



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:43 PM EDT

PDB ID : 6ZZS / pdb_00006zzs
Title : Crystal structure of (R)-3-hydroxybutyrate dehydrogenase from *Acinetobacter baumannii* complexed with NAD⁺ and 3-oxovalerate
Authors : Machado, T.F.G.; da Silva, R.G.; Gloster, T.M.; McMahon, S.A.; Oehler, V.
Deposited on : 2020-08-05
Resolution : 1.85 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

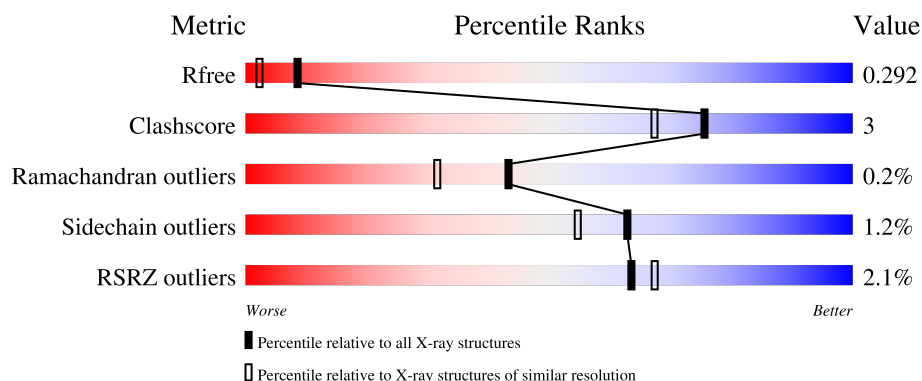
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	
1	B	261	
1	C	261	
1	D	261	
1	E	261	

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Mol	Chain	Length	Quality of chain
1	F	261	3% 85% 11%

2 Entry composition [i](#)

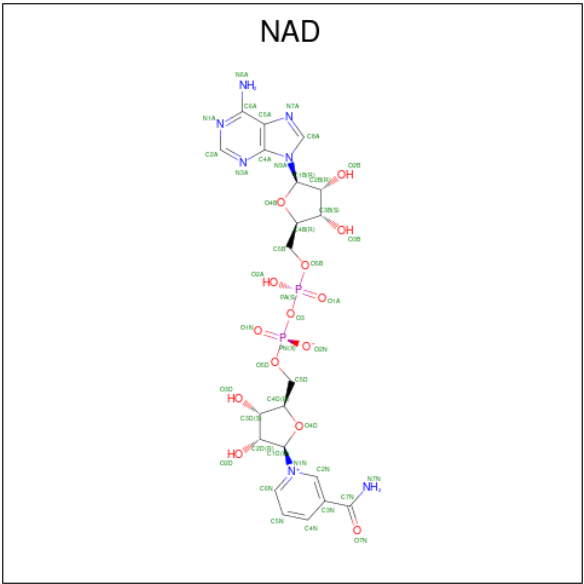
There are 4 unique types of molecules in this entry. The entry contains 12429 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-hydroxybutyrate dehydrogenase.

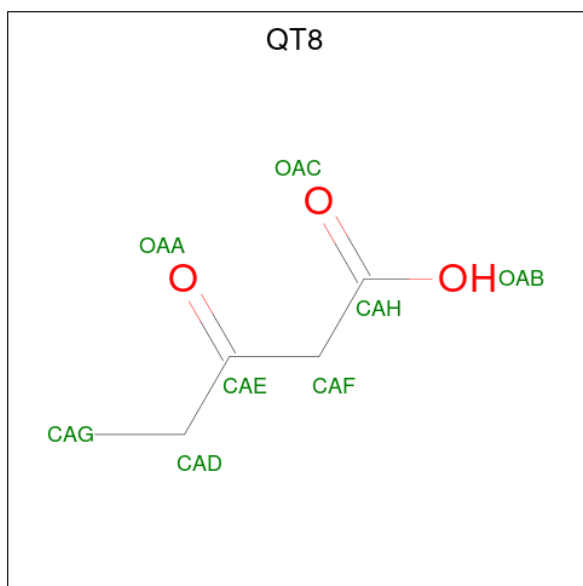
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	4	0
			1900	1208	314	366	12			
1	B	260	Total	C	N	O	S	0	5	0
			1906	1214	314	366	12			
1	C	260	Total	C	N	O	S	0	2	0
			1905	1212	317	365	11			
1	D	261	Total	C	N	O	S	0	3	0
			1906	1210	320	364	12			
1	E	254	Total	C	N	O	S	0	2	0
			1832	1168	302	350	12			
1	F	252	Total	C	N	O	S	0	2	0
			1823	1161	304	348	10			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
2	B	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
2	C	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
2	D	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
2	E	1	Total	C	N	O	P	0	1
			88	42	14	28	4		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is 3-oxidanylidene-pentanoic acid (CCD ID: QT8) (formula: $C_5H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	5	3		
3	B	1	Total	C	O	0	0
			8	5	3		
3	C	1	Total	C	O	0	0
			8	5	3		
3	C	1	Total	C	O	0	0
			8	5	3		
3	D	1	Total	C	O	0	0
			8	5	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			8	5	3		

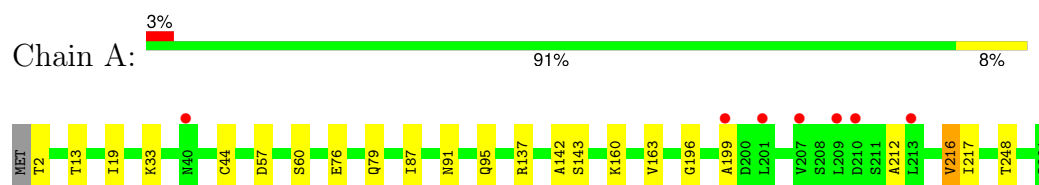
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	122	Total	O	0	2
			124	124		
4	B	123	Total	O	0	6
			129	129		
4	C	108	Total	O	0	5
			113	113		
4	D	118	Total	O	0	7
			125	125		
4	E	75	Total	O	0	1
			76	76		
4	F	57	Total	O	0	1
			58	58		

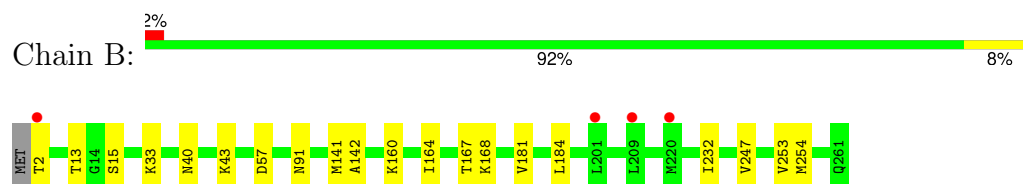
3 Residue-property plots [i](#)

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.

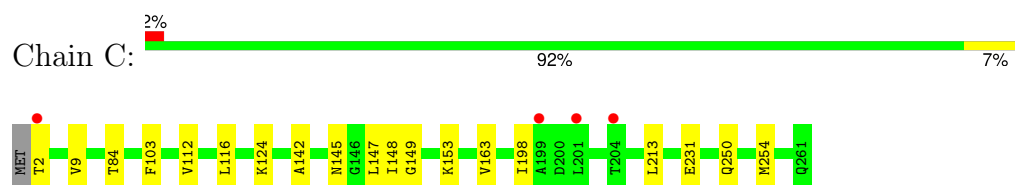
- Molecule 1: 3-hydroxybutyrate dehydrogenase



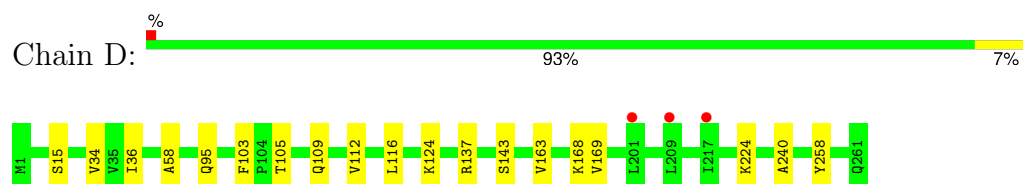
- Molecule 1: 3-hydroxybutyrate dehydrogenase



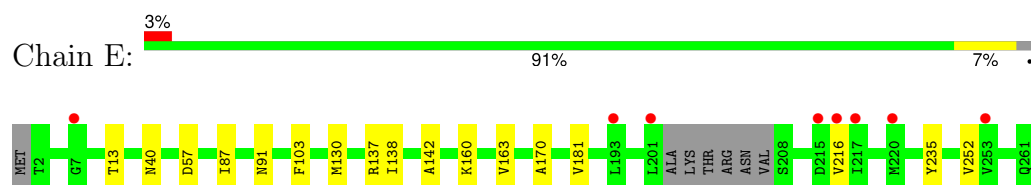
- Molecule 1: 3-hydroxybutyrate dehydrogenase



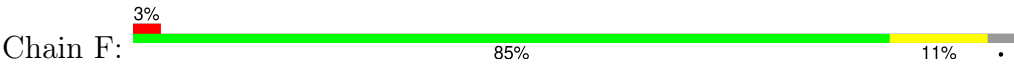
- Molecule 1: 3-hydroxybutyrate dehydrogenase



- Molecule 1: 3-hydroxybutyrate dehydrogenase



- Molecule 1: 3-hydroxybutyrate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.09Å 109.23Å 387.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.16 – 1.85 53.16 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (53.16-1.85) 99.7 (53.16-1.85)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.228 , 0.288 0.235 , 0.292	Depositor DCC
R_{free} test set	5828 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.710	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12429	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 81.17 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.7771e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: QT8, 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	1.07	0/1937	1.44	0/2621
1	B	1.08	0/1946	1.46	0/2632
1	C	1.07	0/1936	1.44	0/2619
1	D	1.07	0/1940	1.45	1/2620 (0.0%)
1	E	1.08	0/1862	1.46	0/2519
1	F	1.09	0/1853	1.46	0/2504
All	All	1.08	0/11474	1.45	1/15515 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	169	VAL	N-CA-C	-5.02	105.60	110.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1900	0	1911	11	0
1	B	1906	0	1929	14	0
1	C	1905	0	1929	15	0
1	D	1906	0	1928	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1832	0	1829	9	0
1	F	1823	0	1830	15	0
2	A	88	0	52	2	0
2	B	88	0	52	2	0
2	C	88	0	52	1	0
2	D	88	0	52	0	0
2	E	88	0	52	1	0
2	F	44	0	26	0	0
3	A	8	0	0	2	0
3	B	8	0	0	0	0
3	C	16	0	0	1	0
3	D	8	0	0	2	0
3	F	8	0	0	0	0
4	A	124	0	0	1	0
4	B	129	0	0	0	0
4	C	113	0	0	1	0
4	D	125	0	0	0	0
4	E	76	0	0	0	0
4	F	58	0	0	0	0
All	All	12429	0	11642	71	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 (71) 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:F:13:THR:O	1:F:91:ASN:HB3	1.84	0.76
1:C:142:ALA:O	2:C:301[A]:NAD:H6N	1.96	0.66
1:E:13:THR:O	1:E:91:ASN:HB3	2.01	0.61
1:D:95:GLN:HE21	3:D:302:QT8:CAH	2.16	0.59
1:A:143:SER:OG	3:A:302:QT8:CAG	2.51	0.58
1:F:8:LYS:HA	1:F:86:ASP:OD2	2.06	0.55
1:B:141[B]:MET:HE1	1:B:184[B]:LEU:HD22	1.89	0.55
1:B:247:VAL:HG22	1:C:254[A]:MET:HG3	1.90	0.54
1:B:142:ALA:O	2:B:301[A]:NAD:H6N	2.08	0.54
1:F:142:ALA:HA	1:F:160:LYS:HD2	1.90	0.53
1:A:76:GLU:HA	1:A:79:GLN:HE21	1.74	0.53
1:F:145:ASN:HB3	1:F:157:ASN:OD1	2.10	0.52
2:A:301[B]:NAD:H52A	4:A:411:HOH:O	2.11	0.51
1:E:235:TYR:CZ	1:E:252:VAL:CG1	2.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ALA:HA	1:B:160:LYS:HD2	1.93	0.50
1:A:142:ALA:HA	1:A:160:LYS:HD2	1.93	0.50
1:F:21:LEU:O	1:F:24:ALA:HB3	2.11	0.49
1:B:40:ASN:CG	1:B:43:LYS:HB2	2.38	0.49
1:A:212:ALA:O	1:A:216:VAL:HG13	2.13	0.49
1:C:124:LYS:NZ	1:D:103:PHE:O	2.39	0.48
1:A:95:GLN:HE21	3:A:302:QT8:CAH	2.26	0.48
1:A:19:ILE:HB	2:A:301[B]:NAD:H51N	1.95	0.48
1:C:103:PHE:O	1:D:124:LYS:NZ	2.38	0.48
1:E:130[B]:MET:HE1	1:E:138:ILE:HD11	1.95	0.48
1:E:103:PHE:O	1:F:124:LYS:NZ	2.42	0.48
1:C:148:ILE:HD12	1:C:148:ILE:C	2.40	0.47
1:F:136:GLY:O	1:F:179:ILE:HA	2.14	0.47
1:B:164[B]:ILE:HG22	1:B:168:LYS:HE3	1.96	0.47
1:D:112:VAL:O	1:D:116:LEU:HB3	2.15	0.47
1:A:196:GLY:O	1:A:199:ALA:HB3	2.14	0.47
1:C:147:LEU:O	1:D:168[A]:LYS:NZ	2.45	0.47
1:E:170:ALA:HB3	1:E:181:VAL:HG11	1.97	0.47
1:B:232:ILE:HA	1:B:254:MET:HE1	1.98	0.46
1:F:228:SER:OG	1:F:231:GLU:HG3	2.16	0.46
1:C:149:GLY:HA3	1:D:168[A]:LYS:HB3	1.98	0.46
1:F:167:THR:HG23	1:F:181:VAL:HG12	1.98	0.45
1:A:87:ILE:HA	1:A:137:ARG:O	2.17	0.45
1:B:160:LYS:O	1:B:164[B]:ILE:HG12	2.16	0.45
1:E:130[B]:MET:HE2	1:E:130[B]:MET:HB2	1.70	0.45
1:D:137:ARG:HG3	1:D:240:ALA:O	2.16	0.44
1:D:105:THR:O	1:D:109[A]:GLN:HG3	2.17	0.44
1:C:145:ASN:HD22	3:C:302:QT8:CAD	2.31	0.44
1:B:13:THR:O	1:B:91:ASN:HB3	2.18	0.44
1:E:142:ALA:HA	1:E:160:LYS:HD2	1.98	0.43
1:A:13:THR:O	1:A:91:ASN:HB3	2.19	0.43
1:C:198:ILE:HD11	1:C:213:LEU:HD13	2.00	0.43
1:C:9:VAL:HG11	1:C:84:THR:O	2.19	0.43
1:C:153:LYS:NZ	4:C:410:HOH:O	2.50	0.43
1:D:34:VAL:O	1:D:58:ALA:HA	2.19	0.43
1:D:258:TYR:CD1	1:D:258:TYR:C	2.97	0.43
1:E:87:ILE:HA	1:E:137:ARG:O	2.19	0.43
1:C:254[B]:MET:HB2	1:C:254[B]:MET:HE2	1.78	0.43
1:F:198:ILE:HD11	1:F:213:LEU:HD13	2.00	0.42
1:D:143:SER:OG	3:D:302:QT8:CAG	2.67	0.42
1:B:33:LYS:HG2	1:B:57:ASP:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:THR:HG23	1:B:181:VAL:HG12	2.02	0.42
1:E:142:ALA:O	2:E:301[B]:NAD:H6N	2.20	0.42
1:C:112:VAL:O	1:C:116:LEU:HB3	2.19	0.42
1:F:137:ARG:HG3	1:F:240:ALA:O	2.20	0.42
1:A:44:CYS:HB3	1:A:60:SER:OG	2.19	0.42
1:F:39:MET:HE1	1:F:64:ASP:OD2	2.19	0.42
1:D:224:LYS:HD3	1:D:224:LYS:HA	1.81	0.41
1:D:15:SER:OG	1:D:36:ILE:HA	2.20	0.41
1:C:231:GLU:O	1:C:254[A]:MET:HE1	2.20	0.41
1:B:142:ALA:O	2:B:301[B]:NAD:H6N	2.19	0.41
1:A:33:LYS:HG2	1:A:57:ASP:HB2	2.03	0.41
1:F:87:ILE:HA	1:F:137:ARG:O	2.21	0.40
1:F:97:VAL:O	1:F:98:ALA:HB2	2.20	0.40
1:F:174:CYS:SG	1:F:179:ILE:CG2	3.09	0.40
1:B:253:VAL:HB	1:C:250:GLN:CD	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	262/261 (100%)	255 (97%)	7 (3%)	0	100	100
1	B	263/261 (101%)	255 (97%)	8 (3%)	0	100	100
1	C	260/261 (100%)	251 (96%)	9 (4%)	0	100	100
1	D	262/261 (100%)	255 (97%)	7 (3%)	0	100	100
1	E	252/261 (97%)	241 (96%)	9 (4%)	2 (1%)	16	6
1	F	250/261 (96%)	238 (95%)	11 (4%)	1 (0%)	30	17
All	All	1549/1566 (99%)	1495 (96%)	51 (3%)	3 (0%)	43	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	40	ASN
1	E	216	VAL
1	F	40	ASN

