



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:21 PM UTC

PDB ID : 8W0O / pdb_00008w0o
Title : GDH-105 crystal structure
Authors : Peat, T.S.; Newman, J.
Deposited on : 2024-02-13
Resolution : 1.66 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:

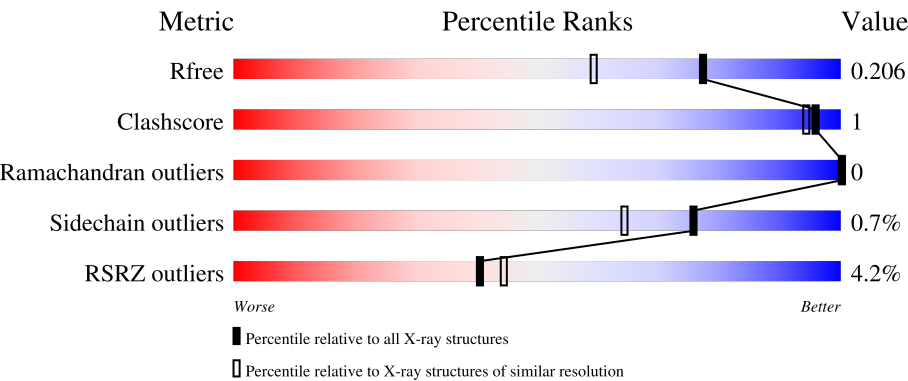
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 1.66 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.



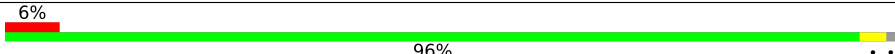
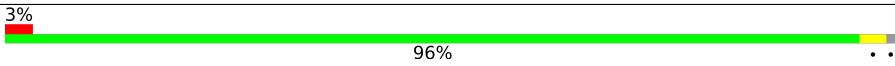
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	261	3% 98% ..
1	B	261	4% 98% ..
1	C	261	5% 98% ..
1	D	261	4% 96% ..
1	E	261	7% 97% ..

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Mol	Chain	Length	Quality of chain
1	F	261	 2% 98% ..
1	G	261	 6% 96% . .
1	H	261	 3% 96% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17193 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 Dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	3	0
			1985	1269	325	380	11			
1	B	259	Total	C	N	O	S	0	5	0
			1999	1280	328	380	11			
1	C	259	Total	C	N	O	S	0	5	0
			1999	1277	329	382	11			
1	D	259	Total	C	N	O	S	0	6	0
			2006	1283	328	384	11			
1	E	259	Total	C	N	O	S	0	6	0
			2007	1283	329	384	11			
1	H	259	Total	C	N	O	S	0	1	0
			1966	1258	322	376	10			
1	F	259	Total	C	N	O	S	0	4	0
			1990	1271	327	381	11			
1	G	259	Total	C	N	O	S	0	11	0
			2046	1306	335	393	12			

There are 32 discrepancies between the modelled and reference sequences:

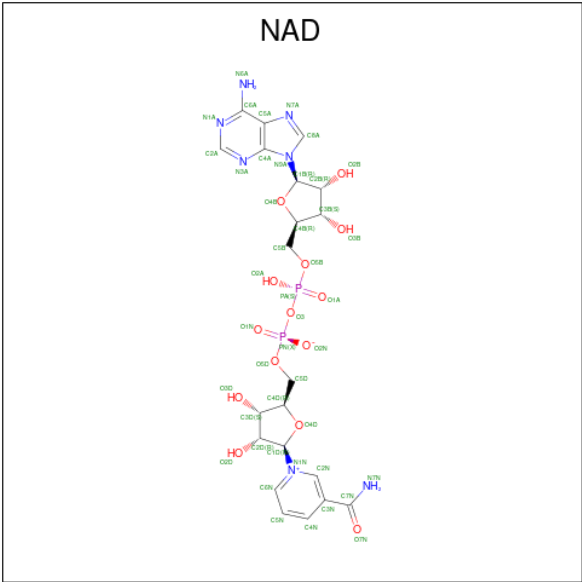
Chain	Residue	Modelled	Actual	Comment	Reference
A	165	MET	ILE	conflict	UNP M9TFE3
A	170	LYS	GLU	conflict	UNP M9TFE3
A	194	THR	PRO	conflict	UNP M9TFE3
A	252	LEU	GLN	conflict	UNP M9TFE3
B	165	MET	ILE	conflict	UNP M9TFE3
B	170	LYS	GLU	conflict	UNP M9TFE3
B	194	THR	PRO	conflict	UNP M9TFE3
B	252	LEU	GLN	conflict	UNP M9TFE3
C	165	MET	ILE	conflict	UNP M9TFE3
C	170	LYS	GLU	conflict	UNP M9TFE3
C	194	THR	PRO	conflict	UNP M9TFE3
C	252	LEU	GLN	conflict	UNP M9TFE3
D	165	MET	ILE	conflict	UNP M9TFE3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	170	LYS	GLU	conflict	UNP M9TFE3
D	194	THR	PRO	conflict	UNP M9TFE3
D	252	LEU	GLN	conflict	UNP M9TFE3
E	165	MET	ILE	conflict	UNP M9TFE3
E	170	LYS	GLU	conflict	UNP M9TFE3
E	194	THR	PRO	conflict	UNP M9TFE3
E	252	LEU	GLN	conflict	UNP M9TFE3
H	165	MET	ILE	conflict	UNP M9TFE3
H	170	LYS	GLU	conflict	UNP M9TFE3
H	194	THR	PRO	conflict	UNP M9TFE3
H	252	LEU	GLN	conflict	UNP M9TFE3
F	165	MET	ILE	conflict	UNP M9TFE3
F	170	LYS	GLU	conflict	UNP M9TFE3
F	194	THR	PRO	conflict	UNP M9TFE3
F	252	LEU	GLN	conflict	UNP M9TFE3
G	165	MET	ILE	conflict	UNP M9TFE3
G	170	LYS	GLU	conflict	UNP M9TFE3
G	194	THR	PRO	conflict	UNP M9TFE3
G	252	LEU	GLN	conflict	UNP M9TFE3

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	E	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	141	Total	O	0	0
			141	141		
4	B	101	Total	O	0	0
			101	101		
4	C	99	Total	O	0	0
			99	99		
4	D	95	Total	O	0	0
			95	95		
4	E	108	Total	O	0	0
			108	108		
4	H	97	Total	O	0	0
			97	97		

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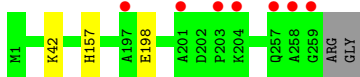
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	104	Total 104	O 104	0	0
4	G	94	Total 94	O 94	0	0

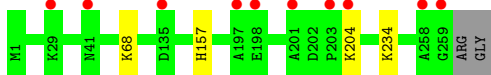
3 Residue-property plots [i](#)

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.

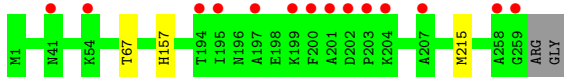
- Molecule 1: Dehydrogenase



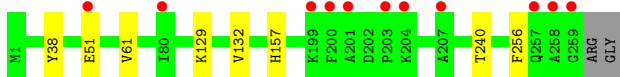
- Molecule 1: Dehydrogenase



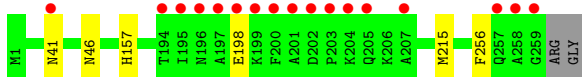
- Molecule 1: Dehydrogenase



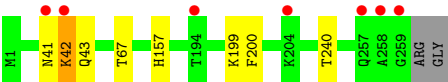
- Molecule 1: Dehydrogenase



- Molecule 1: Dehydrogenase



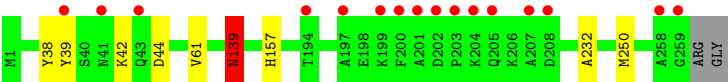
- Molecule 1: Dehydrogenase



● Molecule 1: Dehydrogenase



● Molecule 1: Dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.34Å 120.43Å 125.78Å 90.00° 101.89° 90.00°	Depositor
Resolution (Å)	49.00 – 1.66 49.00 – 1.66	Depositor EDS
% Data completeness (in resolution range)	97.9 (49.00-1.66) 97.9 (49.00-1.66)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 1.66Å)	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.173 , 0.197 0.185 , 0.206	Depositor DCC
R_{free} test set	10634 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 29.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17193	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.42% 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, CL

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	0.58	0/2023	0.82	0/2738
1	B	0.57	0/2037	0.82	0/2757
1	C	0.58	0/2037	0.81	0/2758
1	D	0.58	0/2044	0.83	0/2768
1	E	0.57	0/2045	0.84	1/2769 (0.0%)
1	F	0.57	0/2028	0.83	0/2747
1	G	0.58	0/2084	0.83	1/2820 (0.0%)
1	H	0.60	0/2004	0.85	1/2714 (0.0%)
All	All	0.58	0/16302	0.83	3/22071 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	198	GLU	CB-CA-C	-8.21	97.87	110.92
1	G	139	ASN	CA-CB-CG	6.71	119.31	112.60
1	H	42	LYS	CB-CA-C	-5.24	100.93	110.63

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	139	ASN	Sidechain

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	1985	0	2006	1	0
1	B	1999	0	2029	3	0
1	C	1999	0	2019	4	0
1	D	2006	0	2028	8	0
1	E	2007	0	2027	10	0
1	F	1990	0	2007	1	0
1	G	2046	0	2062	11	0
1	H	1966	0	1988	9	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
2	E	44	0	26	0	0
2	F	44	0	26	0	0
2	G	44	0	26	1	0
2	H	44	0	26	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	141	0	0	1	0
4	B	101	0	0	2	0
4	C	99	0	0	1	0
4	D	95	0	0	1	0
4	E	108	0	0	2	1
4	F	104	0	0	0	0
4	G	94	0	0	1	0
4	H	97	0	0	1	1
All	All	17193	0	16374	35	1

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 1.

