



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:30 PM UTC

PDB ID : 3OJL / pdb_00003ojl
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

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:

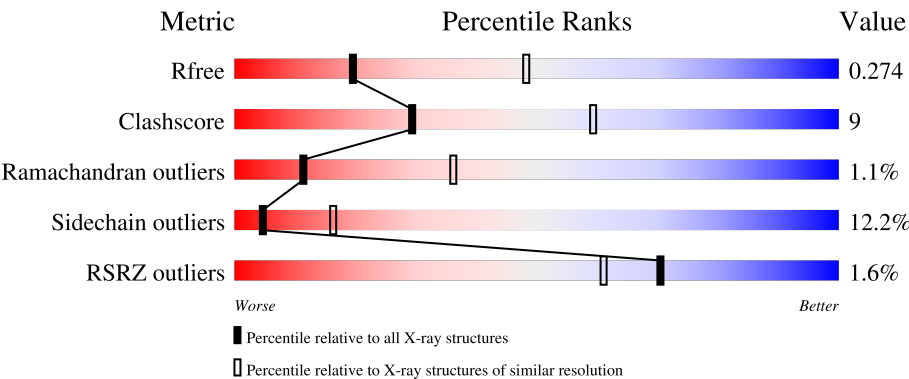
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 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 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			

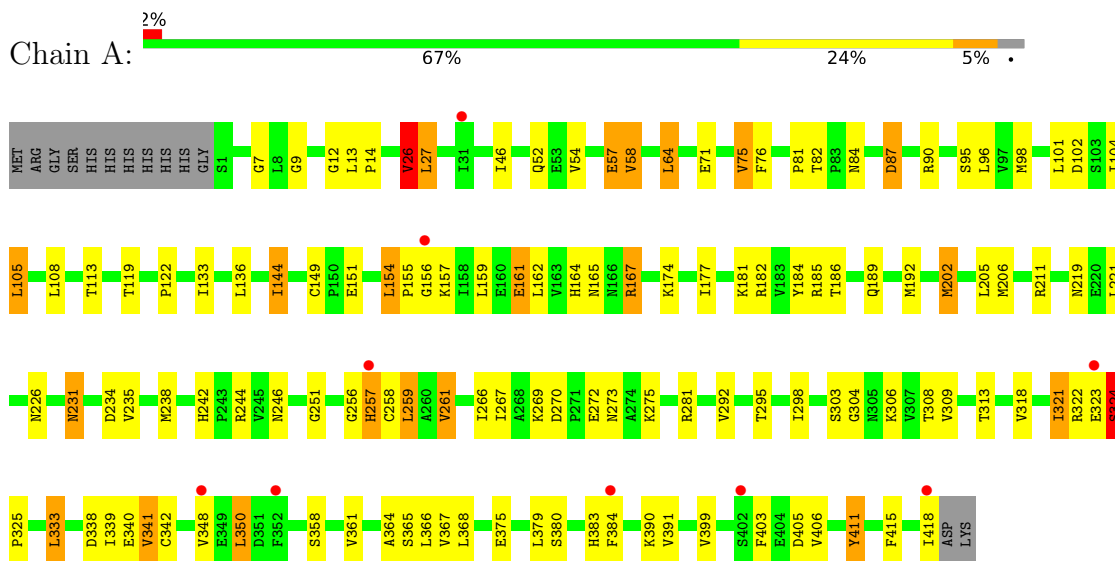
There are 24 discrepancies between the modelled and reference sequences:

