



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:10 PM UTC

PDB ID : 7N29 / pdb_00007n29
Title : Structure of NAD kinase
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Deposited on : 2021-05-28
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

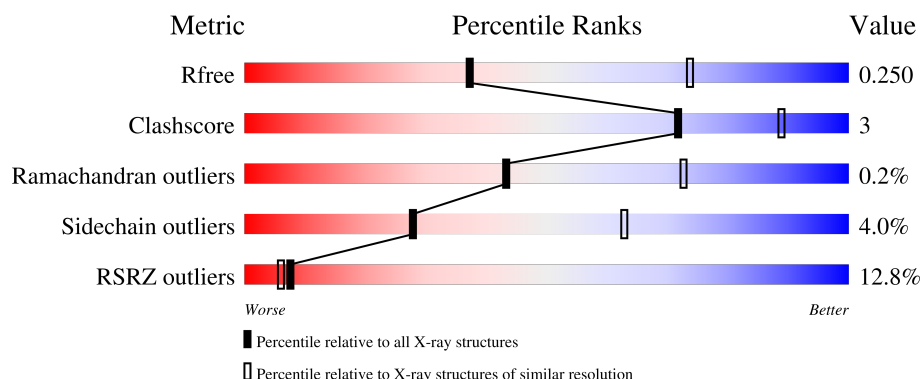
1 Overall quality at a glance

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	398	2% 70% 12% • 17%
1	B	398	5% 76% 11% • 12%
1	C	398	3% 75% 11% • 14%
1	D	398	33% 77% • 20%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10868 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.

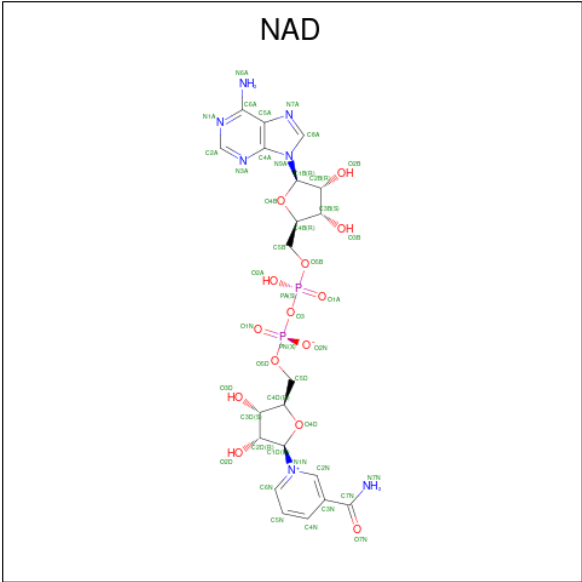
- Molecule 1 is a protein called NAD kinase 2, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	Se	0	0	0
			2572	1611	464	486	7	4			
1	B	350	Total	C	N	O	S	Se	0	0	0
			2740	1716	495	518	7	4			
1	C	342	Total	C	N	O	S	Se	0	0	0
			2679	1677	486	505	7	4			
1	D	318	Total	C	N	O	S	Se	0	0	0
			2499	1568	452	468	7	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	GLY	-	expression tag	UNP Q4G0N4
A	46	PRO	-	expression tag	UNP Q4G0N4
B	45	GLY	-	expression tag	UNP Q4G0N4
B	46	PRO	-	expression tag	UNP Q4G0N4
C	45	GLY	-	expression tag	UNP Q4G0N4
C	46	PRO	-	expression tag	UNP Q4G0N4
D	45	GLY	-	expression tag	UNP Q4G0N4
D	46	PRO	-	expression tag	UNP Q4G0N4

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



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		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

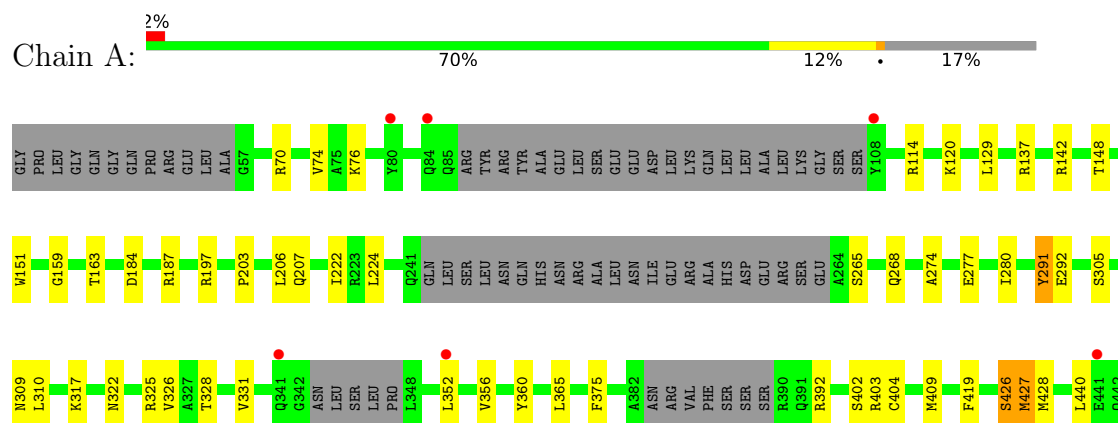
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	63	Total	O	0	0
			63	63		
3	B	71	Total	O	0	0
			71	71		
3	C	68	Total	O	0	0
			68	68		

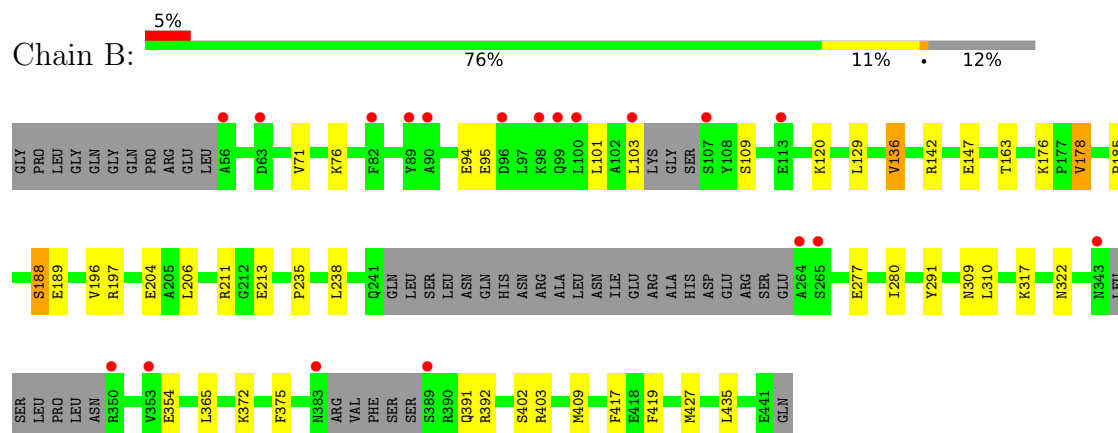
3 Residue-property plots [i](#)

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.