All (35) 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:D:51:GLU:HG2	4:D:436:HOH:O	1.32	1.25
1:G:139:ASN:HD21	1:G:232:ALA:HA	1.34	0.90
1:E:256:PHE:HZ	1:G:250[A]:MET:HE2	1.37	0.90
1:B:68[A]:LYS:HE3	4:B:401:HOH:O	1.78	0.84
1:E:256:PHE:CZ	1:G:250[A]:MET:HE2	2.15	0.80
1:H:41:ASN:O	1:H:43:GLN:O	1.99	0.80
1:E:46[A]:ASN:OD1	4:E:401:HOH:O	2.00	0.80
1:G:139:ASN:ND2	1:G:232:ALA:HA	2.05	0.70
1:E:256:PHE:HZ	1:G:250[A]:MET:CE	2.07	0.68
1:B:68[A]:LYS:CE	4:B:401:HOH:O	2.38	0.68
1:E:215:MET:CE	1:H:240:THR:HB	2.30	0.61
1:E:256:PHE:CZ	1:G:250[A]:MET:CE	2.82	0.61
1:E:215:MET:HE3	1:H:240:THR:CG2	2.32	0.59
1:E:215:MET:HE3	1:H:240:THR:HG22	1.86	0.57
1:G:39:TYR:HB2	2:G:301:NAD:C2A	2.38	0.54
1:G:38:TYR:CE1	1:G:61:VAL:CG1	2.92	0.53
1:D:38:TYR:CE1	1:D:61:VAL:CG1	2.95	0.50
1:H:199:LYS:HE3	1:H:200:PHE:CE1	2.49	0.47
1:C:67:THR:HA	4:C:472:HOH:O	2.15	0.46
1:C:215:MET:HE3	1:D:240:THR:CG2	2.45	0.46
1:C:215:MET:HE3	1:D:240:THR:HG22	1.97	0.45
1:D:256:PHE:CZ	1:F:212:MET:HE2	2.52	0.45
1:D:129:LYS:O	1:D:132[B]:VAL:HG12	2.17	0.45
1:E:41:ASN:OD1	4:E:402:HOH:O	2.21	0.44
1:A:198:GLU:HB3	4:A:460:HOH:O	2.17	0.44
1:C:215:MET:CE	1:D:240:THR:HB	2.48	0.44
1:H:41:ASN:C	1:H:43:GLN:O	2.61	0.43
1:H:42:LYS:O	1:H:42:LYS:HG2	2.17	0.43
1:H:67:THR:HA	4:H:464:HOH:O	2.19	0.43
1:G:38:TYR:CD1	1:G:61:VAL:HG13	2.54	0.42
1:G:139:ASN:HD21	1:G:232:ALA:CA	2.19	0.42
1:E:215:MET:HE2	1:H:240:THR:HB	1.99	0.42
1:G:44:ASP:HA	4:G:414:HOH:O	2.20	0.41
1:D:38:TYR:HE1	1:D:61:VAL:HG12	1.84	0.41
1:B:204:LYS:HA	1:B:204:LYS:HD2	1.95	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:493:HOH:O	4:H:408:HOH:O[1_655]	2.03	0.17

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	260/261 (100%)	252 (97%)	8 (3%)	0	100	100
1	B	262/261 (100%)	253 (97%)	9 (3%)	0	100	100
1	C	262/261 (100%)	253 (97%)	9 (3%)	0	100	100
1	D	263/261 (101%)	254 (97%)	9 (3%)	0	100	100
1	E	263/261 (101%)	254 (97%)	9 (3%)	0	100	100
1	F	261/261 (100%)	251 (96%)	10 (4%)	0	100	100
1	G	268/261 (103%)	256 (96%)	12 (4%)	0	100	100
1	H	258/261 (99%)	250 (97%)	8 (3%)	0	100	100
All	All	2097/2088 (100%)	2023 (96%)	74 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	209/207 (101%)	207 (99%)	2 (1%)	68	52
1	B	211/207 (102%)	209 (99%)	2 (1%)	70	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	211/207 (102%)	210 (100%)	1 (0%)	81	72
1	D	212/207 (102%)	211 (100%)	1 (0%)	81	72
1	E	212/207 (102%)	211 (100%)	1 (0%)	81	72
1	F	210/207 (101%)	209 (100%)	1 (0%)	81	72
1	G	217/207 (105%)	215 (99%)	2 (1%)	70	56
1	H	207/207 (100%)	206 (100%)	1 (0%)	81	72
All	All	1689/1656 (102%)	1678 (99%)	11 (1%)	76	64

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LYS
1	A	157	HIS
1	B	157	HIS
1	B	234	LYS
1	C	157	HIS
1	D	157	HIS
1	E	157	HIS
1	H	157	HIS
1	F	157	HIS
1	G	42	LYS
1	G	157	HIS

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

Mol	Chain	Res	Type
1	A	31	GLN
1	A	41	ASN
1	A	46	ASN
1	B	31	GLN
1	B	46	ASN
1	B	139	ASN
1	B	205	GLN
1	C	31	GLN
1	C	139	ASN
1	C	257	GLN
1	D	139	ASN
1	D	257	GLN
1	E	139	ASN

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Mol	Chain	Res	Type
1	H	46	ASN
1	H	74	ASN
1	H	139	ASN
1	F	46	ASN
1	G	46	ASN
1	G	139	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 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	G	301	-	46,48,48	0.70	1 (2%)	64,73,73	0.98	6 (9%)
2	NAD	E	301	-	46,48,48	0.91	2 (4%)	64,73,73	0.83	3 (4%)
2	NAD	C	301	-	46,48,48	0.89	2 (4%)	64,73,73	0.88	4 (6%)
2	NAD	A	301	-	46,48,48	0.79	2 (4%)	64,73,73	0.89	3 (4%)
2	NAD	D	301	-	46,48,48	0.62	1 (2%)	64,73,73	0.92	3 (4%)
2	NAD	H	301	-	46,48,48	0.68	1 (2%)	64,73,73	0.81	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	F	301	-	46,48,48	0.67	1 (2%)	64,73,73	0.98	4 (6%)
2	NAD	B	301	-	46,48,48	0.71	1 (2%)	64,73,73	0.90	5 (7%)

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	G	301	-	-	8/30/62/62	0/5/5/5
2	NAD	E	301	-	-	7/30/62/62	0/5/5/5
2	NAD	C	301	-	-	10/30/62/62	0/5/5/5
2	NAD	A	301	-	-	7/30/62/62	0/5/5/5
2	NAD	D	301	-	-	8/30/62/62	0/5/5/5
2	NAD	H	301	-	-	8/30/62/62	0/5/5/5
2	NAD	F	301	-	-	9/30/62/62	0/5/5/5
2	NAD	B	301	-	-	8/30/62/62	0/5/5/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	NAD	PN-O3	4.13	1.64	1.59
2	C	301	NAD	C2N-N1N	3.36	1.38	1.35
2	C	301	NAD	PA-O3	3.34	1.63	1.59
2	H	301	NAD	C2N-N1N	3.11	1.38	1.35
2	A	301	NAD	C2N-N1N	3.01	1.38	1.35
2	G	301	NAD	C2N-N1N	2.81	1.38	1.35
2	E	301	NAD	C2N-N1N	2.69	1.37	1.35
2	B	301	NAD	C2N-N1N	2.65	1.37	1.35
2	F	301	NAD	PA-O3	2.61	1.62	1.59
2	A	301	NAD	O4D-C1D	2.53	1.44	1.40
2	D	301	NAD	C2N-N1N	2.30	1.37	1.35