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	193/202 (96%)	188 (97%)	5 (3%)	40	25
1	B	195/202 (96%)	193 (99%)	2 (1%)	68	60
1	C	194/202 (96%)	192 (99%)	2 (1%)	68	60
1	D	193/202 (96%)	192 (100%)	1 (0%)	81	77
1	E	182/202 (90%)	180 (99%)	2 (1%)	65	57
1	F	183/202 (91%)	181 (99%)	2 (1%)	65	57
All	All	1140/1212 (94%)	1126 (99%)	14 (1%)	63	55

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	163	VAL
1	A	216	VAL
1	A	217	ILE
1	A	248	THR
1	B	2	THR
1	B	15	SER
1	C	2	THR
1	C	163	VAL
1	D	163	VAL
1	E	57	ASP
1	E	163	VAL
1	F	197	GLN
1	F	211	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	B	79	GLN
1	B	113	GLN
1	C	73	GLN
1	C	109	GLN
1	C	145	ASN
1	C	157	ASN
1	C	261	GLN
1	D	79	GLN
1	D	250	GLN
1	F	96	HIS
1	F	197	GLN
1	F	223	GLN
1	F	261	GLN

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](#)

17 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	A	301[B]	-	46,48,48	0.90	3 (6%)	64,73,73	0.70	1 (1%)
3	QT8	C	302	-	7,7,7	0.96	0	8,8,8	2.13	1 (12%)
2	NAD	D	301[A]	-	46,48,48	0.84	3 (6%)	64,73,73	0.68	1 (1%)
2	NAD	E	301[A]	-	46,48,48	0.78	2 (4%)	64,73,73	0.77	2 (3%)
2	NAD	A	301[A]	-	46,48,48	0.88	4 (8%)	64,73,73	0.69	1 (1%)
3	QT8	A	302	-	7,7,7	0.96	0	8,8,8	2.57	2 (25%)
3	QT8	B	302	-	7,7,7	1.08	0	8,8,8	1.55	1 (12%)
3	QT8	F	302	-	7,7,7	1.07	0	8,8,8	1.74	1 (12%)
3	QT8	D	302	-	7,7,7	0.75	0	8,8,8	2.45	3 (37%)
2	NAD	E	301[B]	-	46,48,48	0.90	3 (6%)	64,73,73	0.72	1 (1%)
2	NAD	D	301[B]	-	46,48,48	0.72	1 (2%)	64,73,73	0.55	1 (1%)
2	NAD	C	301[B]	-	46,48,48	0.67	1 (2%)	64,73,73	0.61	1 (1%)
2	NAD	F	301	-	46,48,48	0.71	1 (2%)	64,73,73	0.71	1 (1%)
2	NAD	C	301[A]	-	46,48,48	0.77	2 (4%)	64,73,73	0.69	1 (1%)
2	NAD	B	301[B]	-	46,48,48	0.73	2 (4%)	64,73,73	0.70	1 (1%)
3	QT8	C	303	-	7,7,7	1.25	0	8,8,8	1.04	0
2	NAD	B	301[A]	-	46,48,48	0.81	2 (4%)	64,73,73	0.68	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	A	301[B]	-	-	7/30/62/62	0/5/5/5
3	QT8	C	302	-	-	2/6/6/6	-
2	NAD	D	301[A]	-	-	8/30/62/62	0/5/5/5
2	NAD	E	301[A]	-	-	4/30/62/62	0/5/5/5
2	NAD	A	301[A]	-	-	11/30/62/62	0/5/5/5
3	QT8	A	302	-	-	2/6/6/6	-
3	QT8	B	302	-	-	3/6/6/6	-
3	QT8	F	302	-	-	5/6/6/6	-
3	QT8	D	302	-	-	4/6/6/6	-
2	NAD	E	301[B]	-	-	8/30/62/62	0/5/5/5
2	NAD	D	301[B]	-	-	9/30/62/62	0/5/5/5
2	NAD	C	301[B]	-	-	4/30/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	F	301	-	-	3/30/62/62	0/5/5/5
2	NAD	C	301[A]	-	-	3/30/62/62	0/5/5/5
2	NAD	B	301[B]	-	-	6/30/62/62	0/5/5/5
3	QT8	C	303	-	-	4/6/6/6	-
2	NAD	B	301[A]	-	-	8/30/62/62	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301[B]	NAD	C2N-N1N	3.78	1.39	1.35
2	B	301[A]	NAD	C2N-N1N	3.66	1.39	1.35
2	A	301[B]	NAD	C2N-N1N	3.60	1.38	1.35
2	F	301	NAD	C2N-N1N	3.37	1.38	1.35
2	D	301[A]	NAD	C2N-N1N	3.32	1.38	1.35
2	A	301[B]	NAD	O4D-C1D	3.22	1.45	1.40
2	E	301[A]	NAD	C2N-N1N	3.21	1.38	1.35
2	A	301[A]	NAD	C2N-N1N	3.09	1.38	1.35
2	C	301[A]	NAD	O4D-C1D	2.98	1.44	1.40
2	D	301[B]	NAD	C2N-N1N	2.89	1.38	1.35
2	A	301[A]	NAD	PN-O3	2.84	1.62	1.59
2	B	301[B]	NAD	C2N-N1N	2.78	1.38	1.35
2	E	301[B]	NAD	O4D-C1D	2.53	1.44	1.40
2	A	301[A]	NAD	PA-O3	2.51	1.62	1.59
2	C	301[A]	NAD	C2N-N1N	2.47	1.37	1.35
2	D	301[A]	NAD	PN-O3	2.44	1.62	1.59
2	C	301[B]	NAD	O4D-C1D	2.39	1.44	1.40
2	B	301[B]	NAD	O4D-C1D	2.35	1.44	1.40
2	A	301[A]	NAD	O4D-C1D	2.29	1.43	1.40
2	D	301[A]	NAD	O4D-C1D	2.27	1.43	1.40
2	E	301[B]	NAD	PN-O3	2.24	1.61	1.59
2	A	301[B]	NAD	PN-O3	2.16	1.61	1.59
2	B	301[A]	NAD	PN-O3	2.14	1.61	1.59
2	E	301[A]	NAD	PN-O3	2.09	1.61	1.59

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	QT8	CAE-CAF-CAH	-6.32	99.69	112.32
3	D	302	QT8	CAE-CAF-CAH	-5.63	101.07	112.32
3	C	302	QT8	CAE-CAF-CAH	-5.50	101.31	112.32
3	F	302	QT8	CAE-CAF-CAH	-4.45	103.43	112.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301[A]	NAD	C6N-N1N-C2N	-4.18	118.32	121.88
3	B	302	QT8	CAE-CAF-CAH	-3.68	104.96	112.32
2	A	301[A]	NAD	C6N-N1N-C2N	-3.61	118.80	121.88
2	E	301[B]	NAD	C6N-N1N-C2N	-3.56	118.84	121.88
2	F	301	NAD	C6N-N1N-C2N	-3.28	119.08	121.88
2	B	301[B]	NAD	C6N-N1N-C2N	-3.19	119.16	121.88
2	C	301[A]	NAD	C6N-N1N-C2N	-3.00	119.33	121.88
2	B	301[A]	NAD	C6N-N1N-C2N	-2.65	119.62	121.88
2	C	301[B]	NAD	C6N-N1N-C2N	-2.56	119.70	121.88
3	D	302	QT8	OAC-CAH-CAF	-2.53	114.90	122.11
2	A	301[B]	NAD	C6N-N1N-C2N	-2.48	119.77	121.88
2	D	301[A]	NAD	C6N-N1N-C2N	-2.37	119.86	121.88
2	E	301[A]	NAD	C5N-C4N-C3N	-2.35	118.06	120.36
2	D	301[B]	NAD	C6N-N1N-C2N	-2.32	119.91	121.88
3	D	302	QT8	CAG-CAD-CAE	-2.22	102.62	115.21
3	A	302	QT8	OAB-CAH-OAC	2.11	128.76	123.33

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301[A]	NAD	C5D-O5D-PN-O3
2	A	301[A]	NAD	C5D-O5D-PN-O2N
2	A	301[A]	NAD	O4D-C1D-N1N-C2N
2	A	301[A]	NAD	O4D-C1D-N1N-C6N
2	A	301[B]	NAD	C5D-O5D-PN-O2N
2	A	301[B]	NAD	O4D-C1D-N1N-C2N
2	B	301[A]	NAD	C5D-O5D-PN-O3
2	B	301[A]	NAD	C5D-O5D-PN-O2N
2	B	301[A]	NAD	O4D-C1D-N1N-C2N
2	B	301[B]	NAD	C5B-O5B-PA-O1A
2	B	301[B]	NAD	O4D-C1D-N1N-C2N
2	C	301[A]	NAD	C5D-O5D-PN-O2N
2	C	301[A]	NAD	O4D-C1D-N1N-C2N
2	C	301[B]	NAD	C5B-O5B-PA-O1A
2	C	301[B]	NAD	C5B-O5B-PA-O2A
2	C	301[B]	NAD	C5B-O5B-PA-O3
2	C	301[B]	NAD	PA-O3-PN-O5D
2	D	301[A]	NAD	C5B-O5B-PA-O1A
2	D	301[A]	NAD	C5B-O5B-PA-O2A
2	D	301[B]	NAD	C5B-O5B-PA-O1A
2	D	301[B]	NAD	C5B-O5B-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	D	301[B]	NAD	O4B-C4B-C5B-O5B
2	D	301[B]	NAD	O4D-C1D-N1N-C2N
2	E	301[A]	NAD	C5D-O5D-PN-O2N
2	E	301[B]	NAD	C5B-O5B-PA-O1A
2	E	301[B]	NAD	C5B-O5B-PA-O2A
2	E	301[B]	NAD	C5B-O5B-PA-O3
2	E	301[B]	NAD	PA-O3-PN-O5D
2	E	301[B]	NAD	C5D-O5D-PN-O2N
2	E	301[B]	NAD	O4D-C1D-N1N-C2N
2	F	301	NAD	O4D-C1D-N1N-C2N
3	A	302	QT8	CAG-CAD-CAE-CAF
3	C	303	QT8	CAG-CAD-CAE-OAA
3	F	302	QT8	CAG-CAD-CAE-OAA
2	D	301[B]	NAD	C3B-C4B-C5B-O5B
2	A	301[A]	NAD	O4D-C4D-C5D-O5D
2	D	301[A]	NAD	O4B-C4B-C5B-O5B
3	A	302	QT8	CAG-CAD-CAE-OAA
3	C	302	QT8	CAG-CAD-CAE-OAA
3	D	302	QT8	CAG-CAD-CAE-OAA
3	B	302	QT8	CAG-CAD-CAE-CAF
3	C	302	QT8	CAG-CAD-CAE-CAF
3	C	303	QT8	CAG-CAD-CAE-CAF
3	D	302	QT8	CAG-CAD-CAE-CAF
3	F	302	QT8	CAG-CAD-CAE-CAF
2	A	301[A]	NAD	C3D-C4D-C5D-O5D
2	D	301[A]	NAD	C3B-C4B-C5B-O5B
2	A	301[B]	NAD	PA-O3-PN-O5D
2	D	301[A]	NAD	PA-O3-PN-O5D
3	F	302	QT8	CAE-CAF-CAH-OAB
3	B	302	QT8	CAG-CAD-CAE-OAA
2	D	301[B]	NAD	PA-O3-PN-O1N
3	C	303	QT8	CAD-CAE-CAF-CAH
3	D	302	QT8	CAD-CAE-CAF-CAH
3	F	302	QT8	CAD-CAE-CAF-CAH
2	A	301[A]	NAD	C5D-O5D-PN-O1N
2	A	301[B]	NAD	C5D-O5D-PN-O3
2	B	301[A]	NAD	C5D-O5D-PN-O1N
2	D	301[A]	NAD	C5B-O5B-PA-O3
2	D	301[B]	NAD	C5B-O5B-PA-O3
2	E	301[A]	NAD	C5D-O5D-PN-O3
2	E	301[A]	NAD	C5D-O5D-PN-O1N
2	B	301[A]	NAD	O4B-C4B-C5B-O5B

