



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:48 AM UTC

PDB ID : 3OJO / pdb_00003ojo
Title : Derivative structure of the UDP-N-acetyl-mannosamine dehydrogenase Cap5O from *S. aureus*
Authors : Nessler, S.; Gruszczyk, J.; Olivares-Illana, V.; Meyer, P.; Morera, S.
Deposited on : 2010-08-23
Resolution : 2.50 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

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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

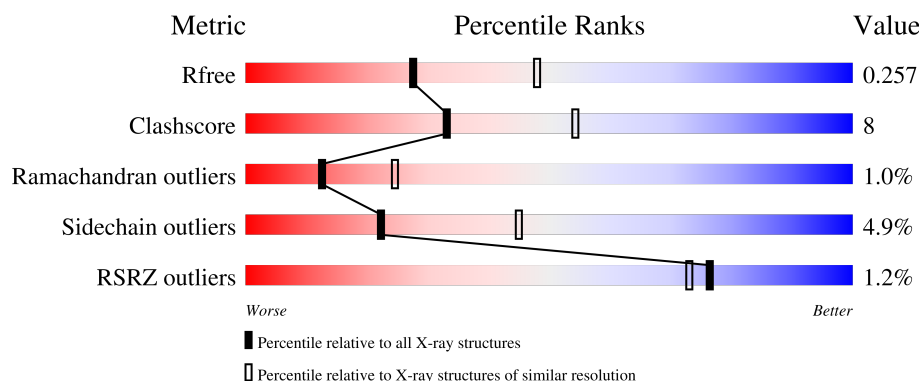
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	431	
1	B	431	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6747 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.

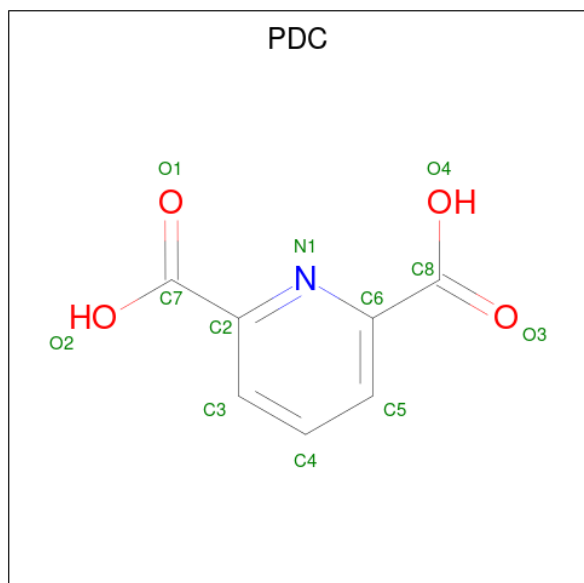
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	0
			3194	2026	531	621	16			
1	B	418	Total	C	N	O	S	0	0	0
			3271	2079	541	635	16			

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

- # NAD

- Molecule 3 is PYRIDINE-2,6-DICARBOXYLIC ACID (CCD ID: PDC) (formula: $C_7H_5NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	7	1	4		
3	A	1	Total	C	N	O	0	0
			12	7	1	4		
3	A	1	Total	C	N	O	0	0
			12	7	1	4		
3	B	1	Total	C	N	O	0	0
			12	7	1	4		
3	B	1	Total	C	N	O	0	0
			12	7	1	4		
3	B	1	Total	C	N	O	0	0
			12	7	1	4		

- Molecule 4 is EUROPIUM ION (CCD ID: EU) (formula: Eu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Eu	0	0
			1	1		
4	B	1	Total	Eu	0	0
			1	1		

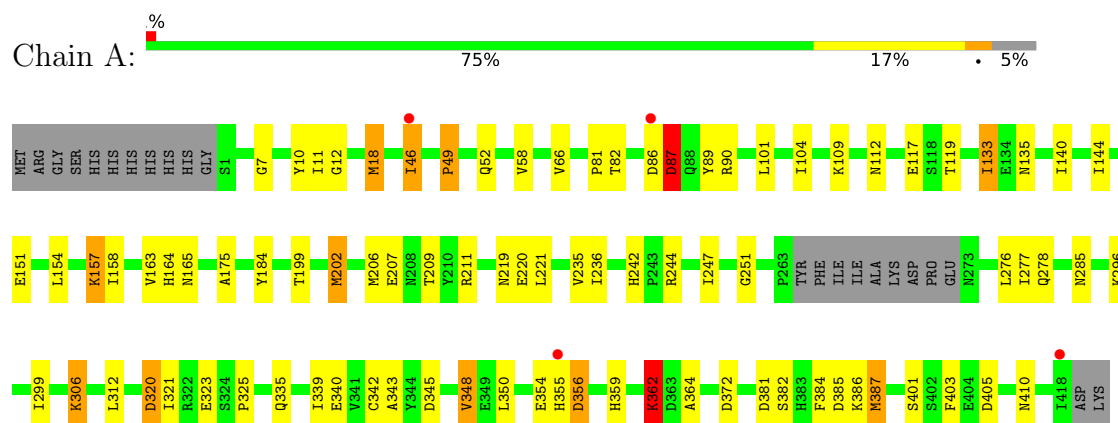
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	57	Total	O	0	0
			57	57		
5	B	63	Total	O	0	0
			63	63		

