



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 02:59 AM GMT

PDB ID : 3OJL
Title : Native structure of the UDP-N-acetyl-mannosaminidehydrogenase 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 validation 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/ValidationPDFNotes.html>

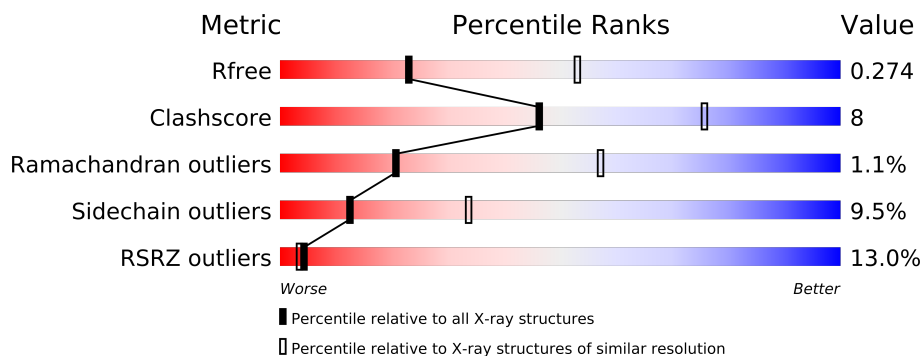
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	431	
1	B	431	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6627 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

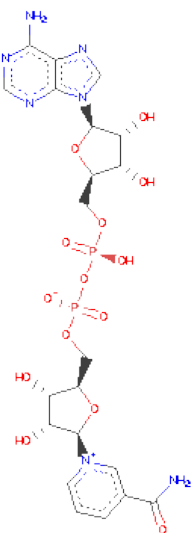
- Molecule 1 is a protein called Cap5O.

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: $C_{21}H_{27}N_7O_{14}P_2$).



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, 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 , 55.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 22319 reflections	Xtriage
F_o, F_c correlation	0.92	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.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (107) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:333:LEU:HB3	1:A:341:VAL:HG11	1.75	0.69
1:A:242:HIS:HD2	1:A:244:ARG:H	1.40	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:206:MET:CE	1:B:221:LEU:HD21	2.28	0.64
1:A:133:ILE:HG21	1:A:144:ILE:HG21	1.78	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:B:139:THR:H	1:B:143:ASP:HB2	1.74	0.52
1:A:105:LEU:HG	1:A:136:LEU:HD11	1.92	0.52
1:A:306:LYS:HE2	1:A:342:CYS:HB2	1.91	0.52
1:A:133:ILE:CG2	1:A:144:ILE:HG21	2.39	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:242:HIS:CD2	1:A:244:ARG:H	2.24	0.50
1:A:7:GLY:O	1:A:12:GLY:HA3	2.11	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:B:7:GLY:O	1:B:12:GLY:HA3	2.11	0.49
1:A:76:PHE:CD1	1:A:104:ILE:HD12	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:390:LYS:HB3	1:B:406:VAL:HG22	1.96	0.48
1:A:54:VAL:HG21	1:A:159:LEU:HD21	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:221:LEU:HD22	1:B:206:MET:HE3	2.00	0.43
1:A:295:THR:HG21	1:A:333:LEU:HD21	2.00	0.43
1:B:314:TYR:CE2	1:B:320:ASP:HB3	2.53	0.43
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:295:THR:HG23	1:B:366:LEU:HD23	2.01	0.42
1:A:81:PRO:HG3	2:A:500:NAD:H51A	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:81:PRO:HG3	2:B:500:NAD:H51A	2.01	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: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%)	19	54
1	B	408/431 (95%)	380 (93%)	24 (6%)	4 (1%)	22	60
All	All	824/862 (96%)	770 (93%)	45 (6%)	9 (1%)	21	57

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%)	14	38
1	B	367/383 (96%)	330 (90%)	37 (10%)	11	30
All	All	739/766 (96%)	669 (90%)	70 (10%)	12	33

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

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

5.3.3 RNA ⓘ

There are no RNA chains 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	-	48,48,48	1.45	3 (6%)	73,73,73	1.62	10 (13%)
2	NAD	B	500	-	48,48,48	1.52	5 (10%)	73,73,73	1.72	9 (12%)

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	-	-	0/30/62/62	0/3/5/5
2	NAD	B	500	-	-	0/30/62/62	0/3/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	NAD	O7N-C7N	7.39	1.41	1.24
2	B	500	NAD	O7N-C7N	7.31	1.41	1.24
2	B	500	NAD	C2A-N3A	3.99	1.40	1.32
2	A	500	NAD	C2A-N3A	3.48	1.39	1.32
2	B	500	NAD	C2A-N1A	2.95	1.39	1.33
2	A	500	NAD	C2A-N1A	2.93	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	NAD	PA-O3	2.33	1.64	1.59
2	B	500	NAD	C2N-N1N	2.24	1.38	1.35

