



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:52 PM UTC

PDB ID : 6R9W / pdb_00006r9w
Title : Crystal structure of InhA in complex with AP-124 inhibitor
Authors : Takebayashi, Y.; Hinchliffe, P.; Spencer, J.
Deposited on : 2019-04-04
Resolution : 1.75 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

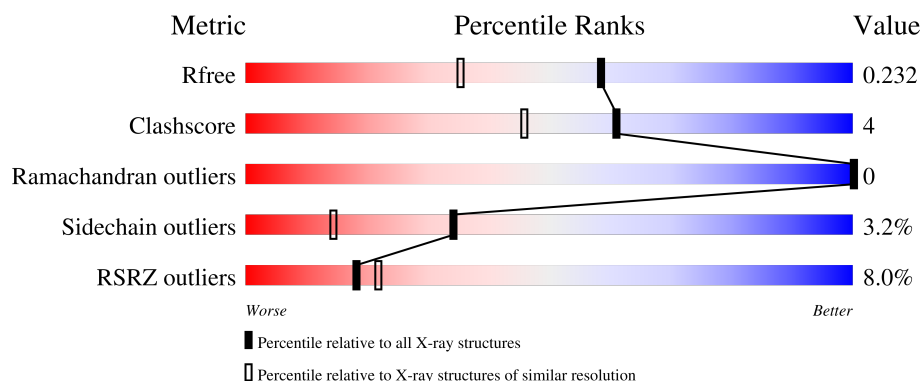
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	272	4% 92% • • •
1	B	272	4% 91% 7% •
1	C	272	4% 91% 5% •
1	D	272	8% 90% 7% • •
1	E	272	13% 88% 8% • •

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Mol	Chain	Length	Quality of chain
1	F	272	12% 77% 10% • 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25144 atoms, of which 12054 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 Enoyl-[acyl-carrier-protein] reductase [NADH].

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	267	Total	C	H	N	O	S	0	3	0
			4032	1269	2026	352	375	10			
1	B	267	Total	C	H	N	O	S	0	2	0
			4008	1263	2013	348	374	10			
1	C	263	Total	C	H	N	O	S	0	2	0
			3951	1246	1984	343	369	9			
1	D	267	Total	C	H	N	O	S	0	3	0
			4019	1266	2018	349	376	10			
1	E	267	Total	C	H	N	O	S	0	2	0
			4008	1263	2013	348	374	10			
1	F	240	Total	C	H	N	O	S	0	2	0
			3632	1149	1824	316	334	9			

There are 18 discrepancies between the modelled and reference sequences:

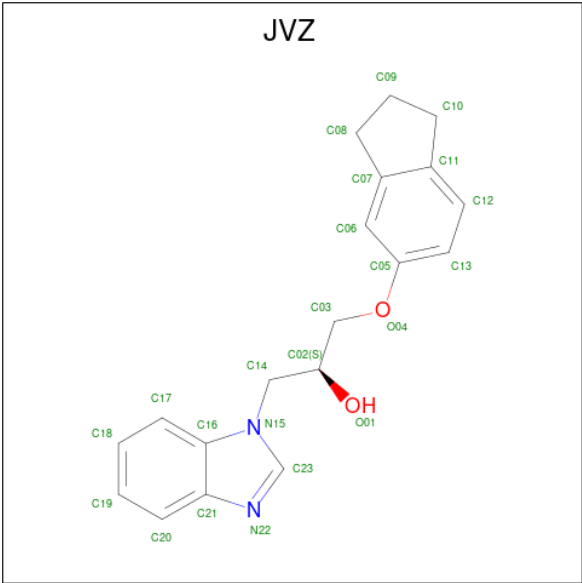
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P9WGR1
A	-1	SER	-	expression tag	UNP P9WGR1
A	0	HIS	-	expression tag	UNP P9WGR1
B	-2	GLY	-	expression tag	UNP P9WGR1
B	-1	SER	-	expression tag	UNP P9WGR1
B	0	HIS	-	expression tag	UNP P9WGR1
C	-2	GLY	-	expression tag	UNP P9WGR1
C	-1	SER	-	expression tag	UNP P9WGR1
C	0	HIS	-	expression tag	UNP P9WGR1
D	-2	GLY	-	expression tag	UNP P9WGR1
D	-1	SER	-	expression tag	UNP P9WGR1
D	0	HIS	-	expression tag	UNP P9WGR1
E	-2	GLY	-	expression tag	UNP P9WGR1
E	-1	SER	-	expression tag	UNP P9WGR1
E	0	HIS	-	expression tag	UNP P9WGR1
F	-2	GLY	-	expression tag	UNP P9WGR1
F	-1	SER	-	expression tag	UNP P9WGR1

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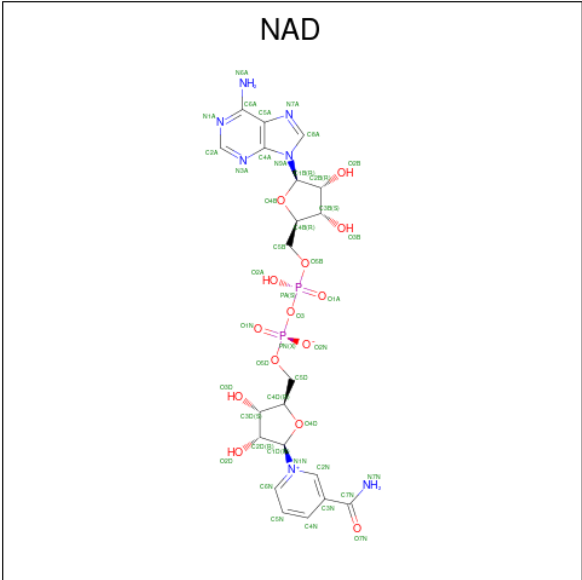
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	HIS	-	expression tag	UNP P9WGR1

- Molecule 2 is (2 {S})-1-(benzimidazol-1-yl)-3-(2,3-dihydro-1 {H}-inden-5-yloxy)propan-2-ol (CCD ID: JVZ) (formula: C₁₉H₂₀N₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
2	A	1	43	19	20	2	2	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
3	B	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
3	C	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
3	D	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
3	E	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
3	F	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		

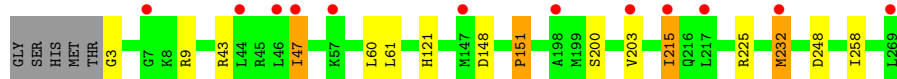
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	222	Total	O	0	0
			222	222		
4	B	218	Total	O	0	0
			218	218		
4	C	191	Total	O	0	0
			191	191		
4	D	139	Total	O	0	0
			139	139		
4	E	128	Total	O	0	0
			128	128		
4	F	133	Total	O	0	0
			133	133		

3 Residue-property plots

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.

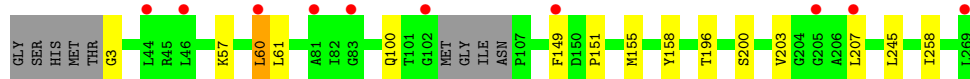
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



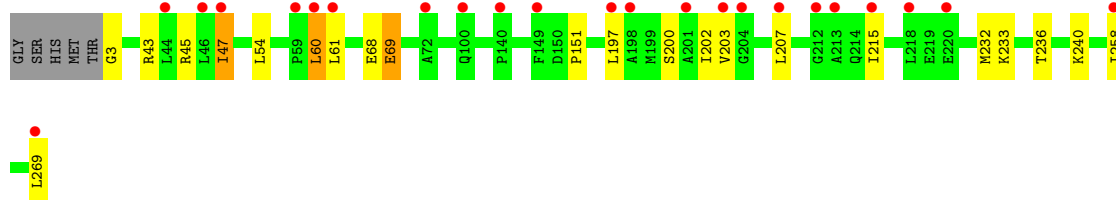
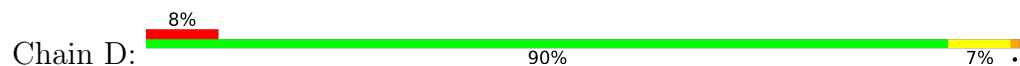
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