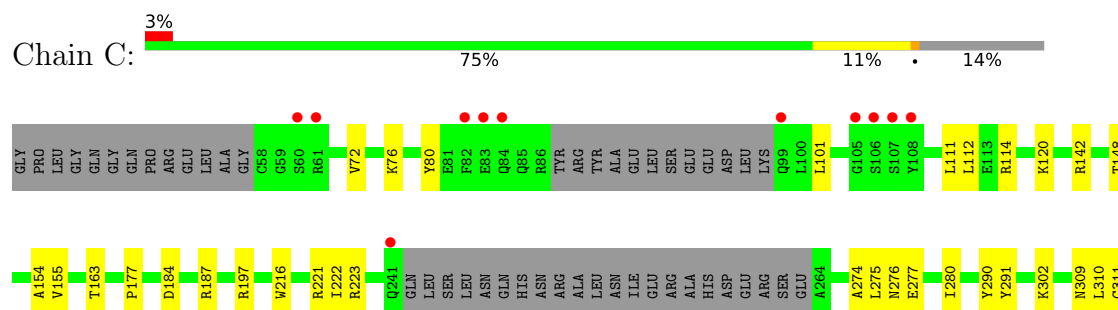
- Molecule 1: NAD kinase 2, mitochondrial

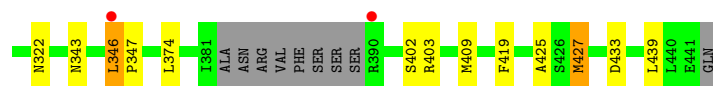


- Molecule 1: NAD kinase 2, mitochondrial

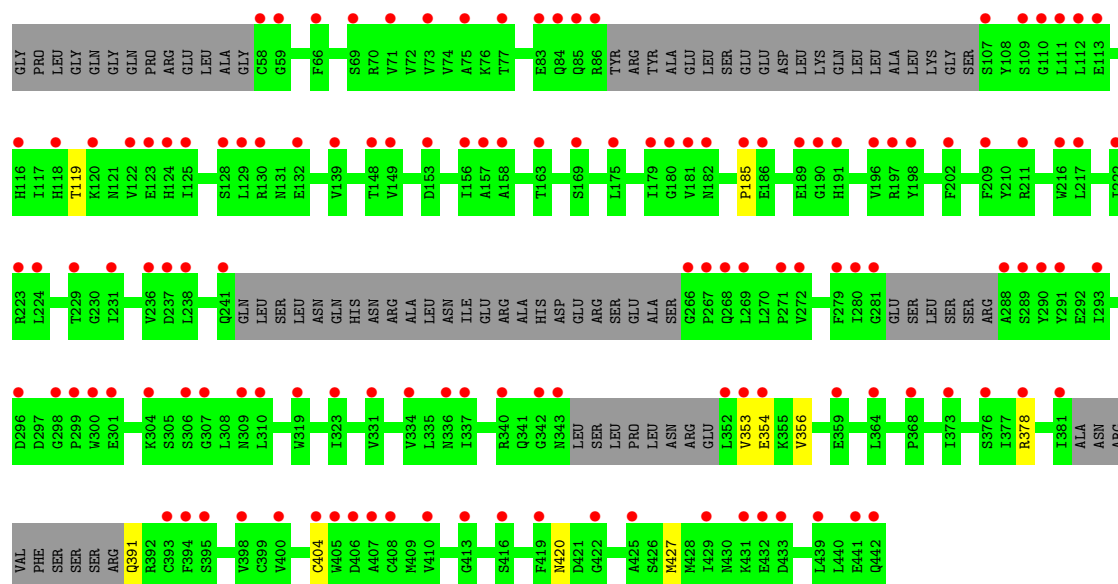
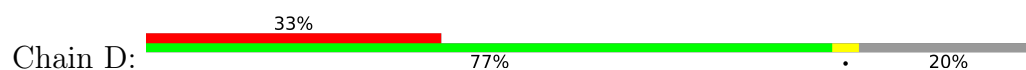


- Molecule 1: NAD kinase 2, mitochondrial





- Molecule 1: NAD kinase 2, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	97.13Å 185.12Å 188.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.79 – 2.80 29.79 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.79-2.80) 99.9 (29.79-2.80)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.80Å)	Xtriage
Refinement program	PHENIX 1.17_3644	Depositor
R, R_{free}	0.191 , 0.249 0.193 , 0.250	Depositor DCC
R_{free} test set	2021 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	47.7	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10868	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.42	0/2613	0.65	0/3525
1	B	0.43	0/2783	0.64	0/3753
1	C	0.39	0/2722	0.61	0/3671
1	D	0.20	0/2539	0.46	0/3423
All	All	0.37	0/10657	0.60	0/14372

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2572	0	2506	24	0
1	B	2740	0	2672	21	0
1	C	2679	0	2637	24	0
1	D	2499	0	2440	0	0
2	A	44	0	26	0	0
2	B	44	0	26	1	0
2	C	44	0	26	1	0
2	D	44	0	24	0	0
3	A	63	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	71	0	0	1	0
3	C	68	0	0	0	0
All	All	10868	0	10357	69	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 3.