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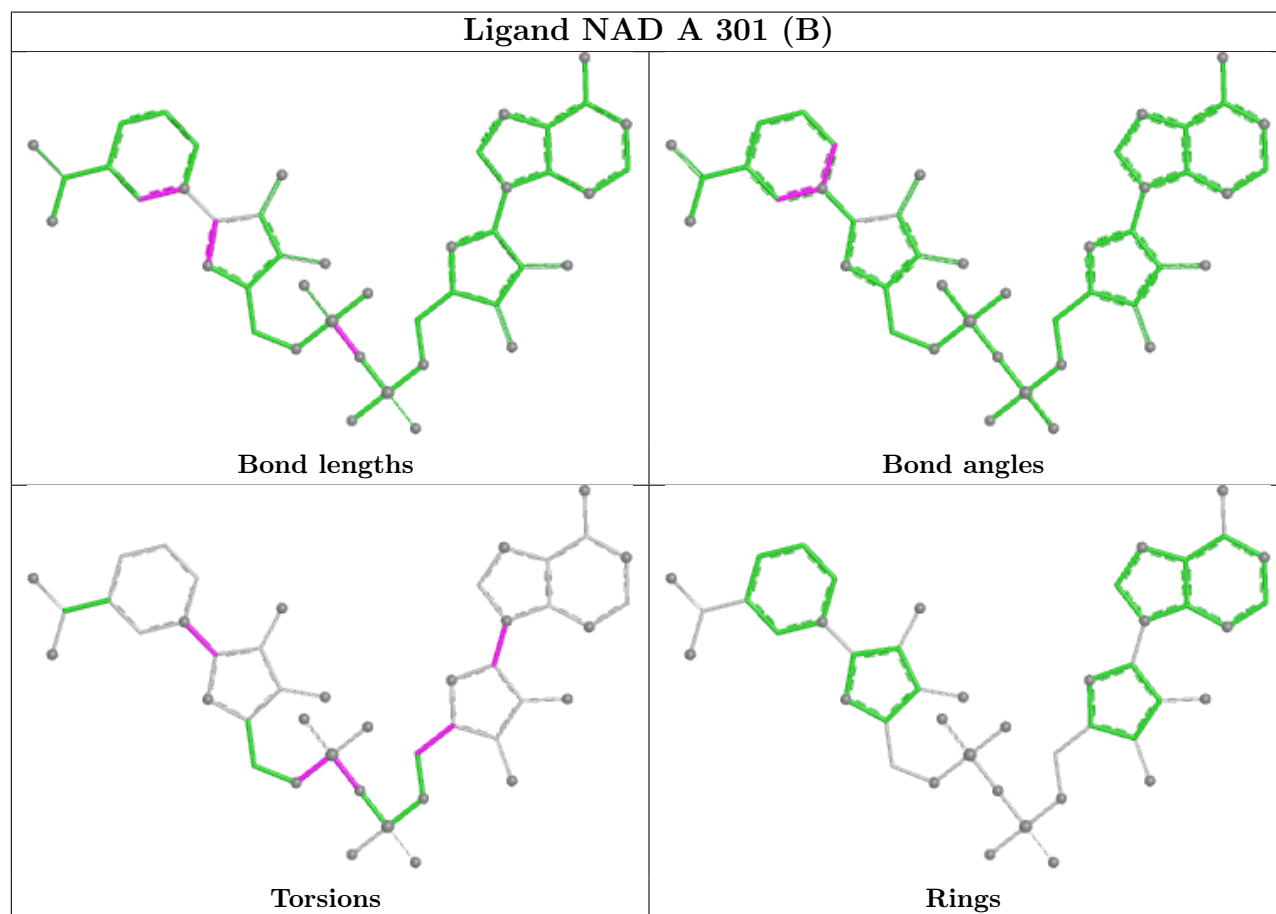
Mol	Chain	Res	Type	Atoms
2	B	301[B]	NAD	O4B-C4B-C5B-O5B
3	F	302	QT8	CAE-CAF-CAH-OAC
2	A	301[A]	NAD	C2D-C1D-N1N-C2N
2	A	301[A]	NAD	C2D-C1D-N1N-C6N
2	A	301[B]	NAD	O4D-C1D-N1N-C6N
2	B	301[A]	NAD	O4D-C1D-N1N-C6N
2	B	301[B]	NAD	O4D-C1D-N1N-C6N
2	C	301[A]	NAD	O4D-C1D-N1N-C6N
2	D	301[A]	NAD	O4D-C1D-N1N-C2N
2	D	301[A]	NAD	O4D-C1D-N1N-C6N
2	D	301[B]	NAD	O4D-C1D-N1N-C6N
2	E	301[A]	NAD	O4D-C1D-N1N-C2N
2	E	301[B]	NAD	O4D-C1D-N1N-C6N
2	F	301	NAD	O4D-C1D-N1N-C6N
3	C	303	QT8	OAA-CAE-CAF-CAH
3	D	302	QT8	OAA-CAE-CAF-CAH
2	A	301[B]	NAD	C2B-C1B-N9A-C8A
2	A	301[A]	NAD	PA-O3-PN-O1N
2	A	301[A]	NAD	PA-O3-PN-O2N
2	B	301[A]	NAD	PA-O3-PN-O1N
2	B	301[A]	NAD	PA-O3-PN-O2N
2	D	301[B]	NAD	PA-O3-PN-O2N
2	E	301[B]	NAD	PN-O3-PA-O1A
3	B	302	QT8	CAD-CAE-CAF-CAH
2	B	301[B]	NAD	C3B-C4B-C5B-O5B
2	F	301	NAD	O4B-C4B-C5B-O5B
2	B	301[B]	NAD	C2B-C1B-N9A-C8A
2	A	301[B]	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

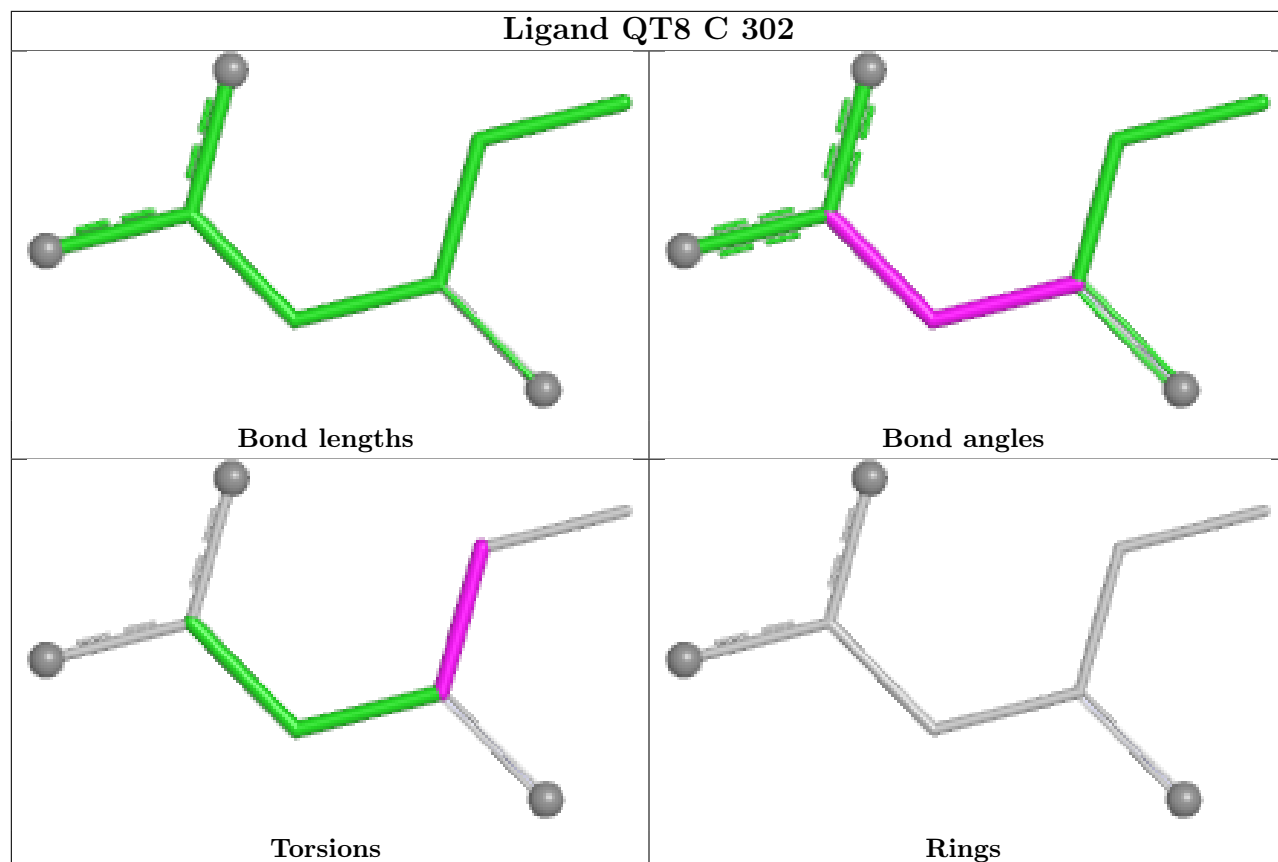
8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301[B]	NAD	2	0
3	C	302	QT8	1	0
3	A	302	QT8	2	0
3	D	302	QT8	2	0
2	E	301[B]	NAD	1	0
2	C	301[A]	NAD	1	0
2	B	301[B]	NAD	1	0
2	B	301[A]	NAD	1	0

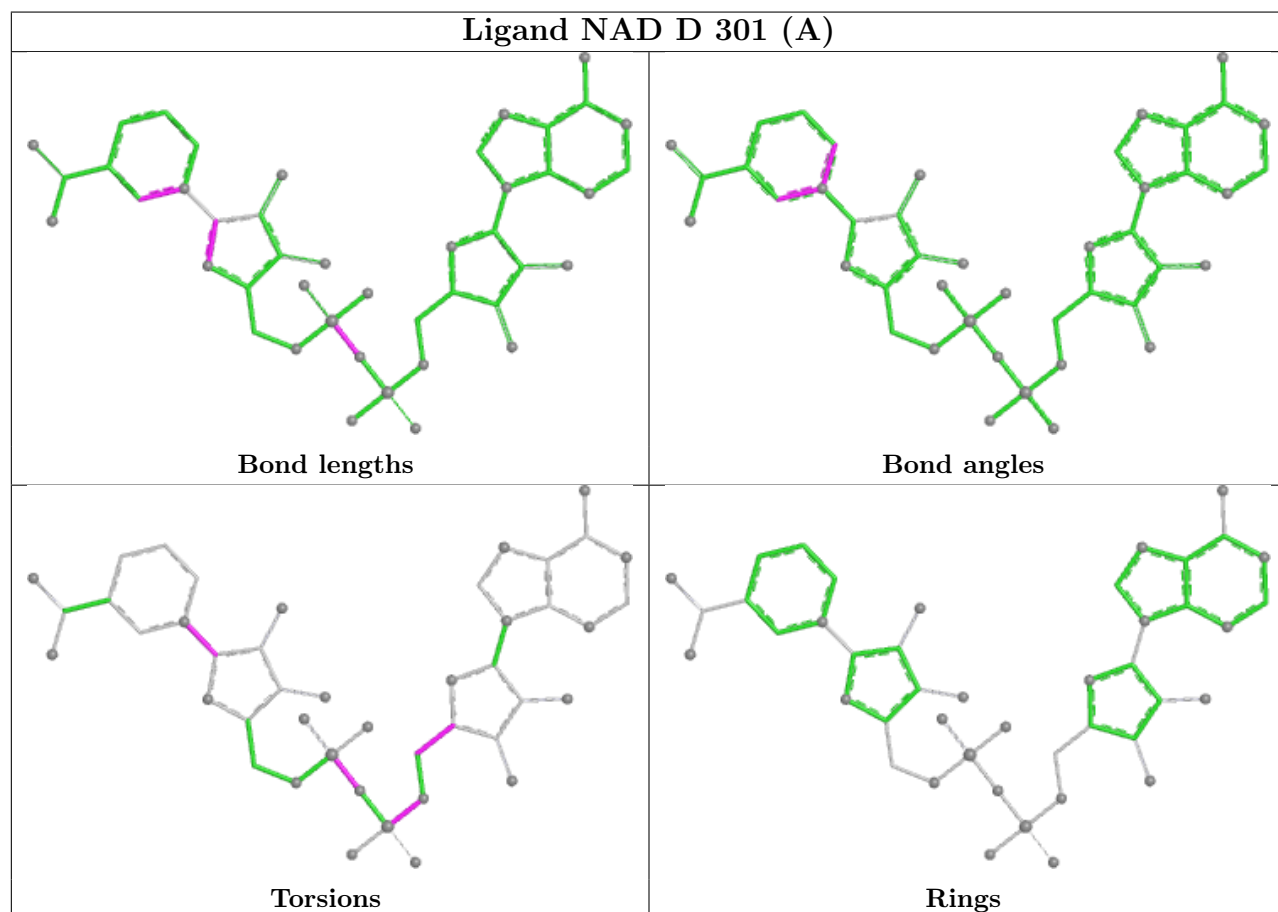
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