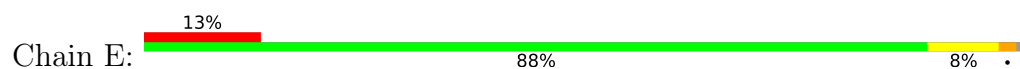
- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

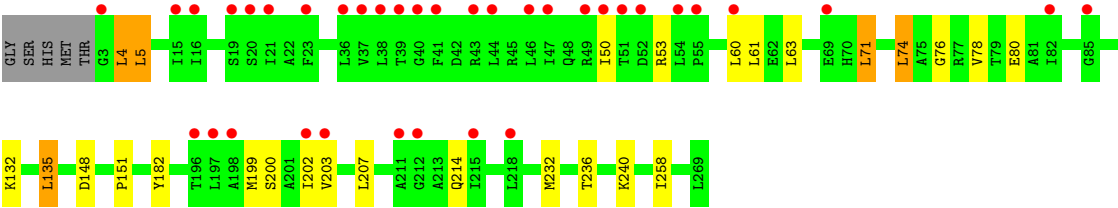


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]

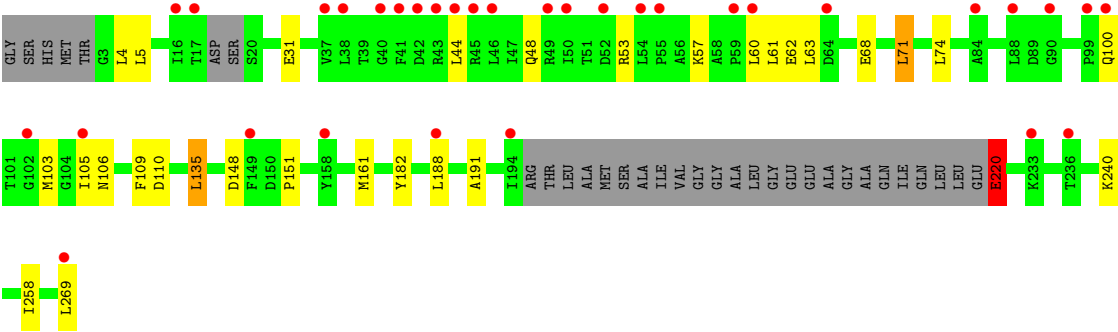
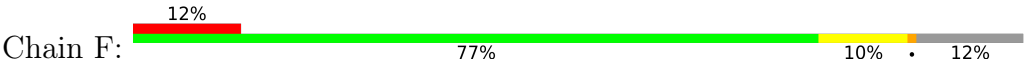


- Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]





● Molecule 1: Enoyl-[acyl-carrier-protein] reductase [NADH]



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	100.90Å 81.60Å 189.41Å 90.00° 95.52° 90.00°	Depositor
Resolution (Å)	43.32 – 1.75 43.32 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.2 (43.32-1.75) 99.2 (43.32-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 1.75Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.187 , 0.227 0.194 , 0.232	Depositor DCC
R_{free} test set	7638 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25144	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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, JVZ

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	0.76	1/2055 (0.0%)	0.90	2/2787 (0.1%)
1	B	0.78	2/2044 (0.1%)	0.89	0/2773
1	C	0.66	0/2015	0.86	0/2732
1	D	0.64	0/2050	0.88	1/2781 (0.0%)
1	E	0.64	0/2044	0.85	1/2773 (0.0%)
1	F	0.79	2/1855 (0.1%)	0.86	2/2515 (0.1%)
All	All	0.71	5/12063 (0.0%)	0.87	6/16361 (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	F	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	220	GLU	CD-OE2	15.85	1.55	1.25
1	F	220	GLU	CD-OE1	12.76	1.49	1.25
1	A	121	HIS	CE1-NE2	8.83	1.41	1.32
1	B	70	HIS	CE1-NE2	5.53	1.38	1.32
1	B	210	GLU	CD-OE2	5.10	1.35	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	69	GLU	CB-CA-C	6.02	121.08	110.85
1	A	148	ASP	CA-CB-CG	5.29	117.89	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	220	GLU	CG-CD-OE1	-5.26	106.30	118.40
1	F	148	ASP	CA-CB-CG	5.09	117.69	112.60
1	E	148	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	151	PRO	N-CA-CB	-5.04	97.96	103.25

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	220	GLU	Sidechain

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5.2 Torsion angles

5.2.1 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	268/272 (98%)	258 (96%)	10 (4%)	0	100	100
1	B	267/272 (98%)	257 (96%)	10 (4%)	0	100	100
1	C	261/272 (96%)	250 (96%)	11 (4%)	0	100	100
1	D	268/272 (98%)	257 (96%)	11 (4%)	0	100	100
1	E	267/272 (98%)	257 (96%)	10 (4%)	0	100	100
1	F	236/272 (87%)	225 (95%)	11 (5%)	0	100	100
All	All	1567/1632 (96%)	1504 (96%)	63 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.2.2 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	206/207 (100%)	202 (98%)	4 (2%)	50	31
1	B	205/207 (99%)	200 (98%)	5 (2%)	43	23
1	C	202/207 (98%)	199 (98%)	3 (2%)	57	41
1	D	206/207 (100%)	199 (97%)	7 (3%)	32	13
1	E	205/207 (99%)	198 (97%)	7 (3%)	32	13
1	F	187/207 (90%)	175 (94%)	12 (6%)	16	3
All	All	1211/1242 (98%)	1173 (97%)	38 (3%)	34	15

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ILE
1	A	151	PRO
1	A	215	ILE
1	A	232	MET
1	B	53	ARG
1	B	151	PRO
1	B	210	GLU
1	B	215	ILE
1	B	216	GLN
1	C	57	LYS
1	C	60	LEU
1	C	151	PRO
1	D	45	ARG
1	D	47	ILE
1	D	60	LEU
1	D	68	GLU
1	D	151	PRO
1	D	232	MET
1	D	269	LEU
1	E	4	LEU
1	E	5	LEU
1	E	71	LEU
1	E	74	LEU
1	E	135	LEU
1	E	151	PRO
1	E	232	MET

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Mol	Chain	Res	Type
1	F	4	LEU
1	F	5	LEU
1	F	53	ARG
1	F	57	LYS
1	F	71	LEU
1	F	74	LEU
1	F	105	ILE
1	F	135	LEU
1	F	151	PRO
1	F	188	LEU
1	F	220	GLU
1	F	269	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	B	35	GLN
1	B	66	GLN
1	B	100	GLN
1	B	224	GLN
1	C	66	GLN
1	D	66	GLN
1	D	100	GLN
1	D	121	HIS
1	E	66	GLN
1	F	224	GLN

5.2.3 RNA ⓘ

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.4 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.5 Ligand geometry

7 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$
3	NAD	D	301	-	46,48,48	1.11	4 (8%)	64,73,73	0.91	2 (3%)
3	NAD	E	301	-	46,48,48	0.72	1 (2%)	64,73,73	0.91	4 (6%)
3	NAD	C	301	-	46,48,48	1.18	3 (6%)	64,73,73	0.90	2 (3%)
3	NAD	F	301	-	46,48,48	0.58	1 (2%)	64,73,73	0.80	1 (1%)
2	JVZ	A	301	-	26,26,26	1.97	9 (34%)	36,36,36	1.37	5 (13%)
3	NAD	A	302	-	46,48,48	0.86	2 (4%)	64,73,73	0.96	2 (3%)
3	NAD	B	301	-	46,48,48	1.00	3 (6%)	64,73,73	1.09	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
3	NAD	D	301	-	-	9/30/62/62	0/5/5/5
3	NAD	E	301	-	-	8/30/62/62	0/5/5/5
3	NAD	C	301	-	-	8/30/62/62	0/5/5/5
3	NAD	F	301	-	-	11/30/62/62	0/5/5/5
2	JVZ	A	301	-	-	1/9/15/15	0/4/4/4
3	NAD	A	302	-	-	11/30/62/62	0/5/5/5
3	NAD	B	301	-	-	8/30/62/62	0/5/5/5

