



# Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

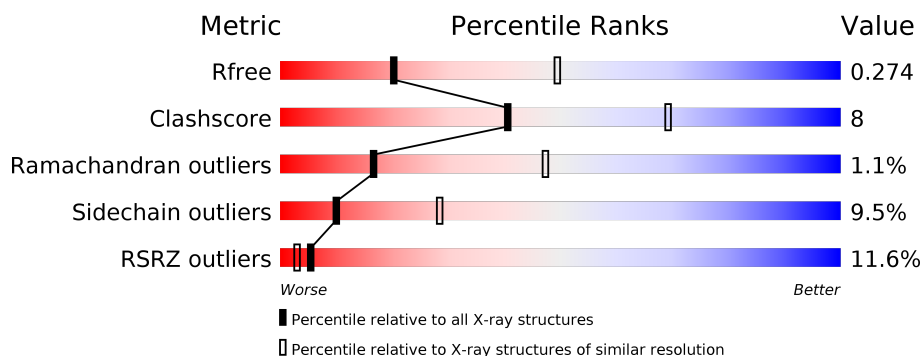
# 1 Overall quality at a glance

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  $\geq 3$ , 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.

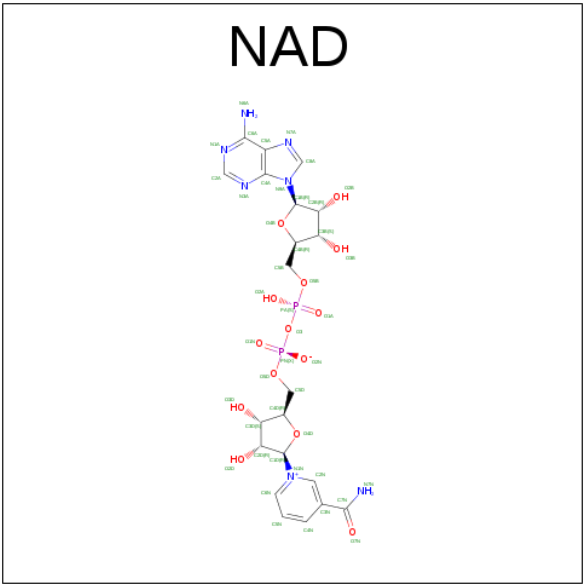
- Molecule 1 is a protein called Cap5O.

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: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	63.1	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 71.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

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

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.