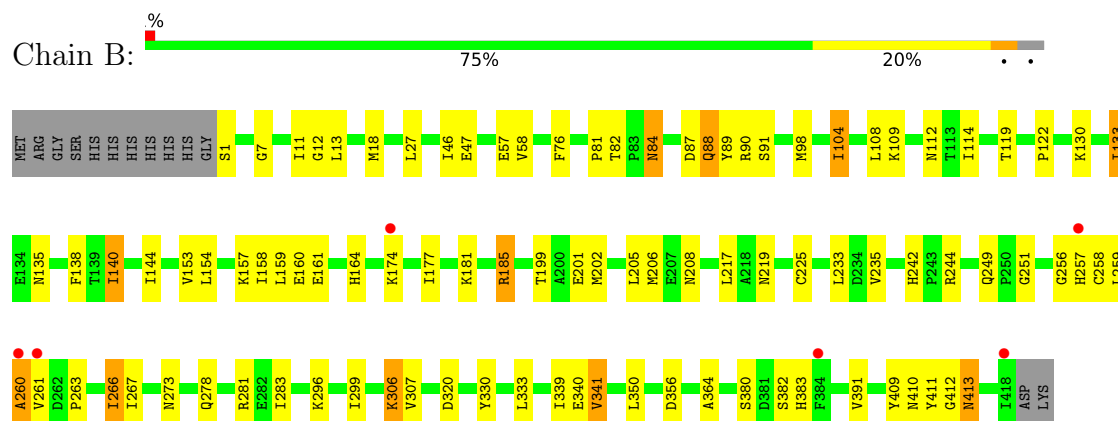
3 Residue-property plots [i](#)

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: Cap50



• Molecule 1: Cap50



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	40.22Å 131.50Å 158.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.63 – 2.50 29.63 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.63-2.50) 99.6 (29.63-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.201 , 0.246 0.206 , 0.257	Depositor DCC
R_{free} test set	1525 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	46.5	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.9	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	0.94	EDS
Total number of atoms	6747	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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: EU, PDC, 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	0.88	3/3250 (0.1%)	1.45	27/4408 (0.6%)
1	B	0.85	2/3331 (0.1%)	1.42	24/4520 (0.5%)
All	All	0.86	5/6581 (0.1%)	1.44	51/8928 (0.6%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	18	MET	SD-CE	-8.21	1.59	1.79
1	A	387	MET	SD-CE	-7.27	1.61	1.79
1	B	140	ILE	CG1-CD1	-6.42	1.26	1.51
1	A	202	MET	SD-CE	-5.80	1.65	1.79
1	B	98	MET	SD-CE	-5.61	1.65	1.79

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	ASP	CA-C-N	7.71	135.59	121.70
1	A	86	ASP	C-N-CA	7.71	135.59	121.70
1	A	356	ASP	CA-C-N	7.38	135.64	121.54
1	A	356	ASP	C-N-CA	7.38	135.64	121.54
1	A	158	ILE	N-CA-C	6.73	117.23	110.23
1	B	266	ILE	N-CA-C	6.71	117.88	111.91
1	B	259	LEU	N-CA-C	6.40	119.87	110.59
1	B	411	TYR	N-CA-C	-6.29	105.09	112.89
1	B	185	ARG	CA-C-N	6.08	128.71	120.38
1	B	185	ARG	C-N-CA	6.08	128.71	120.38
1	B	208	ASN	CA-C-N	6.00	128.60	120.44
1	B	208	ASN	C-N-CA	6.00	128.60	120.44
1	A	403	PHE	N-CA-C	5.99	118.40	108.99
1	A	320	ASP	CA-CB-CG	5.93	118.53	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	87	ASP	CA-C-N	5.89	128.97	120.79
1	B	87	ASP	C-N-CA	5.89	128.97	120.79
1	A	164	HIS	N-CA-C	5.88	120.18	112.89
1	A	323	GLU	CA-C-N	5.79	128.53	120.65
1	A	323	GLU	C-N-CA	5.79	128.53	120.65
1	B	164	HIS	N-CA-C	5.78	120.40	113.23
1	B	88	GLN	CA-C-N	5.72	129.75	120.60
1	B	88	GLN	C-N-CA	5.72	129.75	120.60
1	A	381	ASP	CA-C-N	5.69	128.69	120.38
1	A	381	ASP	C-N-CA	5.69	128.69	120.38
1	A	362	LYS	N-CA-C	5.51	122.53	110.80
1	A	52	GLN	CA-C-N	5.42	127.49	120.44
1	A	52	GLN	C-N-CA	5.42	127.49	120.44
1	A	325	PRO	CA-C-N	5.35	127.39	120.44
1	A	325	PRO	C-N-CA	5.35	127.39	120.44
1	B	256	GLY	CA-C-N	5.34	131.73	121.54
1	B	256	GLY	C-N-CA	5.34	131.73	121.54
1	B	138	PHE	N-CA-C	5.30	117.88	109.50
1	B	356	ASP	CA-C-N	5.29	127.68	120.54
1	B	356	ASP	C-N-CA	5.29	127.68	120.54
1	B	201	GLU	CA-C-N	5.24	127.30	120.28
1	B	201	GLU	C-N-CA	5.24	127.30	120.28
1	A	306	LYS	N-CA-C	5.19	117.22	109.59
1	A	184	TYR	N-CA-C	5.17	117.82	111.82
1	A	49	PRO	N-CA-C	5.17	123.12	112.47
1	B	330	TYR	CA-C-N	5.16	127.19	120.28
1	B	330	TYR	C-N-CA	5.16	127.19	120.28
1	A	410	ASN	CA-CB-CG	5.14	117.74	112.60
1	B	306	LYS	N-CA-C	5.12	117.12	109.59
1	A	175	ALA	CA-C-N	5.11	127.12	120.28
1	A	175	ALA	C-N-CA	5.11	127.12	120.28
1	A	165	ASN	CA-CB-CG	5.08	117.68	112.60
1	A	87	ASP	CA-C-N	5.03	131.42	122.06
1	A	87	ASP	C-N-CA	5.03	131.42	122.06
1	A	372	ASP	CA-CB-CG	5.03	117.63	112.60
1	B	57	GLU	CA-C-N	5.00	127.53	120.42
1	B	57	GLU	C-N-CA	5.00	127.53	120.42