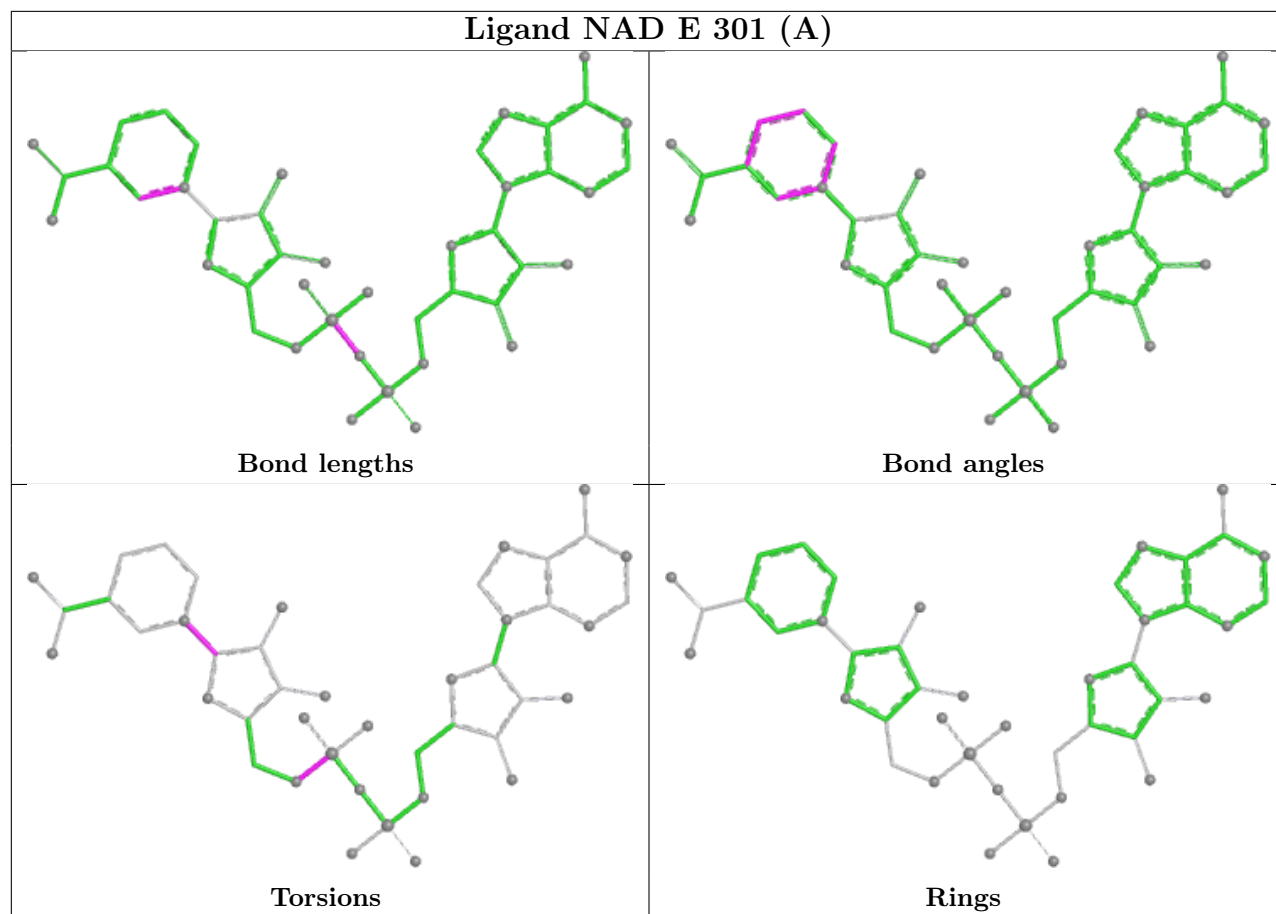


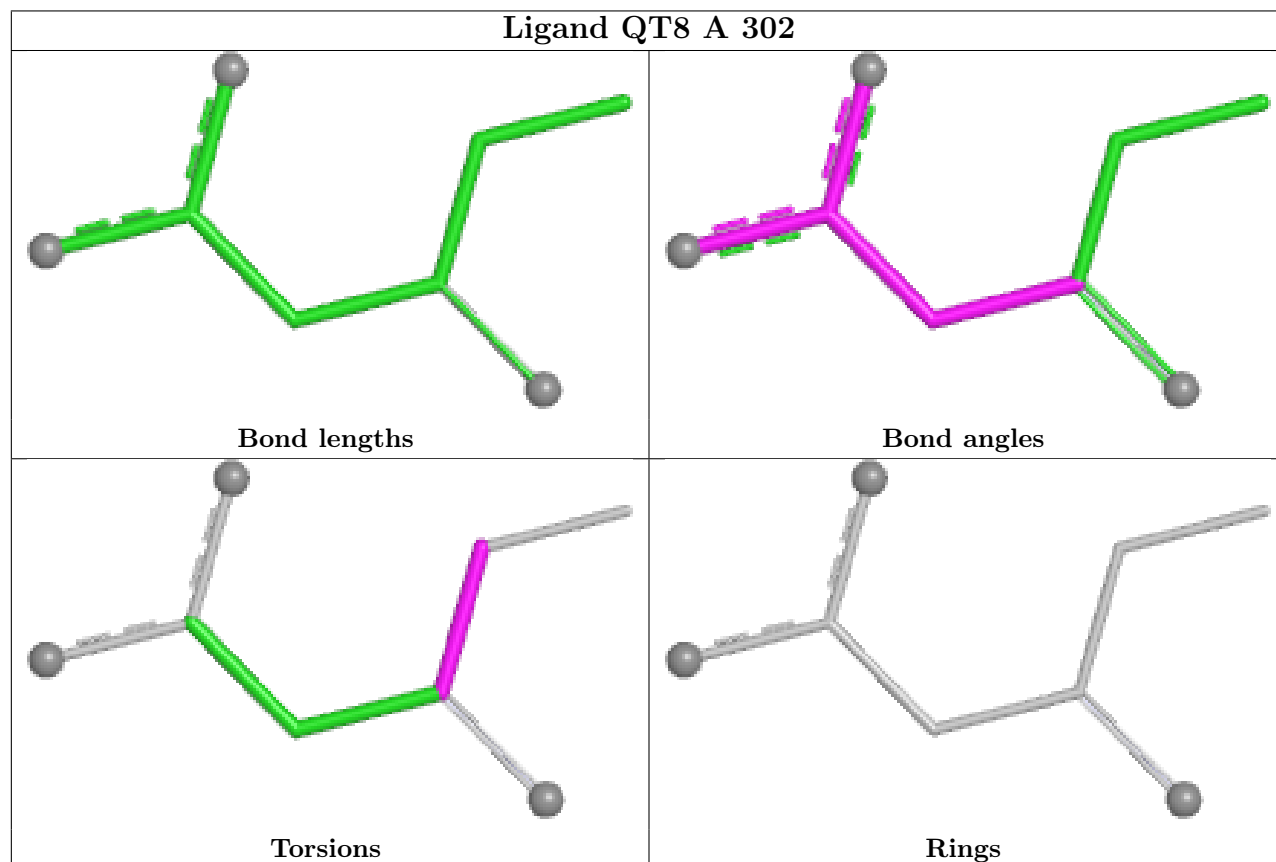
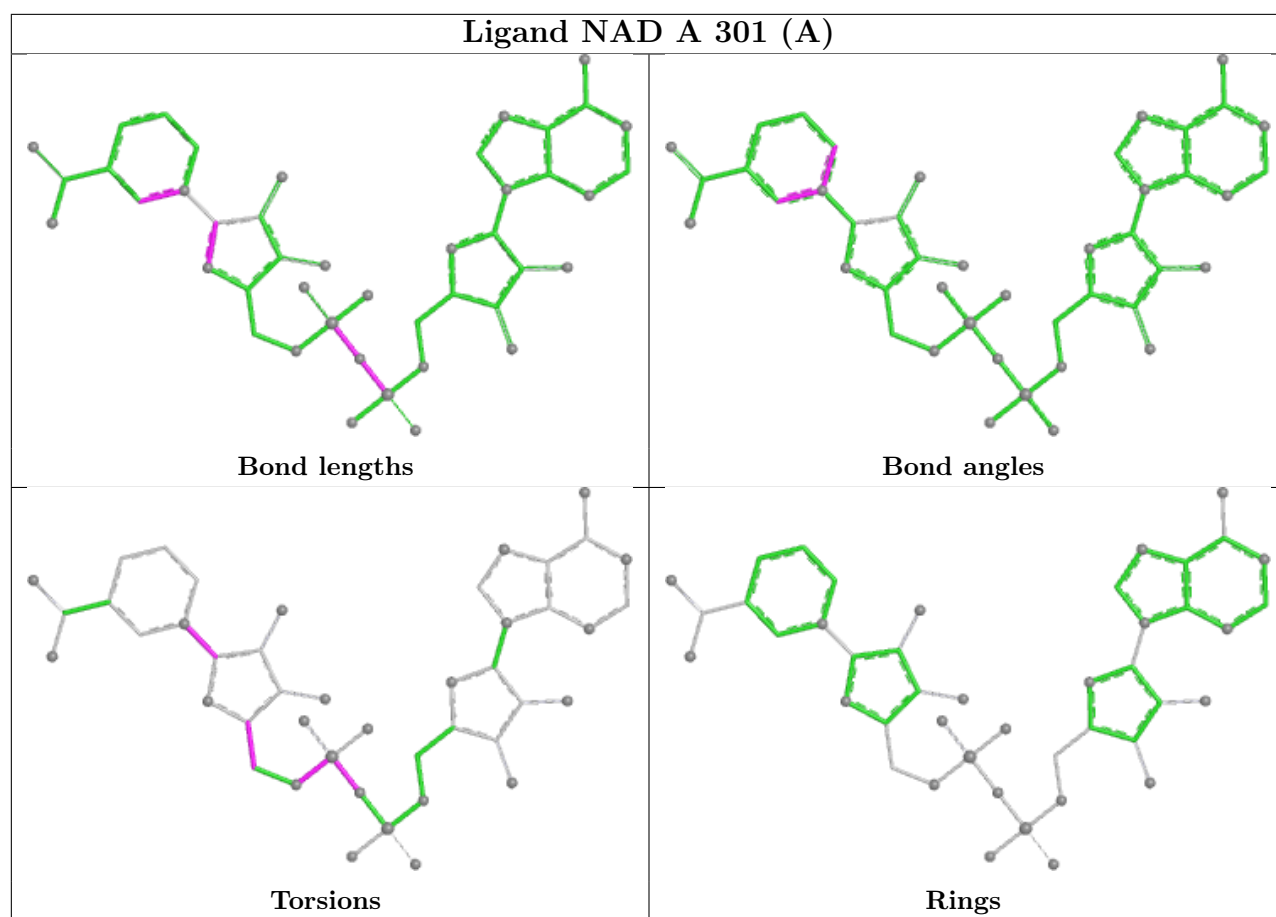
Ligand QT8 C 302



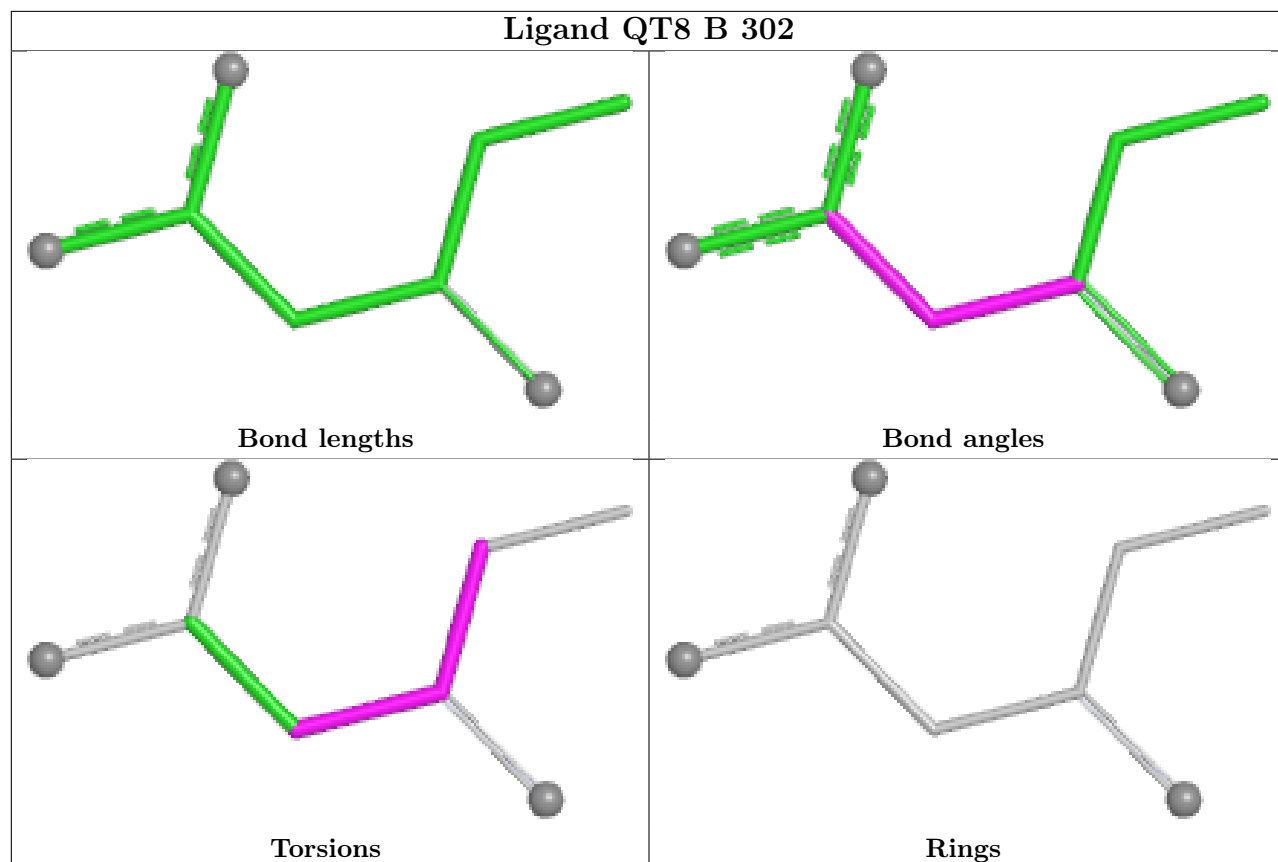
Ligand NAD D 301 (A)