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	NAD	C2N-N1N	5.06	1.40	1.35
3	D	301	NAD	C2N-N1N	4.86	1.40	1.35
3	B	301	NAD	C2N-N1N	4.40	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	JVZ	C14-N15	4.21	1.52	1.46
2	A	301	JVZ	C08-C07	3.99	1.57	1.51
2	A	301	JVZ	C10-C11	3.72	1.56	1.51
3	C	301	NAD	O4D-C1D	3.55	1.45	1.40
3	B	301	NAD	O4D-C1D	3.34	1.45	1.40
3	D	301	NAD	PA-O3	3.23	1.63	1.59
3	A	302	NAD	C2N-N1N	3.10	1.38	1.35
2	A	301	JVZ	C06-C05	3.08	1.44	1.39
3	C	301	NAD	PA-O3	2.99	1.62	1.59
3	A	302	NAD	O4D-C1D	2.77	1.44	1.40
3	D	301	NAD	O4D-C1D	2.59	1.44	1.40
2	A	301	JVZ	C19-C18	2.59	1.43	1.38
2	A	301	JVZ	C16-N15	2.51	1.43	1.39
2	A	301	JVZ	C16-C21	2.17	1.43	1.40
2	A	301	JVZ	C03-C02	2.11	1.58	1.51
3	F	301	NAD	C2N-N1N	2.09	1.37	1.35
3	E	301	NAD	C4N-C3N	2.07	1.42	1.39
2	A	301	JVZ	O01-C02	-2.05	1.37	1.43
3	B	301	NAD	C2N-C3N	2.01	1.42	1.39
3	D	301	NAD	C4N-C3N	2.01	1.42	1.39

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	NAD	C6N-N1N-C2N	-3.89	118.56	121.88
3	B	301	NAD	C5N-C4N-C3N	-2.94	117.47	120.36
3	F	301	NAD	O2B-C2B-C1B	2.86	119.97	110.10
3	A	302	NAD	O4B-C1B-N9A	2.85	113.56	108.09
2	A	301	JVZ	C10-C09-C08	-2.63	101.97	107.08
3	C	301	NAD	C4B-O4B-C1B	-2.63	103.66	109.47
3	A	302	NAD	O3-PN-O1N	-2.62	102.83	110.70
3	D	301	NAD	O7N-C7N-C3N	-2.61	116.40	119.60
3	E	301	NAD	C4D-O4D-C1D	-2.45	107.68	109.92
3	E	301	NAD	O7N-C7N-C3N	-2.41	116.65	119.60
2	A	301	JVZ	O04-C03-C02	2.37	111.92	107.64
3	E	301	NAD	O4B-C1B-N9A	2.36	112.62	108.09
3	B	301	NAD	O3-PN-O1N	-2.33	103.69	110.70
3	E	301	NAD	C2N-C3N-C4N	2.31	120.95	118.26
3	B	301	NAD	O2N-PN-O3	2.31	113.52	107.27
2	A	301	JVZ	C09-C08-C07	2.29	106.79	103.79
2	A	301	JVZ	C09-C10-C11	2.23	106.71	103.79
3	C	301	NAD	C6N-N1N-C2N	-2.14	120.06	121.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	NAD	O4B-C1B-N9A	2.08	112.08	108.09
3	D	301	NAD	C4D-O4D-C1D	-2.04	108.06	109.92
2	A	301	JVZ	C20-C21-N22	2.01	133.33	129.62

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	NAD	C5B-O5B-PA-O2A
3	A	302	NAD	PN-O3-PA-O5B
3	A	302	NAD	C5D-O5D-PN-O3
3	A	302	NAD	C5D-O5D-PN-O1N
3	A	302	NAD	C5D-O5D-PN-O2N
3	A	302	NAD	O4D-C1D-N1N-C2N
3	A	302	NAD	O4D-C1D-N1N-C6N
3	A	302	NAD	C2D-C1D-N1N-C6N
3	B	301	NAD	C5D-O5D-PN-O3
3	B	301	NAD	C5D-O5D-PN-O1N
3	B	301	NAD	C5D-O5D-PN-O2N
3	B	301	NAD	O4D-C1D-N1N-C2N
3	B	301	NAD	O4D-C1D-N1N-C6N
3	B	301	NAD	C2D-C1D-N1N-C2N
3	B	301	NAD	C2D-C1D-N1N-C6N
3	C	301	NAD	C5D-O5D-PN-O3
3	C	301	NAD	C5D-O5D-PN-O1N
3	C	301	NAD	C5D-O5D-PN-O2N
3	C	301	NAD	O4D-C1D-N1N-C2N
3	C	301	NAD	O4D-C1D-N1N-C6N
3	C	301	NAD	C2D-C1D-N1N-C2N
3	C	301	NAD	C2D-C1D-N1N-C6N
3	D	301	NAD	C5B-O5B-PA-O2A
3	D	301	NAD	C5D-O5D-PN-O3
3	D	301	NAD	C5D-O5D-PN-O1N
3	D	301	NAD	C5D-O5D-PN-O2N
3	D	301	NAD	O4D-C1D-N1N-C2N
3	E	301	NAD	C5B-O5B-PA-O1A
3	E	301	NAD	PN-O3-PA-O5B
3	E	301	NAD	C5D-O5D-PN-O3
3	E	301	NAD	C5D-O5D-PN-O1N
3	E	301	NAD	C5D-O5D-PN-O2N
3	E	301	NAD	O4D-C1D-N1N-C2N
3	E	301	NAD	O4D-C1D-N1N-C6N

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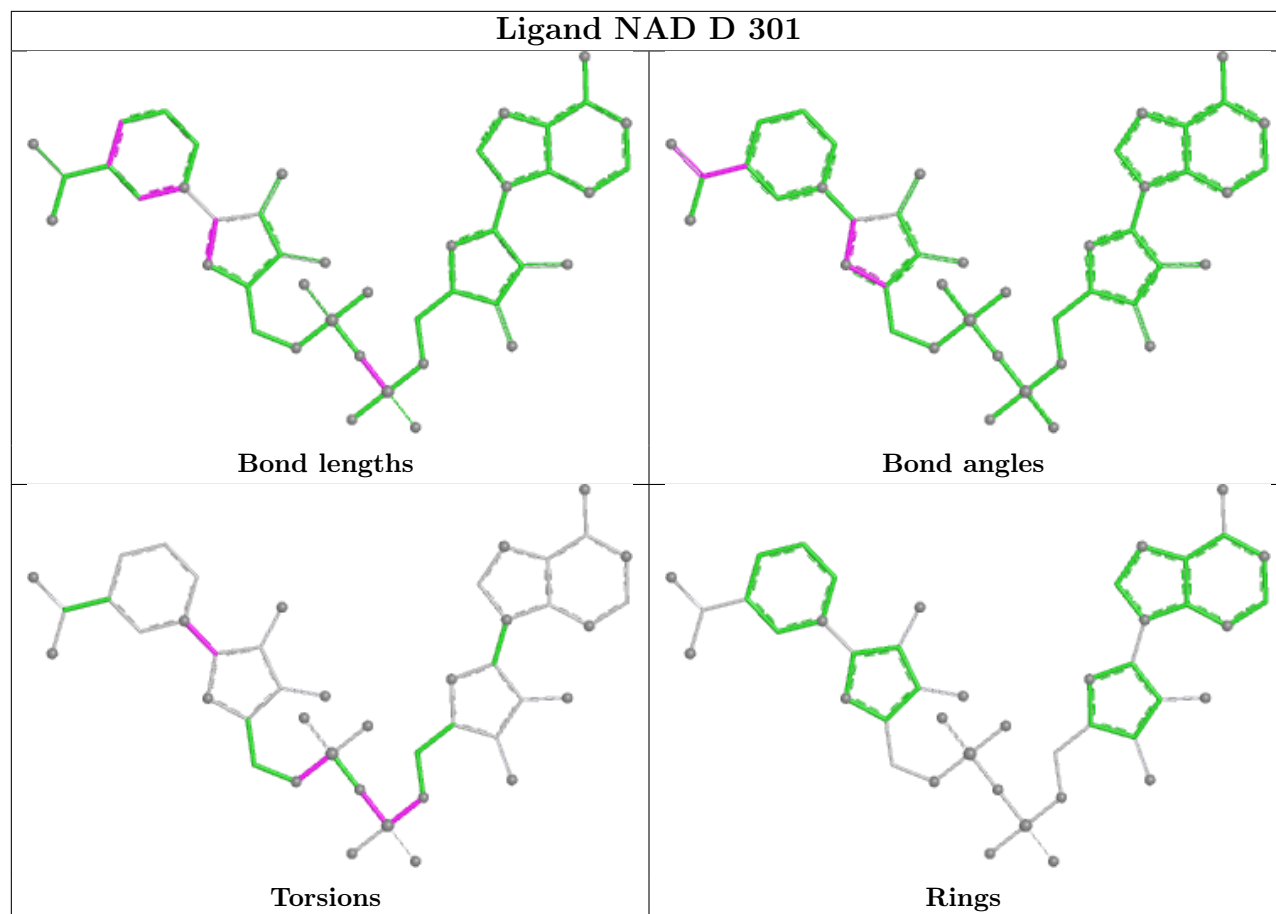
Mol	Chain	Res	Type	Atoms
3	F	301	NAD	C5B-O5B-PA-O2A
3	F	301	NAD	PN-O3-PA-O5B
3	F	301	NAD	C5D-O5D-PN-O3
3	F	301	NAD	C5D-O5D-PN-O2N
3	F	301	NAD	O4D-C1D-N1N-C2N
3	F	301	NAD	O4D-C1D-N1N-C6N
3	F	301	NAD	C2D-C1D-N1N-C2N
3	F	301	NAD	C2D-C1D-N1N-C6N
3	C	301	NAD	PN-O3-PA-O5B
3	D	301	NAD	PN-O3-PA-O5B
2	A	301	JVZ	C02-C03-O04-C05
3	A	302	NAD	C5B-O5B-PA-O1A
3	A	302	NAD	C5B-O5B-PA-O3
3	D	301	NAD	C5B-O5B-PA-O1A
3	D	301	NAD	C5B-O5B-PA-O3
3	F	301	NAD	C5B-O5B-PA-O1A
3	F	301	NAD	C5B-O5B-PA-O3
3	F	301	NAD	C5D-O5D-PN-O1N
3	A	302	NAD	C2D-C1D-N1N-C2N
3	E	301	NAD	C2D-C1D-N1N-C6N
3	D	301	NAD	O4D-C1D-N1N-C6N
3	B	301	NAD	O4B-C4B-C5B-O5B