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

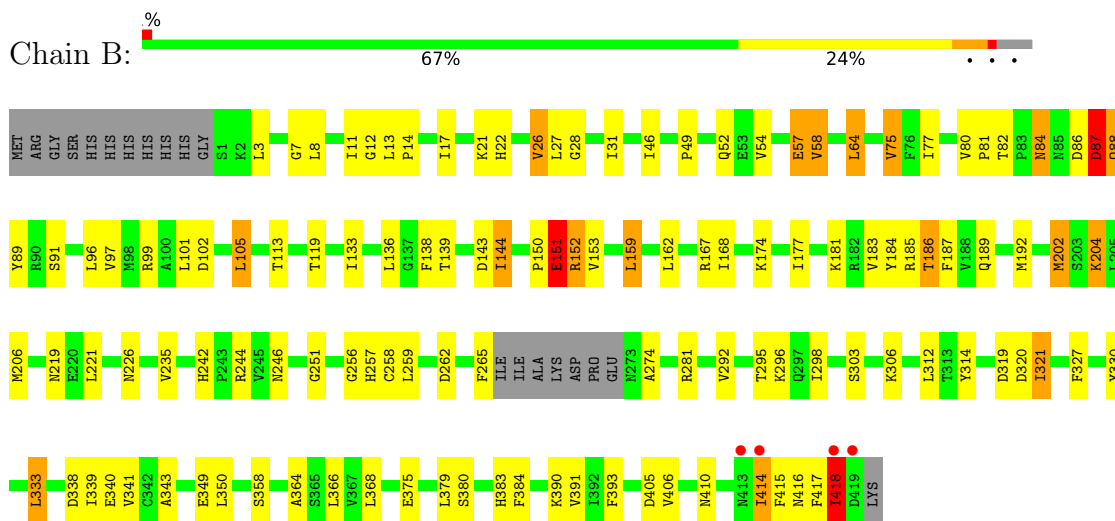
3 Residue-property plots [i](#)

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	77.90Å 87.26Å 131.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.12 – 2.80 29.12 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.12-2.80) 98.2 (29.12-2.80)	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 (3.63%)	wwPDB-VP
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 , 68.3	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	0.92	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.

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

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	0.87	0/3331	1.44	20/4520 (0.4%)
1	B	0.88	1/3283 (0.0%)	1.44	20/4453 (0.4%)
All	All	0.87	1/6614 (0.0%)	1.44	40/8973 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	80	VAL	CA-C	5.51	1.58	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	87	ASP	CA-CB-CG	7.28	119.88	112.60
1	B	84	ASN	CA-CB-CG	7.25	119.85	112.60
1	B	88	GLN	N-CA-C	-7.13	104.59	112.72
1	B	417	PHE	CA-C-N	6.79	134.19	121.97
1	B	417	PHE	C-N-CA	6.79	134.19	121.97
1	A	259	LEU	N-CA-C	6.15	119.62	111.75
1	A	52	GLN	CA-C-N	6.07	128.33	120.44
1	A	52	GLN	C-N-CA	6.07	128.33	120.44
1	A	26	VAL	N-CA-C	6.03	117.28	108.53
1	A	324	SER	N-CA-C	6.02	119.03	109.64
1	A	411	TYR	N-CA-C	-5.88	106.07	113.18
1	B	265	PHE	CA-CB-CG	5.82	119.62	113.80
1	B	52	GLN	CA-C-N	5.80	127.99	120.44
1	B	52	GLN	C-N-CA	5.80	127.99	120.44
1	A	164	HIS	N-CA-C	5.54	119.75	112.89
1	B	97	VAL	N-CA-C	-5.53	105.33	110.53
1	B	341	VAL	N-CA-C	5.48	116.47	108.53
1	A	261	VAL	CA-C-N	5.43	129.01	120.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	VAL	C-N-CA	5.43	129.01	120.97
1	B	151	GLU	CA-C-N	5.43	128.93	121.33
1	B	151	GLU	C-N-CA	5.43	128.93	121.33
1	A	267	ILE	N-CA-CB	5.36	116.24	110.62
1	A	341	VAL	N-CA-C	5.34	115.64	108.17
1	A	161	GLU	CA-C-N	5.29	127.90	120.28
1	A	161	GLU	C-N-CA	5.29	127.90	120.28
1	A	87	ASP	CA-C-N	5.25	127.27	120.44
1	A	87	ASP	C-N-CA	5.25	127.27	120.44
1	B	327	PHE	CA-CB-CG	-5.24	108.56	113.80
1	B	274	ALA	CA-C-N	5.23	127.24	120.44
1	B	274	ALA	C-N-CA	5.23	127.24	120.44
1	A	57	GLU	CA-C-N	5.12	127.48	120.46
1	A	57	GLU	C-N-CA	5.12	127.48	120.46
1	A	350	LEU	CA-C-N	5.11	127.08	120.44
1	A	350	LEU	C-N-CA	5.11	127.08	120.44
1	B	99	ARG	CA-C-N	5.05	127.05	120.28
1	B	99	ARG	C-N-CA	5.05	127.05	120.28
1	B	57	GLU	CA-C-N	5.05	127.38	120.46
1	B	57	GLU	C-N-CA	5.05	127.38	120.46
1	B	417	PHE	CB-CA-C	5.02	117.45	111.22
1	A	257	HIS	N-CA-C	-5.01	105.47	111.03