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	NAD	N3A-C2A-N1A	-9.25	120.98	128.71
2	A	500	NAD	N3A-C2A-N1A	-8.85	121.31	128.71
2	B	500	NAD	O4D-C1D-N1N	5.50	113.58	107.95
2	A	500	NAD	O4D-C1D-N1N	4.80	112.86	107.95
2	B	500	NAD	C2D-C1D-N1N	-3.77	107.47	113.86
2	B	500	NAD	N3A-C4A-N9A	3.59	131.92	125.43
2	A	500	NAD	N3A-C4A-N9A	3.44	131.65	125.43
2	A	500	NAD	C4A-C5A-N7A	-3.31	106.69	109.52
2	A	500	NAD	C2D-C1D-N1N	-2.94	108.88	113.86
2	B	500	NAD	C6N-N1N-C2N	-2.55	119.16	122.04
2	B	500	NAD	PN-O3-PA	-2.38	122.74	132.95
2	A	500	NAD	PN-O3-PA	-2.37	122.79	132.95
2	A	500	NAD	C5A-C4A-N3A	-2.35	120.57	125.70
2	A	500	NAD	N7A-C8A-N9A	-2.21	108.12	114.36
2	A	500	NAD	C6N-N1N-C2N	-2.14	119.62	122.04
2	B	500	NAD	N7A-C8A-N9A	-2.13	108.33	114.36
2	B	500	NAD	C5A-C4A-N3A	-2.06	121.22	125.70
2	B	500	NAD	C4A-C5A-N7A	-2.04	107.77	109.52
2	A	500	NAD	C8A-N7A-C5A	2.01	109.82	103.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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%)	0.74	76 (18%) 2 2	30, 70, 118, 136	0
1	B	412/431 (95%)	0.41	32 (7%) 13 11	30, 66, 94, 117	0
All	All	830/862 (96%)	0.58	108 (13%) 4 3	30, 67, 113, 136	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	257	HIS	6.7
1	A	401	SER	6.3
1	A	43	GLN	5.4
1	B	264	TYR	5.2
1	A	77	ILE	4.6
1	A	323	GLU	4.5
1	A	156	GLY	4.4
1	A	382	SER	4.4
1	A	347	HIS	4.4
1	A	335	GLN	4.2
1	A	5	VAL	4.2
1	A	320	ASP	4.1
1	B	86	ASP	3.9
1	A	15	THR	3.9
1	A	86	ASP	3.8
1	A	402	SER	3.7
1	B	164	HIS	3.5
1	A	115	ILE	3.5
1	A	89	TYR	3.5
1	A	350	LEU	3.4
1	A	363	ASP	3.4
1	B	77	ILE	3.4
1	A	378	ASN	3.4
1	A	317	ASP	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	154	LEU	3.3
1	B	12	GLY	3.3
1	A	395	THR	3.3
1	B	57	GLU	3.2
1	A	404	GLU	3.1
1	A	322	ARG	3.1
1	A	78	ILE	3.1
1	A	407	LEU	3.1
1	A	59	LEU	3.1
1	B	89	TYR	3.0
1	A	349	GLU	3.0
1	A	352	PHE	3.0
1	B	359	HIS	2.9
1	A	403	PHE	2.9
1	B	418	ILE	2.9
1	A	351	ASP	2.9
1	B	155	PRO	2.8
1	B	88	GLN	2.8
1	A	331	GLU	2.8
1	A	384	PHE	2.8
1	A	85	ASN	2.8
1	A	337	PRO	2.8
1	B	47	GLU	2.8
1	A	418	ILE	2.8
1	A	303	SER	2.8
1	A	370	LEU	2.8
1	A	416	ASN	2.7
1	A	11	ILE	2.7
1	A	327	PHE	2.7
1	A	319	ASP	2.7
1	A	379	LEU	2.7
1	A	396	LYS	2.6
1	A	340	GLU	2.6
1	A	41	ASN	2.6
1	A	116	VAL	2.6
1	A	117	GLU	2.6
1	B	53	GLU	2.6
1	A	328	ASP	2.6
1	B	156	GLY	2.6
1	A	417	PHE	2.5
1	A	374	SER	2.5
1	A	34	GLN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	15	THR	2.5
1	B	11	ILE	2.5
1	A	4	THR	2.5
1	A	369	ILE	2.5
1	B	117	GLU	2.5
1	A	79	ALA	2.4
1	A	42	GLY	2.4
1	B	349	GLU	2.4
1	A	375	GLU	2.4
1	A	31	ILE	2.4
1	B	160	GLU	2.3
1	A	339	ILE	2.3
1	A	348	VAL	2.3
1	A	342	CYS	2.3
1	B	78	ILE	2.3
1	A	309	VAL	2.3
1	A	261	VAL	2.3
1	A	301	ALA	2.2
1	A	300	LYS	2.2
1	B	402	SER	2.2
1	B	79	ALA	2.2
1	B	85	ASN	2.2
1	A	304	GLY	2.2
1	A	368	LEU	2.2
1	B	308	THR	2.2
1	B	118	SER	2.1
1	B	385	ASP	2.1
1	A	16	SER	2.1
1	A	359	HIS	2.1
1	A	332	LEU	2.1
1	A	65	LYS	2.1
1	A	6	VAL	2.1
1	A	12	GLY	2.1
1	B	137	GLY	2.1
1	A	260	ALA	2.0
1	B	115	ILE	2.0
1	A	344	TYR	2.0
1	B	367	VAL	2.0
1	B	149	CYS	2.0
1	A	62	GLY	2.0
1	A	60	SER	2.0
1	B	65	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAD	B	500	44/44	0.23	-0.23	52,63,109,110	0
2	NAD	A	500	44/44	0.19	-0.79	64,76,90,95	0

6.5 Other polymers

There are no such residues in this entry.