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	3194	0	3198	54	0
1	B	3271	0	3274	61	0
2	A	44	0	26	3	0
2	B	44	0	26	2	0
3	A	36	0	11	3	0
3	B	36	0	10	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	57	0	0	2	0
5	B	63	0	0	0	0
All	All	6747	0	6545	102	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 (102) 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:B:133:ILE:HG21	1:B:144:ILE:HD11	1.46	0.96
1:A:11:ILE:HG22	2:A:500:NAD:O2N	1.68	0.93
1:A:221:LEU:HD21	1:B:206:MET:SD	2.10	0.90
1:A:384:PHE:HB3	1:A:387:MET:HE3	1.58	0.86
1:A:355:HIS:HB2	1:A:359:HIS:HB3	1.58	0.85
1:A:312:LEU:HD21	1:A:343:ALA:HB1	1.61	0.82
1:A:219:ASN:HD21	1:A:251:GLY:H	1.28	0.80
1:B:219:ASN:HD21	1:B:251:GLY:H	1.29	0.79
1:A:384:PHE:HB3	1:A:387:MET:CE	2.13	0.78
1:B:242:HIS:HD2	1:B:244:ARG:H	1.34	0.75
1:A:90:ARG:HH12	1:A:285:ASN:HD21	1.36	0.74
1:A:242:HIS:HD2	1:A:244:ARG:H	1.35	0.74
1:A:362:LYS:HA	1:A:386:LYS:HB3	1.71	0.71
1:B:409:TYR:HA	1:B:413:ASN:HD21	1.55	0.71
1:B:108:LEU:HD21	1:B:114:ILE:HD11	1.73	0.70
1:B:89:TYR:HB3	1:B:261:VAL:HG21	1.74	0.70
1:B:82:THR:HG21	1:B:119:THR:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:VAL:HG12	1:B:206:MET:SD	2.32	0.69
1:A:18:MET:HE2	1:A:163:VAL:HG23	1.75	0.69
1:A:82:THR:HG21	1:A:119:THR:O	1.93	0.69
1:A:247:ILE:HD13	1:B:206:MET:HE3	1.75	0.67
1:B:333:LEU:HB3	1:B:341:VAL:HG11	1.77	0.67
1:A:209:THR:HG22	1:B:217:LEU:HD11	1.77	0.65
1:B:133:ILE:HG21	1:B:144:ILE:CD1	2.25	0.65
1:A:209:THR:CG2	1:B:217:LEU:HD11	2.29	0.63
1:A:206:MET:SD	1:B:235:VAL:HG12	2.39	0.62
1:A:133:ILE:HG21	1:A:140:ILE:HD11	1.82	0.62
1:A:81:PRO:HG3	2:A:500:NAD:H51A	1.81	0.61
1:A:18:MET:CE	1:A:163:VAL:HG23	2.30	0.61
1:B:81:PRO:HG3	2:B:500:NAD:H51A	1.83	0.61
1:B:122:PRO:HD3	1:B:205:LEU:HD12	1.83	0.59
1:A:306:LYS:HB3	1:A:364:ALA:HA	1.85	0.59
1:B:174:LYS:HA	1:B:177:ILE:HD12	1.85	0.59
1:A:89:TYR:CE1	1:A:278:GLN:HB2	2.38	0.58
1:A:11:ILE:HG13	1:A:151:GLU:HG2	1.87	0.57
1:A:18:MET:CE	1:A:163:VAL:CG2	2.83	0.56
1:B:306:LYS:HB3	1:B:364:ALA:HA	1.86	0.56
1:B:119:THR:OG1	2:B:500:NAD:H6N	2.05	0.56
1:B:130:LYS:HG3	1:B:140:ILE:HD13	1.87	0.56
1:A:133:ILE:CG2	1:A:140:ILE:HD11	2.35	0.56
1:A:221:LEU:CD2	1:B:206:MET:SD	2.90	0.55
1:B:18:MET:HE2	1:B:159:LEU:HD22	1.89	0.55
1:B:413:ASN:C	1:B:413:ASN:HD22	2.14	0.55
1:B:296:LYS:HG2	1:B:339:ILE:HD11	1.87	0.55
1:A:209:THR:HG23	1:A:277:ILE:HG12	1.88	0.55
1:B:410:ASN:HB3	1:B:412:GLY:H	1.72	0.54
1:A:296:LYS:HG2	1:A:339:ILE:HD11	1.90	0.54
1:A:119:THR:OG1	2:A:500:NAD:H6N	2.08	0.54
1:A:11:ILE:HG23	5:A:467:HOH:O	2.09	0.52
1:A:11:ILE:HD11	1:A:117:GLU:HB3	1.93	0.51
1:B:261:VAL:HA	1:B:266:ILE:HD11	1.92	0.51
1:A:202:MET:HG3	1:B:235:VAL:HG11	1.93	0.51
1:A:242:HIS:CD2	1:A:244:ARG:H	2.23	0.51
1:B:154:LEU:HD22	1:B:157:LYS:HB2	1.92	0.51
1:A:236:ILE:HA	1:B:206:MET:HE1	1.93	0.51
1:B:84:ASN:HD21	1:B:258:CYS:HB3	1.76	0.50
1:A:154:LEU:HD22	1:A:157:LYS:HG3	1.94	0.49
1:A:235:VAL:HG11	1:B:202:MET:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:SER:H	1:B:383:HIS:CD2	2.31	0.49
1:A:89:TYR:HE1	1:A:278:GLN:HB2	1.78	0.48
1:B:11:ILE:HD13	1:B:153:VAL:HG13	1.95	0.48
1:B:333:LEU:HB3	1:B:341:VAL:CG1	2.42	0.48
1:A:202:MET:HE2	1:B:225:CYS:SG	2.52	0.48
1:B:89:TYR:CE1	1:B:278:GLN:HB2	2.48	0.48
1:B:242:HIS:CD2	1:B:244:ARG:H	2.24	0.48
1:A:355:HIS:HB2	1:A:359:HIS:CB	2.38	0.48
1:A:11:ILE:HD11	1:A:151:GLU:HB3	1.95	0.47
1:B:153:VAL:HB	1:B:158:ILE:HG12	1.96	0.47
1:A:109:LYS:H	1:A:112:ASN:ND2	2.13	0.47
1:B:181:LYS:O	1:B:185:ARG:HB2	2.14	0.46
1:B:333:LEU:CB	1:B:341:VAL:HG11	2.43	0.46
3:B:504:PDC:O2	3:B:503:PDC:O4	2.34	0.46
1:B:88:GLN:H	1:B:88:GLN:CD	2.24	0.46
1:A:207:GLU:O	3:A:504:PDC:H4	2.17	0.45
1:B:109:LYS:H	1:B:112:ASN:ND2	2.15	0.45
1:B:307:VAL:HG11	1:B:333:LEU:HD13	1.99	0.44
1:A:220:GLU:HG3	1:B:273:ASN:O	2.18	0.44
1:A:306:LYS:HA	1:A:340:GLU:O	2.18	0.44
1:A:10:TYR:CE2	1:A:46:ILE:HG13	2.51	0.44
1:B:13:LEU:HD23	1:B:46:ILE:HG12	1.99	0.43
1:B:263:PRO:HA	1:B:267:ILE:HD12	1.99	0.43
1:A:7:GLY:O	1:A:12:GLY:HA3	2.17	0.43
1:A:199:THR:HG23	1:B:235:VAL:HG22	2.01	0.43
1:A:11:ILE:CD1	1:A:151:GLU:HB3	2.49	0.43
1:B:90:ARG:O	1:B:90:ARG:HG3	2.19	0.42
1:B:205:LEU:HB3	1:B:260:ALA:HA	2.00	0.42
3:A:504:PDC:O1	1:B:244:ARG:NH1	2.52	0.42
1:B:84:ASN:ND2	1:B:258:CYS:HB3	2.34	0.42
1:A:320:ASP:HA	5:A:443:HOH:O	2.20	0.42
1:A:101:LEU:HD11	1:A:133:ILE:HD11	2.01	0.42
1:A:276:LEU:HB2	1:B:283:ILE:CD1	2.49	0.42
1:B:333:LEU:C	1:B:341:VAL:HG11	2.45	0.41
1:B:7:GLY:O	1:B:12:GLY:HA3	2.20	0.41
1:A:235:VAL:HG22	1:B:199:THR:HG23	2.01	0.41
1:A:345:ASP:HB3	1:A:348:VAL:HG22	2.02	0.41
1:A:112:ASN:HB2	1:A:144:ILE:HD13	2.03	0.41
3:A:502:PDC:O4	3:A:504:PDC:O4	2.39	0.41
1:B:154:LEU:HB2	1:B:161:GLU:CD	2.45	0.41
1:B:233:LEU:HD22	1:B:249:GLN:HE22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:LYS:HA	1:B:340:GLU:O	2.21	0.41
1:B:205:LEU:HB3	1:B:260:ALA:CA	2.51	0.40
1:B:76:PHE:CD1	1:B:104:ILE:HG12	2.56	0.40

