



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 05:49 am GMT

PDB ID : 3OJL
Title : Native structure of the UDP-N-acetyl-mannosamine dehydrogenase Cap5O from *Staphylococcus aureus*
Authors : Nessler, S.; Gruszczyk, J.; Olivares-Illana, V.; Meyer, P.; Morera, S.; Grangeasse, C.; Fleurie, A.
Deposited on : 2010-08-23
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

<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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

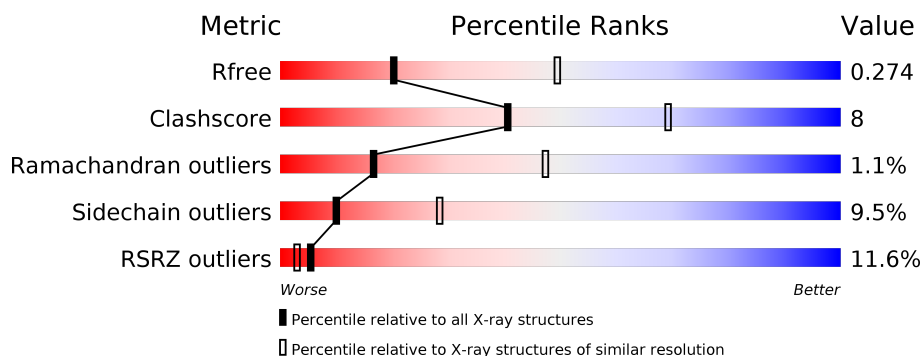
1 Overall quality at a glance

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))
R_{free}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (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 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.

Mol	Chain	Length	Quality of chain
1	A	431	<div> <div>16%</div> <div> <div></div> <div>71%</div> <div>23%</div> <div>• •</div> </div> </div>
1	B	431	<div> <div>7%</div> <div> <div></div> <div>71%</div> <div>23%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6627 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.

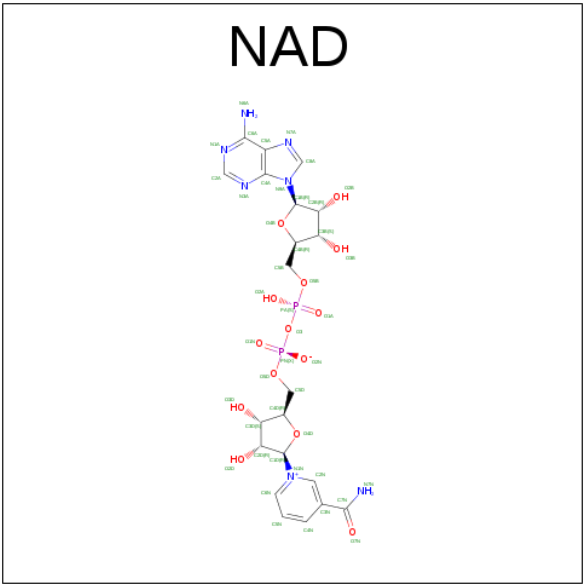
- Molecule 1 is a protein called Cap5O.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			3271	2079	541	635	16			
1	B	412	Total	C	N	O	S	0	0	0
			3225	2048	534	627	16			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	EXPRESSION TAG	UNP P95708
A	-9	ARG	-	EXPRESSION TAG	UNP P95708
A	-8	GLY	-	EXPRESSION TAG	UNP P95708
A	-7	SER	-	EXPRESSION TAG	UNP P95708
A	-6	HIS	-	EXPRESSION TAG	UNP P95708
A	-5	HIS	-	EXPRESSION TAG	UNP P95708
A	-4	HIS	-	EXPRESSION TAG	UNP P95708
A	-3	HIS	-	EXPRESSION TAG	UNP P95708
A	-2	HIS	-	EXPRESSION TAG	UNP P95708
A	-1	HIS	-	EXPRESSION TAG	UNP P95708
A	0	GLY	-	EXPRESSION TAG	UNP P95708
A	1	SER	-	EXPRESSION TAG	UNP P95708
B	-10	MET	-	EXPRESSION TAG	UNP P95708
B	-9	ARG	-	EXPRESSION TAG	UNP P95708
B	-8	GLY	-	EXPRESSION TAG	UNP P95708
B	-7	SER	-	EXPRESSION TAG	UNP P95708
B	-6	HIS	-	EXPRESSION TAG	UNP P95708
B	-5	HIS	-	EXPRESSION TAG	UNP P95708
B	-4	HIS	-	EXPRESSION TAG	UNP P95708
B	-3	HIS	-	EXPRESSION TAG	UNP P95708
B	-2	HIS	-	EXPRESSION TAG	UNP P95708
B	-1	HIS	-	EXPRESSION TAG	UNP P95708
B	0	GLY	-	EXPRESSION TAG	UNP P95708
B	1	SER	-	EXPRESSION TAG	UNP P95708

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total	O	0	0
			15	15		
3	B	28	Total	O	0	0
			28	28		

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

Chain A:

16% 71% 23%

MET ARG GLY SER HIS HIS HIS HIS HIS GLY S1 T4 V5 V6 G7 I8 G9 Y10 I11 G12 L13 P14 T15 S16 V26 L27 T31 Q34 R41 C42 Q43 V54 E57 V58 L59 G62 K63 L64 E71 V75 F76 I77 I78 A79 V80 P81 T82 P83 R84 R85 D86 D87 Q88 Y89 R90 S91 C92 S95 L96 W97 M98 L101 D102 S103 I104 L105 L108 T113 I114 I115 V116 E117 S118 T119 P122 I133 L136 I144 C149 P150 E151 L154 P155 G156 L159 E160 E161 L162 N165 M166 R167 K174 P81 I177 V181 R185 R186 T186 Q189 M202 L205 M206 R211 N219 E220 L221 N226 N231 D234 V235 H242 P243 R244 V245 N246 T247 H248 G251 G256 H257 A260 V261 I266 K269 R281 V292 T295 I298 S303 G304 N305 K306 V307 T308 T313 G316 D317 V318 D319 D320 I321 R322 E323 S324 S325 P326 K326 F327 D328 E331 L332 L333 N334 Q335 E336 P337 D338 L339 V340 C341 C342 V347 V348 E349 L350 D351 F352 S358 V361 K362 D363 A364 S365 L366 V367 L368 T369 L370 S374 N375 L379 S380 D381 S382 R383 F384 V390