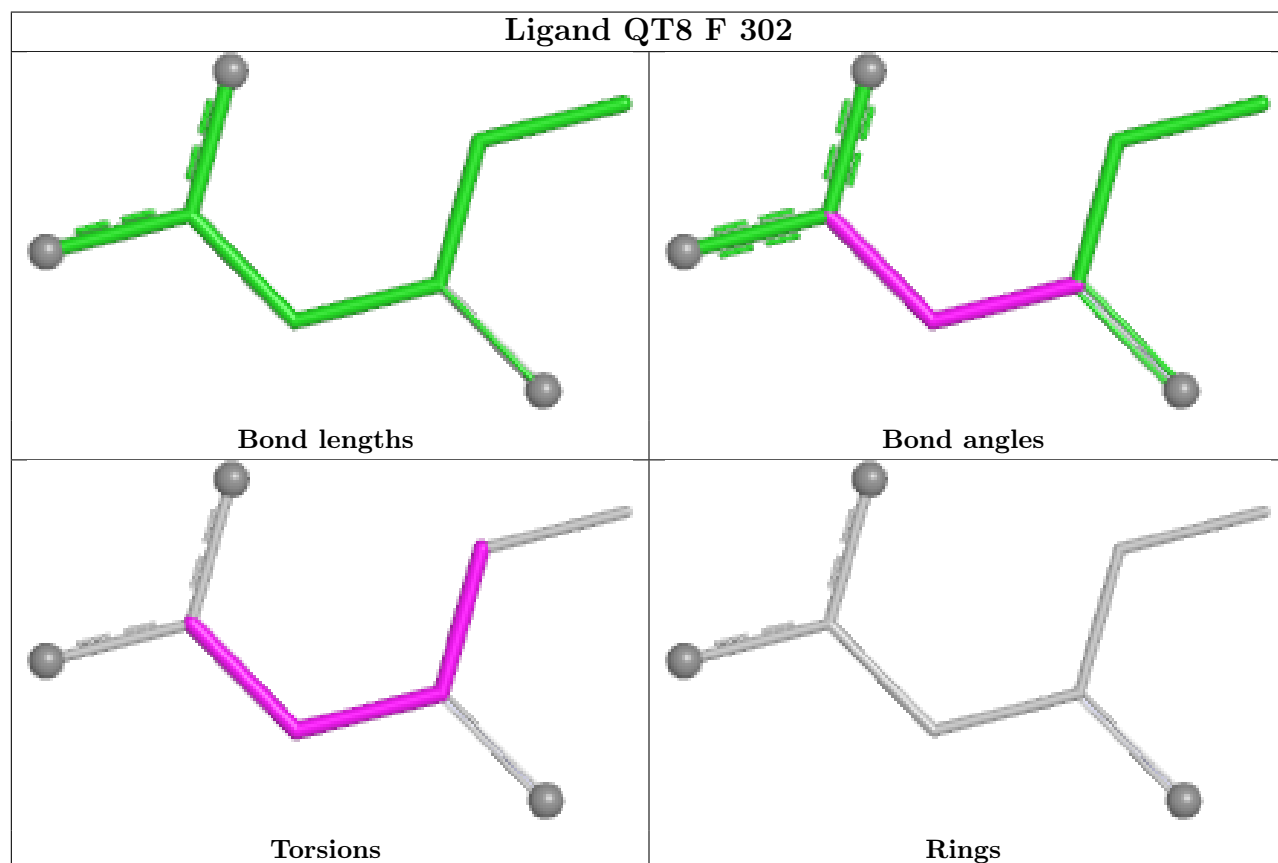


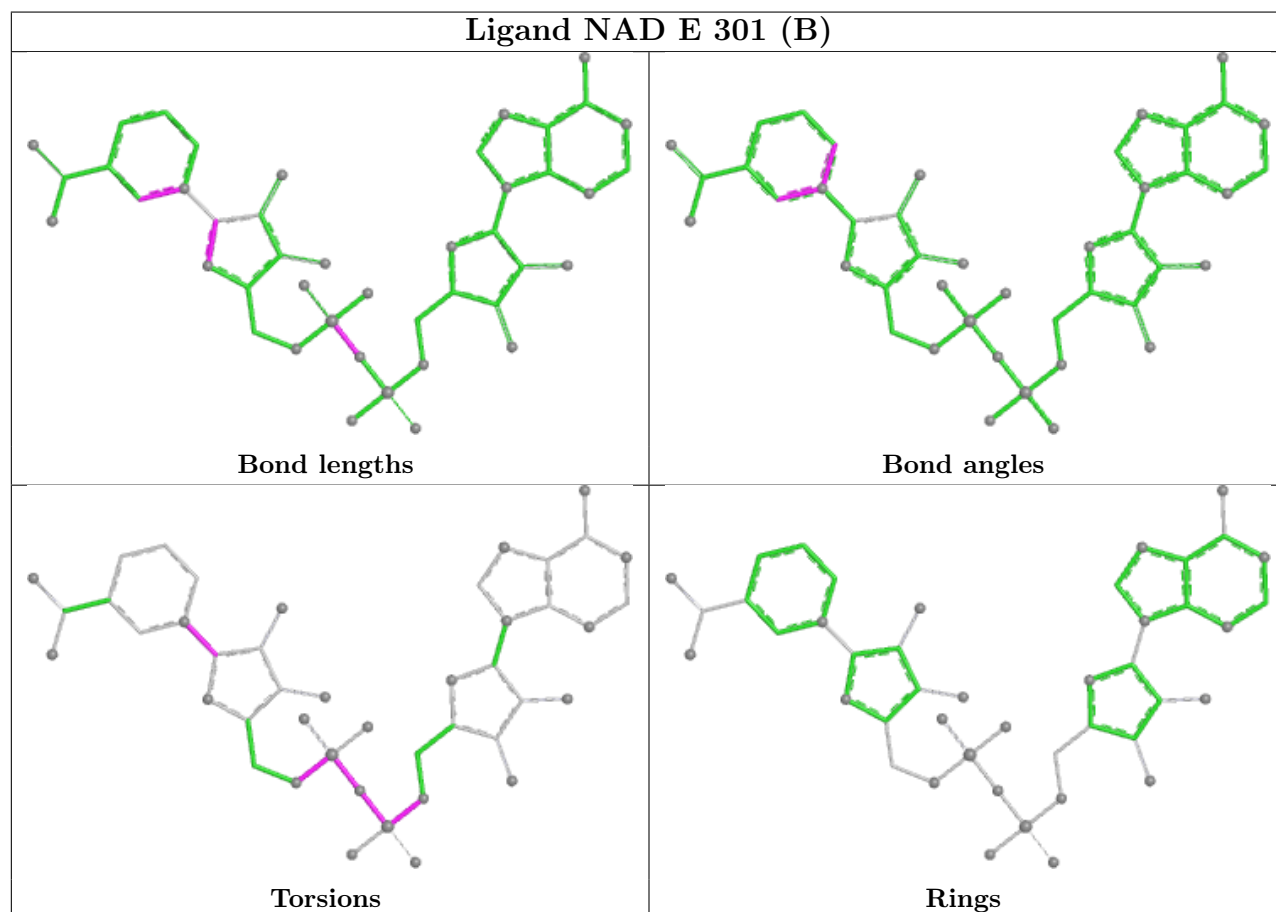
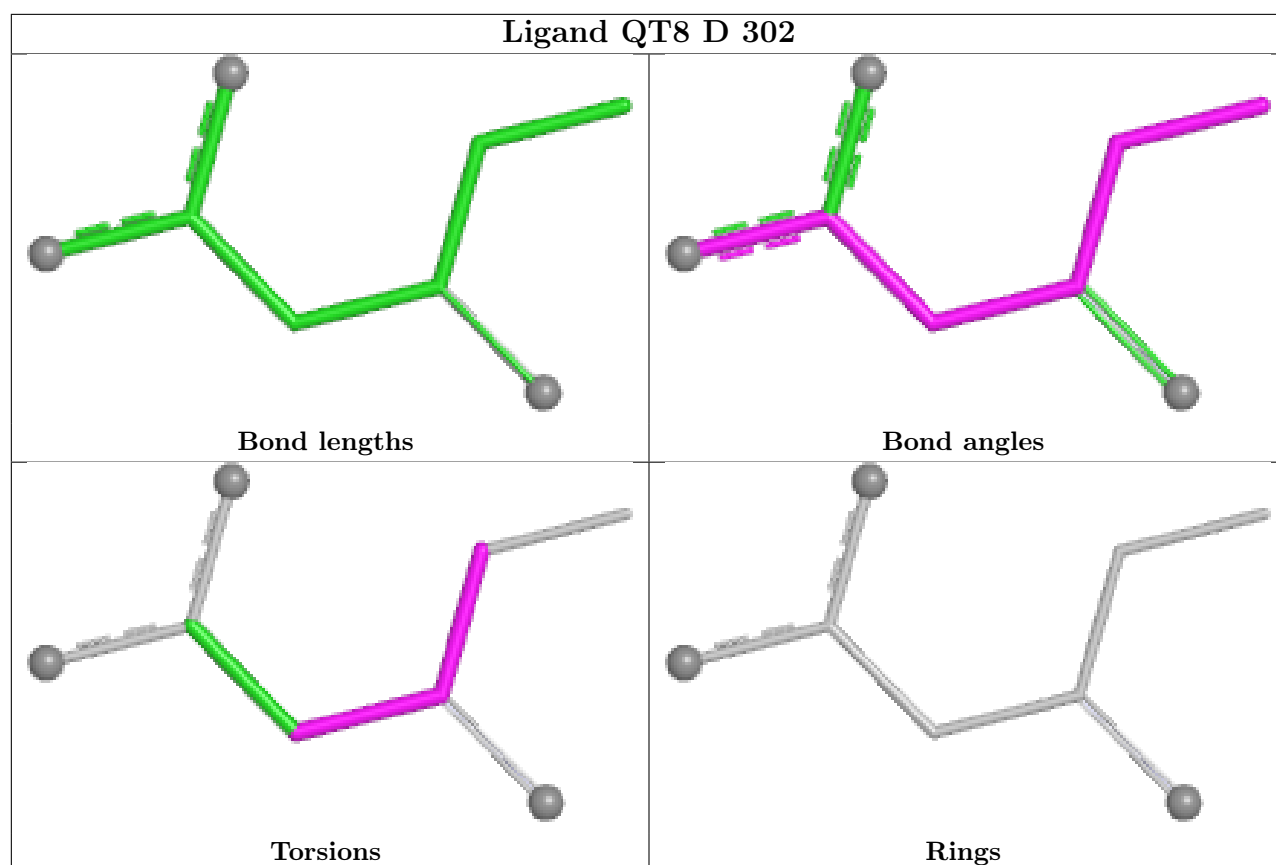


