	C	253	HIS
1	B	116	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	249/281 (88%)	1.01	33 (13%) 7 8	17, 24, 47, 58	0
1	B	252/281 (89%)	1.12	34 (13%) 7 8	17, 26, 45, 58	0
1	C	248/281 (88%)	1.04	35 (14%) 6 7	15, 25, 51, 77	0
1	D	243/281 (86%)	1.07	38 (15%) 5 6	15, 26, 49, 64	0
All	All	992/1124 (88%)	1.06	140 (14%) 6 7	15, 25, 48, 77	0

The worst 5 of 140 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	72	GLY	7.0
1	C	90	ALA	7.0
1	B	2	SER	6.6
1	A	168	GLY	6.4
1	B	202	LYS	5.4

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.