All (69) 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:280:ILE:HG12	1:B:409:MSE:HG2	1.74	0.70
1:A:224:LEU:HG	1:A:427:MSE:HE2	1.77	0.67
1:C:76:LYS:HB2	1:C:163:THR:HG21	1.75	0.67
1:C:280:ILE:HG12	1:C:409:MSE:HG2	1.77	0.66
1:A:76:LYS:HB2	1:A:163:THR:HG21	1.80	0.63
1:A:426:SER:C	1:A:427:MSE:HE3	2.24	0.62
1:A:70:ARG:NH1	1:A:151:TRP:O	2.33	0.61
1:A:114:ARG:HD2	1:A:187:ARG:HD2	1.81	0.61
1:B:197:ARG:NH2	1:B:204:GLU:OE2	2.33	0.61
1:A:426:SER:O	1:A:427:MSE:HE3	2.02	0.60
1:A:331:VAL:HG11	1:A:356:VAL:HG23	1.85	0.59
1:A:159:GLY:HA3	1:A:163:THR:HG21	1.87	0.57
1:B:76:LYS:HB2	1:B:163:THR:HG21	1.87	0.56
1:A:203:PRO:O	1:A:207:GLN:HG3	2.06	0.55
1:C:80:TYR:CE1	1:C:112:LEU:HD13	2.41	0.54
1:C:114:ARG:HD2	1:C:187:ARG:HD2	1.89	0.54
1:A:291:TYR:OH	1:A:305:SER:OG	2.26	0.54
1:C:114:ARG:NH1	1:C:184:ASP:OD1	2.40	0.54
1:A:280:ILE:HG12	1:A:409:MSE:HG2	1.90	0.52
1:C:310:LEU:HD22	1:C:427:MSE:HG3	1.90	0.52
1:B:310:LEU:HG	1:B:375:PHE:HD1	1.74	0.52
1:B:188:SER:O	1:B:188:SER:OG	2.22	0.52
1:A:402:SER:HB2	1:A:419:PHE:CE2	2.46	0.51
1:C:222:ILE:HB	1:C:274:ALA:HB3	1.92	0.51
1:A:114:ARG:NH1	1:A:184:ASP:OD1	2.44	0.51
1:A:222:ILE:HB	1:A:274:ALA:HB3	1.93	0.51
1:A:317:LYS:HG3	1:A:365:LEU:HD22	1.93	0.51
1:C:346:LEU:HD12	1:C:347:PRO:HD2	1.94	0.50
1:B:322:ASN:OD1	2:B:501:NAD:N7N	2.44	0.50
1:B:211:ARG:NH2	1:B:213:GLU:OE1	2.43	0.49
1:A:137:ARG:NH1	1:A:148:THR:HG22	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:PRO:HB3	1:C:216:TRP:CZ3	2.48	0.48
1:B:317:LYS:HG3	1:B:365:LEU:HD22	1.95	0.48
1:B:392:ARG:NH2	3:B:606:HOH:O	2.46	0.48
1:C:223:ARG:HB3	1:C:433:ASP:OD2	2.13	0.47
1:C:425:ALA:CB	1:C:427:MSE:HE1	2.44	0.47
1:C:154:ALA:HB2	1:C:177:PRO:HG2	1.96	0.47
1:C:277:GLU:HG3	1:C:309:ASN:OD1	2.14	0.47
1:C:120:LYS:HE2	1:C:120:LYS:HB3	1.58	0.47
1:C:177:PRO:HB3	1:C:216:TRP:HZ3	1.80	0.47
1:B:120:LYS:HB3	1:B:120:LYS:HE2	1.66	0.46
1:A:277:GLU:HG3	1:A:309:ASN:OD1	2.15	0.46
1:A:292:GLU:OE2	1:A:403:ARG:NH1	2.49	0.45
1:B:403:ARG:HD3	1:B:403:ARG:HA	1.79	0.45
1:C:221:ARG:HG2	1:C:275:LEU:HA	1.99	0.44
1:C:402:SER:HB2	1:C:419:PHE:CE2	2.52	0.44
1:B:235:PRO:HB3	1:B:417:PHE:CE1	2.53	0.44
1:B:176:LYS:HB2	1:B:176:LYS:HE3	1.76	0.43
1:C:403:ARG:HA	1:C:403:ARG:HD3	1.88	0.43
1:A:322:ASN:HD22	1:A:325:ARG:HE	1.66	0.43
1:C:311:CYS:SG	1:C:374:LEU:HB3	2.58	0.43
1:B:71:VAL:O	1:B:136:VAL:HA	2.19	0.43
1:C:322:ASN:OD1	2:C:501:NAD:N7N	2.52	0.43
1:B:402:SER:HB2	1:B:419:PHE:CE2	2.53	0.43
1:C:439:LEU:HD23	1:C:439:LEU:HA	1.80	0.42
1:A:310:LEU:HD22	1:A:427:MSE:HG3	2.01	0.42
1:B:129:LEU:HD23	1:B:206:LEU:HD11	2.00	0.42
1:C:276:ASN:HB3	1:C:277:GLU:OE1	2.20	0.42
1:A:375:PHE:O	1:A:392:ARG:HA	2.19	0.42
1:C:290:TYR:OH	1:C:302:LYS:HD3	2.19	0.42
1:A:428:MSE:HE2	1:A:428:MSE:HB3	2.01	0.41
1:A:129:LEU:HD23	1:A:206:LEU:HD11	2.02	0.41
1:B:178:VAL:HG11	1:B:435:LEU:HD11	2.01	0.41
1:B:277:GLU:HG3	1:B:309:ASN:OD1	2.20	0.41
1:B:76:LYS:CB	1:B:163:THR:HG21	2.50	0.41
1:A:326:VAL:HG22	1:A:360:TYR:CD2	2.55	0.41
1:B:185:PRO:HB3	1:B:196:VAL:HG22	2.03	0.41
1:B:238:LEU:HD23	1:B:238:LEU:HA	1.90	0.40
1:C:72:VAL:HG13	1:C:155:VAL:HG13	2.03	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	320/398 (80%)	309 (97%)	11 (3%)	0	100	100
1	B	340/398 (85%)	324 (95%)	16 (5%)	0	100	100
1	C	334/398 (84%)	320 (96%)	14 (4%)	0	100	100
1	D	306/398 (77%)	290 (95%)	13 (4%)	3 (1%)	12	38
All	All	1300/1592 (82%)	1243 (96%)	54 (4%)	3 (0%)	43	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	185	PRO
1	D	353	VAL
1	D	354	GLU

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	273/341 (80%)	260 (95%)	13 (5%)	23	56
1	B	289/341 (85%)	273 (94%)	16 (6%)	19	51
1	C	288/341 (84%)	279 (97%)	9 (3%)	35	70
1	D	266/341 (78%)	259 (97%)	7 (3%)	40	75
All	All	1116/1364 (82%)	1071 (96%)	45 (4%)	28	63

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	VAL
1	A	120	LYS
1	A	142	ARG
1	A	197	ARG
1	A	265	SER
1	A	268	GLN
1	A	291	TYR
1	A	328	THR
1	A	352	LEU
1	A	404	CYS
1	A	426	SER
1	A	427	MSE
1	A	440	LEU
1	B	94	GLU
1	B	95	GLU
1	B	101	LEU
1	B	103	LEU
1	B	109	SER
1	B	136	VAL
1	B	142	ARG
1	B	147	GLU
1	B	178	VAL
1	B	188	SER
1	B	189	GLU
1	B	291	TYR
1	B	354	GLU
1	B	372	LYS
1	B	391	GLN
1	B	427	MSE
1	C	101	LEU
1	C	111	LEU
1	C	142	ARG
1	C	148	THR
1	C	197	ARG
1	C	291	TYR
1	C	343	ASN
1	C	346	LEU
1	C	427	MSE
1	D	119	THR
1	D	356	VAL
1	D	378	ARG
1	D	391	GLN
1	D	404	CYS

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Mol	Chain	Res	Type
1	D	420	ASN
1	D	427	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	HIS
1	B	239	HIS
1	C	329	GLN
1	D	336	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 ⓘ

4 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	C	501	-	46,48,48	0.63	2 (4%)	64,73,73	0.64	1 (1%)
2	NAD	D	501	-	46,48,48	0.69	2 (4%)	64,73,73	0.70	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	A	501	-	46,48,48	0.63	1 (2%)	64,73,73	0.68	1 (1%)
2	NAD	B	501	-	46,48,48	0.64	1 (2%)	64,73,73	0.61	1 (1%)

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	C	501	-	-	9/30/62/62	0/5/5/5
2	NAD	D	501	-	-	7/30/62/62	0/5/5/5
2	NAD	A	501	-	-	7/30/62/62	0/5/5/5
2	NAD	B	501	-	-	7/30/62/62	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAD	C2N-N1N	3.13	1.38	1.35
2	D	501	NAD	C2N-N1N	2.71	1.38	1.35
2	C	501	NAD	PA-O3	2.22	1.61	1.59
2	A	501	NAD	PA-O3	2.12	1.61	1.59
2	C	501	NAD	C2N-N1N	2.11	1.37	1.35
2	D	501	NAD	PN-O3	2.00	1.61	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	NAD	C6N-N1N-C2N	-2.69	119.59	121.88
2	A	501	NAD	C6N-N1N-C2N	-2.61	119.66	121.88
2	B	501	NAD	C6N-N1N-C2N	-2.57	119.69	121.88
2	D	501	NAD	C6N-N1N-C2N	-2.17	120.03	121.88