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	NAD	O3-PN-O1N	-3.12	101.32	110.70
2	F	301	NAD	O2A-PA-O1A	3.09	126.82	112.44
2	A	301	NAD	C6N-N1N-C2N	-2.90	119.41	121.88
2	D	301	NAD	O2N-PN-O3	2.82	114.89	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	NAD	O2A-PA-O1A	2.76	125.27	112.44
2	G	301	NAD	O3-PA-O1A	-2.72	102.52	110.70
2	F	301	NAD	C4D-O4D-C1D	-2.69	107.46	109.92
2	B	301	NAD	O3-PA-O1A	-2.62	102.83	110.70
2	G	301	NAD	C2N-C3N-C4N	2.48	121.14	118.26
2	C	301	NAD	C6N-N1N-C2N	-2.42	119.82	121.88
2	B	301	NAD	O2N-PN-O1N	2.33	123.27	112.44
2	D	301	NAD	C3N-C7N-N7N	2.30	120.58	117.74
2	C	301	NAD	O2A-PA-O1A	2.30	123.14	112.44
2	A	301	NAD	O3-PN-O1N	-2.27	103.89	110.70
2	A	301	NAD	C2N-C3N-C4N	2.24	120.87	118.26
2	G	301	NAD	O3-PN-O1N	-2.23	104.00	110.70
2	F	301	NAD	O3-PA-O1A	-2.22	104.03	110.70
2	F	301	NAD	C2N-C3N-C4N	2.22	120.83	118.26
2	E	301	NAD	C3N-C7N-N7N	2.16	120.41	117.74
2	H	301	NAD	O2N-PN-O3	2.14	113.05	107.27
2	G	301	NAD	C6N-N1N-C2N	-2.11	120.08	121.88
2	B	301	NAD	O3-PN-O1N	-2.11	104.37	110.70
2	E	301	NAD	C4N-C3N-C7N	-2.09	115.35	121.06
2	G	301	NAD	C4D-O4D-C1D	-2.06	108.04	109.92
2	H	301	NAD	C2N-C3N-C4N	2.05	120.65	118.26
2	B	301	NAD	O2A-PA-O1A	2.05	121.97	112.44
2	C	301	NAD	O3-PN-O1N	-2.04	104.56	110.70
2	B	301	NAD	O7N-C7N-C3N	-2.03	117.11	119.60
2	H	301	NAD	C6N-N1N-C2N	-2.03	120.15	121.88
2	C	301	NAD	O3-PA-O1A	-2.02	104.64	110.70
2	E	301	NAD	O2A-PA-O1A	2.01	121.81	112.44

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NAD	C5B-O5B-PA-O1A
2	A	301	NAD	C5B-O5B-PA-O3
2	A	301	NAD	C5D-O5D-PN-O3
2	A	301	NAD	C5D-O5D-PN-O1N
2	A	301	NAD	C5D-O5D-PN-O2N
2	B	301	NAD	C5B-O5B-PA-O1A
2	B	301	NAD	C5B-O5B-PA-O3
2	B	301	NAD	PN-O3-PA-O5B
2	B	301	NAD	C5D-O5D-PN-O3
2	B	301	NAD	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
2	B	301	NAD	C5D-O5D-PN-O2N
2	C	301	NAD	C5B-O5B-PA-O1A
2	C	301	NAD	C5B-O5B-PA-O3
2	C	301	NAD	C5D-O5D-PN-O3
2	C	301	NAD	C5D-O5D-PN-O1N
2	C	301	NAD	C5D-O5D-PN-O2N
2	D	301	NAD	C5B-O5B-PA-O1A
2	D	301	NAD	C5B-O5B-PA-O3
2	D	301	NAD	C5D-O5D-PN-O3
2	D	301	NAD	C5D-O5D-PN-O1N
2	D	301	NAD	C5D-O5D-PN-O2N
2	E	301	NAD	C5B-O5B-PA-O1A
2	E	301	NAD	C5D-O5D-PN-O3
2	E	301	NAD	C5D-O5D-PN-O1N
2	E	301	NAD	C5D-O5D-PN-O2N
2	H	301	NAD	C5B-O5B-PA-O1A
2	H	301	NAD	C5B-O5B-PA-O3
2	H	301	NAD	C5D-O5D-PN-O3
2	H	301	NAD	C5D-O5D-PN-O1N
2	H	301	NAD	C5D-O5D-PN-O2N
2	F	301	NAD	C5B-O5B-PA-O1A
2	F	301	NAD	C5B-O5B-PA-O3
2	F	301	NAD	C5D-O5D-PN-O3
2	F	301	NAD	C5D-O5D-PN-O1N
2	F	301	NAD	C5D-O5D-PN-O2N
2	G	301	NAD	C5B-O5B-PA-O1A
2	G	301	NAD	C5B-O5B-PA-O3
2	G	301	NAD	C5D-O5D-PN-O3
2	G	301	NAD	C5D-O5D-PN-O1N
2	G	301	NAD	C5D-O5D-PN-O2N
2	A	301	NAD	PN-O3-PA-O5B
2	C	301	NAD	PN-O3-PA-O5B
2	D	301	NAD	PN-O3-PA-O5B
2	E	301	NAD	PN-O3-PA-O5B
2	H	301	NAD	PN-O3-PA-O5B
2	F	301	NAD	PN-O3-PA-O5B
2	G	301	NAD	PN-O3-PA-O5B
2	A	301	NAD	C5B-O5B-PA-O2A
2	B	301	NAD	C5B-O5B-PA-O2A
2	C	301	NAD	C5B-O5B-PA-O2A
2	D	301	NAD	C5B-O5B-PA-O2A
2	E	301	NAD	C5B-O5B-PA-O2A

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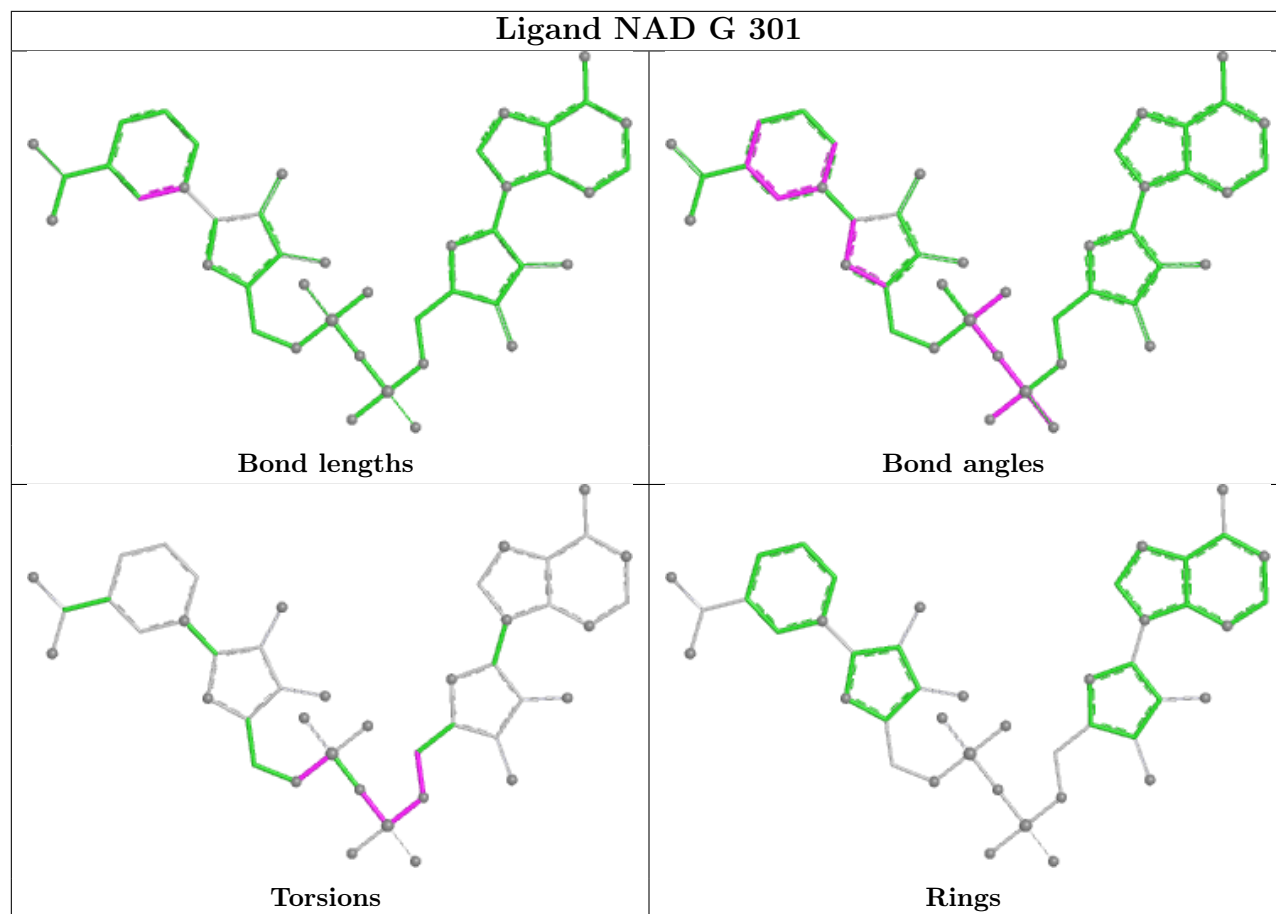
Mol	Chain	Res	Type	Atoms
2	E	301	NAD	C5B-O5B-PA-O3
2	H	301	NAD	C5B-O5B-PA-O2A
2	F	301	NAD	C5B-O5B-PA-O2A
2	G	301	NAD	C5B-O5B-PA-O2A
2	D	301	NAD	C4B-C5B-O5B-PA
2	F	301	NAD	PN-O3-PA-O1A
2	F	301	NAD	C4B-C5B-O5B-PA
2	G	301	NAD	C4B-C5B-O5B-PA
2	C	301	NAD	PN-O3-PA-O1A
2	C	301	NAD	O4B-C4B-C5B-O5B
2	H	301	NAD	C4B-C5B-O5B-PA
2	C	301	NAD	C4B-C5B-O5B-PA
2	B	301	NAD	PA-O3-PN-O2N