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	405/431 (94%)	386 (95%)	13 (3%)	6 (2%)	8	16
1	B	416/431 (96%)	397 (95%)	17 (4%)	2 (0%)	24	43
All	All	821/862 (95%)	783 (95%)	30 (4%)	8 (1%)	12	24

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	PRO
1	A	356	ASP
1	A	362	LYS
1	B	257	HIS
1	A	354	GLU
1	A	405	ASP
1	A	87	ASP
1	B	260	ALA

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	364/383 (95%)	346 (95%)	18 (5%)	22	45
1	B	372/383 (97%)	354 (95%)	18 (5%)	23	46
All	All	736/766 (96%)	700 (95%)	36 (5%)	22	45

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ILE
1	A	58	VAL
1	A	66	VAL
1	A	87	ASP
1	A	104	ILE
1	A	133	ILE
1	A	135	ASN
1	A	157	LYS
1	A	211	ARG
1	A	299	ILE
1	A	321	ILE
1	A	335	GLN
1	A	342	CYS
1	A	348	VAL
1	A	350	LEU
1	A	382	SER
1	A	385	ASP
1	A	401	SER
1	B	1	SER
1	B	27	LEU
1	B	47	GLU
1	B	58	VAL
1	B	84	ASN
1	B	91	SER
1	B	104	ILE
1	B	133	ILE
1	B	135	ASN
1	B	160	GLU
1	B	281	ARG
1	B	299	ILE
1	B	320	ASP
1	B	341	VAL
1	B	350	LEU

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Mol	Chain	Res	Type
1	B	382	SER
1	B	391	VAL
1	B	413	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	40	GLN
1	A	43	GLN
1	A	52	GLN
1	A	112	ASN
1	A	164	HIS
1	A	214	ASN
1	A	219	ASN
1	A	226	ASN
1	A	242	HIS
1	A	248	HIS
1	A	257	HIS
1	A	278	GLN
1	A	285	ASN
1	A	297	GLN
1	A	305	ASN
1	A	335	GLN
1	A	359	HIS
1	A	383	HIS
1	B	22	HIS
1	B	43	GLN
1	B	52	GLN
1	B	84	ASN
1	B	88	GLN
1	B	112	ASN
1	B	165	ASN
1	B	214	ASN
1	B	219	ASN
1	B	226	ASN
1	B	242	HIS
1	B	248	HIS
1	B	249	GLN
1	B	273	ASN
1	B	278	GLN
1	B	305	ASN