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAD	C5B-O5B-PA-O1A
2	A	501	NAD	C5B-O5B-PA-O3
2	A	501	NAD	C5D-O5D-PN-O1N
2	A	501	NAD	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
2	B	501	NAD	C5B-O5B-PA-O1A
2	B	501	NAD	O4D-C1D-N1N-C6N
2	C	501	NAD	C5B-O5B-PA-O1A
2	C	501	NAD	C5B-O5B-PA-O3
2	C	501	NAD	C5D-O5D-PN-O1N
2	C	501	NAD	O4D-C1D-N1N-C6N
2	D	501	NAD	O4D-C4D-C5D-O5D
2	D	501	NAD	C3D-C4D-C5D-O5D
2	A	501	NAD	C3B-C4B-C5B-O5B
2	D	501	NAD	PA-O3-PN-O1N
2	B	501	NAD	PN-O3-PA-O5B
2	A	501	NAD	O4B-C4B-C5B-O5B
2	B	501	NAD	PA-O3-PN-O2N
2	B	501	NAD	C5D-O5D-PN-O1N
2	D	501	NAD	C5B-O5B-PA-O1A
2	D	501	NAD	C5D-O5D-PN-O1N
2	C	501	NAD	PA-O3-PN-O1N
2	D	501	NAD	PA-O3-PN-O2N
2	B	501	NAD	O4B-C4B-C5B-O5B
2	A	501	NAD	C4B-C5B-O5B-PA
2	C	501	NAD	C4B-C5B-O5B-PA
2	B	501	NAD	PA-O3-PN-O1N
2	C	501	NAD	PA-O3-PN-O2N
2	C	501	NAD	O4B-C4B-C5B-O5B
2	C	501	NAD	C3B-C4B-C5B-O5B
2	D	501	NAD	O4B-C4B-C5B-O5B

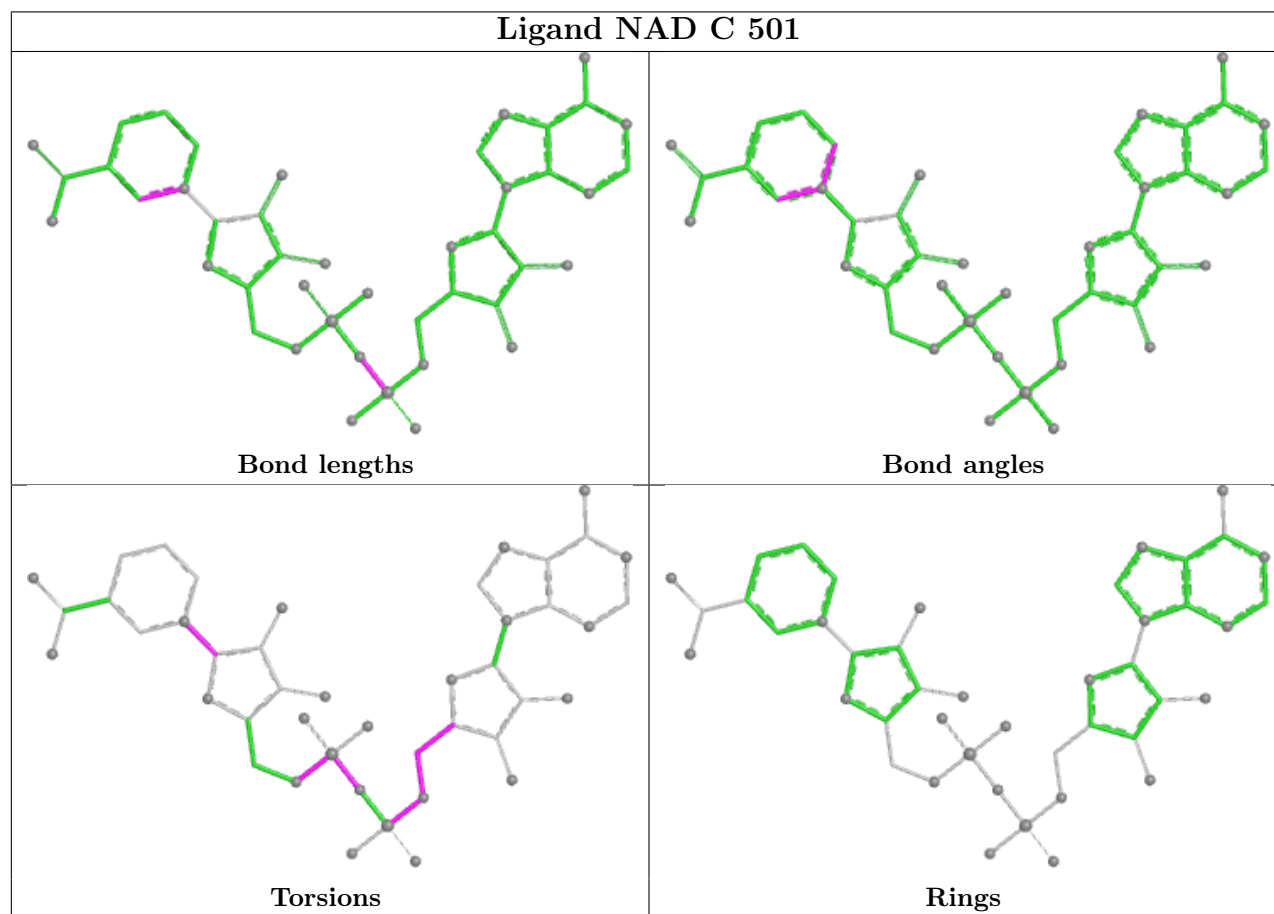
There are no ring outliers.