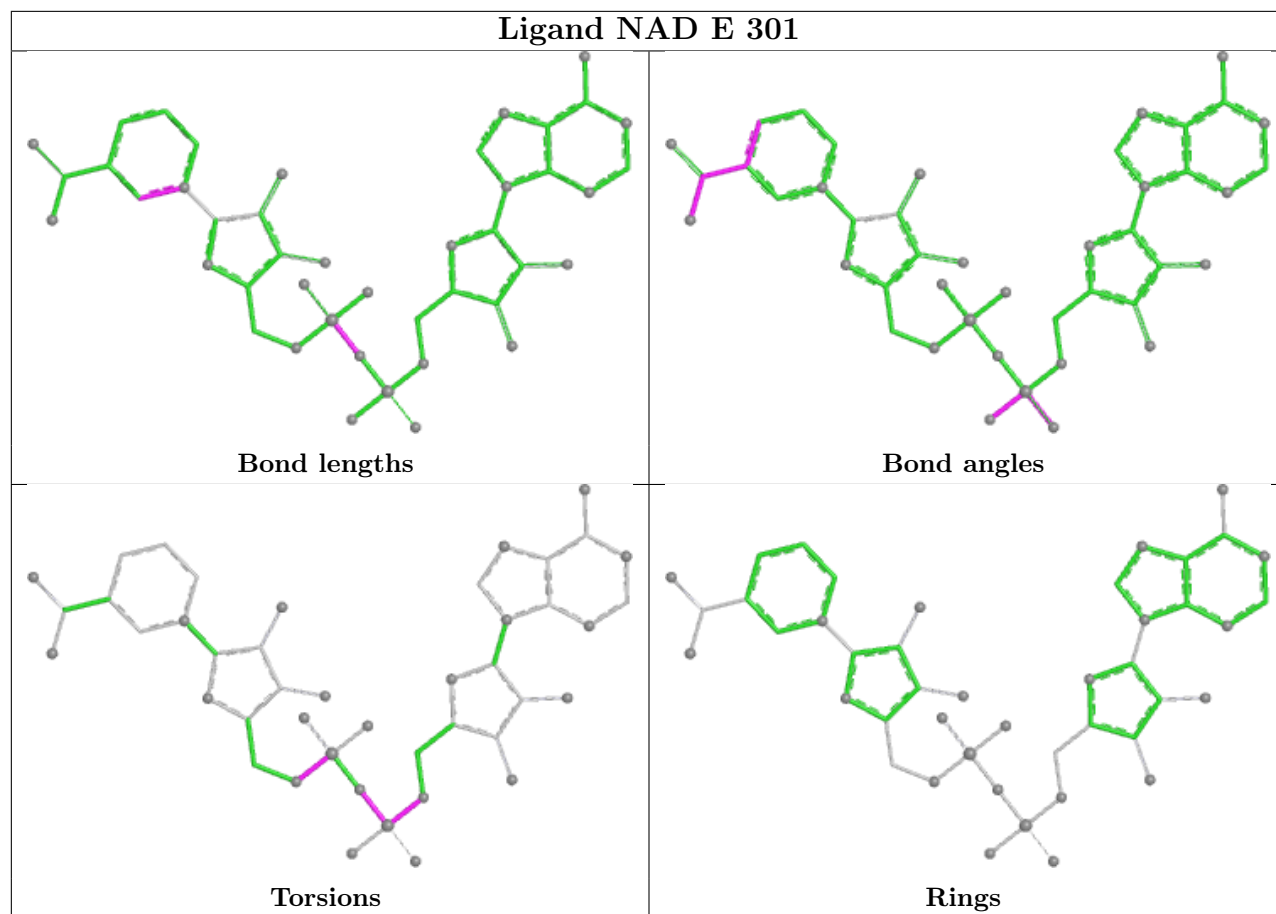
There are no ring outliers.

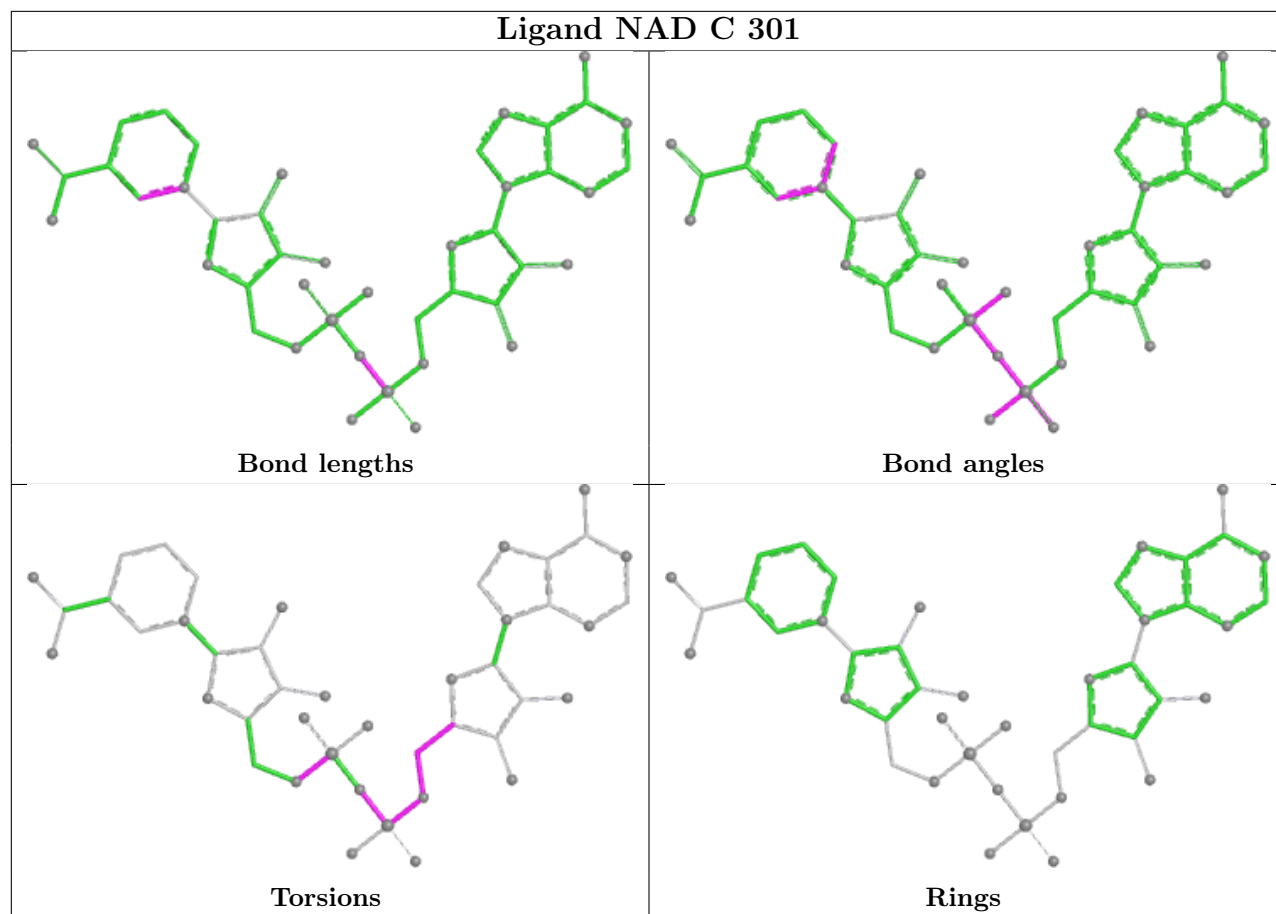
1 monomer is involved in 1 short contact:

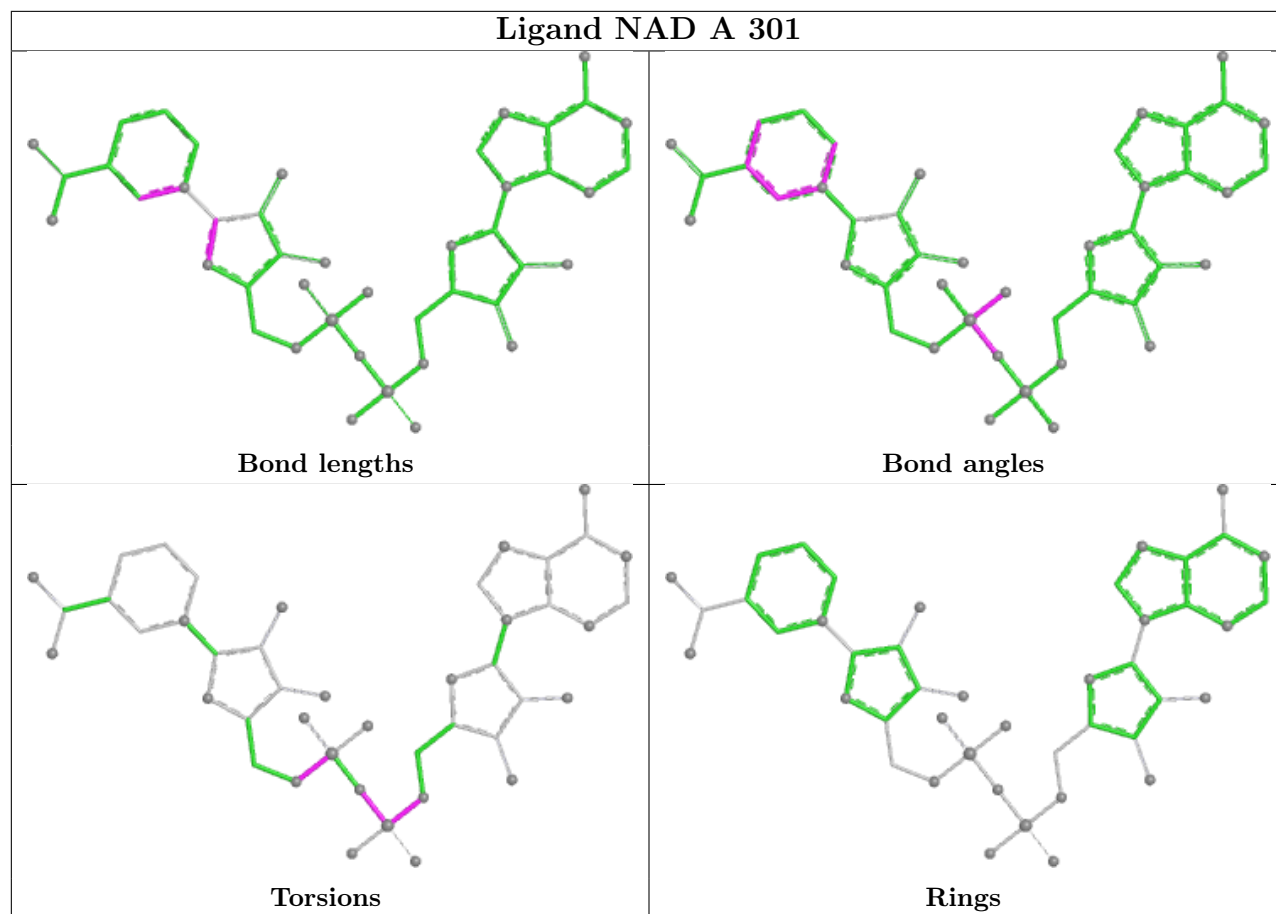
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	301	NAD	1	0

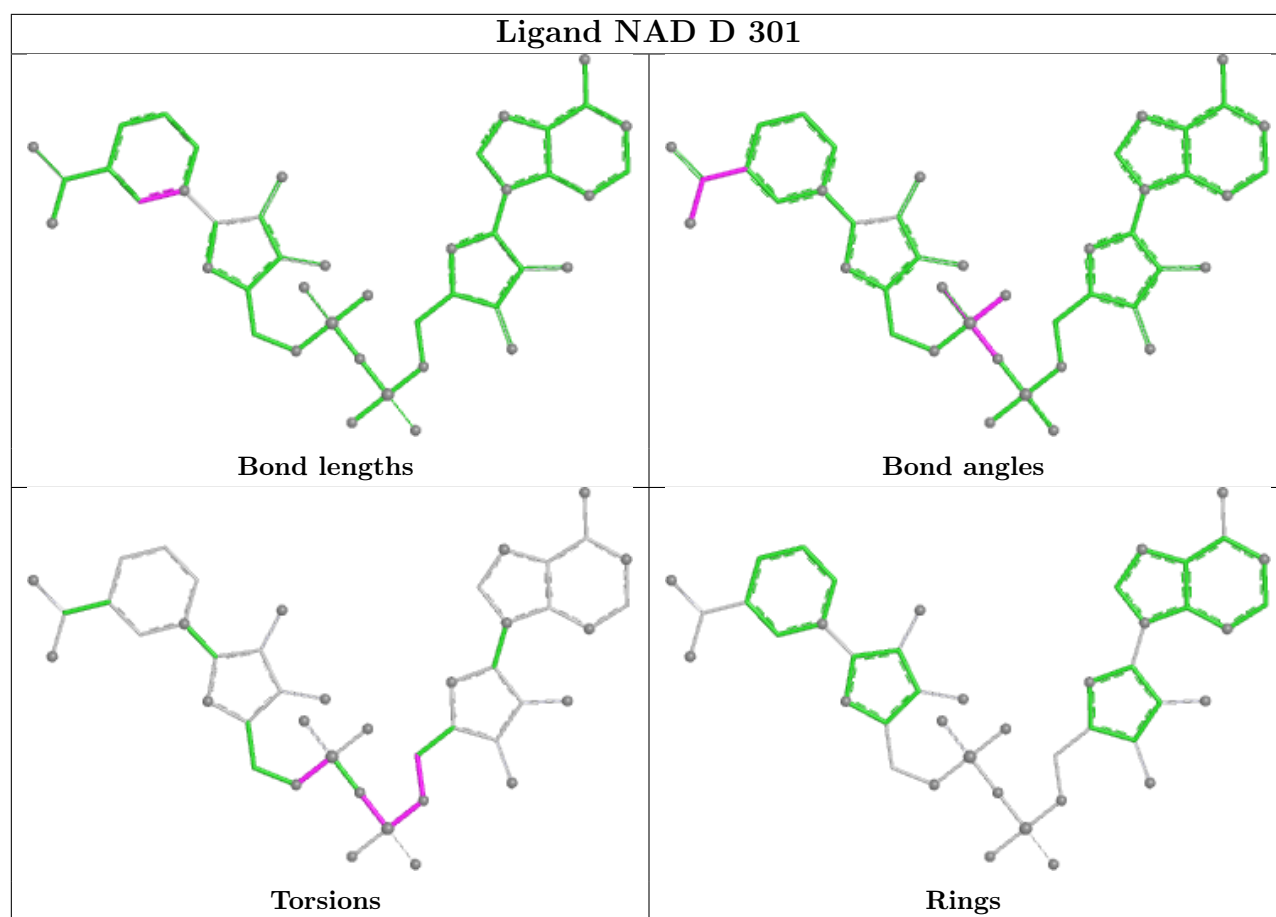
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