All (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
1:B:150:PRO:HB2	1:B:204:LYS:HG3	1.74	0.68
1:A:304:GLY:HA3	1:A:365:SER:OG	1.94	0.68
1:B:298:ILE:HG21	1:B:366:LEU:HD13	1.78	0.65
1:A:306:LYS:HB3	1:A:364:ALA:HA	1.79	0.65
1:B:306:LYS:HB3	1:B:364:ALA:HA	1.79	0.65
1:B:242:HIS:HD2	1:B:244:ARG:H	1.45	0.64
1:A:133:ILE:HG21	1:A:144:ILE:HG21	1.78	0.64
1:A:206:MET:CE	1:B:221:LEU:HD21	2.28	0.64
1:A:84:ASN:HD22	1:A:90:ARG:HB3	1.64	0.61
1:A:226:ASN:HD22	1:A:415:PHE:HD2	1.49	0.61
1:B:219:ASN:HD21	1:B:251:GLY:H	1.49	0.60
1:A:27:LEU:HD12	1:A:71:GLU:HG2	1.83	0.59
1:A:219:ASN:HD21	1:A:251:GLY:H	1.51	0.58
1:B:312:LEU:HB3	1:B:321:ILE:HD11	1.85	0.58
1:A:205:LEU:CB	1:A:266:ILE:HD11	2.34	0.57
1:B:226:ASN:HD22	1:B:415:PHE:HD2	1.51	0.57
1:B:416:ASN:C	1:B:418:ILE:H	2.07	0.57
1:B:183:VAL:O	1:B:186:THR:HG23	2.06	0.56
1:A:211:ARG:HG2	1:A:259:LEU:HD11	1.87	0.55
1:A:231:ASN:HD22	1:A:234:ASP:H	1.54	0.54
1:A:154:LEU:HG	1:A:156:GLY:H	1.72	0.53
1:A:235:VAL:CG1	1:B:206:MET:SD	2.97	0.53
1:B:393:PHE:CE1	1:B:414:ILE:HG12	2.44	0.53
1:A:105:LEU:HG	1:A:136:LEU:HD11	1.92	0.52
1:B:139:THR:H	1:B:143:ASP:HB2	1.74	0.52
1:A:133:ILE:CG2	1:A:144:ILE:HG21	2.39	0.52
1:A:306:LYS:HE2	1:A:342:CYS:HB2	1.91	0.52
1:A:306:LYS:HA	1:A:340:GLU:HB3	1.92	0.52
1:A:321:ILE:HD11	1:A:348:VAL:HG11	1.93	0.51
1:A:101:LEU:HD11	1:A:133:ILE:HD11	1.93	0.51
1:A:206:MET:SD	1:B:221:LEU:HD21	2.52	0.50
1:A:7:GLY:O	1:A:12:GLY:HA3	2.11	0.50
1:A:242:HIS:CD2	1:A:244:ARG:H	2.24	0.50
1:B:242:HIS:CD2	1:B:244:ARG:H	2.29	0.50
1:B:105:LEU:HG	1:B:136:LEU:HD11	1.94	0.49
1:A:76:PHE:CD1	1:A:104:ILE:HD12	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:GLY:O	1:B:12:GLY:HA3	2.11	0.49
1:A:108:LEU:HD22	1:A:144:ILE:HD11	1.94	0.49
1:B:87:ASP:HB2	1:B:89:TYR:H	1.78	0.48
1:B:174:LYS:HA	1:B:177:ILE:HD12	1.95	0.48
1:A:161:GLU:O	1:A:165:ASN:HB2	2.13	0.48
1:A:174:LYS:HA	1:A:177:ILE:HD12	1.94	0.48
1:A:54:VAL:HG21	1:A:159:LEU:HD21	1.96	0.48
1:B:390:LYS:HB3	1:B:406:VAL:HG22	1.96	0.48
1:A:390:LYS:HB3	1:A:406:VAL:HG22	1.95	0.48
1:A:205:LEU:HB3	1:A:266:ILE:CD1	2.42	0.48
1:A:308:THR:HG23	1:A:367:VAL:HG22	1.95	0.48
1:B:181:LYS:O	1:B:185:ARG:HB2	2.14	0.48
1:B:54:VAL:HG21	1:B:159:LEU:HD21	1.96	0.47
1:A:231:ASN:ND2	1:A:234:ASP:H	2.11	0.47
1:B:292:VAL:HG22	1:B:333:LEU:HD13	1.96	0.47
1:B:306:LYS:HA	1:B:340:GLU:HB3	1.95	0.47
1:A:221:LEU:HD22	1:B:206:MET:CE	2.44	0.47