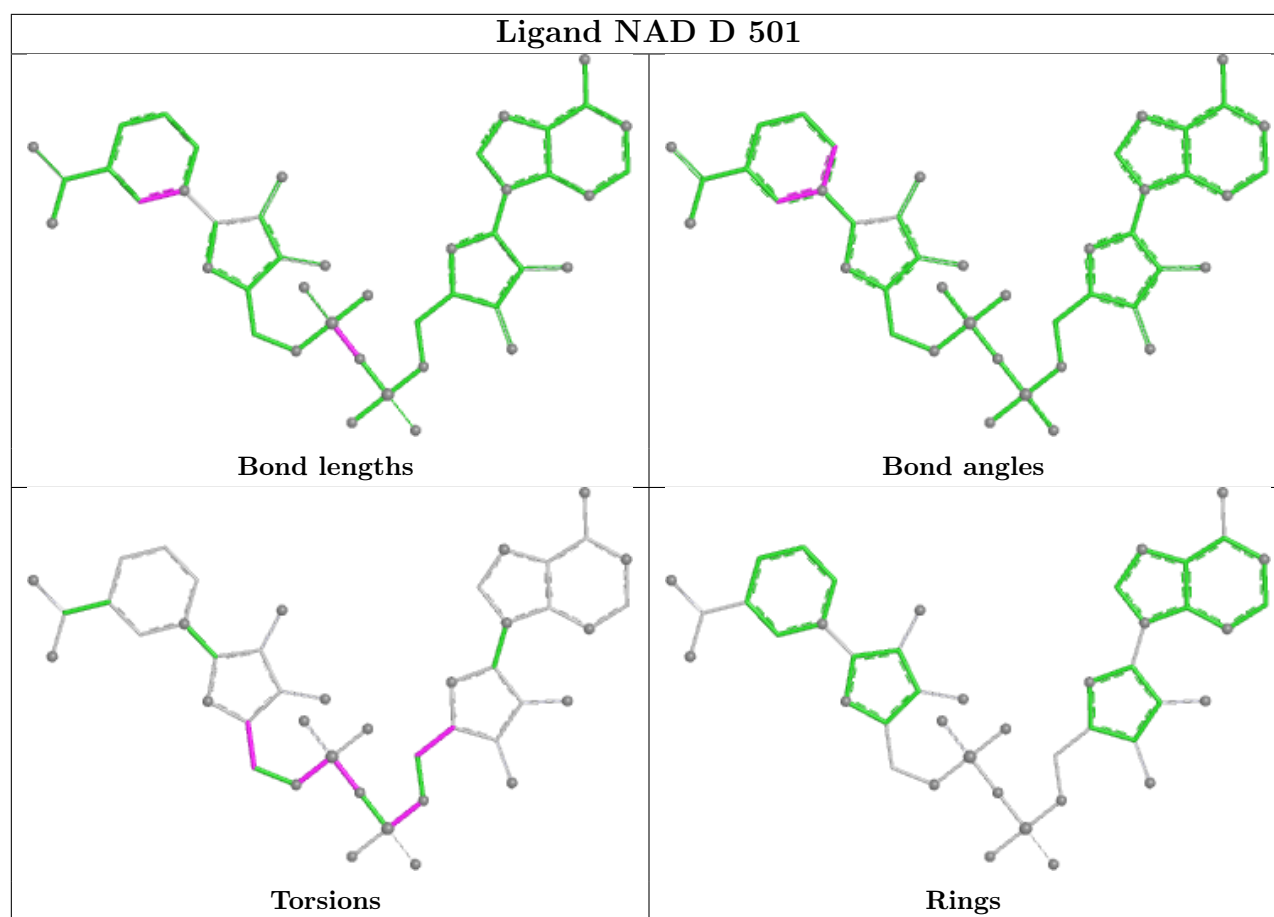
2 monomers are involved in 2 short contacts:

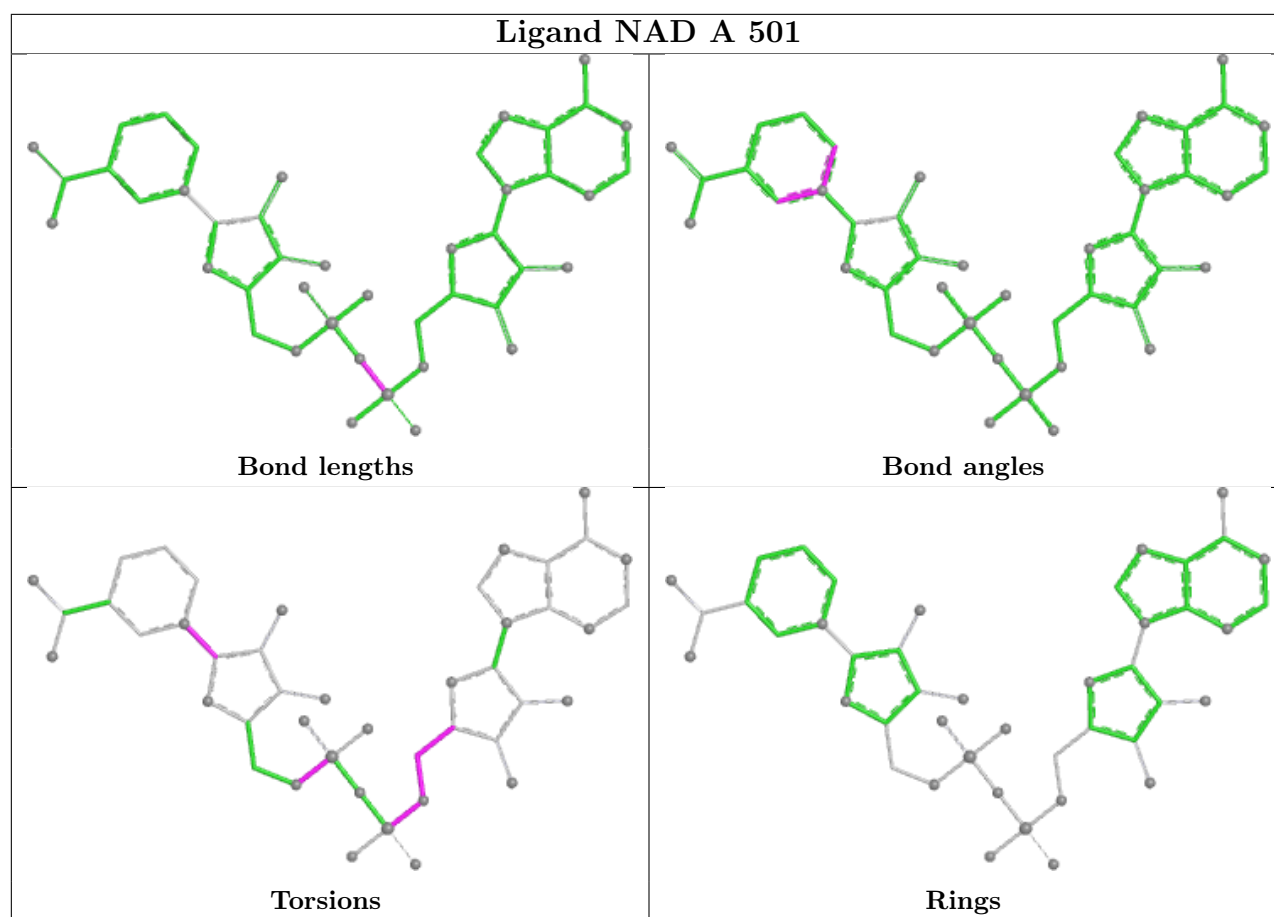
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	NAD	1	0
2	B	501	NAD	1	0