Ligand QT8 B 302

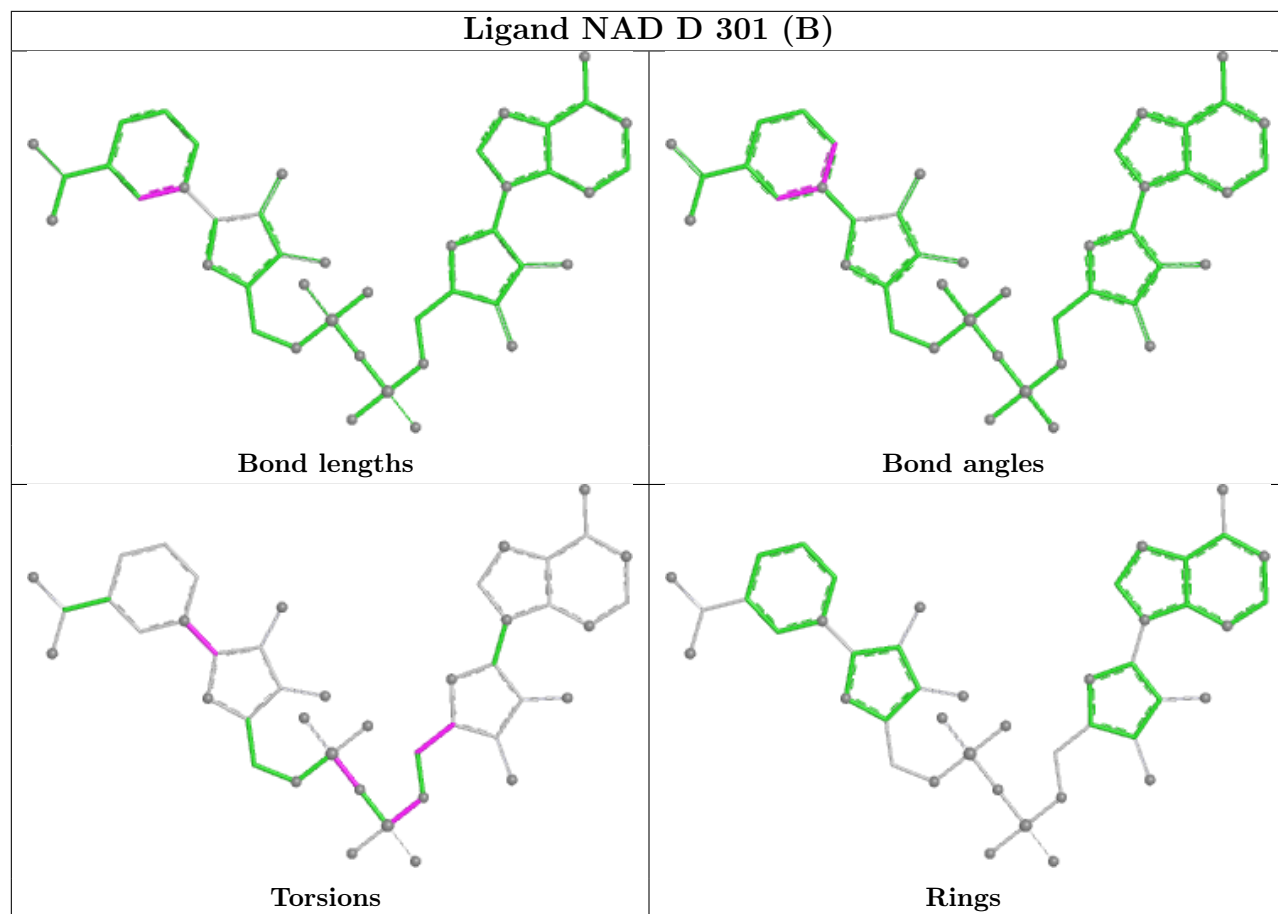


Ligand QT8 F 302

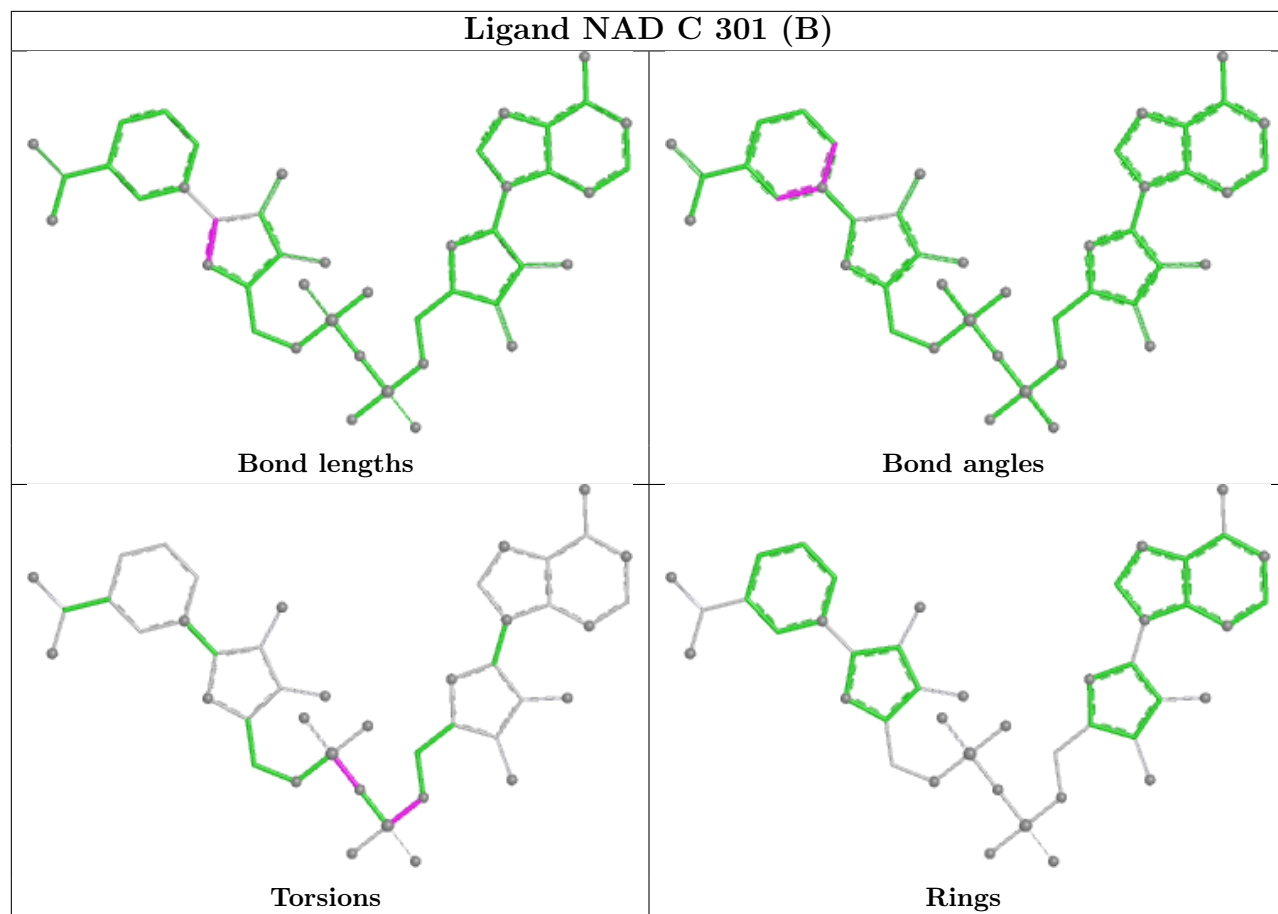


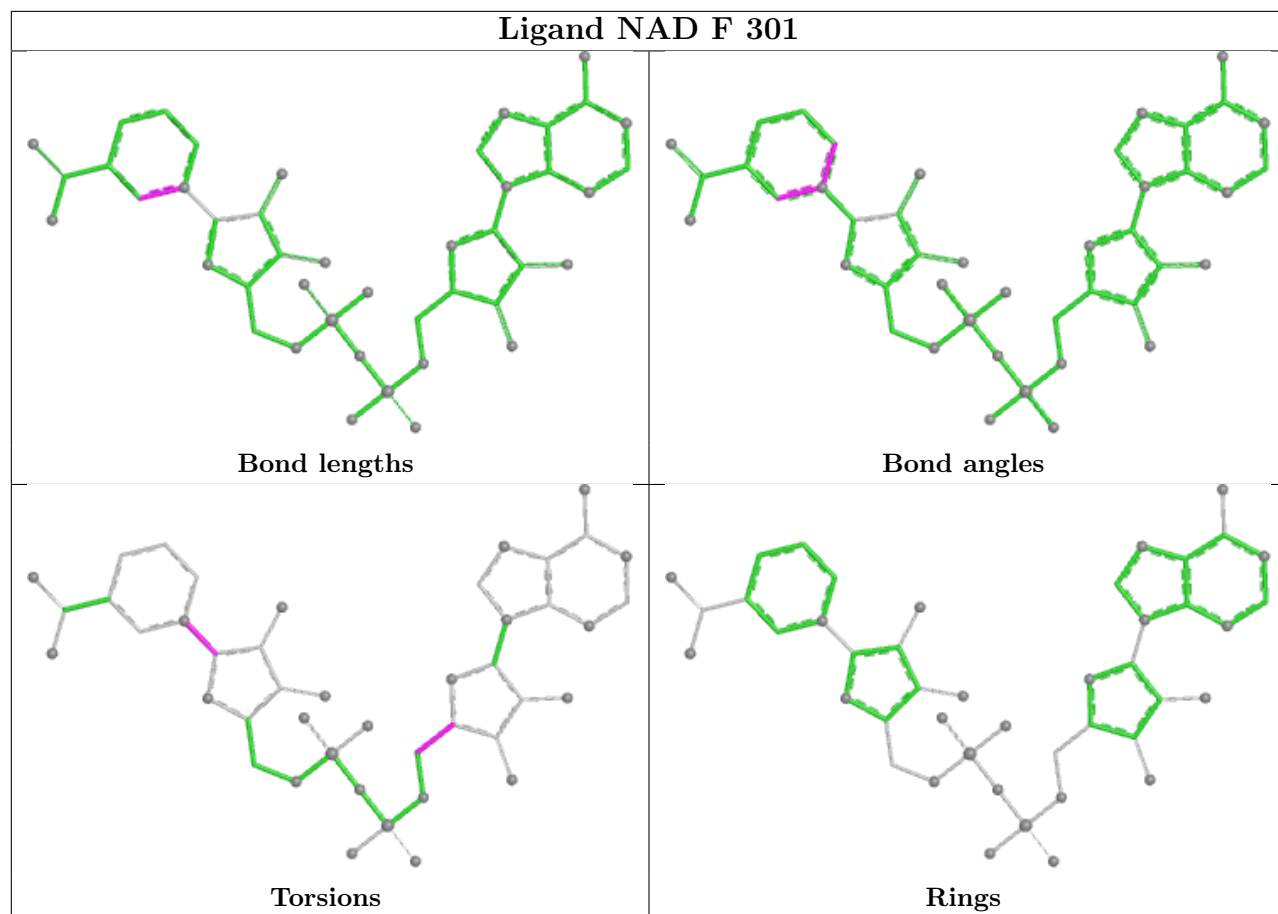


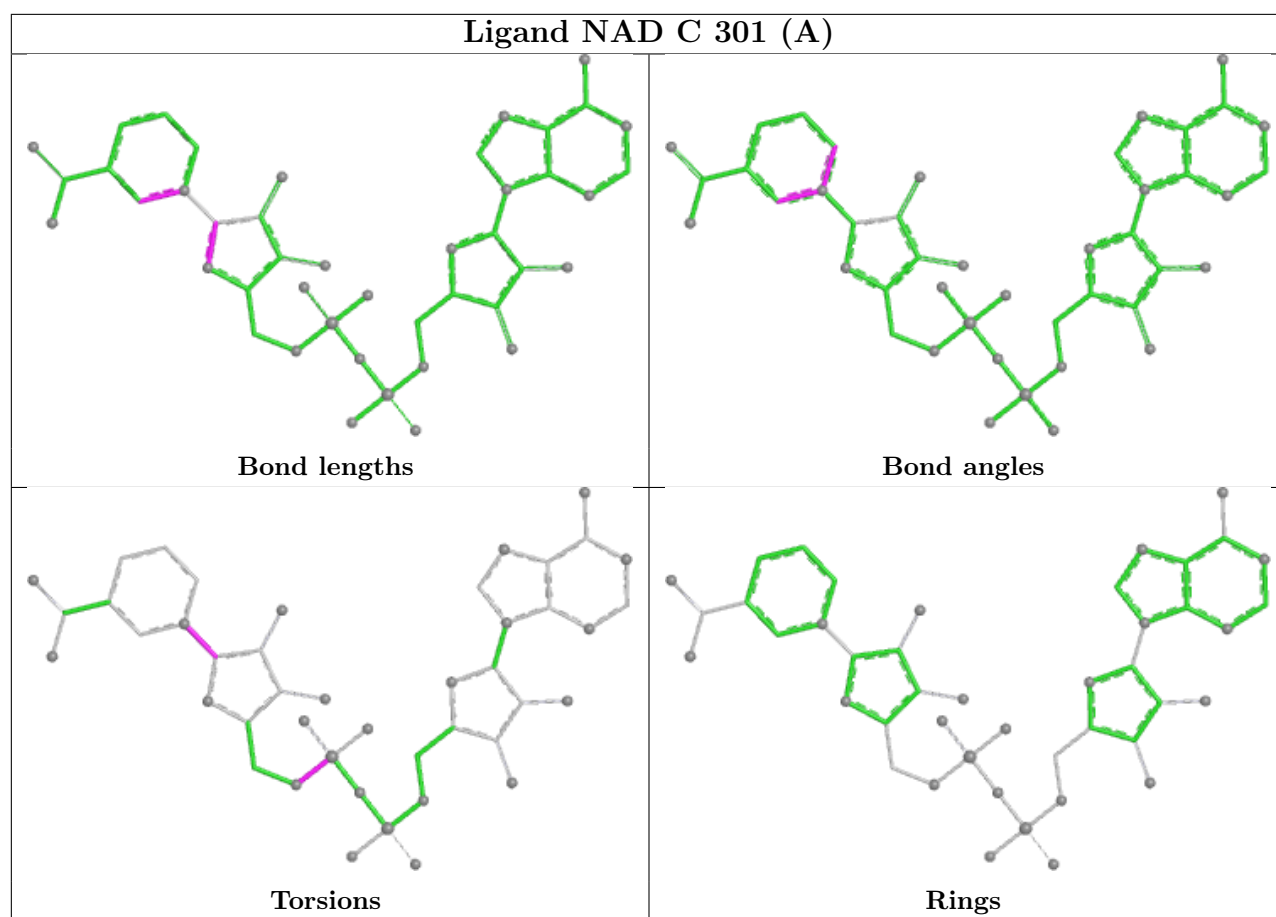
Ligand NAD D 301 (B)



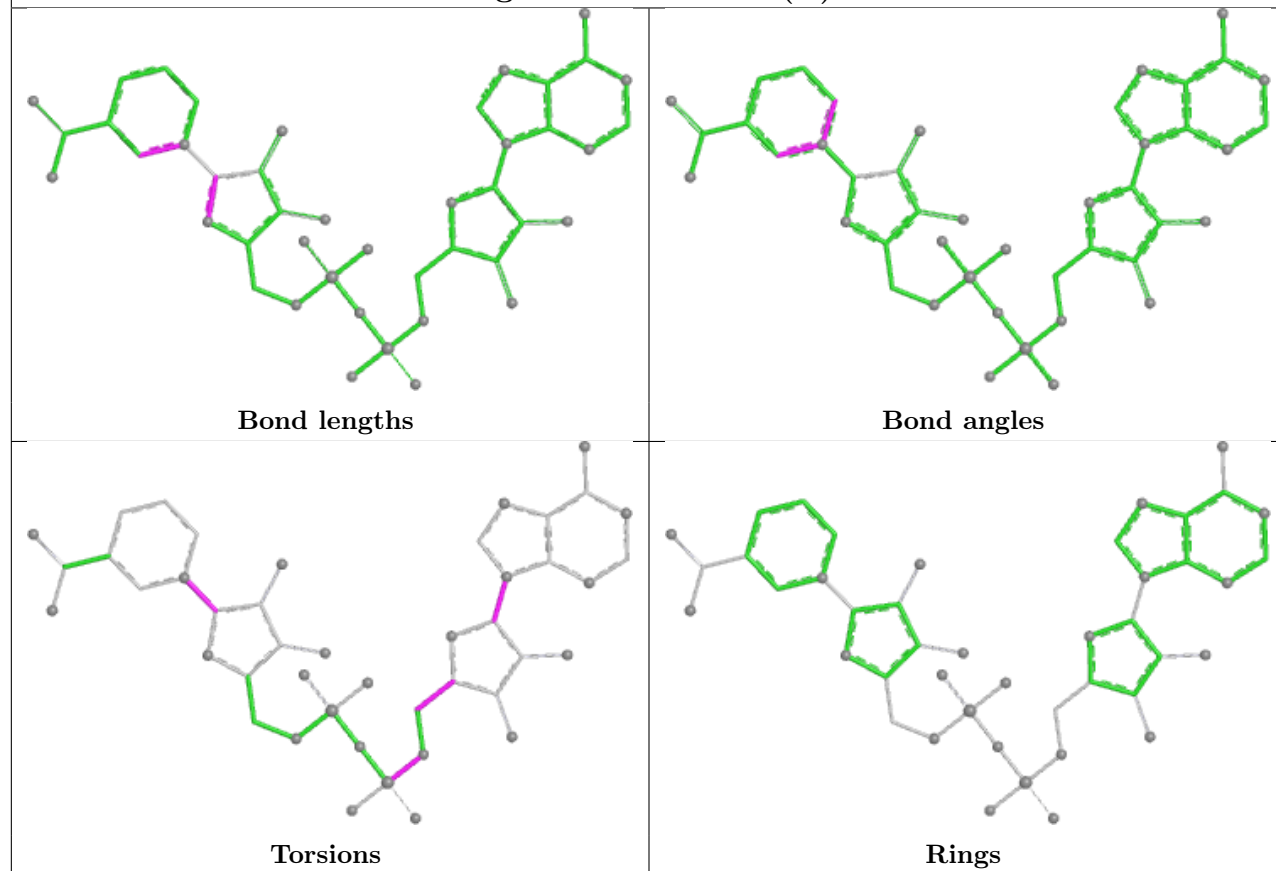
Ligand NAD C 301 (B)