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Mol	Chain	Res	Type
1	B	383	HIS
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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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	-	46,48,48	1.88	6 (13%)	64,73,73	1.50	9 (14%)
3	PDC	B	503	4	12,12,12	1.52	3 (25%)	16,16,16	2.96	5 (31%)
3	PDC	A	503	4	12,12,12	1.79	4 (33%)	16,16,16	1.70	3 (18%)
3	PDC	B	504	4	12,12,12	1.66	4 (33%)	16,16,16	2.59	6 (37%)
3	PDC	B	502	4	12,12,12	1.60	3 (25%)	16,16,16	1.63	3 (18%)
3	PDC	A	504	4	12,12,12	1.20	2 (16%)	16,16,16	2.29	6 (37%)
3	PDC	A	502	4	12,12,12	1.67	4 (33%)	16,16,16	1.43	2 (12%)
2	NAD	B	500	-	46,48,48	1.84	6 (13%)	64,73,73	1.57	9 (14%)

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	-	-	4/30/62/62	0/5/5/5
3	PDC	B	503	4	-	0/8/8/8	0/1/1/1
3	PDC	A	503	4	-	0/8/8/8	0/1/1/1
3	PDC	B	504	4	-	0/8/8/8	0/1/1/1
3	PDC	B	502	4	-	0/8/8/8	0/1/1/1
3	PDC	A	504	4	-	0/8/8/8	0/1/1/1
3	PDC	A	502	4	-	0/8/8/8	0/1/1/1
2	NAD	B	500	-	-	4/30/62/62	0/5/5/5

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	NAD	O7N-C7N	9.74	1.42	1.24
2	B	500	NAD	O7N-C7N	9.55	1.41	1.24
3	A	503	PDC	O2-C7	3.37	1.40	1.30
3	B	502	PDC	C2-C7	-3.35	1.44	1.50
2	A	500	NAD	C2A-N1A	3.25	1.39	1.33
3	A	503	PDC	C3-C2	3.23	1.45	1.39
3	B	503	PDC	C6-N1	-3.03	1.30	1.34
2	A	500	NAD	C2N-N1N	3.00	1.38	1.35
2	B	500	NAD	C2N-N1N	2.90	1.38	1.35
2	B	500	NAD	C2A-N1A	2.87	1.39	1.33
3	B	502	PDC	O2-C7	2.83	1.38	1.30
2	A	500	NAD	C2A-N3A	2.70	1.38	1.33
2	B	500	NAD	PA-O3	2.70	1.62	1.59
3	B	504	PDC	C2-C7	-2.67	1.45	1.50
3	A	504	PDC	O4-C8	2.64	1.38	1.30
3	A	502	PDC	O4-C8	2.63	1.38	1.30
2	B	500	NAD	C2A-N3A	2.61	1.38	1.33
3	A	503	PDC	C2-C7	-2.55	1.46	1.50
3	B	504	PDC	C2-N1	2.51	1.38	1.34
3	B	504	PDC	C3-C2	2.46	1.43	1.39
3	B	503	PDC	O2-C7	2.40	1.37	1.30
2	A	500	NAD	PN-O3	2.40	1.62	1.59
3	A	502	PDC	C6-C8	-2.35	1.46	1.50
2	A	500	NAD	PA-O3	2.25	1.61	1.59
3	B	504	PDC	C5-C6	2.21	1.43	1.39
3	B	502	PDC	C6-C8	-2.20	1.46	1.50
3	A	504	PDC	C6-C8	-2.13	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	PDC	C3-C2	2.13	1.43	1.39
3	A	503	PDC	C5-C6	2.07	1.43	1.39
3	A	502	PDC	C4-C3	2.06	1.42	1.38
3	B	503	PDC	C4-C3	2.06	1.42	1.38
2	B	500	NAD	C8A-N7A	2.05	1.35	1.31

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	PDC	C6-N1-C2	8.31	127.83	117.54
2	B	500	NAD	N3A-C2A-N1A	-5.76	119.86	128.58
3	B	504	PDC	O4-C8-O3	-5.16	112.26	123.35
2	A	500	NAD	N3A-C2A-N1A	-5.02	120.98	128.58
3	B	503	PDC	C3-C2-N1	-4.90	117.20	122.92
3	A	504	PDC	C6-N1-C2	4.68	123.33	117.54
3	B	504	PDC	C5-C6-N1	-4.51	117.66	122.92
2	A	500	NAD	C5A-C4A-N3A	-4.22	120.90	126.72
3	A	504	PDC	C3-C2-N1	-4.16	118.07	122.92
2	B	500	NAD	C5A-C4A-N3A	-4.13	121.03	126.72
3	B	504	PDC	O4-C8-C6	3.85	123.85	114.71
3	B	504	PDC	C8-C6-N1	3.82	122.17	116.46
3	A	503	PDC	O2-C7-O1	3.70	131.30	123.35
2	B	500	NAD	N9A-C8A-N7A	-3.66	108.74	113.94
3	B	503	PDC	C3-C2-C7	3.56	126.52	120.32
3	B	504	PDC	C4-C5-C6	3.54	122.86	118.63
2	A	500	NAD	N9A-C8A-N7A	-3.48	109.00	113.94
3	B	503	PDC	C5-C6-C8	3.44	126.31	120.32
2	B	500	NAD	C2A-N3A-C4A	3.39	120.11	111.83
2	B	500	NAD	N3A-C4A-N9A	3.36	132.88	127.17
3	B	503	PDC	C5-C6-N1	-3.21	119.18	122.92
3	B	504	PDC	C6-N1-C2	3.20	121.50	117.54
2	A	500	NAD	C5A-N7A-C8A	3.19	108.46	103.45
3	A	504	PDC	O2-C7-C2	3.09	122.05	114.71
2	A	500	NAD	C2A-N3A-C4A	3.06	119.31	111.83
2	A	500	NAD	N3A-C4A-N9A	3.01	132.28	127.17
2	B	500	NAD	C5A-N7A-C8A	2.83	107.90	103.45
3	B	502	PDC	O1-C7-C2	-2.82	115.62	121.30
3	A	504	PDC	C4-C5-C6	-2.67	115.44	118.63
3	A	502	PDC	C6-N1-C2	2.58	120.73	117.54
3	A	504	PDC	O1-C7-C2	-2.49	116.28	121.30
3	B	502	PDC	O4-C8-O3	-2.42	118.14	123.35
3	A	502	PDC	O2-C7-C2	2.42	120.46	114.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	PDC	C4-C5-C6	2.36	121.45	118.63
2	B	500	NAD	C4A-N9A-C8A	2.33	108.19	105.74
2	A	500	NAD	C6A-C5A-C4A	2.28	120.30	117.18
3	B	502	PDC	O2-C7-O1	2.23	128.16	123.35
2	A	500	NAD	C4A-C5A-N7A	-2.23	108.03	110.58
3	A	503	PDC	C7-C2-N1	2.20	119.76	116.46
3	A	504	PDC	C5-C4-C3	2.19	123.05	120.24
2	A	500	NAD	C6N-N1N-C2N	-2.09	120.10	121.88
2	B	500	NAD	C6N-N1N-C2N	-2.08	120.11	121.88
2	B	500	NAD	O2A-PA-O3	2.00	112.69	107.27