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	68	0
1	B	3225	0	3220	56	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	113	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 9.

All (113) 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:221:LEU:HD22	1:B:206:MET:HE2	1.63	0.79
1:A:206:MET:SD	1:B:221:LEU:HD11	2.25	0.77
1:A:206:MET:HE3	1:B:221:LEU:HD21	1.65	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:B:416:ASN:C	1:B:418:ILE:H	2.07	0.62
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:26:VAL:HG22	1:A:64:LEU:HG	1.97	0.47
1:B:184:TYR:HB2	1:B:192:MET:HE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:184:TYR:HB2	1:A:192:MET:HE1	2.00	0.43
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:154:LEU:C	1:A:156:GLY:H	2.26	0.43
1:A:238:MET:HE1	1:B:168:ILE:HG12	2.01	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
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: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:B:82:THR:HG21	1:B:119:THR:O	2.19	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:8:LEU:HD11	1:B:28:GLY:HA3	2.02	0.41
1:B:26:VAL:HG22	1:B:64:LEU:HG	2.03	0.41
1:A:82:THR:HG21	1:A:119:THR:O	2.21	0.40
1:A:308:THR:HG21	1:A:361:VAL:HG12	2.03	0.40
1:B:138:PHE:HD2	1:B:143:ASP:HB3	1.87	0.40
1:A:221:LEU:HD22	1:B:206:MET:CE	2.44	0.40
1:A:270:ASP:CG	1:A:273:ASN:HD22	2.29	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 [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%)	10	34
1	B	408/431 (95%)	380 (93%)	24 (6%)	4 (1%)	12	38
All	All	824/862 (96%)	770 (93%)	45 (6%)	9 (1%)	11	36

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 [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%)	329 (88%)	43 (12%)	5	18
1	B	367/383 (96%)	320 (87%)	47 (13%)	4	15
All	All	739/766 (96%)	649 (88%)	90 (12%)	5	16

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	VAL
1	A	27	LEU
1	A	46	ILE
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	157	LYS
1	A	162	LEU
1	A	167	ARG
1	A	182	ARG
1	A	186	THR
1	A	189	GLN
1	A	202	MET
1	A	231	ASN
1	A	246	ASN
1	A	257	HIS
1	A	258	CYS
1	A	261	VAL
1	A	272	GLU
1	A	275	LYS
1	A	281	ARG
1	A	303	SER
1	A	309	VAL
1	A	323	GLU
1	A	324	SER
1	A	333	LEU
1	A	338	ASP
1	A	350	LEU
1	A	358	SER
1	A	368	LEU
1	A	375	GLU
1	A	391	VAL
1	A	405	ASP
1	A	411	TYR

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Mol	Chain	Res	Type
1	A	418	ILE
1	B	26	VAL
1	B	27	LEU
1	B	31	ILE
1	B	46	ILE
1	B	57	GLU
1	B	58	VAL
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	144	ILE
1	B	151	GLU
1	B	152	ARG
1	B	153	VAL
1	B	159	LEU
1	B	162	LEU
1	B	167	ARG
1	B	186	THR
1	B	189	GLN
1	B	202	MET
1	B	204	LYS
1	B	246	ASN
1	B	257	HIS
1	B	258	CYS
1	B	259	LEU
1	B	262	ASP
1	B	281	ARG
1	B	296	LYS
1	B	303	SER
1	B	319	ASP
1	B	321	ILE
1	B	333	LEU
1	B	338	ASP
1	B	349	GLU
1	B	350	LEU
1	B	358	SER
1	B	368	LEU