1:A:26:VAL:HG22	1:A:64:LEU:HG	1.97	0.47
1:B:58:VAL:HG13	1:B:64:LEU:HB2	1.98	0.46
1:B:379:LEU:HD13	1:B:384:PHE:HZ	1.81	0.46
1:A:58:VAL:HG13	1:A:64:LEU:HB2	1.99	0.45
1:B:330:TYR:CE1	1:B:343:ALA:HB2	2.52	0.45
1:A:9:GLY:HA3	2:A:500:NAD:O5B	2.16	0.45
1:B:11:ILE:HD12	1:B:151:GLU:HG2	1.98	0.45
1:A:202:MET:HG3	1:B:235:VAL:HG11	1.99	0.45
1:B:380:SER:H	1:B:383:HIS:CD2	2.34	0.45
1:A:13:LEU:HB3	1:A:14:PRO:HD3	1.99	0.45
1:A:181:LYS:O	1:A:185:ARG:HB2	2.16	0.45
1:A:399:VAL:HG11	1:A:403:PHE:HE2	1.81	0.45
1:A:81:PRO:HD2	1:A:96:LEU:HD13	1.99	0.44
1:B:81:PRO:HD2	1:B:96:LEU:HD13	1.98	0.44
1:A:122:PRO:HD2	1:A:269:LYS:HG3	1.98	0.44
1:B:101:LEU:HD11	1:B:133:ILE:HD11	1.99	0.44
1:A:380:SER:H	1:A:383:HIS:CD2	2.35	0.44
1:A:75:VAL:HB	1:A:113:THR:HB	1.98	0.44
1:B:17:ILE:O	1:B:21:LYS:HB2	2.17	0.44
1:B:13:LEU:HB3	1:B:14:PRO:HD3	1.98	0.44
1:A:298:ILE:HG21	1:A:366:LEU:HD13	1.99	0.43
1:A:295:THR:HG21	1:A:333:LEU:HD21	2.00	0.43
1:A:221:LEU:HD22	1:B:206:MET:HE3	2.00	0.43
1:B:314:TYR:CE2	1:B:320:ASP:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:VAL:HB	1:B:113:THR:HB	2.00	0.43
1:A:149:CYS:SG	1:A:167:ARG:HG2	2.59	0.43
1:A:242:HIS:HD2	1:A:244:ARG:N	2.13	0.43
1:B:3:LEU:HD21	1:B:77:ILE:HD12	2.00	0.43
1:A:81:PRO:HG3	2:A:500:NAD:H51A	2.01	0.42
1:B:295:THR:HG23	1:B:366:LEU:HD23	2.01	0.42
1:B:138:PHE:HB3	1:B:144:ILE:HG13	2.01	0.42
1:A:235:VAL:HG11	1:B:202:MET:HG3	2.01	0.42
1:B:152:ARG:HE	1:B:152:ARG:HB2	1.71	0.42
1:B:82:THR:HG21	1:B:119:THR:O	2.19	0.42
1:B:22:HIS:CD2	1:B:187:PHE:HB3	2.53	0.42
1:B:81:PRO:HG3	2:B:500:NAD:H51A	2.01	0.42
1:A:379:LEU:HD13	1:A:384:PHE:HZ	1.84	0.42
1:B:133:ILE:CG2	1:B:144:ILE:HD11	2.50	0.42
1:A:324:SER:HA	1:A:325:PRO:HD3	1.98	0.42
1:A:333:LEU:HB3	1:A:341:VAL:CG1	2.47	0.41
1:A:313:THR:HG21	1:A:318:VAL:O	2.19	0.41
1:A:292:VAL:HG22	1:A:333:LEU:HD13	2.01	0.41
1:B:26:VAL:HG22	1:B:64:LEU:HG	2.03	0.41
1:B:8:LEU:HD11	1:B:28:GLY:HA3	2.02	0.41
1:A:308:THR:HG21	1:A:361:VAL:HG12	2.03	0.40
1:A:82:THR:HG21	1:A:119:THR:O	2.21	0.40
1:B:138:PHE:HD2	1:B:143:ASP:HB3	1.87	0.40
1:A:333:LEU:HG	1:A:339:ILE:HG21	2.03	0.40
1:B:333:LEU:HG	1:B:339:ILE:HG21	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (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
1	B	418	ILE
1	A	87	ASP
1	A	321	ILE
1	A	155	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	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