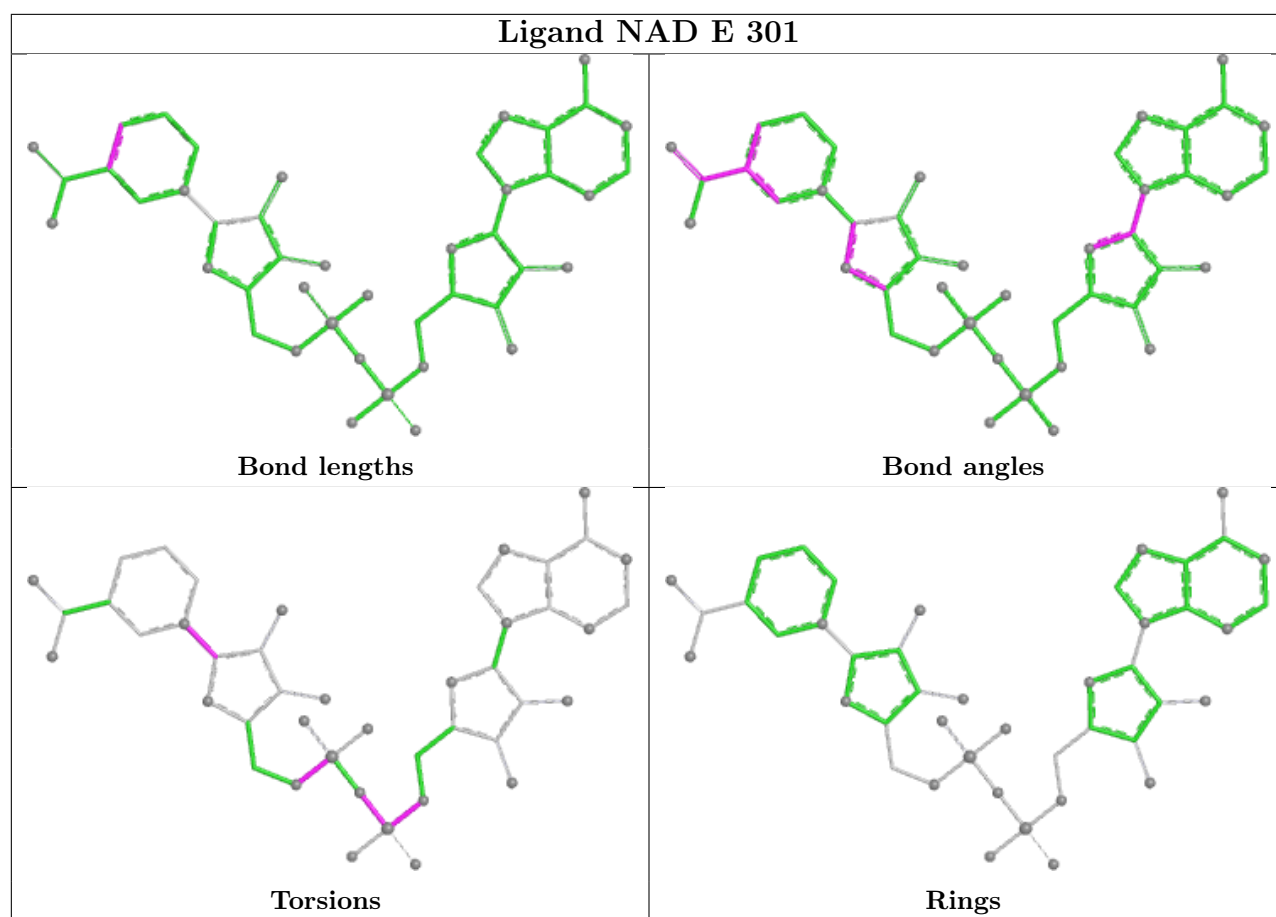
There are no ring outliers.

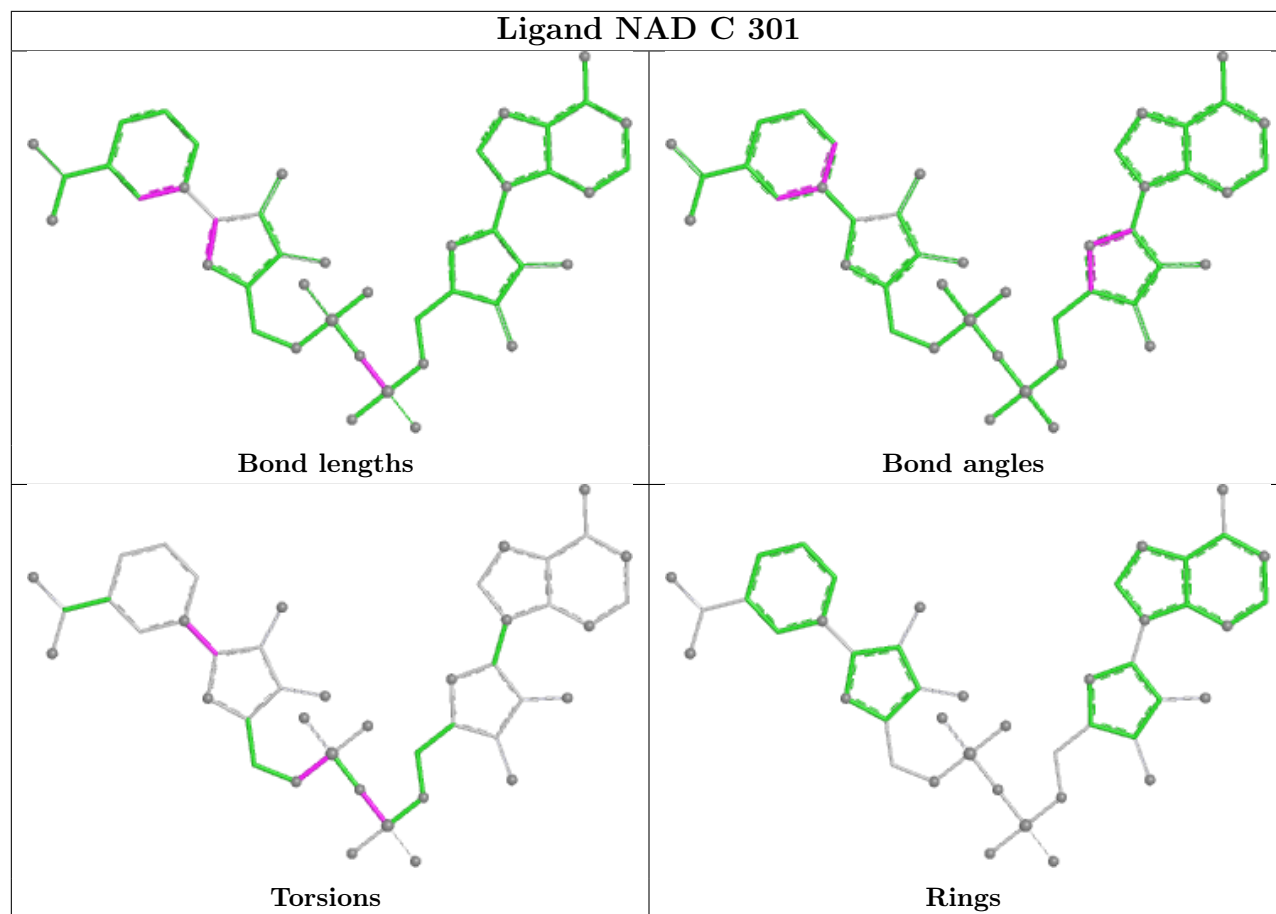
2 monomers are involved in 3 short contacts:

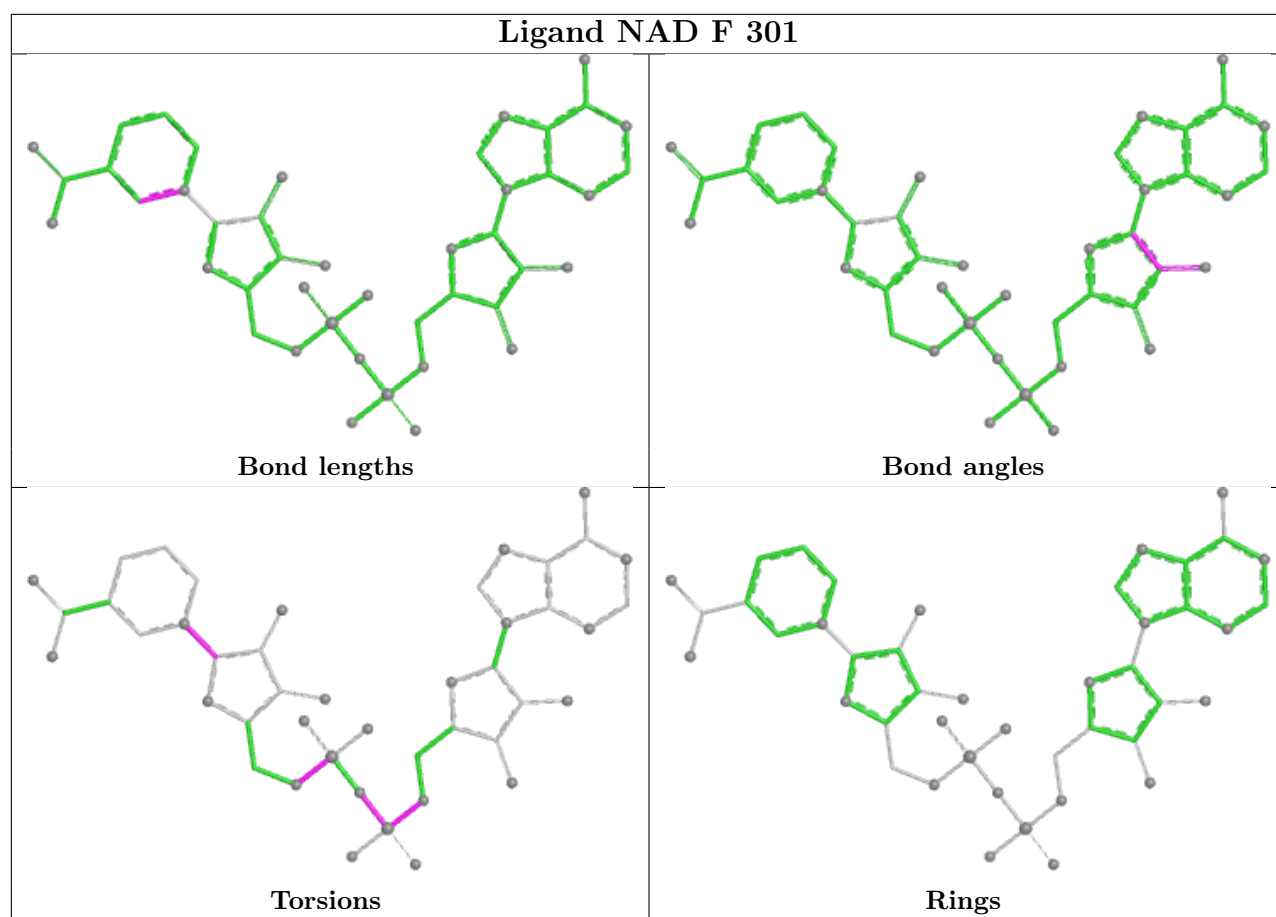
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	NAD	1	0
3	F	301	NAD	2	0

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.