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Mol	Chain	Res	Type
1	B	375	GLU
1	B	391	VAL
1	B	405	ASP
1	B	410	ASN
1	B	414	ILE
1	B	418	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	32	ASN
1	A	34	GLN
1	A	84	ASN
1	A	208	ASN
1	A	219	ASN
1	A	226	ASN
1	A	231	ASN
1	A	242	HIS
1	A	249	GLN
1	A	273	ASN
1	A	334	ASN
1	A	383	HIS
1	A	410	ASN
1	A	413	ASN
1	B	22	HIS
1	B	32	ASN
1	B	34	GLN
1	B	85	ASN
1	B	135	ASN
1	B	219	ASN
1	B	226	ASN
1	B	242	HIS
1	B	249	GLN
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 ⓘ

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	-	46,48,48	1.82	7 (15%)	64,73,73	1.54	9 (14%)
2	NAD	B	500	-	46,48,48	1.95	7 (15%)	64,73,73	1.52	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
2	NAD	B	500	-	-	4/30/62/62	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	NAD	O7N-C7N	9.33	1.41	1.24
2	B	500	NAD	O7N-C7N	9.23	1.41	1.24
2	B	500	NAD	PA-O3	4.25	1.64	1.59
2	B	500	NAD	C2A-N3A	3.45	1.40	1.33
2	B	500	NAD	C2A-N1A	3.26	1.39	1.33
2	A	500	NAD	C2A-N1A	3.23	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	NAD	C2A-N3A	2.88	1.39	1.33
2	B	500	NAD	C2N-N1N	2.87	1.38	1.35
2	A	500	NAD	C2N-N1N	2.57	1.37	1.35
2	B	500	NAD	PN-O3	2.48	1.62	1.59
2	A	500	NAD	C5A-N7A	-2.40	1.34	1.39
2	B	500	NAD	C8A-N7A	2.24	1.36	1.31
2	A	500	NAD	PN-O3	2.23	1.61	1.59
2	A	500	NAD	C8A-N7A	2.00	1.35	1.31

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	NAD	N3A-C2A-N1A	-5.02	120.98	128.58
2	A	500	NAD	N3A-C2A-N1A	-4.80	121.31	128.58
2	A	500	NAD	C5A-C4A-N3A	-4.46	120.57	126.72
2	A	500	NAD	N9A-C8A-N7A	-4.10	108.12	113.94
2	A	500	NAD	C5A-N7A-C8A	4.05	109.82	103.45
2	B	500	NAD	C5A-C4A-N3A	-3.99	121.22	126.72
2	B	500	NAD	N9A-C8A-N7A	-3.95	108.33	113.94
2	A	500	NAD	C4A-C5A-N7A	-3.40	106.69	110.58
2	B	500	NAD	C5A-N7A-C8A	3.35	108.71	103.45
2	B	500	NAD	C6N-N1N-C2N	-3.20	119.16	121.88
2	A	500	NAD	C2A-N3A-C4A	3.09	119.38	111.83
2	B	500	NAD	C2A-N3A-C4A	3.04	119.25	111.83
2	B	500	NAD	N3A-C4A-N9A	2.79	131.92	127.17
2	A	500	NAD	C6N-N1N-C2N	-2.65	119.62	121.88
2	A	500	NAD	N3A-C4A-N9A	2.64	131.65	127.17
2	A	500	NAD	C6A-C5A-C4A	2.46	120.54	117.18
2	B	500	NAD	C4A-C5A-N7A	-2.46	107.77	110.58
2	B	500	NAD	C4A-N9A-C8A	2.45	108.31	105.74