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	57	GLU
1	A	58	VAL
1	A	64	LEU
1	A	75	VAL
1	A	95	SER
1	A	98	MET

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Mol	Chain	Res	Type
1	A	102	ASP
1	A	105	LEU
1	A	144	ILE
1	A	151	GLU
1	A	154	LEU
1	A	162	LEU
1	A	167	ARG
1	A	186	THR
1	A	189	GLN
1	A	202	MET
1	A	231	ASN
1	A	246	ASN
1	A	248	HIS
1	A	257	HIS
1	A	258	CYS
1	A	281	ARG
1	A	303	SER
1	A	324	SER
1	A	338	ASP
1	A	350	LEU
1	A	358	SER
1	A	368	LEU
1	A	382	SER
1	A	405	ASP
1	A	411	TYR
1	A	418	ILE
1	B	27	LEU
1	B	31	ILE
1	B	57	GLU
1	B	64	LEU
1	B	75	VAL
1	B	84	ASN
1	B	87	ASP
1	B	88	GLN
1	B	91	SER
1	B	102	ASP
1	B	105	LEU
1	B	151	GLU
1	B	152	ARG
1	B	162	LEU
1	B	167	ARG
1	B	186	THR

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Mol	Chain	Res	Type
1	B	189	GLN
1	B	202	MET
1	B	246	ASN
1	B	248	HIS
1	B	257	HIS
1	B	258	CYS
1	B	262	ASP
1	B	281	ARG
1	B	303	SER
1	B	319	ASP
1	B	321	ILE
1	B	338	ASP
1	B	349	GLU
1	B	350	LEU
1	B	358	SER
1	B	368	LEU
1	B	382	SER
1	B	405	ASP
1	B	410	ASN
1	B	414	ILE
1	B	418	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	219	ASN
1	A	226	ASN
1	A	231	ASN
1	A	242	HIS
1	A	249	GLN
1	A	297	GLN
1	A	334	ASN
1	A	383	HIS
1	B	85	ASN
1	B	219	ASN
1	B	226	ASN
1	B	242	HIS
1	B	249	GLN
1	B	297	GLN
1	B	334	ASN
1	B	383	HIS

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Mol	Chain	Res	Type
1	B	410	ASN
1	B	413	ASN

### 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

All (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
2	A	500	NAD	O7N-C7N	8.40	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	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

All (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
1	A	347	HIS	4.4
1	A	156	GLY	4.3
1	A	323	GLU	4.1
1	A	382	SER	4.0
1	A	402	SER	3.9
1	A	5	VAL	3.9
1	A	407	LEU	3.9
1	A	335	GLN	3.9
1	A	317	ASP	3.8
1	A	15	THR	3.8
1	B	86	ASP	3.8
1	A	320	ASP	3.7
1	A	115	ILE	3.5
1	B	77	ILE	3.5
1	A	86	ASP	3.3
1	A	363	ASP	3.3
1	A	395	THR	3.3
1	A	89	TYR	3.2
1	B	57	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	352	PHE	3.1
1	B	156	GLY	3.1
1	B	418	ILE	3.0
1	B	12	GLY	3.0
1	B	164	HIS	3.0
1	A	322	ARG	3.0
1	A	319	ASP	3.0
1	A	331	GLU	2.9
1	A	404	GLU	2.9
1	B	88	GLN	2.9
1	A	351	ASP	2.9
1	A	78	ILE	2.9
1	A	350	LEU	2.9
1	A	59	LEU	2.8
1	A	304	GLY	2.8
1	A	378	ASN	2.7
1	B	154	LEU	2.7
1	A	303	SER	2.7
1	B	117	GLU	2.7
1	B	359	HIS	2.7
1	A	117	GLU	2.6
1	B	155	PRO	2.6
1	B	89	TYR	2.6
1	A	42	GLY	2.6
1	A	349	GLU	2.6
1	A	370	LEU	2.6
1	A	11	ILE	2.6
1	A	384	PHE	2.6
1	A	116	VAL	2.5
1	A	337	PRO	2.5
1	A	31	ILE	2.5
1	A	368	LEU	2.5
1	B	53	GLU	2.5
1	B	11	ILE	2.5
1	A	396	LYS	2.5
1	A	416	ASN	2.5
1	A	418	ILE	2.5
1	A	403	PHE	2.5
1	B	15	THR	2.5
1	A	79	ALA	2.4
1	B	78	ILE	2.4
1	A	4	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	34	GLN	2.4
1	A	92	CYS	2.4
1	B	118	SER	2.4
1	A	374	SER	2.3
1	A	62	GLY	2.3
1	A	41	ASN	2.3
1	B	47	GLU	2.3
1	A	85	ASN	2.3
1	A	316	GLY	2.3
1	A	328	ASP	2.3
1	A	369	ILE	2.3
1	B	79	ALA	2.2
1	B	265	PHE	2.2
1	A	332	LEU	2.2
1	A	417	PHE	2.2
1	B	402	SER	2.2
1	B	385	ASP	2.1
1	B	115	ILE	2.1
1	A	340	GLU	2.1
1	A	261	VAL	2.1
1	A	16	SER	2.1
1	A	12	GLY	2.1
1	B	85	ASN	2.1
1	B	160	GLU	2.1
1	A	327	PHE	2.1
1	A	342	CYS	2.0
1	B	5	VAL	2.0
1	B	349	GLU	2.0
1	A	318	VAL	2.0
1	A	348	VAL	2.0

## 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	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.