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	NAD	C2N-C3N-C7N-O7N
2	A	500	NAD	C2N-C3N-C7N-N7N
2	B	500	NAD	C2N-C3N-C7N-O7N
2	B	500	NAD	C2N-C3N-C7N-N7N
2	A	500	NAD	O4B-C4B-C5B-O5B
2	B	500	NAD	O4B-C4B-C5B-O5B
2	A	500	NAD	C3B-C4B-C5B-O5B
2	B	500	NAD	C3B-C4B-C5B-O5B

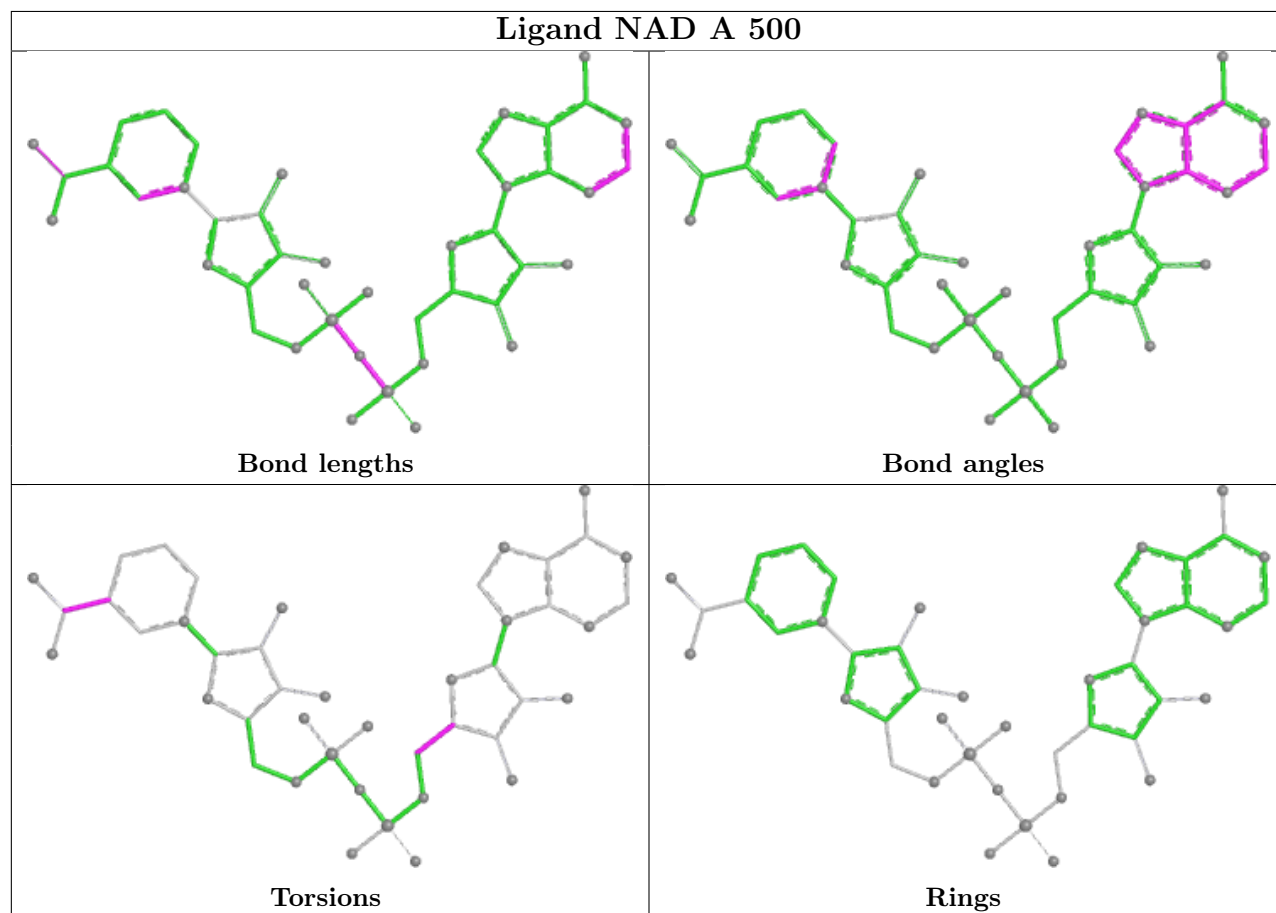
There are no ring outliers.