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	NAD	C2N-C3N-C7N-N7N
2	B	500	NAD	C2N-C3N-C7N-N7N
2	A	500	NAD	C4N-C3N-C7N-O7N
2	A	500	NAD	C4N-C3N-C7N-N7N
2	B	500	NAD	C4N-C3N-C7N-O7N
2	B	500	NAD	C4N-C3N-C7N-N7N
2	A	500	NAD	C2N-C3N-C7N-O7N

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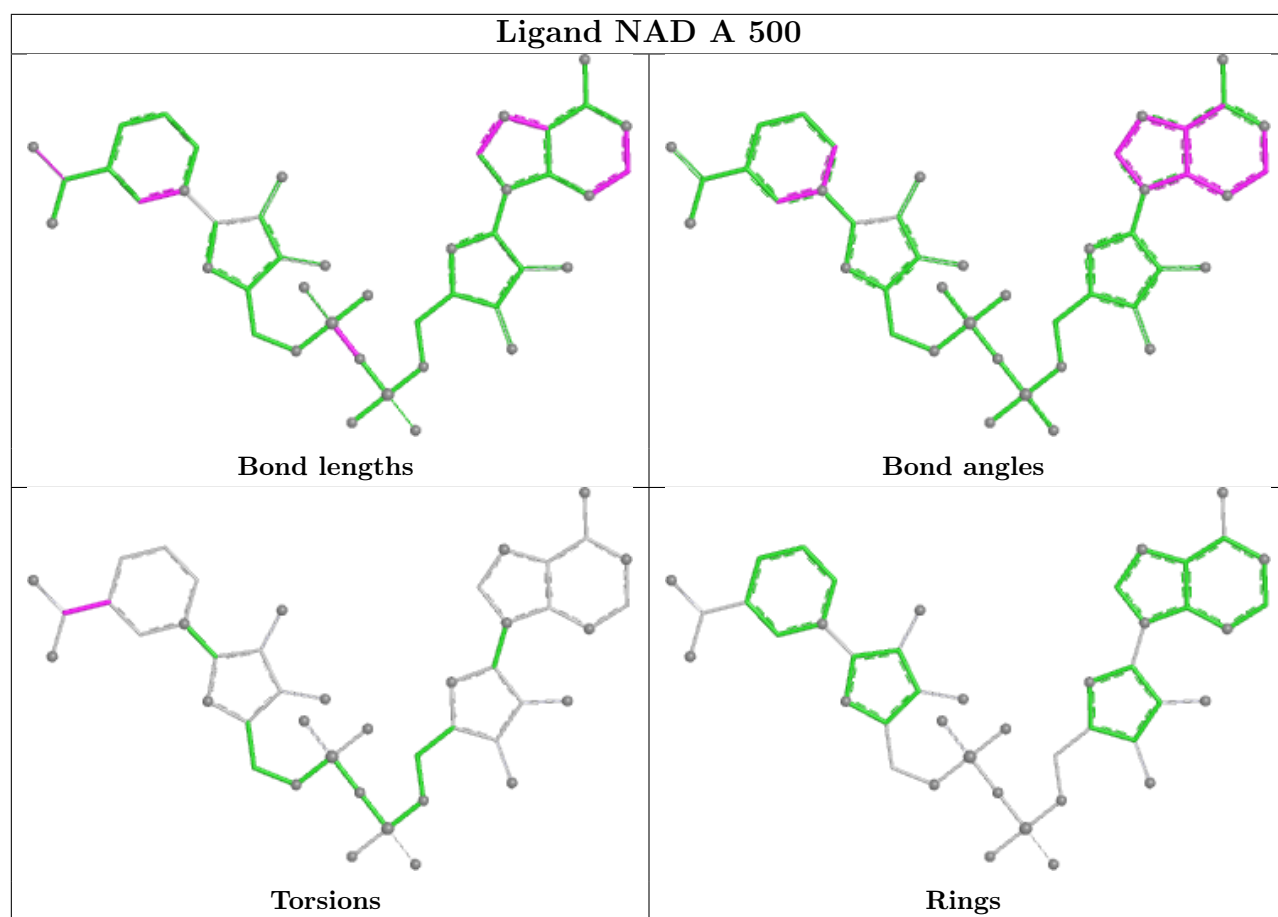
Mol	Chain	Res	Type	Atoms
2	B	500	NAD	C2N-C3N-C7N-O7N