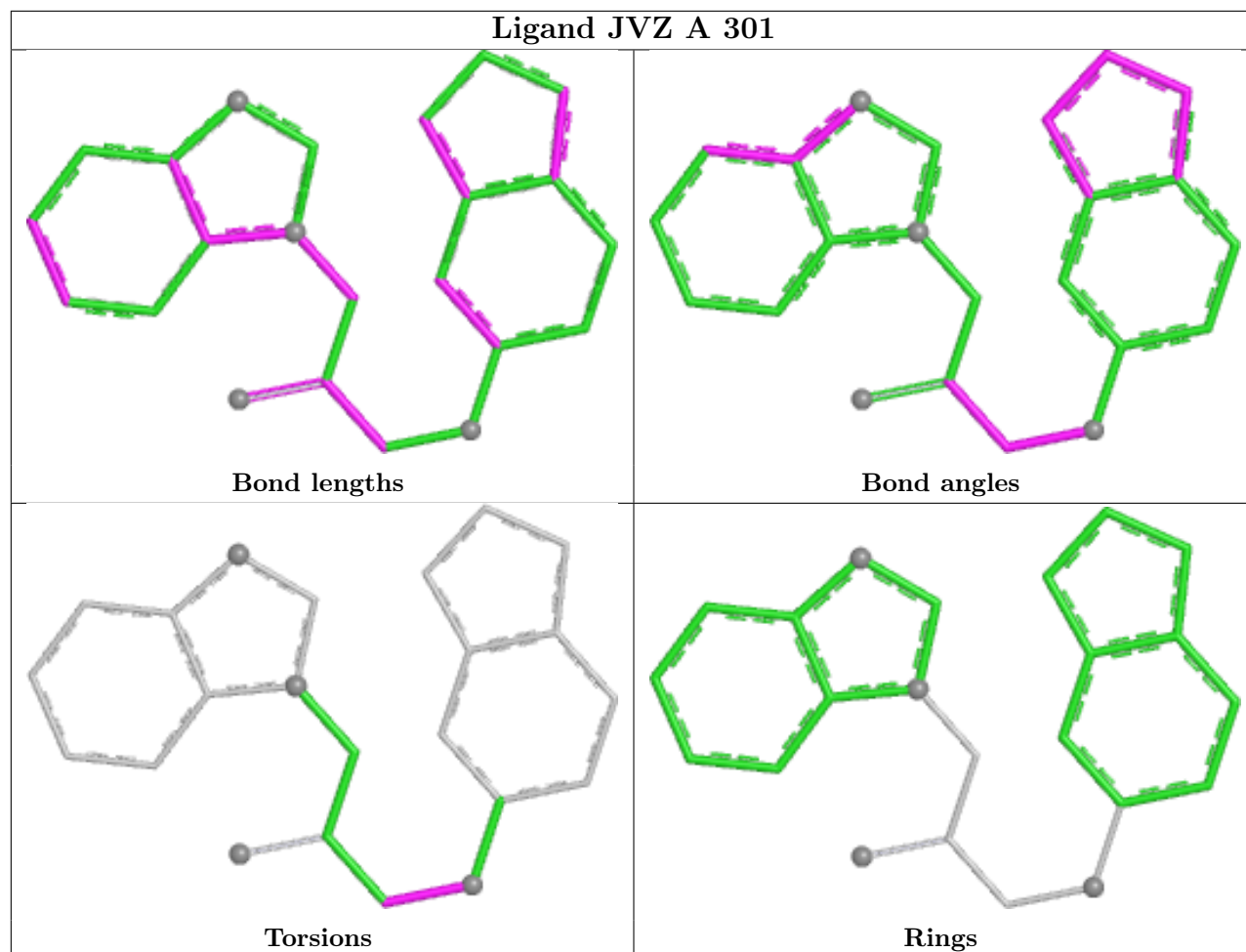


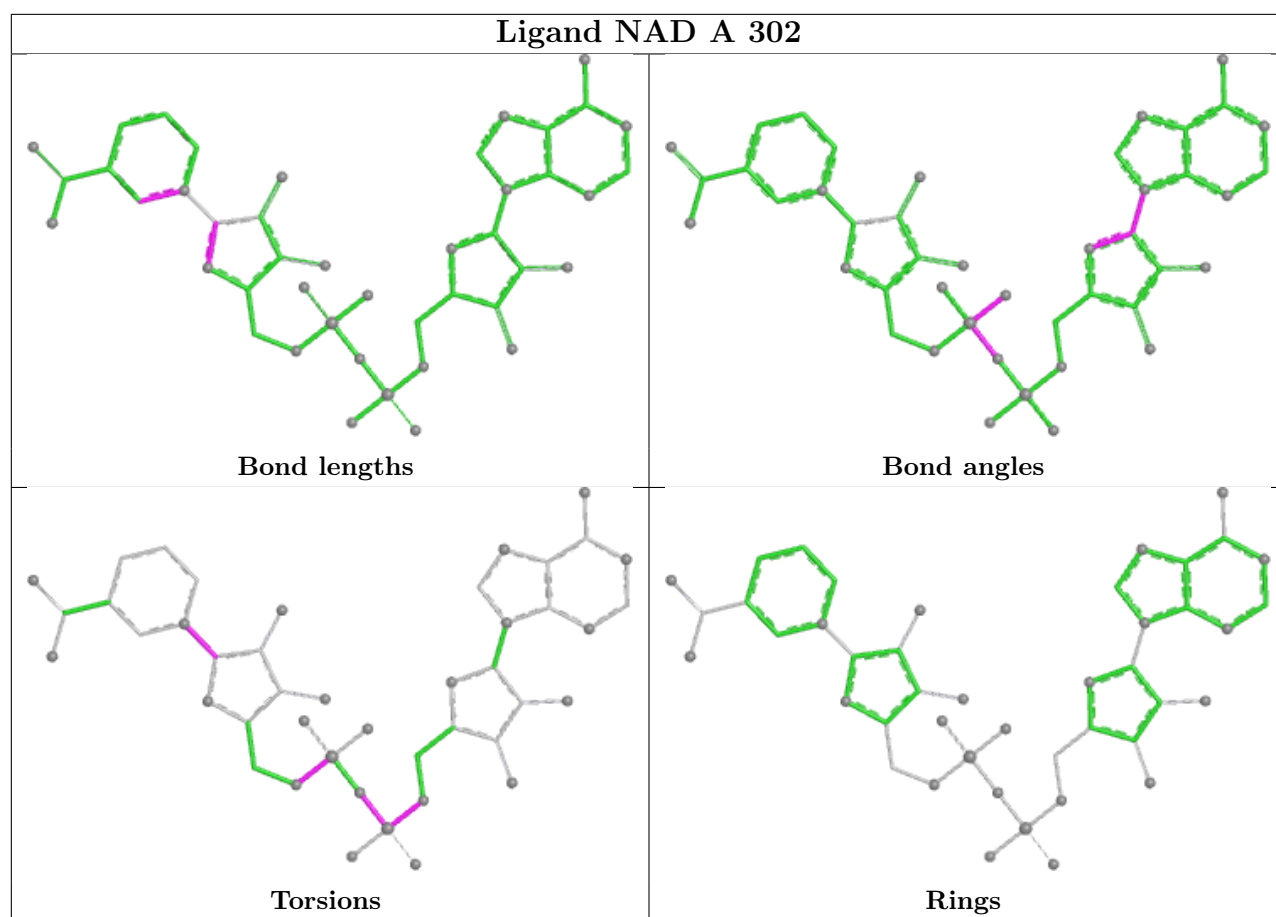


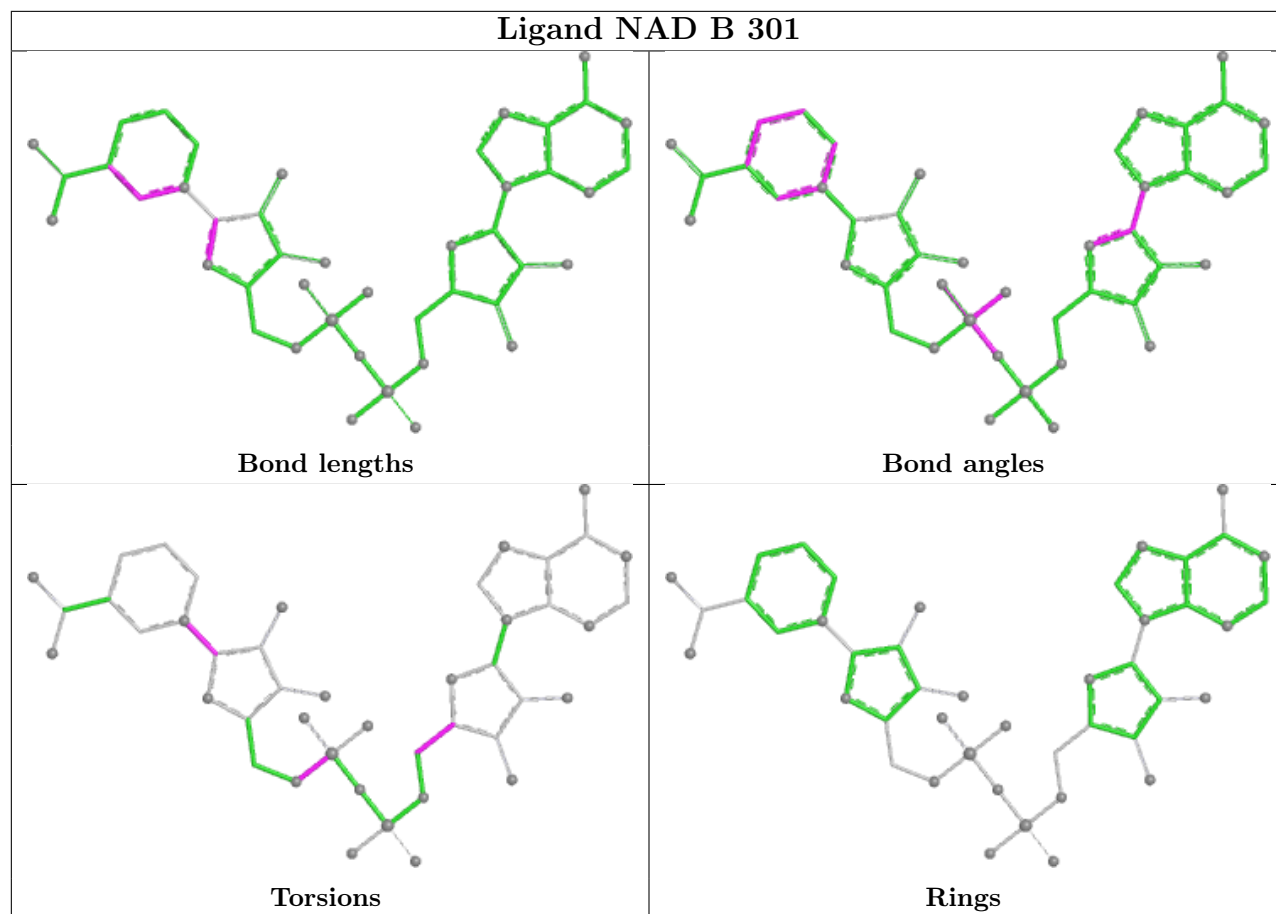




Ligand JVZ A 301







5.6 Other polymers [i](#)

There are no such residues in this entry.