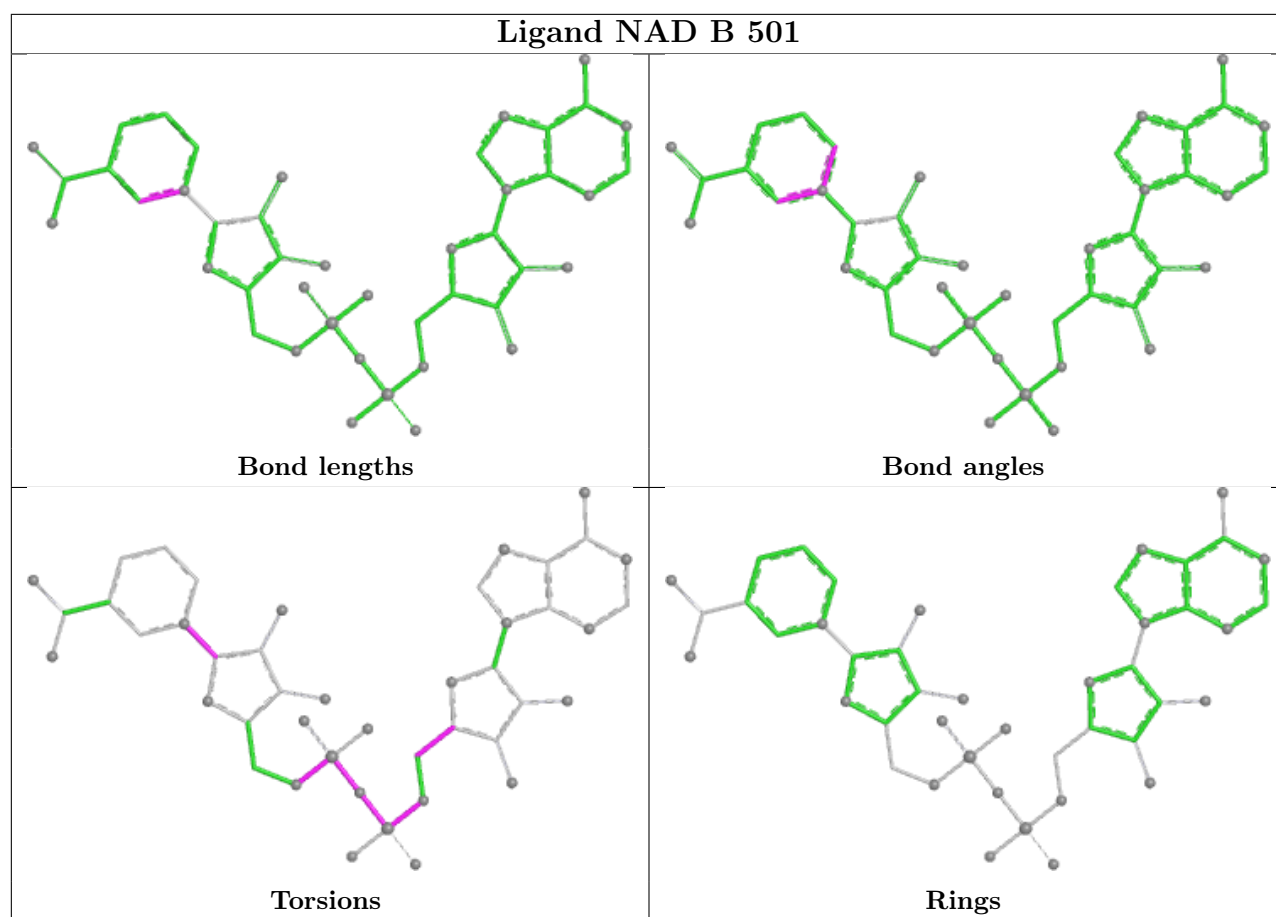
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

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	326/398 (81%)	-0.27	6 (1%) 67 58	17, 45, 99, 190	0
1	B	346/398 (86%)	-0.23	19 (5%) 30 23	18, 40, 99, 203	0
1	C	338/398 (84%)	-0.16	13 (3%) 44 35	25, 47, 112, 152	0
1	D	314/398 (78%)	2.07	131 (41%) 0 0	12, 29, 44, 60	314 (100%)
All	All	1324/1592 (83%)	0.32	169 (12%) 7 6	12, 40, 99, 203	314 (23%)

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	376	SER	8.4
1	D	129	LEU	6.5
1	D	224	LEU	6.4
1	D	158	ALA	6.0
1	D	309	ASN	6.0
1	D	222	ILE	5.8
1	D	125	ILE	5.7
1	D	353	VAL	5.6
1	D	299	PRO	5.5
1	D	209	PHE	5.4
1	D	442	GLN	5.3
1	D	405	TRP	5.3
1	D	128	SER	5.2
1	D	395	SER	5.2
1	D	280	ILE	5.0
1	D	281	GLY	4.7
1	D	236	VAL	4.6
1	D	306	SER	4.6
1	D	181	VAL	4.5
1	C	82	PHE	4.5
1	D	185	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	113	GLU	4.2
1	D	85	GLN	4.1
1	D	439	LEU	4.1
1	D	288	ALA	4.1
1	D	123	GLU	4.0
1	D	266	GLY	4.0
1	D	272	VAL	3.9
1	D	118	HIS	3.9
1	D	156	ILE	3.8
1	D	343	ASN	3.8
1	C	106	SER	3.7
1	B	56	ALA	3.7
1	D	398	VAL	3.7
1	D	364	LEU	3.7
1	D	408	CYS	3.6
1	D	381	ILE	3.6
1	D	354	GLU	3.6
1	D	296	ASP	3.6
1	D	86	ARG	3.5
1	D	425	ALA	3.5
1	D	116	HIS	3.5
1	D	109	SER	3.5
1	D	290	TYR	3.5
1	D	301	GLU	3.5
1	D	319	TRP	3.5
1	B	343	ASN	3.5
1	C	390	ARG	3.4
1	D	238	LEU	3.4
1	D	229	THR	3.4
1	D	310	LEU	3.3
1	D	289	SER	3.3
1	D	189	GLU	3.3
1	D	323	ILE	3.3
1	D	298	GLY	3.3
1	D	191	HIS	3.2
1	D	340	ARG	3.2
1	D	432	GLU	3.2
1	D	307	GLY	3.2
1	D	267	PRO	3.2
1	B	103	LEU	3.2
1	D	84	GLN	3.2
1	D	279	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	410	VAL	3.1
1	D	163	THR	3.1
1	D	122	VAL	3.1
1	D	352	LEU	3.1
1	D	336	ASN	3.0
1	D	293	ILE	3.0
1	D	304	LYS	3.0
1	D	378	ARG	3.0
1	A	441	GLU	3.0
1	D	110	GLY	3.0
1	D	120	LYS	2.9
1	D	334	VAL	2.9
1	B	99	GLN	2.9
1	D	186	GLU	2.9
1	D	75	ALA	2.9
1	D	416	SER	2.9
1	D	271	PRO	2.8
1	D	394	PHE	2.8
1	B	89	TYR	2.8
1	D	71	VAL	2.8
1	D	149	VAL	2.8
1	D	124	HIS	2.8
1	B	107	SER	2.8
1	D	413	GLY	2.8
1	D	58	CYS	2.8
1	A	84	GLN	2.8
1	D	211	ARG	2.8
1	B	96	ASP	2.8
1	D	241	GLN	2.8
1	C	99	GLN	2.7
1	D	66	PHE	2.7
1	D	393	CYS	2.7
1	D	431	LYS	2.7
1	D	359	GLU	2.7
1	D	373	ILE	2.7
1	D	268	GLN	2.7
1	D	182	ASN	2.6
1	D	190	GLY	2.6
1	D	429	ILE	2.6
1	D	69	SER	2.6
1	D	112	LEU	2.6
1	D	169	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	80	TYR	2.5
1	D	269	LEU	2.5
1	D	73	VAL	2.5
1	D	400	VAL	2.5
1	D	441	GLU	2.5
1	B	389	SER	2.5
1	C	60	SER	2.5
1	B	63	ASP	2.5
1	D	153	ASP	2.5
1	A	352	LEU	2.5
1	D	139	VAL	2.5
1	A	341	GLN	2.5
1	B	90	ALA	2.5
1	D	223	ARG	2.5
1	D	407	ALA	2.5
1	D	217	LEU	2.4
1	D	107	SER	2.4
1	D	291	TYR	2.4
1	D	300	TRP	2.4
1	B	100	LEU	2.4
1	C	107	SER	2.4
1	D	132	GLU	2.4
1	D	422	GLY	2.4
1	B	113	GLU	2.4
1	D	231	ILE	2.4
1	C	83	GLU	2.3
1	D	198	TYR	2.3
1	D	337	ILE	2.3
1	B	350	ARG	2.3
1	D	196	VAL	2.3
1	D	83	GLU	2.3
1	D	148	THR	2.3
1	C	61	ARG	2.3
1	C	105	GLY	2.3
1	D	419	PHE	2.2
1	C	84	GLN	2.2
1	C	241	GLN	2.2
1	D	237	ASP	2.2
1	D	433	ASP	2.2
1	D	216	TRP	2.2
1	D	331	VAL	2.2
1	D	368	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	342	GLY	2.2
1	D	175	LEU	2.2
1	D	59	GLY	2.2
1	B	353	VAL	2.2
1	D	180	GLY	2.2
1	A	108	TYR	2.2
1	B	82	PHE	2.2
1	B	98	LYS	2.1
1	D	197	ARG	2.1
1	D	111	LEU	2.1
1	D	202	PHE	2.1
1	B	264	ALA	2.1
1	C	108	TYR	2.1
1	D	404	CYS	2.1
1	D	130	ARG	2.1
1	D	406	ASP	2.1
1	D	157	ALA	2.1
1	B	265	SER	2.0
1	B	383	ASN	2.0
1	D	77	THR	2.0
1	D	179	ILE	2.0
1	C	346	LEU	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 [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. 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	D	501	44/44	0.40	0.22	63,93,108,118	44