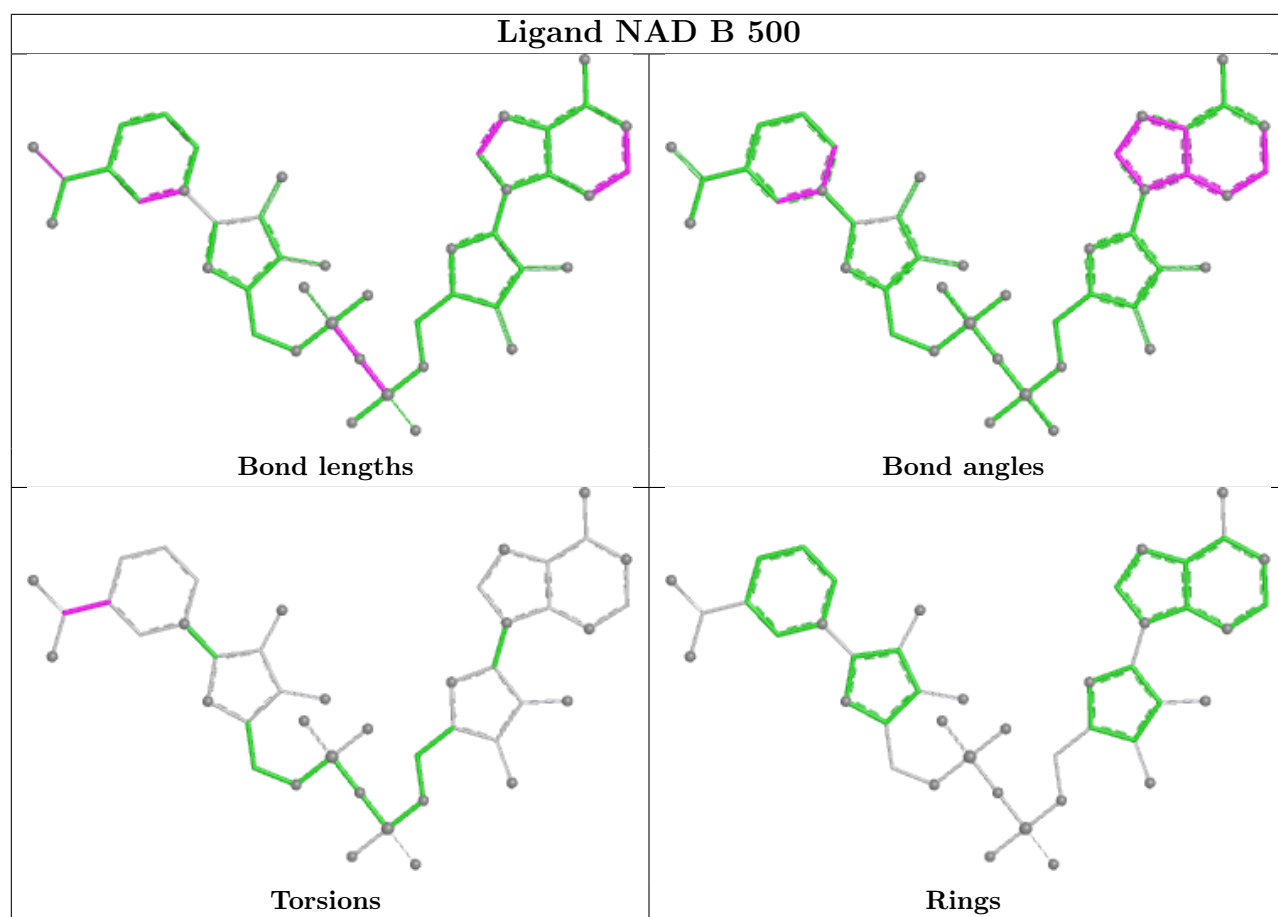
There are no ring outliers.