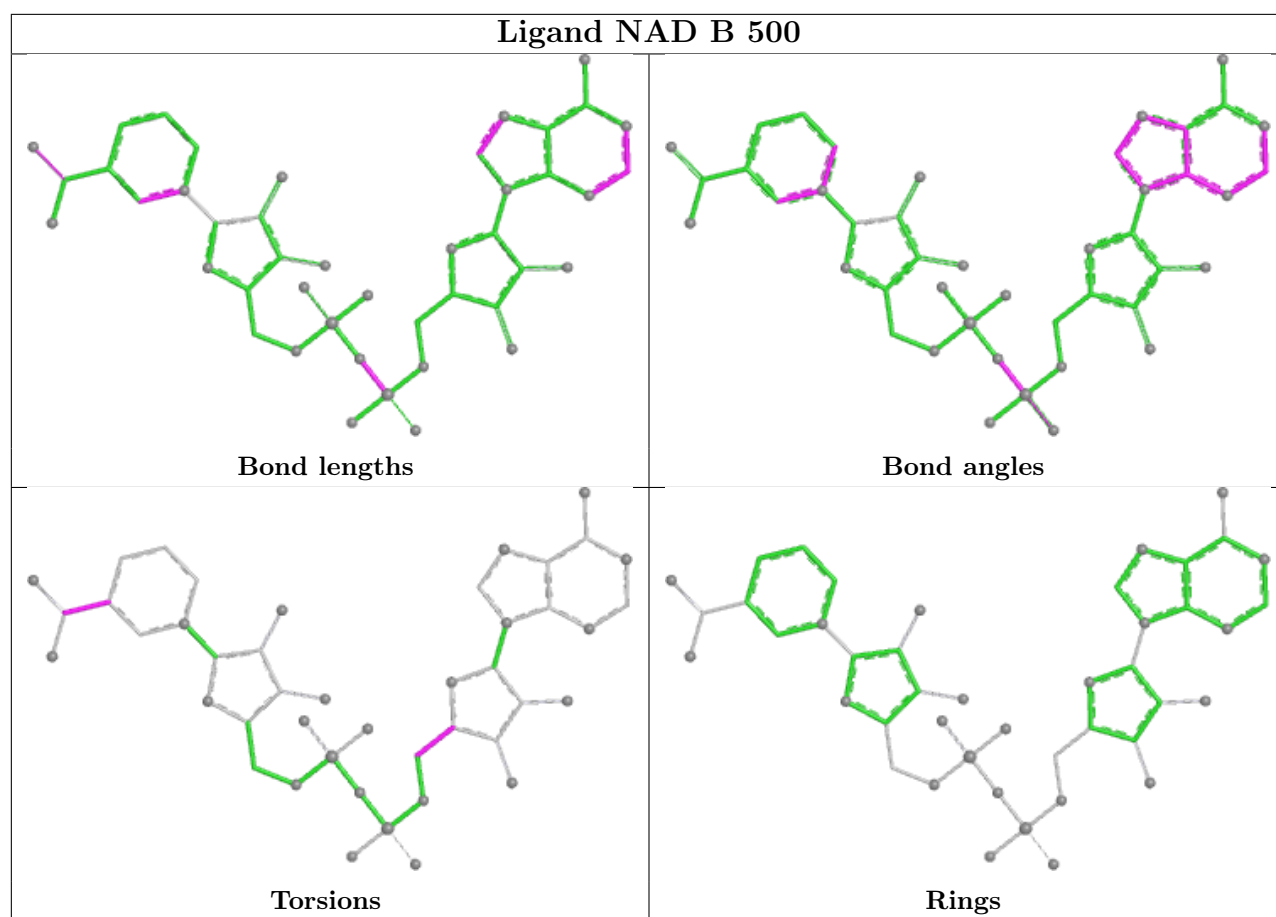
6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	NAD	3	0
3	B	503	PDC	1	0
3	B	504	PDC	1	0
3	A	504	PDC	3	0
3	A	502	PDC	1	0
2	B	500	NAD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	409/431 (94%)	0.09	4 (0%) 79 76	32, 54, 89, 101	0
1	B	418/431 (96%)	0.13	6 (1%) 73 70	31, 55, 84, 99	0
All	All	827/862 (95%)	0.11	10 (1%) 76 73	31, 55, 87, 101	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	261	VAL	4.2
1	B	260	ALA	3.5
1	A	418	ILE	3.4
1	B	257	HIS	3.3
1	B	418	ILE	3.2
1	B	384	PHE	2.8
1	A	86	ASP	2.6
1	A	355	HIS	2.6
1	B	174	LYS	2.5
1	A	46	ILE	2.4

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](#)

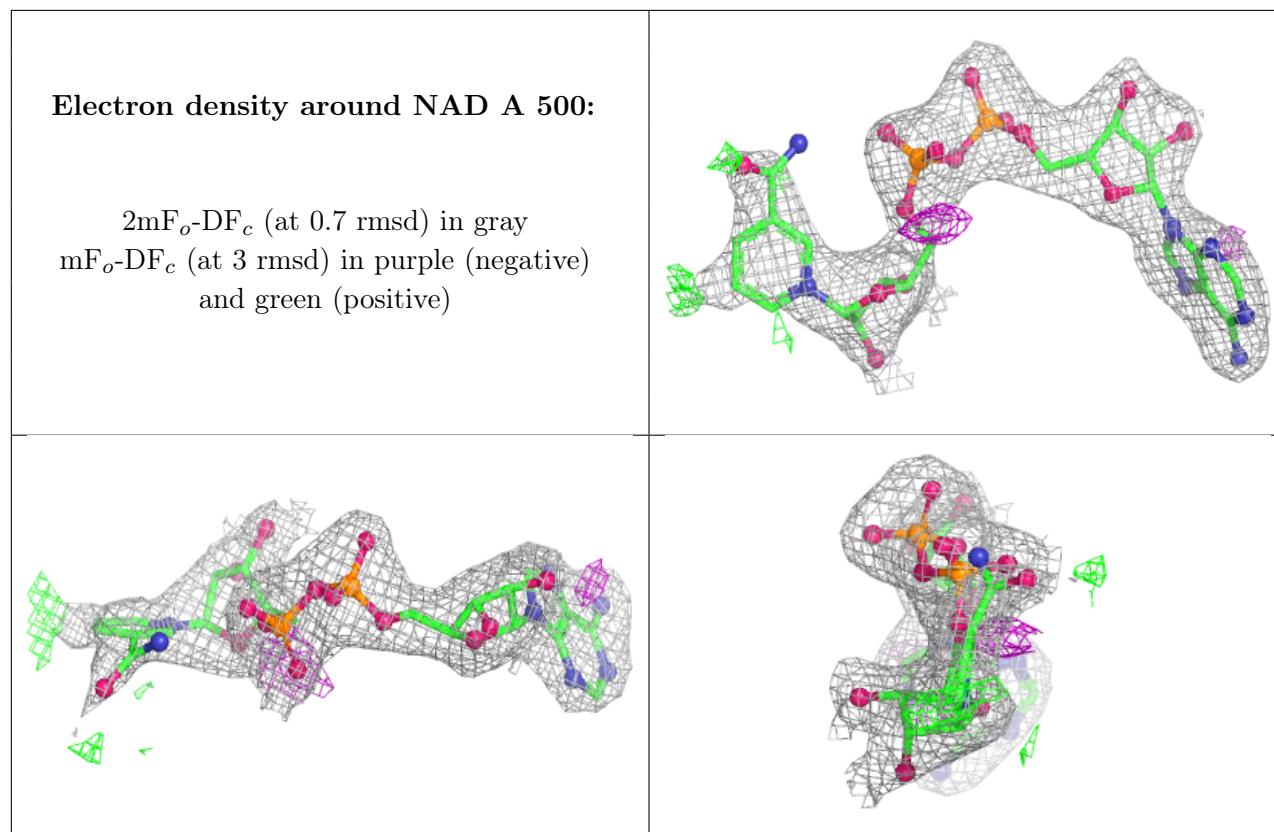
There are no oligosaccharides in this entry.