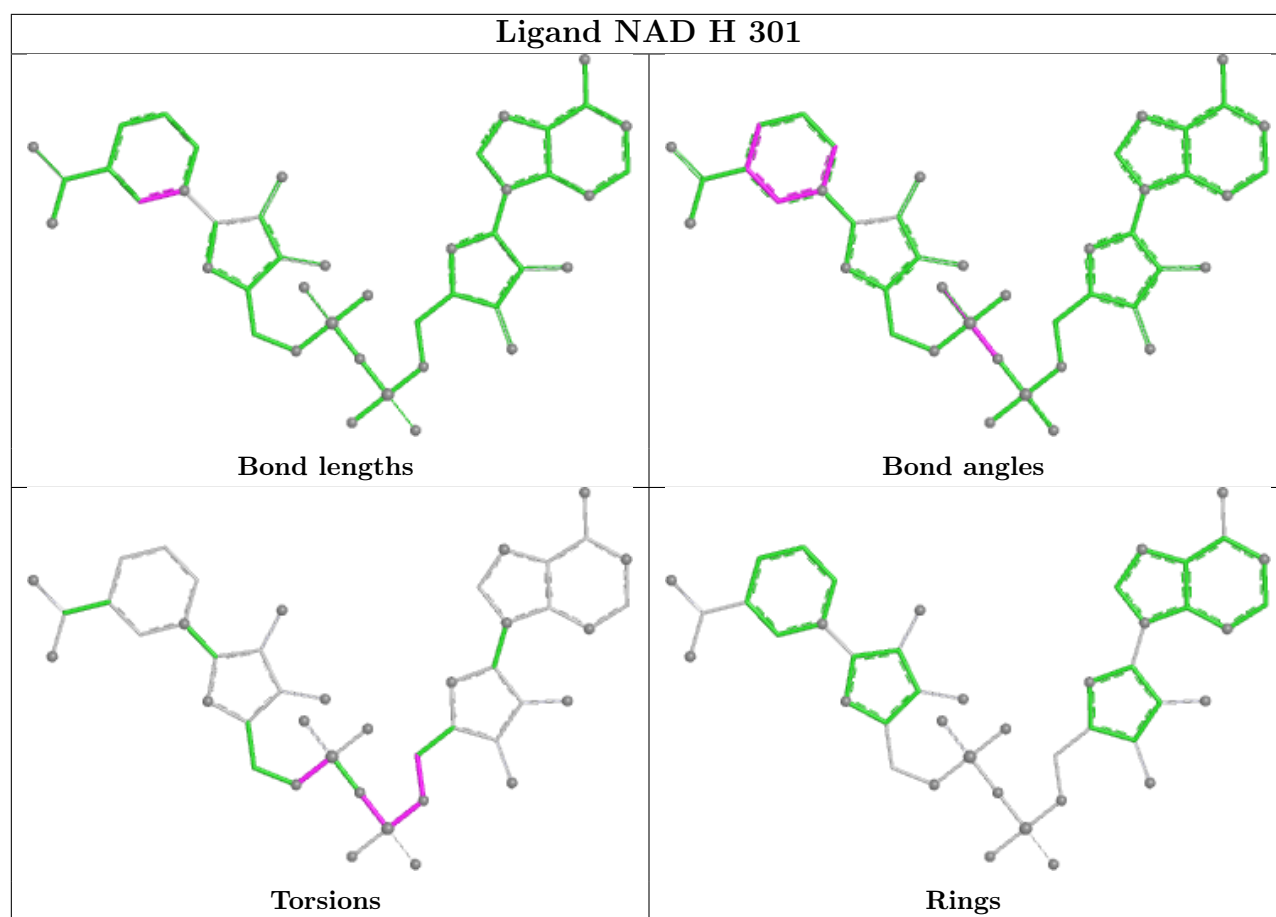


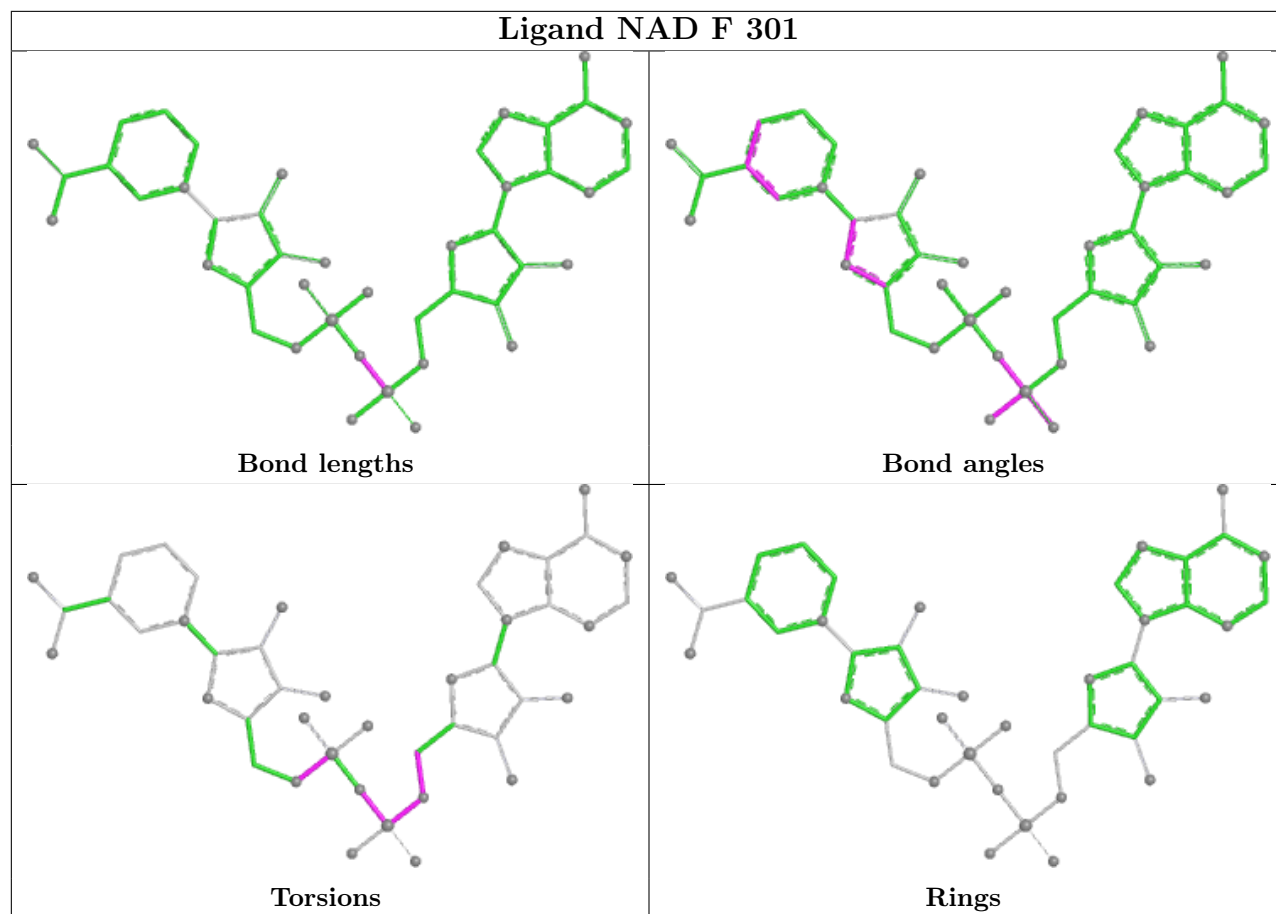


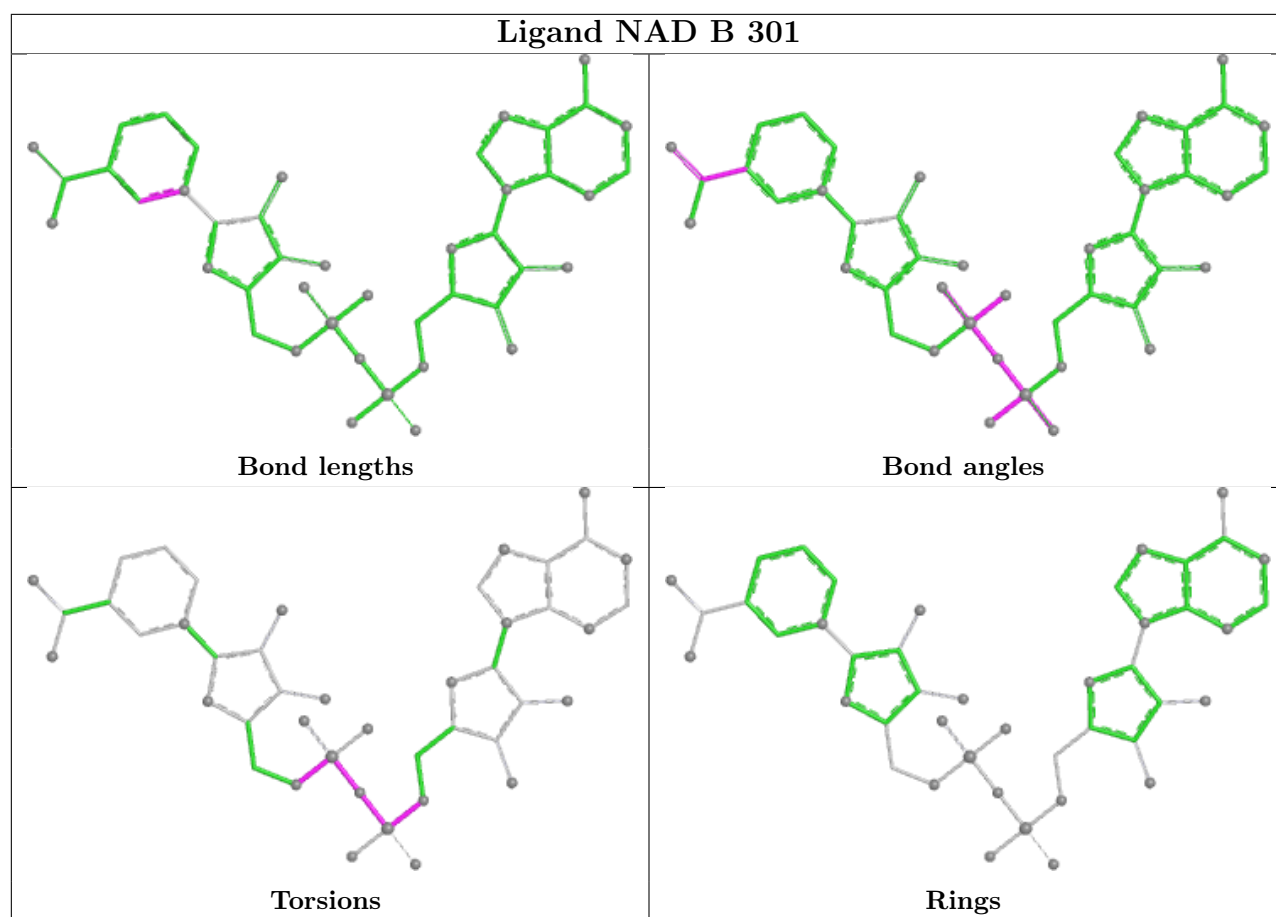












5.7 Other polymers [i](#)

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	259/261 (99%)	-0.18	7 (2%) 56 61	10, 18, 37, 73	3 (1%)
1	B	259/261 (99%)	-0.06	10 (3%) 43 48	8, 18, 43, 81	5 (1%)
1	C	259/261 (99%)	0.23	14 (5%) 31 35	9, 21, 44, 73	5 (1%)
1	D	259/261 (99%)	0.09	11 (4%) 40 44	8, 20, 40, 70	6 (2%)
1	E	259/261 (99%)	0.08	17 (6%) 24 27	9, 20, 51, 124	6 (2%)
1	F	259/261 (99%)	0.16	5 (1%) 66 71	8, 21, 40, 61	4 (1%)
1	G	259/261 (99%)	0.12	16 (6%) 26 30	8, 19, 48, 70	11 (4%)
1	H	259/261 (99%)	0.06	7 (2%) 56 61	8, 21, 39, 74	1 (0%)
All	All	2072/2088 (99%)	0.06	87 (4%) 40 44	8, 20, 43, 124	41 (1%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	259	GLY	7.3
1	F	259	GLY	6.6
1	C	258	ALA	5.6
1	E	201	ALA	5.3
1	A	259	GLY	5.3
1	A	258	ALA	5.0
1	E	197	ALA	4.9
1	H	259	GLY	4.9
1	H	41	ASN	4.7
1	C	201	ALA	4.7
1	G	259	GLY	4.6
1	E	200	PHE	4.6
1	D	259	GLY	4.5
1	G	41[A]	ASN	4.4
1	G	39	TYR	4.2
1	E	198	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	258	ALA	4.0
1	F	258	ALA	4.0
1	C	259	GLY	3.8
1	G	258	ALA	3.7
1	B	201	ALA	3.6
1	E	258	ALA	3.6
1	B	197	ALA	3.6
1	H	258	ALA	3.6
1	A	201	ALA	3.5
1	B	258	ALA	3.4
1	F	41	ASN	3.4
1	G	201	ALA	3.4
1	E	195	ILE	3.4
1	E	203	PRO	3.3
1	C	203	PRO	3.2
1	E	199	LYS	3.1
1	E	204	LYS	3.1
1	D	203	PRO	3.0
1	B	41	ASN	3.0
1	B	203	PRO	3.0
1	G	199	LYS	2.9
1	G	194[A]	THR	2.9
1	G	197	ALA	2.9
1	E	259	GLY	2.9
1	C	207	ALA	2.8
1	B	204	LYS	2.8
1	C	197	ALA	2.8
1	C	41	ASN	2.7
1	C	202	ASP	2.7
1	G	208[A]	ASP	2.7