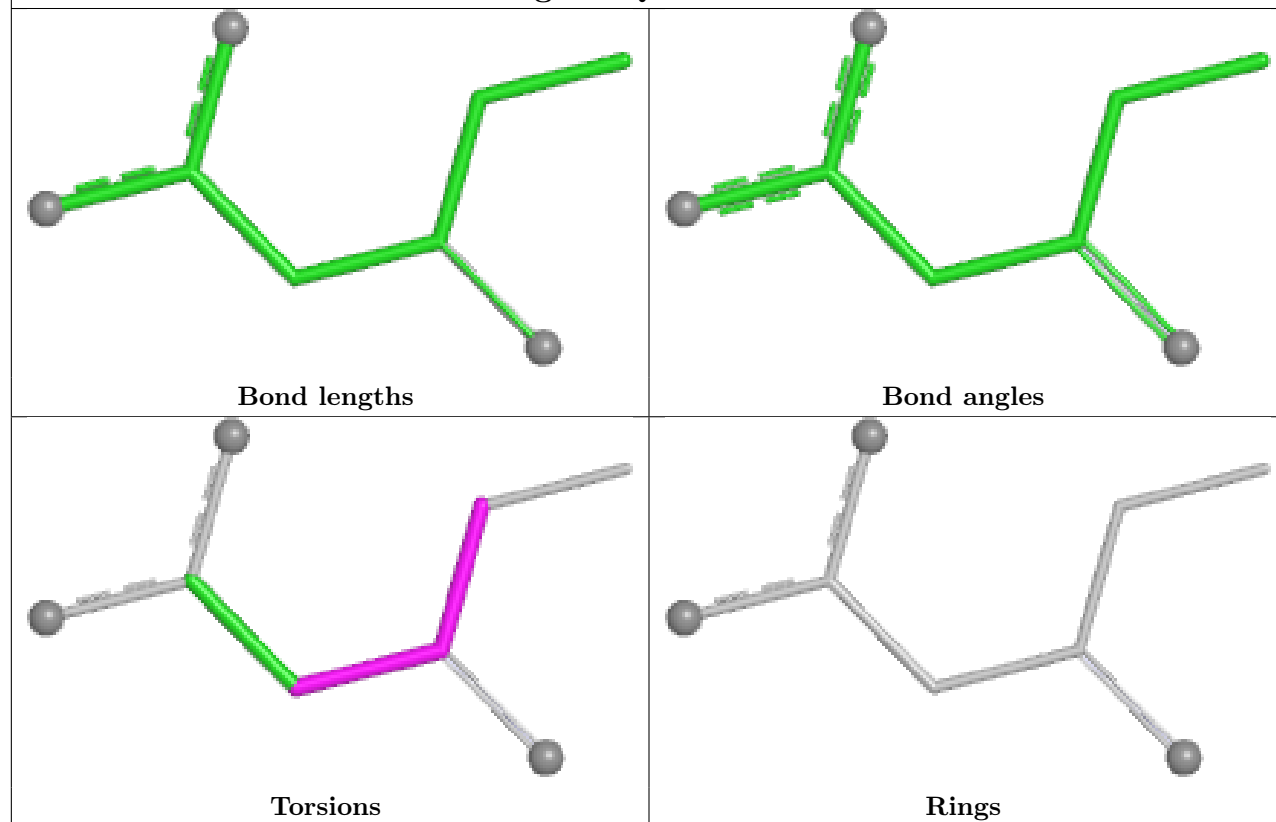


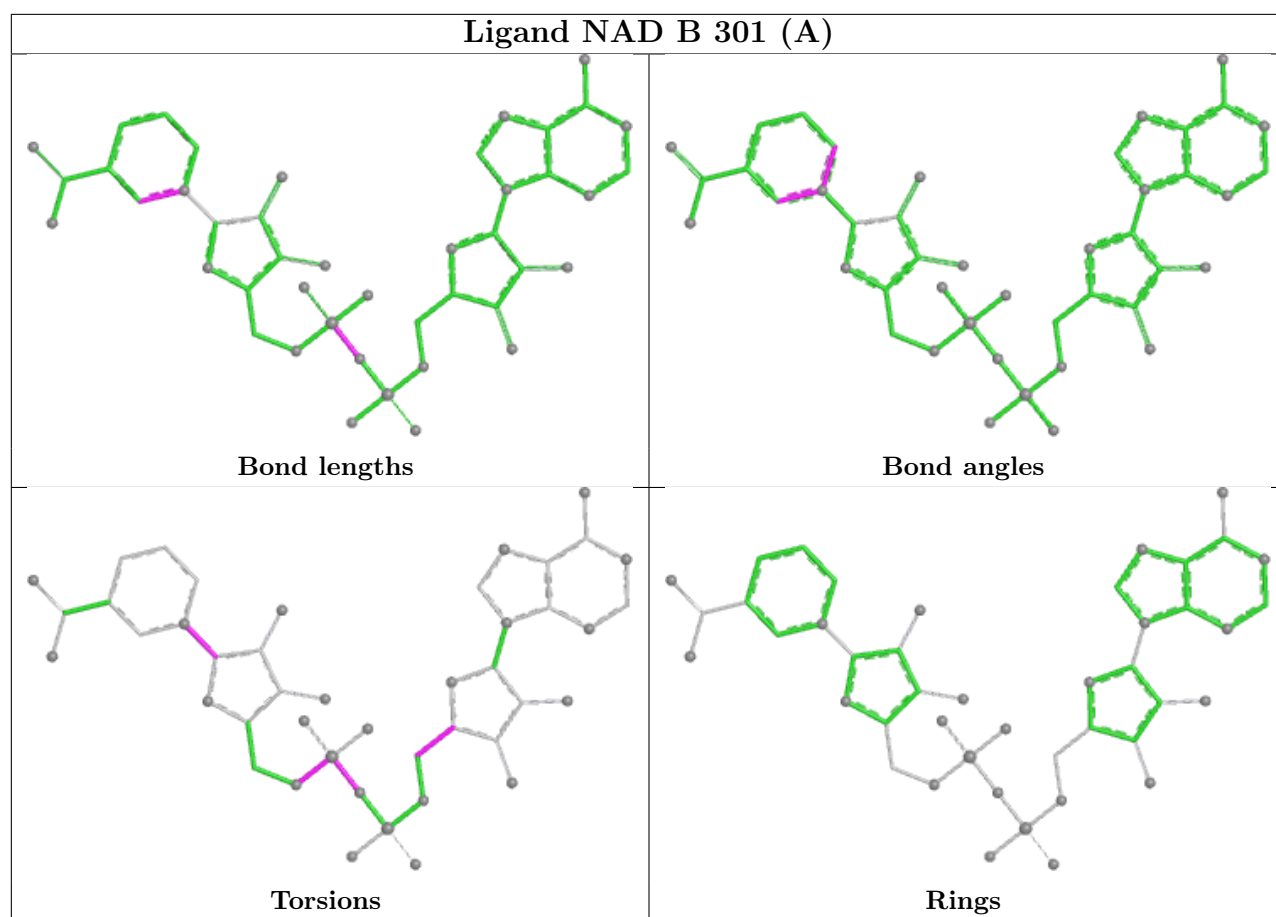


Ligand NAD B 301 (B)



Ligand QT8 C 303





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	260/261 (99%)	0.31	7 (2%)	56	59	13, 29, 52, 77	4 (1%)
1	B	260/261 (99%)	0.39	4 (1%)	72	76	12, 28, 52, 70	5 (1%)
1	C	260/261 (99%)	0.31	4 (1%)	72	76	16, 30, 52, 73	2 (0%)
1	D	261/261 (100%)	0.25	3 (1%)	78	81	15, 30, 52, 70	3 (1%)
1	E	254/261 (97%)	0.58	8 (3%)	51	55	20, 37, 56, 69	2 (0%)
1	F	252/261 (96%)	0.69	7 (2%)	55	58	23, 38, 55, 69	2 (0%)
All	All	1547/1566 (98%)	0.42	33 (2%)	63	67	12, 32, 53, 77	18 (1%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	7	GLY	3.9
1	F	216	VAL	3.8
1	F	201	LEU	3.7
1	E	201	LEU	3.4
1	E	217	ILE	3.3
1	B	201	LEU	3.0
1	F	209	LEU	3.0
1	E	216	VAL	2.9
1	E	220	MET	2.9
1	B	220[A]	MET	2.8
1	A	209	LEU	2.7
1	E	215	ASP	2.5
1	F	7	GLY	2.5
1	D	217	ILE	2.5
1	A	213	LEU	2.5
1	E	193	LEU	2.4
1	C	199	ALA	2.4
1	F	193	LEU	2.4
1	F	100	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	201	LEU	2.3
1	C	201	LEU	2.3
1	A	199	ALA	2.3
1	A	207	VAL	2.3
1	A	210	ASP	2.2
1	B	2	THR	2.2
1	F	40	ASN	2.2
1	C	2	THR	2.2
1	E	253	VAL	2.1
1	D	201	LEU	2.1
1	A	40	ASN	2.1
1	D	209	LEU	2.1
1	C	204	THR	2.1
1	B	209	LEU	2.1

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($\text{\AA}^2$)	Q<0.9
3	QT8	C	303	8/8	0.66	0.19	55,62,64,73	0
3	QT8	D	302	8/8	0.69	0.19	48,58,60,65	0
3	QT8	A	302	8/8	0.71	0.21	53,62,66,77	0
3	QT8	F	302	8/8	0.71	0.20	67,70,71,74	0
3	QT8	C	302	8/8	0.78	0.20	56,60,66,73	0
3	QT8	B	302	8/8	0.81	0.18	64,67,68,73	0
2	NAD	E	301[A]	44/44	0.82	0.12	35,44,59,61	44
2	NAD	E	301[B]	44/44	0.82	0.12	27,32,37,39	44
2	NAD	A	301[A]	44/44	0.84	0.13	31,44,55,56	44

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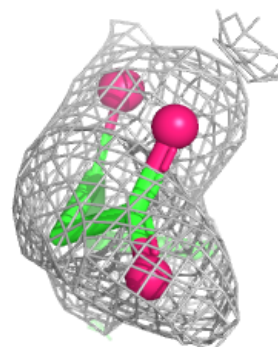
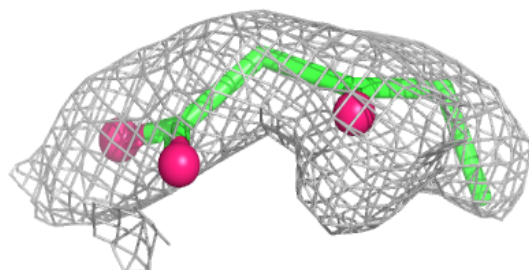
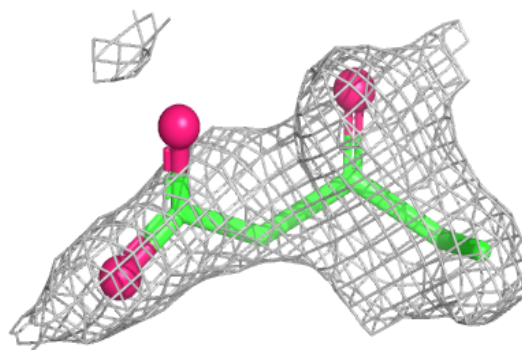
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAD	A	301[B]	44/44	0.84	0.13	20,25,29,31	44
2	NAD	B	301[A]	44/44	0.86	0.09	24,32,36,38	44
2	NAD	B	301[B]	44/44	0.86	0.09	23,29,34,35	44
2	NAD	D	301[A]	44/44	0.89	0.08	24,30,34,34	44
2	NAD	D	301[B]	44/44	0.89	0.08	34,40,45,48	44
2	NAD	C	301[A]	44/44	0.90	0.08	25,36,41,43	44
2	NAD	C	301[B]	44/44	0.90	0.08	26,33,43,44	44
2	NAD	F	301	44/44	0.90	0.09	33,45,58,73	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.