5.7 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	267/272 (98%)	-0.13	12 (4%)	38	44	7, 23, 61, 89	2 (0%)
1	B	267/272 (98%)	-0.04	11 (4%)	41	47	7, 23, 61, 81	1 (0%)
1	C	263/272 (96%)	0.43	10 (3%)	44	50	11, 37, 62, 80	1 (0%)
1	D	267/272 (98%)	0.71	23 (8%)	16	19	12, 39, 77, 94	2 (0%)
1	E	267/272 (98%)	0.92	36 (13%)	7	8	13, 46, 77, 103	1 (0%)
1	F	240/272 (88%)	0.95	33 (13%)	6	7	15, 47, 76, 103	1 (0%)
All	All	1571/1632 (96%)	0.47	125 (7%)	18	22	7, 36, 72, 103	8 (0%)

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	215	ILE	6.2
1	A	147	MET	5.1
1	A	269	LEU	5.0
1	C	102	GLY	4.9
1	B	203	VAL	4.9
1	D	218	LEU	4.7
1	E	197	LEU	4.7
1	B	269	LEU	4.3
1	D	203	VAL	4.2
1	E	46	LEU	4.1
1	E	203	VAL	3.8
1	C	269	LEU	3.7
1	E	60	LEU	3.6
1	F	158	TYR	3.6
1	F	38	LEU	3.6
1	F	269	LEU	3.6
1	E	215	ILE	3.5
1	D	46	LEU	3.5
1	B	210	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	215	ILE	3.3
1	F	194	ILE	3.3
1	D	269	LEU	3.3
1	A	232	MET	3.3
1	F	60	LEU	3.3
1	E	49	ARG	3.3
1	E	50	ILE	3.2
1	F	44	LEU	3.2
1	D	47	ILE	3.2
1	D	60	LEU	3.1
1	F	99	PRO	3.1
1	C	46	LEU	3.1
1	D	213	ALA	3.1
1	A	203	VAL	3.1
1	B	46	LEU	3.1
1	E	198	ALA	3.0
1	D	220	GLU	3.0
1	F	49	ARG	3.0
1	F	17	THR	2.9
1	E	218	LEU	2.9
1	D	201	ALA	2.9
1	D	197	LEU	2.9
1	D	212	GLY	2.9
1	D	44	LEU	2.9
1	E	44	LEU	2.9
1	D	140	PRO	2.8
1	D	100	GLN	2.7
1	C	205	GLY	2.6
1	E	3	GLY	2.6
1	F	90	GLY	2.6
1	E	19	SER	2.6
1	C	83	GLY	2.6
1	C	44	LEU	2.6
1	E	36	LEU	2.6
1	F	16	ILE	2.6
1	F	50	ILE	2.6
1	F	105	ILE	2.6
1	F	45	ARG	2.6
1	F	149	PHE	2.6
1	A	217	LEU	2.6
1	F	102	GLY	2.5
1	E	38	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	46	LEU	2.5
1	F	233	LYS	2.5
1	A	215	ILE	2.5
1	F	55	PRO	2.5
1	F	42	ASP	2.5
1	E	196	THR	2.5
1	D	61	LEU	2.5
1	F	37	VAL	2.5
1	E	47	ILE	2.5
1	C	149	PHE	2.5
1	E	41	PHE	2.4
1	B	200	SER	2.4
1	B	57	LYS	2.4
1	D	198	ALA	2.4
1	E	39	THR	2.4
1	A	44	LEU	2.4
1	C	207	LEU	2.4
1	F	52	ASP	2.4
1	A	47	ILE	2.4
1	E	212	GLY	2.3
1	F	188	LEU	2.3
1	E	37	VAL	2.3
1	D	149	PHE	2.3
1	E	82	ILE	2.3
1	E	202	ILE	2.3
1	A	198	ALA	2.3
1	B	197	LEU	2.3
1	B	218	LEU	2.3
1	E	52	ASP	2.3
1	E	85	GLY	2.3
1	F	236	THR	2.2
1	E	69	GLU	2.2
1	E	211	ALA	2.2
1	D	207	LEU	2.2
1	E	23	PHE	2.2
1	D	59	PRO	2.2
1	E	54	LEU	2.2
1	F	54	LEU	2.2
1	A	7	GLY	2.2
1	B	49	ARG	2.2
1	E	55	PRO	2.2
1	F	41	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	81	ALA	2.1
1	D	204	GLY	2.1
1	B	42	ASP	2.1
1	D	258	ILE	2.1
1	E	16	ILE	2.1
1	E	21	ILE	2.1
1	A	46	LEU	2.1
1	E	51	THR	2.1
1	E	40	GLY	2.1
1	C	60	LEU	2.1
1	F	43	ARG	2.1
1	F	88	LEU	2.1
1	F	59	PRO	2.1
1	F	40	GLY	2.0
1	D	72	ALA	2.0
1	F	100	GLN	2.0
1	E	20	SER	2.0
1	E	15	ILE	2.0
1	E	43	ARG	2.0
1	F	64	ASP	2.0
1	F	84	ALA	2.0
1	A	57	LYS	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	JVZ	A	301	23/23	0.88	0.12	20,31,40,44	43

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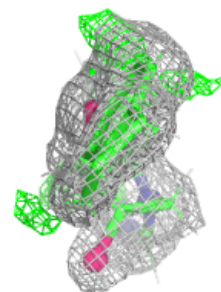
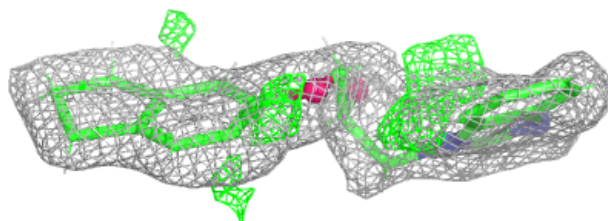
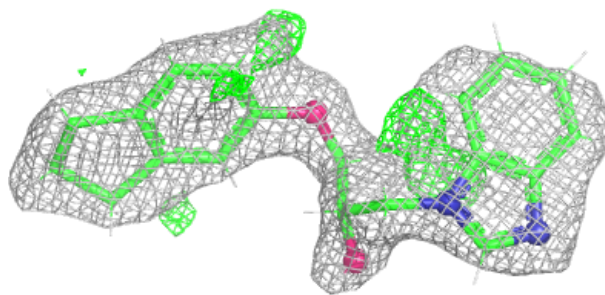
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAD	F	301	44/44	0.89	0.14	30,40,49,52	70
3	NAD	E	301	44/44	0.94	0.08	33,42,51,53	0
3	NAD	D	301	44/44	0.96	0.07	28,33,42,44	0
3	NAD	B	301	44/44	0.96	0.07	18,29,39,45	0
3	NAD	C	301	44/44	0.96	0.06	22,29,34,37	0
3	NAD	A	302	44/44	0.98	0.05	19,22,28,29	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.