1	D	201	ALA	2.7
1	E	202	ASP	2.6
1	D	257	GLN	2.6
1	G	205	GLN	2.6
1	C	194	THR	2.6
1	F	70	GLU	2.6
1	H	42	LYS	2.6
1	E	205	GLN	2.5
1	A	204	LYS	2.5
1	H	204	LYS	2.5
1	B	135	ASP	2.5
1	G	200	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	41	ASN	2.4
1	H	257	GLN	2.4
1	G	207	ALA	2.4
1	G	43	GLN	2.4
1	C	195	ILE	2.4
1	F	80	ILE	2.4
1	D	199	LYS	2.3
1	D	51	GLU	2.3
1	E	194	THR	2.3
1	D	207	ALA	2.2
1	G	202	ASP	2.2
1	A	197	ALA	2.2
1	G	204	LYS	2.2
1	E	257	GLN	2.2
1	B	29[A]	LYS	2.2
1	C	199	LYS	2.2
1	E	207	ALA	2.1
1	A	203	PRO	2.1
1	G	203	PRO	2.1
1	C	200	PHE	2.1
1	H	194	THR	2.1
1	C	54	LYS	2.1
1	D	80	ILE	2.1
1	B	198	GLU	2.0
1	C	204	LYS	2.0
1	D	204	LYS	2.0
1	E	196	ASN	2.0
1	A	257	GLN	2.0
1	D	200	PHE	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

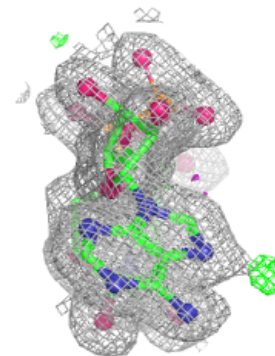
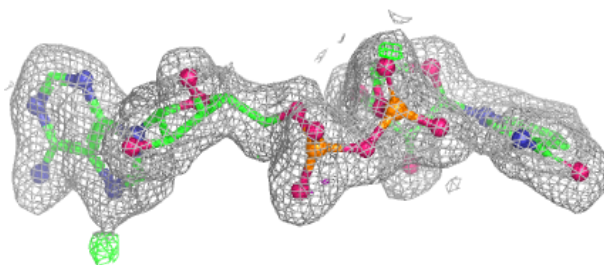
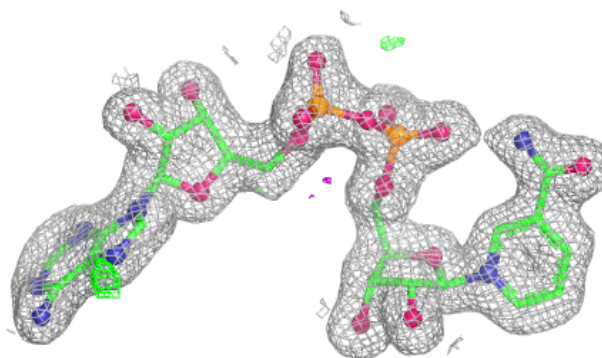
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	C	301	44/44	0.97	0.05	18,21,25,28	0
3	CL	D	302	1/1	0.97	0.06	22,22,22,22	0
2	NAD	A	301	44/44	0.98	0.05	16,18,20,21	0
2	NAD	D	301	44/44	0.98	0.05	16,19,20,24	0
2	NAD	E	301	44/44	0.98	0.05	18,20,23,25	0
2	NAD	H	301	44/44	0.98	0.05	17,20,23,26	0
2	NAD	F	301	44/44	0.98	0.05	15,20,23,25	0
2	NAD	G	301	44/44	0.98	0.05	17,20,24,26	0
3	CL	B	302	1/1	0.98	0.04	21,21,21,21	0
2	NAD	B	301	44/44	0.98	0.04	14,18,20,21	0
3	CL	A	302	1/1	0.99	0.04	21,21,21,21	0
3	CL	E	302	1/1	0.99	0.03	22,22,22,22	0

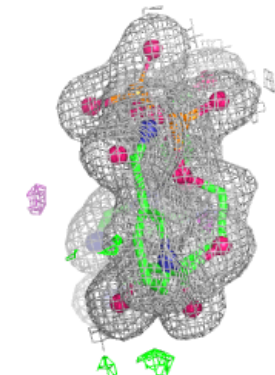
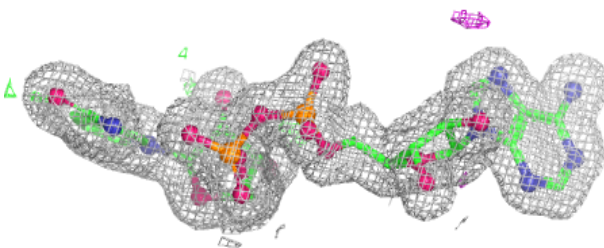
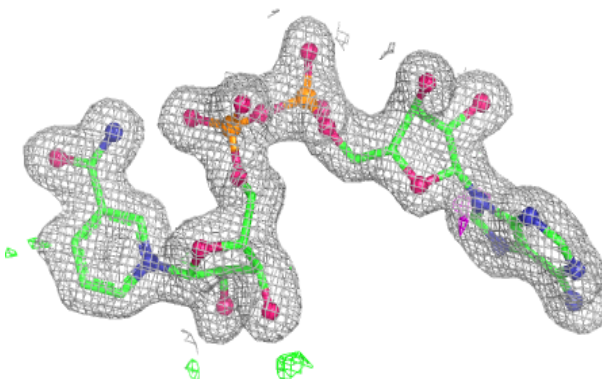
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD C 301:

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

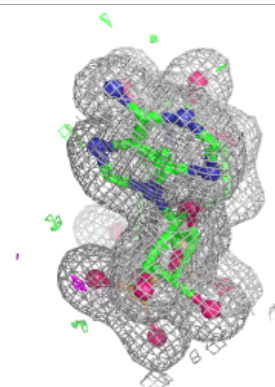
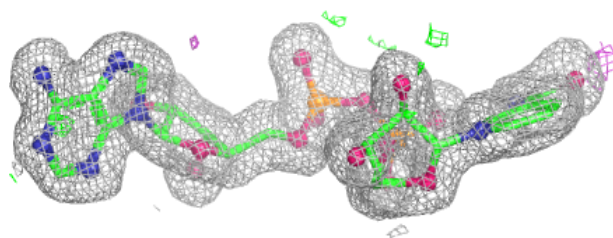
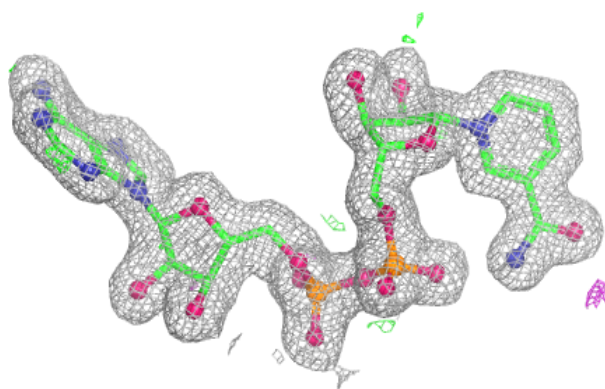
**Electron density around NAD A 301:**

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

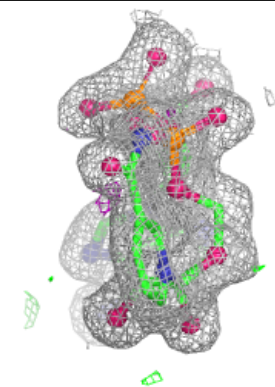
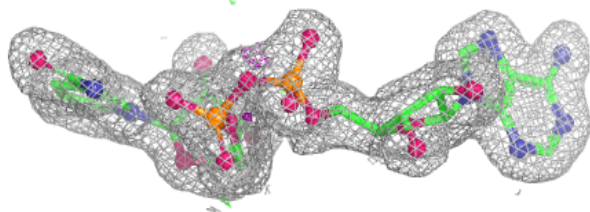
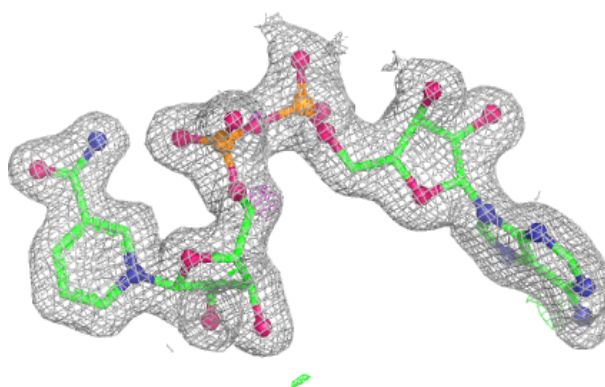


Electron density around NAD D 301:

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

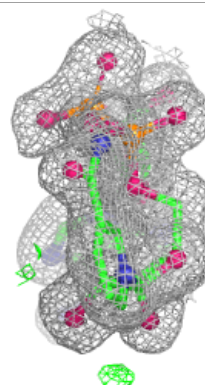
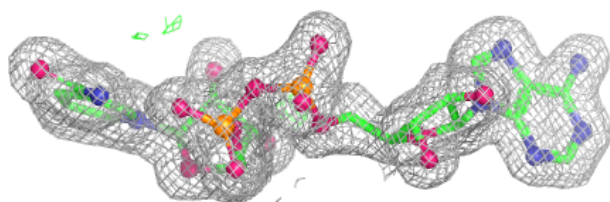
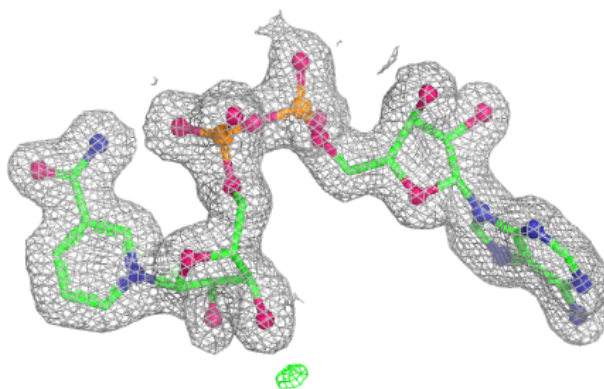
**Electron density around NAD E 301:**

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

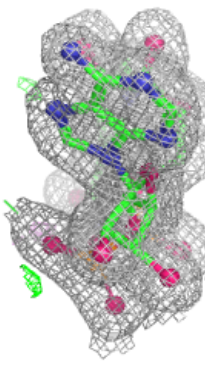
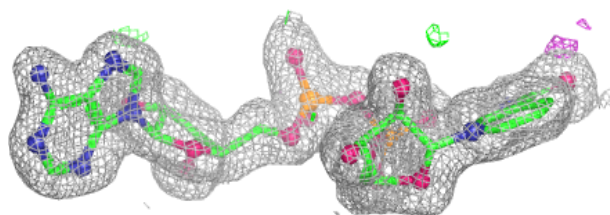
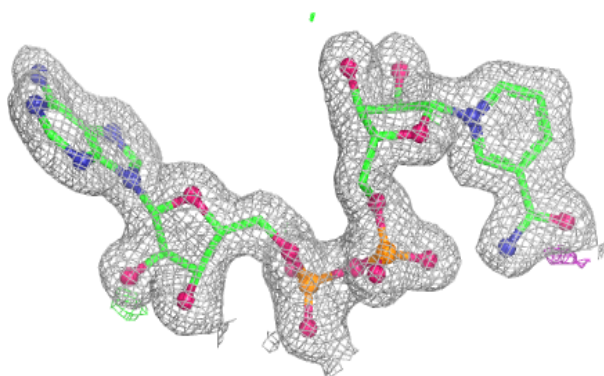


Electron density around NAD H 301:

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

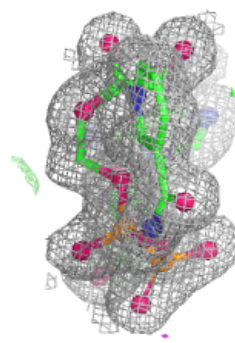
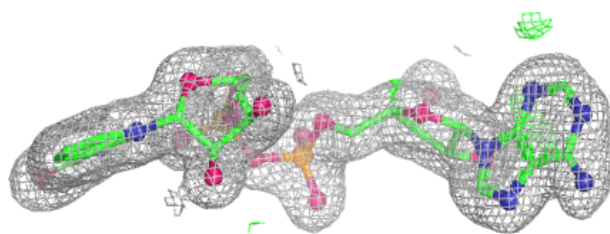
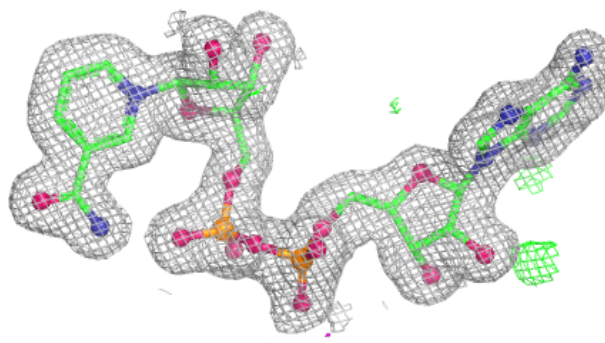
**Electron density around NAD F 301:**

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

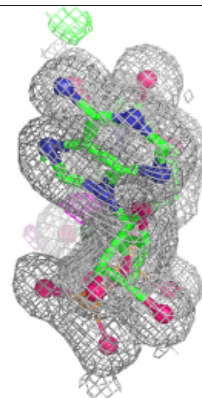
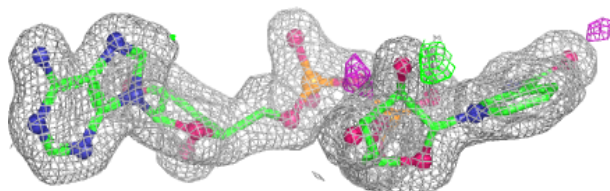
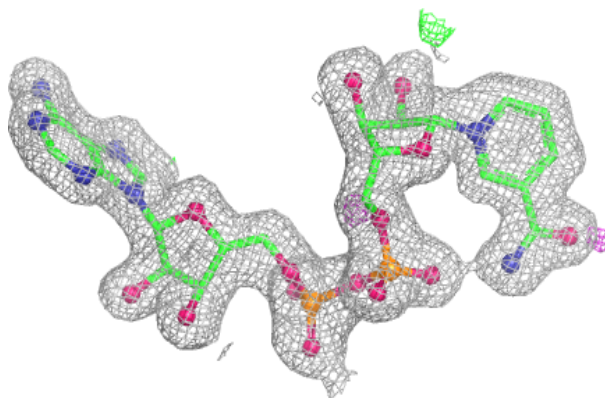


Electron density around NAD G 301:

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

**Electron density around NAD B 301:**

$2mF_o-DF_c$ (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.