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

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	418/431 (96%)	0.36	9 (2%) 62 52	30, 70, 118, 136	0
1	B	412/431 (95%)	0.17	4 (0%) 79 72	30, 66, 94, 117	0
All	All	830/862 (96%)	0.27	13 (1%) 70 61	30, 67, 113, 136	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	384	PHE	3.1
1	A	348	VAL	2.8
1	A	352	PHE	2.6
1	B	413	ASN	2.4
1	A	402	SER	2.4
1	A	156	GLY	2.3
1	B	418	ILE	2.1
1	A	257	HIS	2.1
1	B	414	ILE	2.1
1	A	31	ILE	2.1
1	B	419	ASP	2.1
1	A	323	GLU	2.1
1	A	418	ILE	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](#)

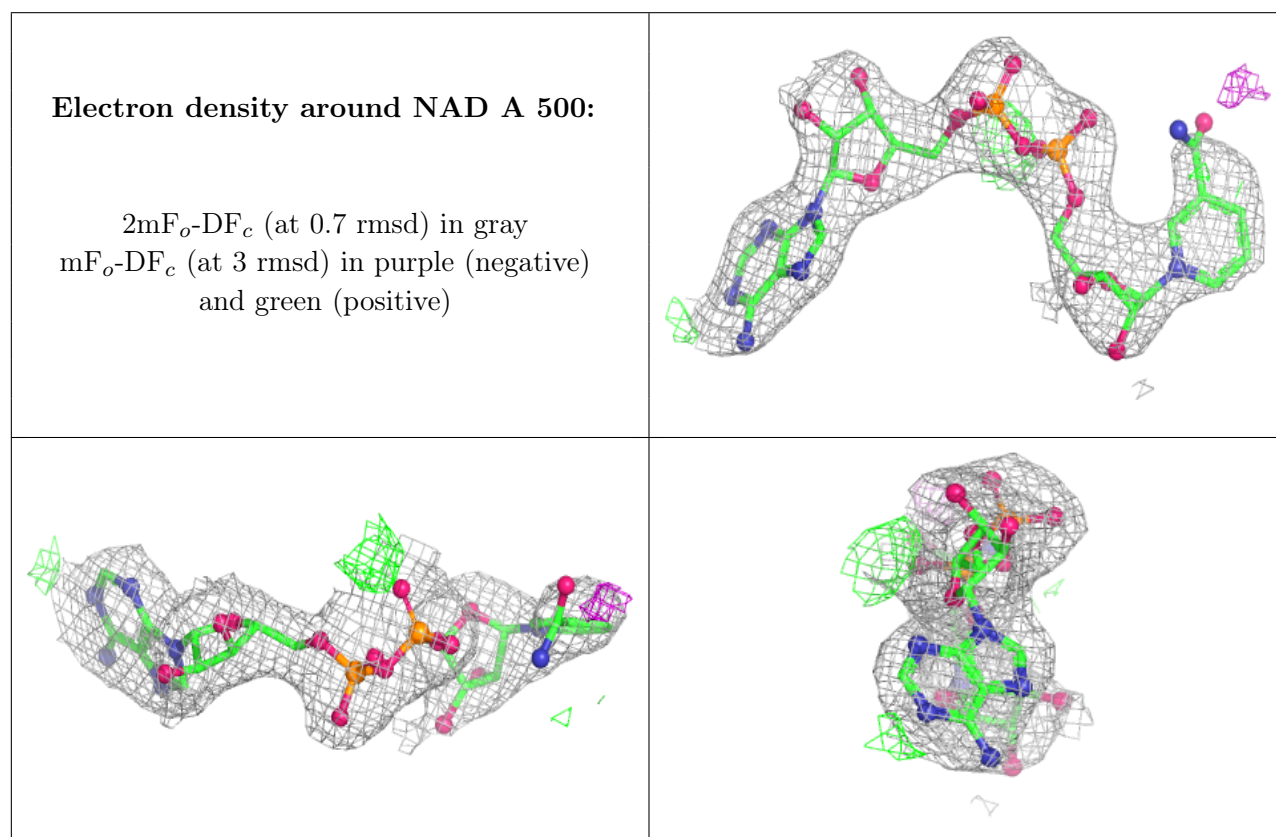
There are no oligosaccharides in this entry.