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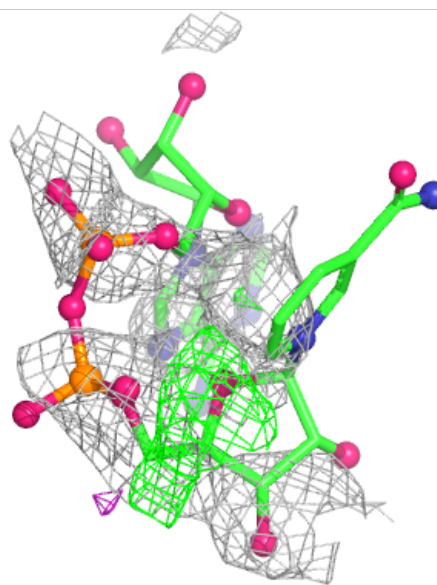
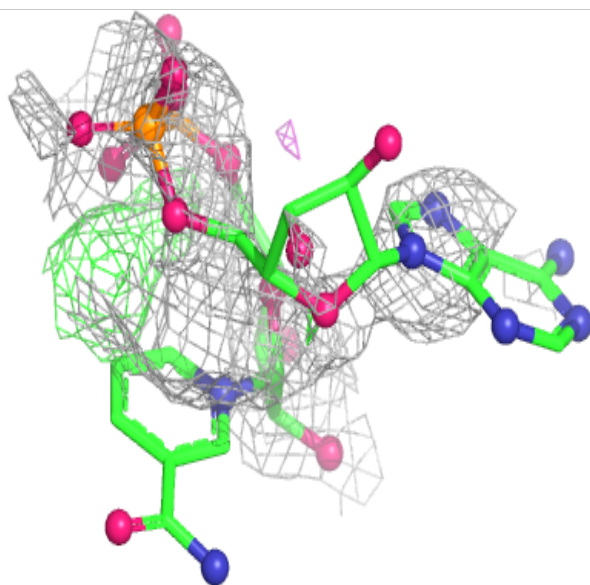
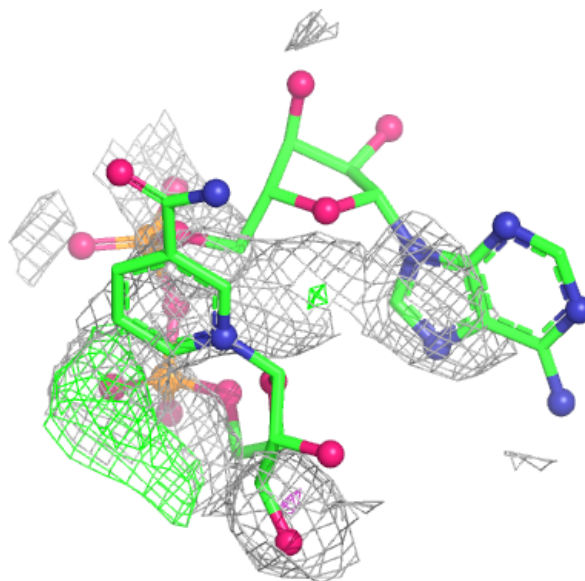
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	C	501	44/44	0.93	0.09	25,40,91,118	0
2	NAD	A	501	44/44	0.93	0.09	24,42,86,111	0
2	NAD	B	501	44/44	0.94	0.08	17,30,82,104	0

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.