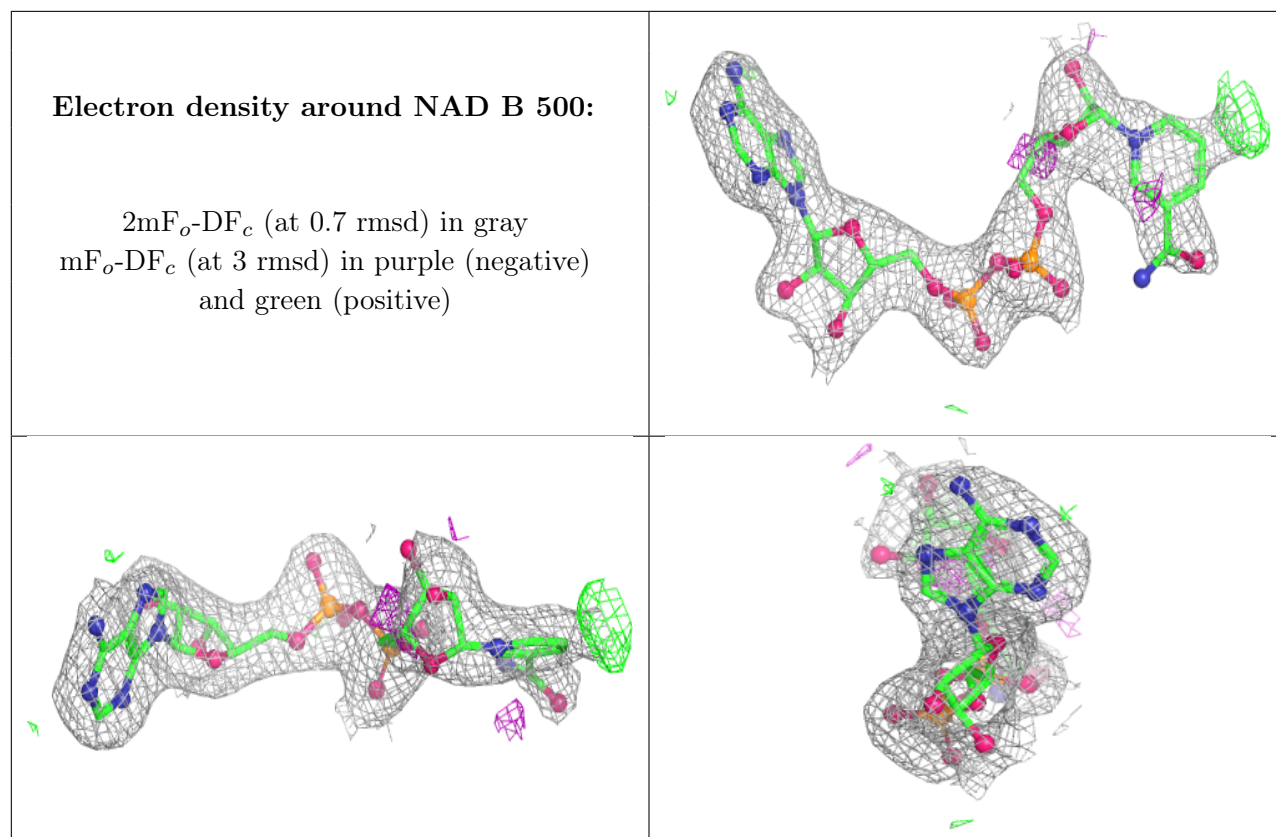
6.4 Ligands ⓘ

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. 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	B-factors(Å ²)	Q<0.9
2	NAD	A	500	44/44	0.90	0.10	44,60,77,82	0
3	PDC	B	504	12/12	0.91	0.15	72,75,78,79	0
3	PDC	A	503	12/12	0.92	0.12	36,39,42,42	6
3	PDC	A	504	12/12	0.92	0.13	36,39,41,43	5
3	PDC	A	502	12/12	0.92	0.11	48,51,53,55	2
3	PDC	B	503	12/12	0.92	0.10	48,51,54,54	0
3	PDC	B	502	12/12	0.94	0.12	43,46,50,52	4
2	NAD	B	500	44/44	0.94	0.09	33,42,78,79	0
4	EU	A	501	1/1	0.99	0.12	22,22,22,22	1
4	EU	B	501	1/1	1.00	0.09	33,33,33,33	1

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.