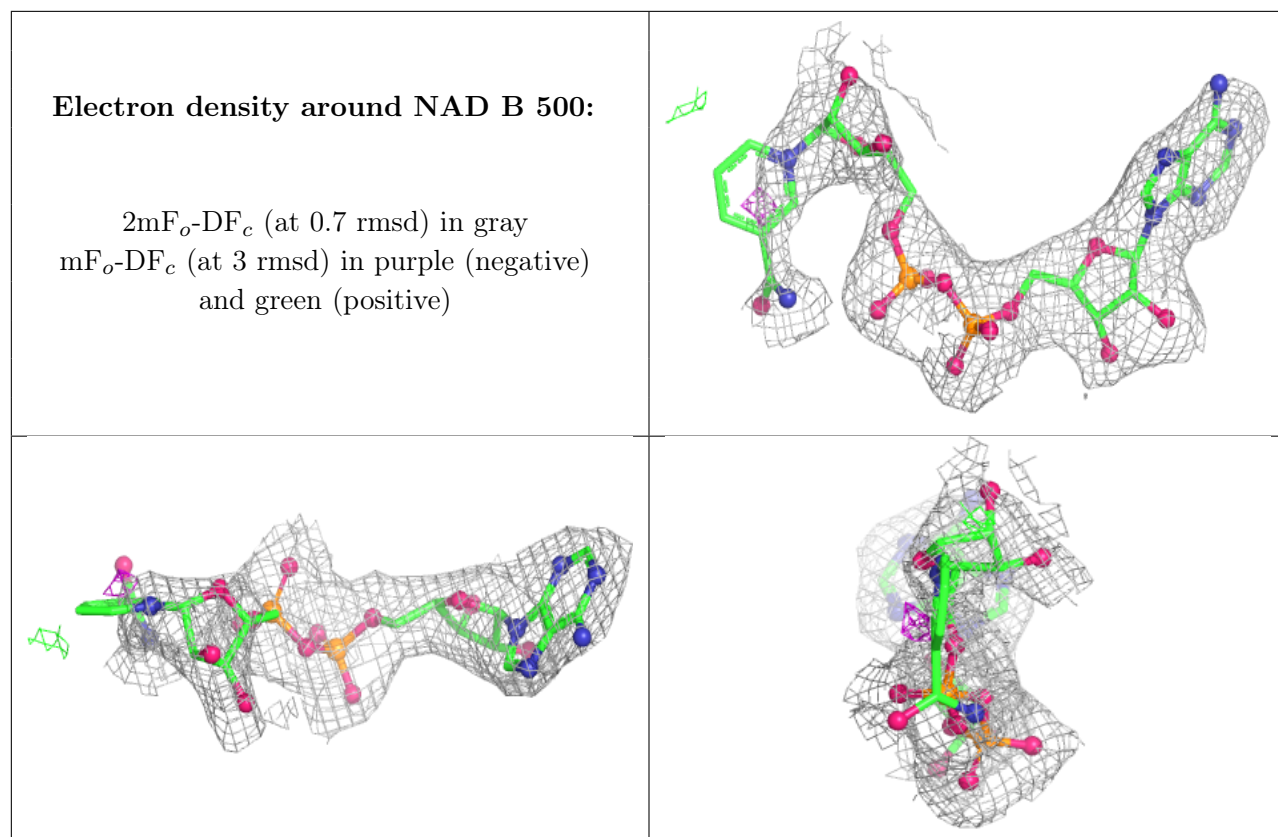
6.4 Ligands ⓘ

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	0.88	0.11	64,76,90,95	0
2	NAD	B	500	44/44	0.92	0.10	52,63,109,110	0

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.