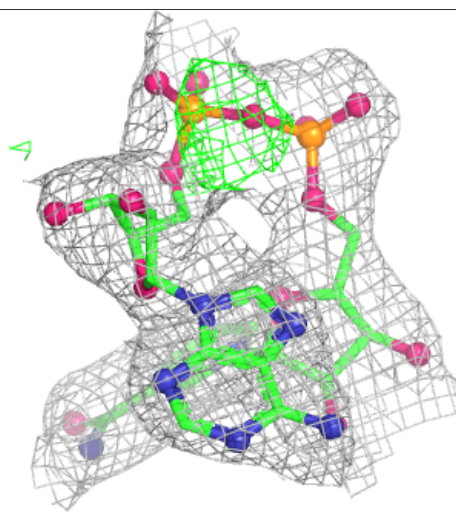
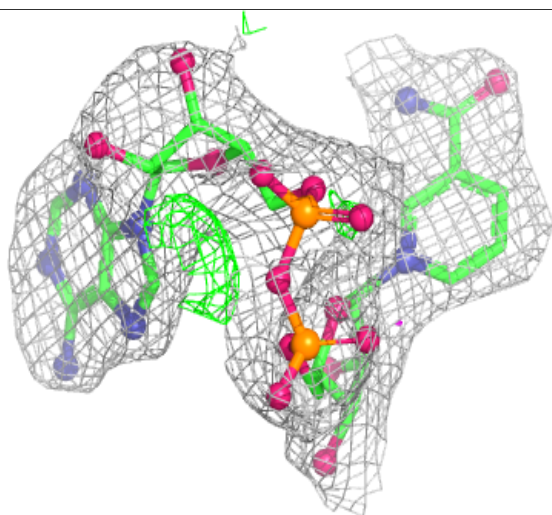
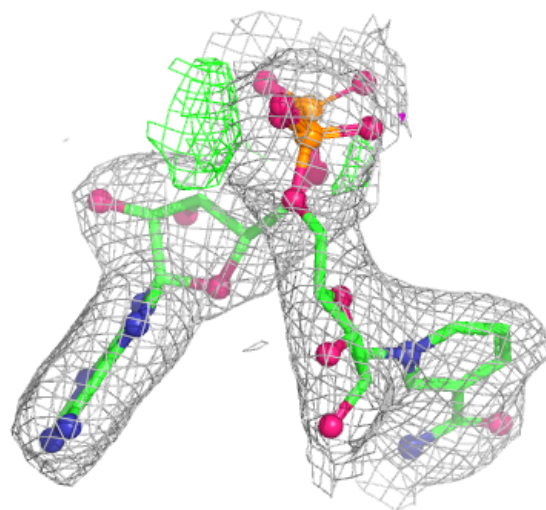
Electron density around NAD D 501:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



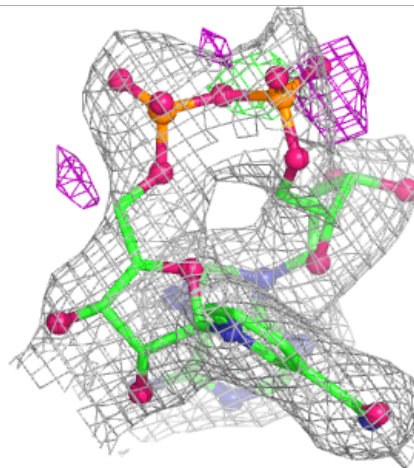
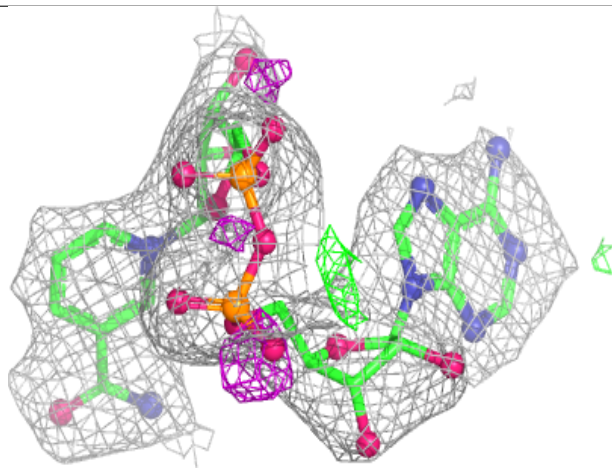
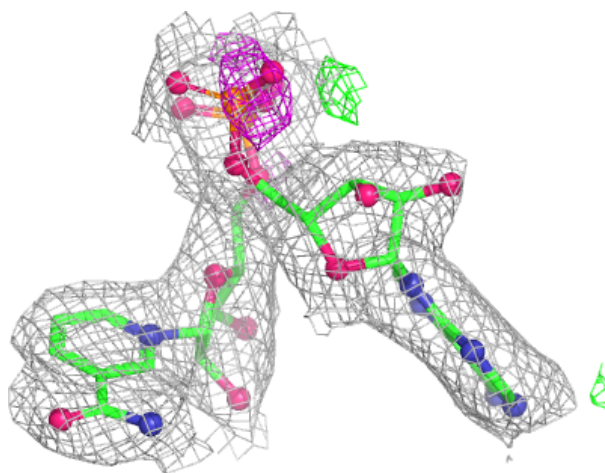
Electron density around NAD C 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



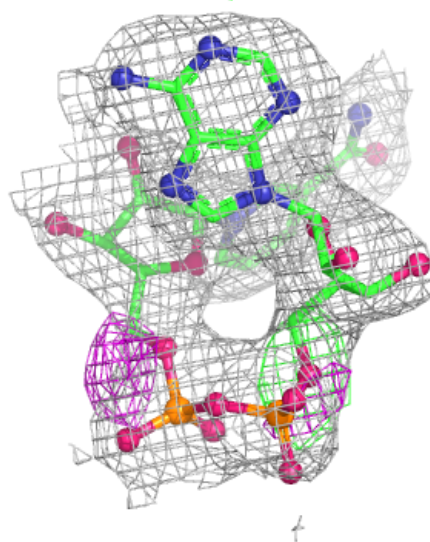
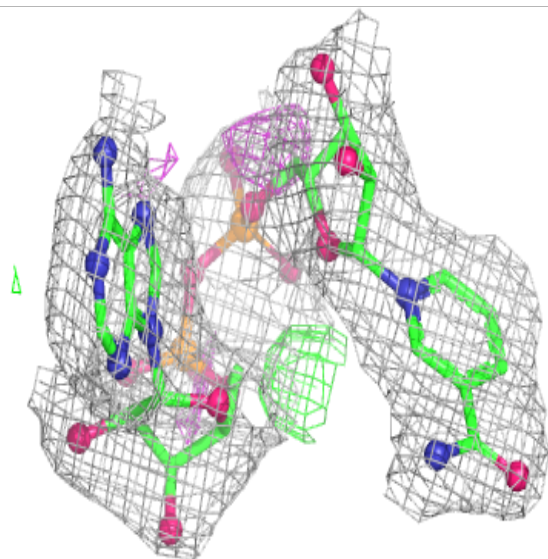
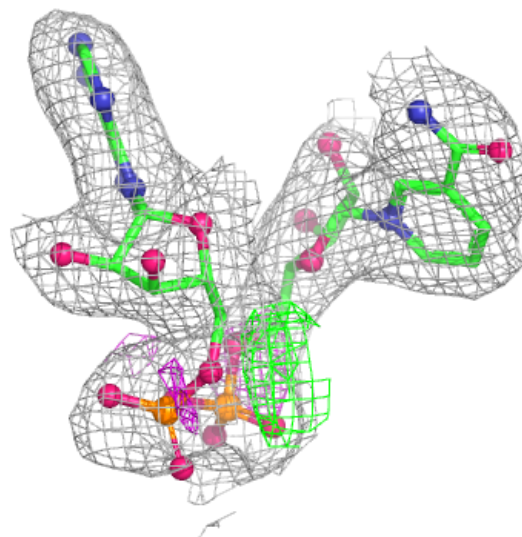
Electron density around NAD A 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NAD B 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.