Chain B:

71% 23%

7%

MET ARG GLY SER HIS HIS HIS HIS HIS GLY S1 K2 L3 T4 V5 V6 G7 L8 I11 G12 L13 P14 T15 S16 I17 K21 H22 V26 L27 G28 I31 E47 E48 P49 E53 V54 E57 V58 L64 V75 F76 I77 I78 A79 V80 T82 P81 T83 P83 N84 N85 W86 D86 D87 Q88 Y89 S91 L96 L101 D102 L105 T113 I114 I115 V116 E117 T119 I133 L136 G137 F138 T139 D143 I144 P150 E151 R152 V153 L154 P155 G156 L159 E160 E161 L162 V163 H164 R167 K174 I177 K181 R182 V183 V184 R185 T186 F187 V188 Q189 M202 S203 K204 L205 M206 N219 E220 L221 W226 V235 H242 P243 R244 N245 L247 H248 G251 G256 H257 C258 D262 P263 Y264 F265 ILE ILE ALA LYS ASP PRO GLU R273 R281 V292 T295 I298 S303 K306 L312 T313 R315 Y314 D319 D320 I321 Y330 L333 D338 L339 E340 A343 E349 L350 S358 R359 A364 S365 L366 V367 L368 L379 S380 D381 S382 H383 F384 D385 K390 F393 S402 D405 V406 N410 I414 F415 N416 F417 D418 LYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.90Å 87.26Å 131.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.12 – 2.80 29.06 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.12-2.80) 98.3 (29.06-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.80Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.217 , 0.263 0.228 , 0.274	Depositor DCC
R_{free} test set	810 reflections (3.77%)	DCC
Wilson B-factor (Å ²)	63.1	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 71.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6627	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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](#)

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

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	0/3331	0.73	0/4520
1	B	0.50	0/3283	0.74	0/4453
All	All	0.50	0/6614	0.73	0/8973

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	3271	0	3276	63	0
1	B	3225	0	3220	53	0
2	A	44	0	26	2	0
2	B	44	0	26	1	0
3	A	15	0	0	0	0
3	B	28	0	0	0	0
All	All	6627	0	6548	107	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 8.

The worst 5 of 107 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:206:MET:SD	1:B:221:LEU:HD11	2.25	0.77
1:A:235:VAL:HG12	1:B:206:MET:SD	2.30	0.71
1:A:205:LEU:HB3	1:A:266:ILE:HD11	1.72	0.71
1:A:242:HIS:HD2	1:A:244:ARG:H	1.40	0.69
1:A:333:LEU:HB3	1:A:341:VAL:HG11	1.75	0.69

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	416/431 (96%)	390 (94%)	21 (5%)	5 (1%)	15	44
1	B	408/431 (95%)	380 (93%)	24 (6%)	4 (1%)	18	50
All	All	824/862 (96%)	770 (93%)	45 (6%)	9 (1%)	17	47

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	ARG
1	B	86	ASP
1	A	256	GLY
1	B	49	PRO
1	B	256	GLY

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	372/383 (97%)	339 (91%)	33 (9%)	11	32
1	B	367/383 (96%)	330 (90%)	37 (10%)	9	25
All	All	739/766 (96%)	669 (90%)	70 (10%)	10	28

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	411	TYR
1	B	87	ASP
1	B	368	LEU
1	A	418	ILE
1	B	57	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	383	HIS
1	B	219	ASN
1	B	334	ASN
1	A	334	ASN
1	B	383	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAD	A	500	-	41,48,48	1.71	3 (7%)	43,73,73	1.57	2 (4%)
2	NAD	B	500	-	41,48,48	1.74	3 (7%)	43,73,73	1.62	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	500	-	-	0/22/62/62	0/5/5/5
2	NAD	B	500	-	-	0/22/62/62	0/5/5/5

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	NAD	C2A-N1A	3.07	1.39	1.33
2	B	500	NAD	C2A-N1A	3.10	1.39	1.33
2	A	500	NAD	C2A-N3A	4.13	1.39	1.32
2	B	500	NAD	C2A-N3A	4.74	1.40	1.32
2	B	500	NAD	O7N-C7N	8.31	1.41	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	NAD	N3A-C2A-N1A	-9.05	120.98	128.86
2	A	500	NAD	N3A-C2A-N1A	-8.66	121.31	128.86
2	A	500	NAD	C4A-C5A-N7A	-2.82	106.69	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	NAD	2	0
2	B	500	NAD	1	0

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	418/431 (96%)	0.70	67 (16%) 2 1	30, 70, 118, 136	0
1	B	412/431 (95%)	0.40	29 (7%) 17 10	30, 66, 94, 117	0
All	All	830/862 (96%)	0.55	96 (11%) 5 3	30, 67, 113, 136	0

The worst 5 of 96 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	401	SER	6.4
1	A	257	HIS	5.9
1	B	264	TYR	4.9
1	A	77	ILE	4.6
1	A	43	GLN	4.6

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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAD	B	500	44/44	0.92	0.24	-0.23	52,63,109,110	0
2	NAD	A	500	44/44	0.92	0.19	-0.81	64,76,90,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.