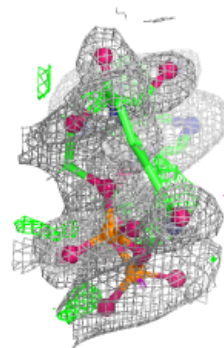
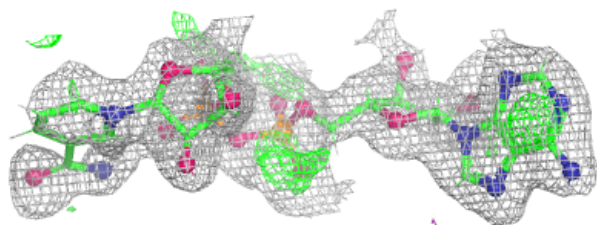
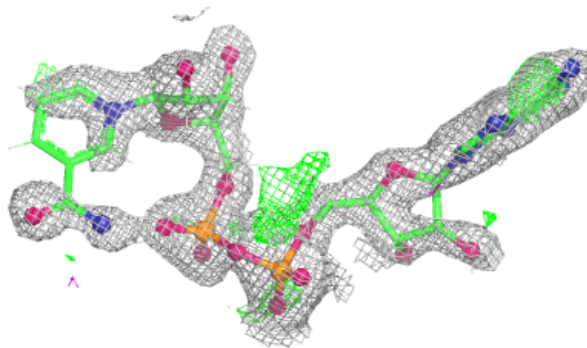
Electron density around JVZ A 301:

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

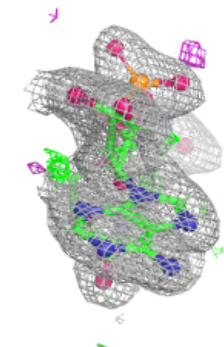
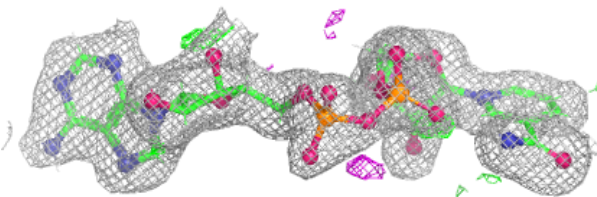
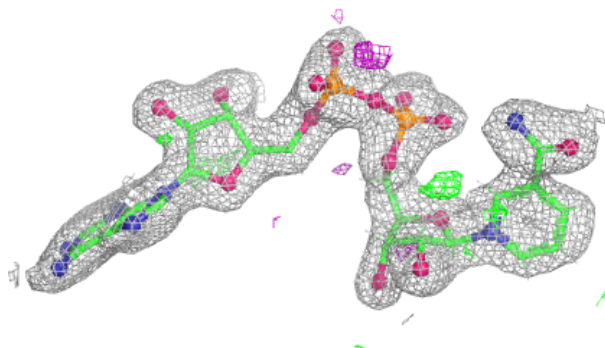


Electron density around NAD F 301:

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

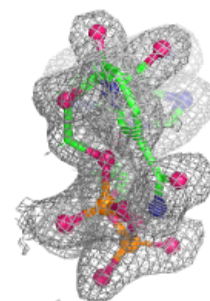
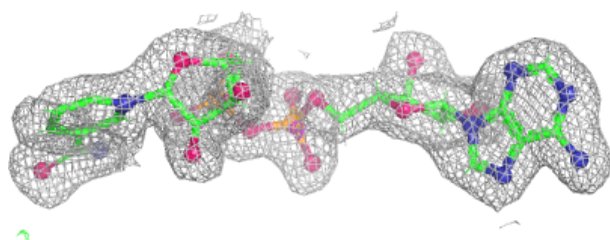
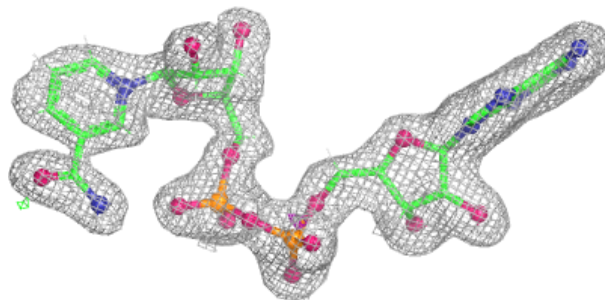
**Electron density around NAD E 301:**

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

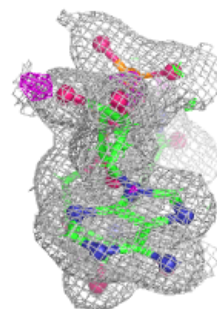
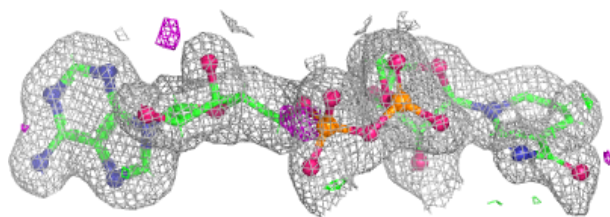
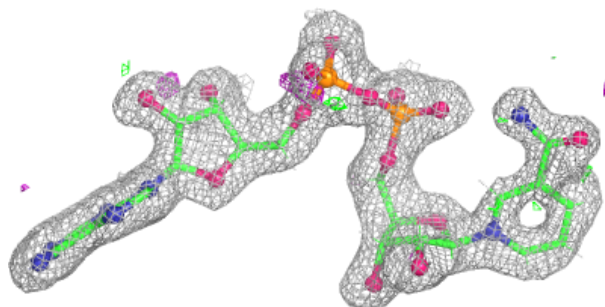


Electron density around NAD D 301:

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

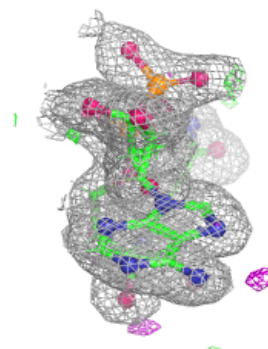
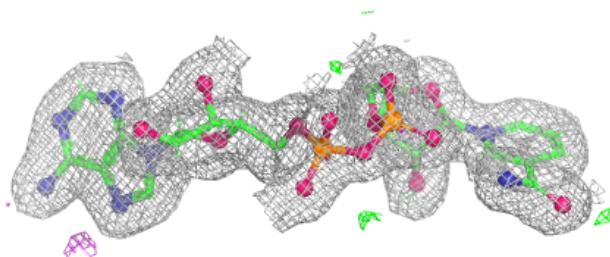
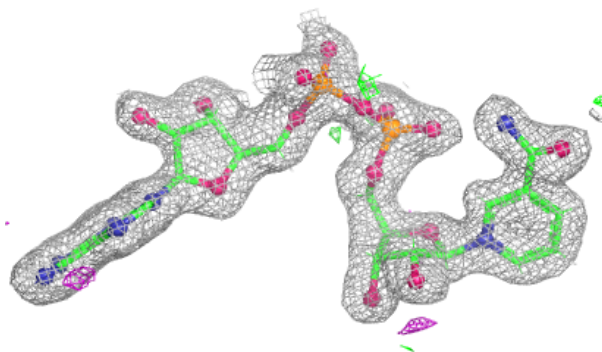
**Electron density around NAD B 301:**

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

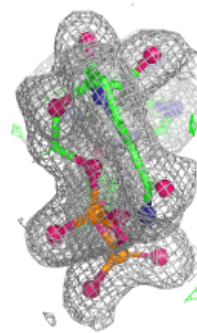
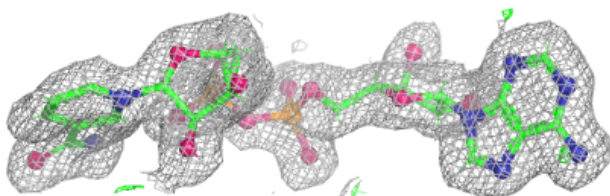
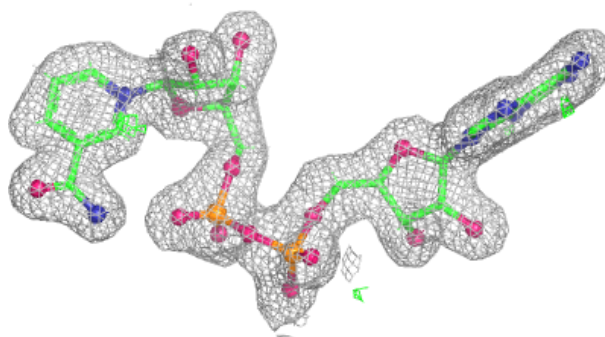


Electron density around NAD C 301:

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

**Electron density around NAD A 302:**

$2mF_o-DF_c$ (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.