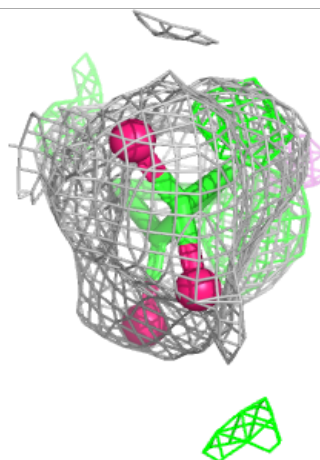
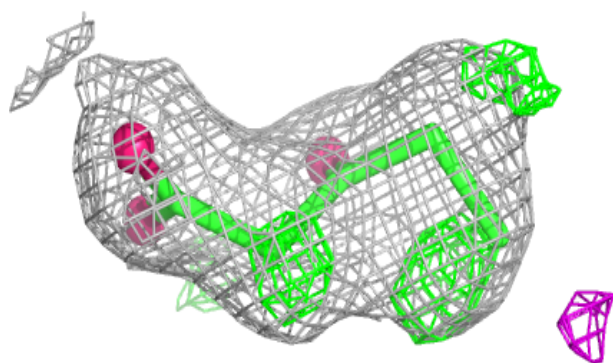
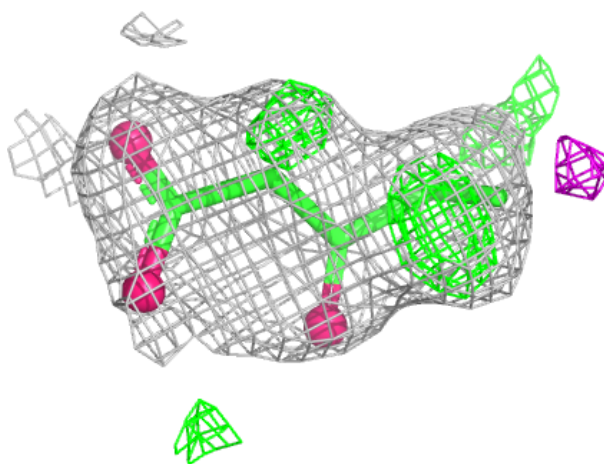
Electron density around QT8 C 303:

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



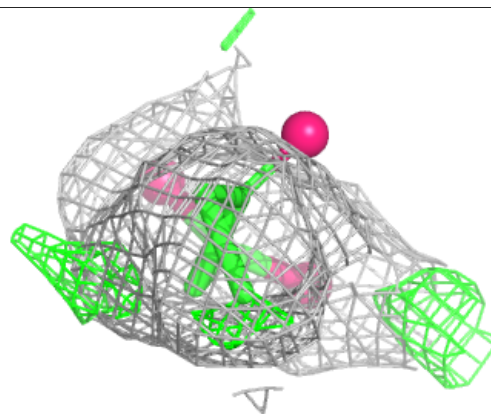
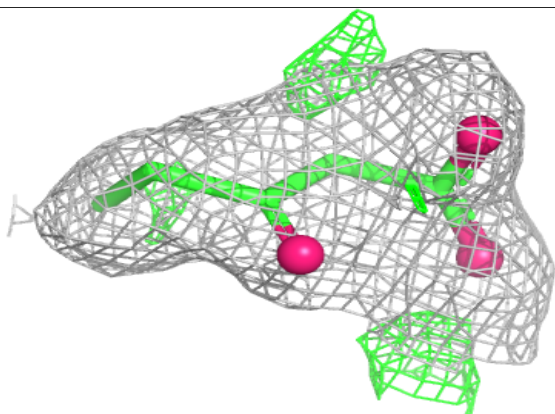
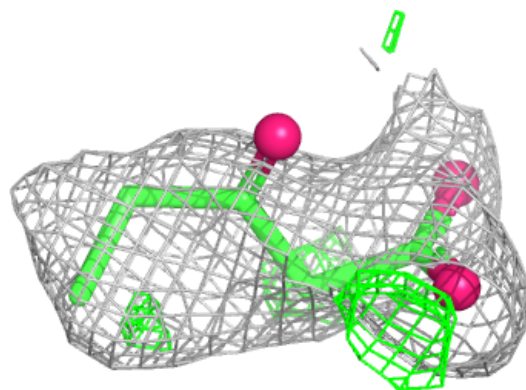
Electron density around QT8 D 302:

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



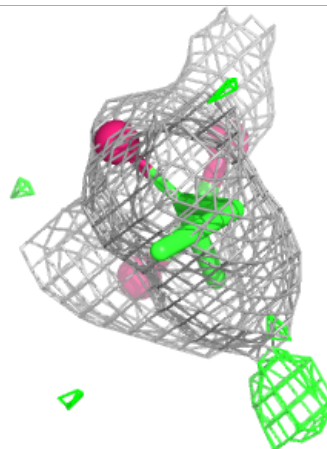
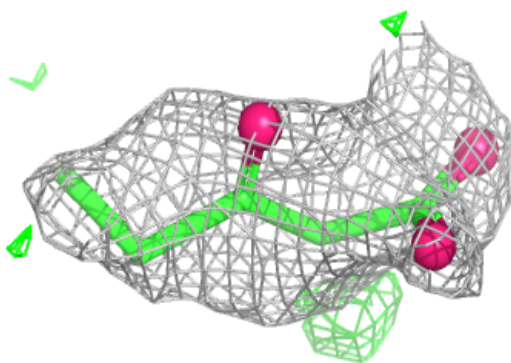
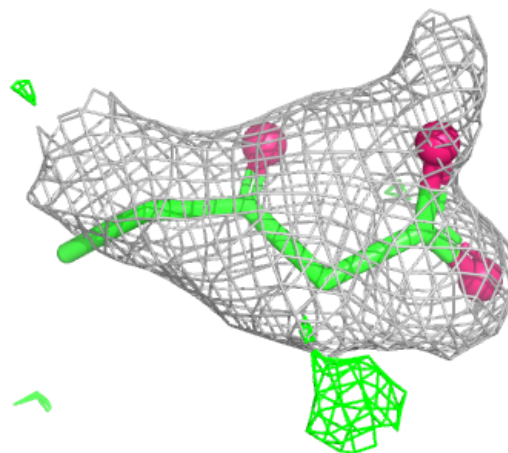
Electron density around QT8 A 302:

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and green (positive)



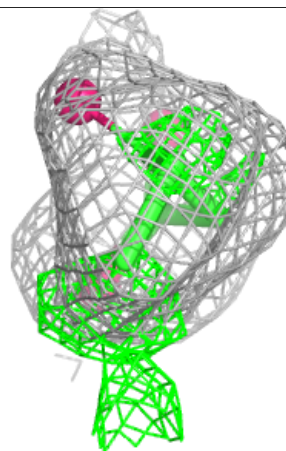
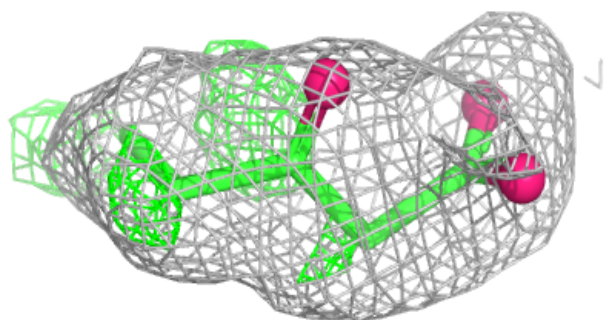
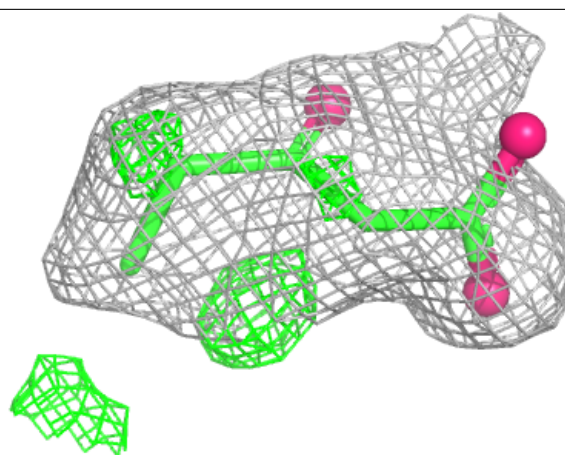
Electron density around QT8 F 302:

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and green (positive)



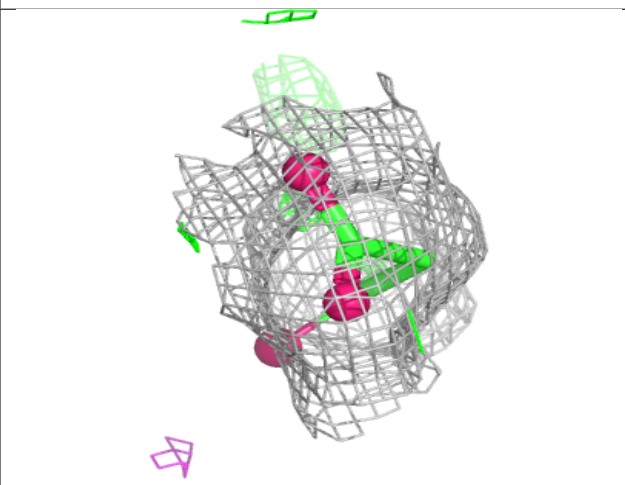
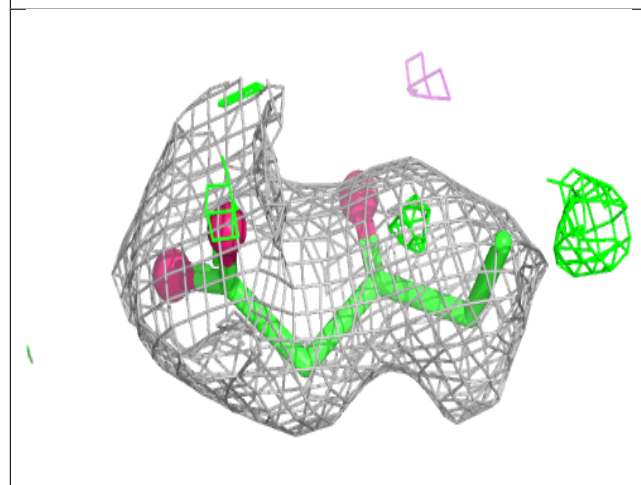
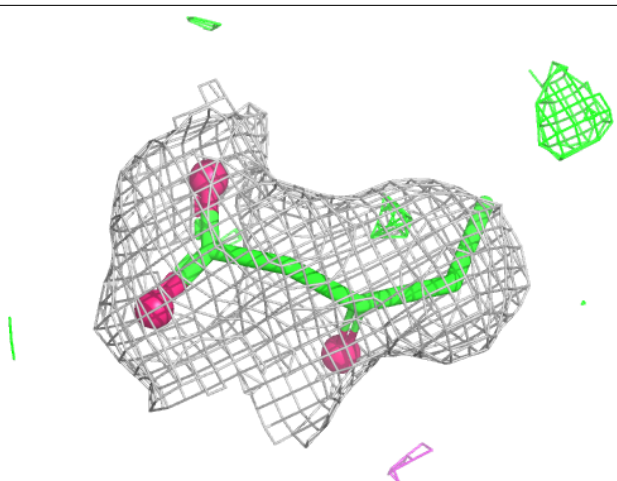
Electron density around QT8 C 302:

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



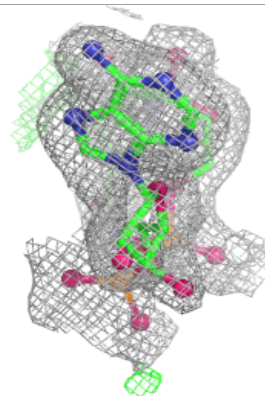
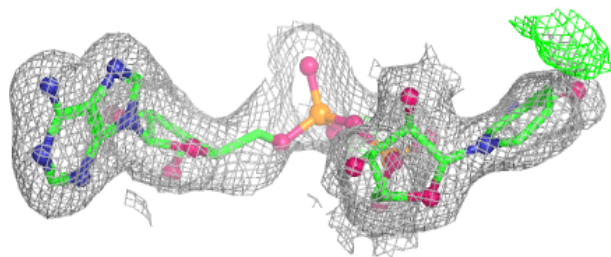
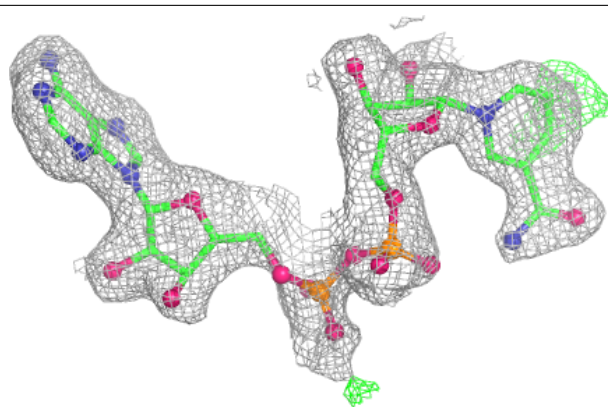
Electron density around QT8 B 302:

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

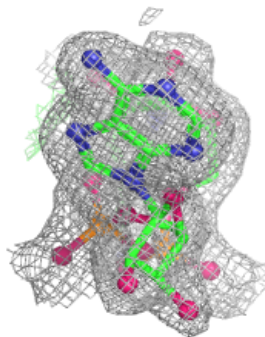
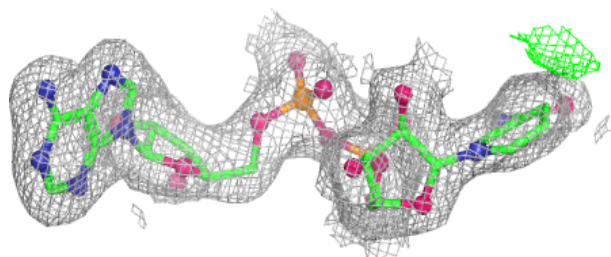
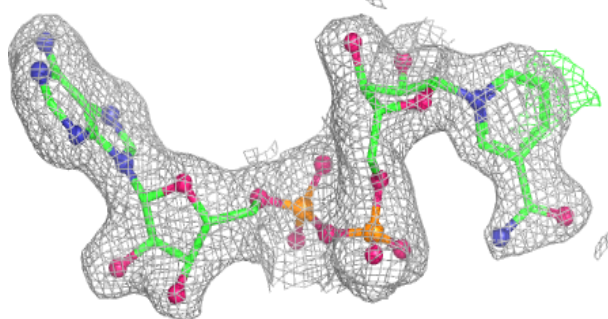


Electron density around NAD E 301 (A):

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

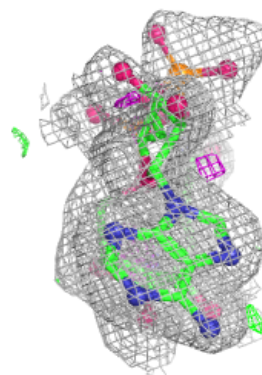
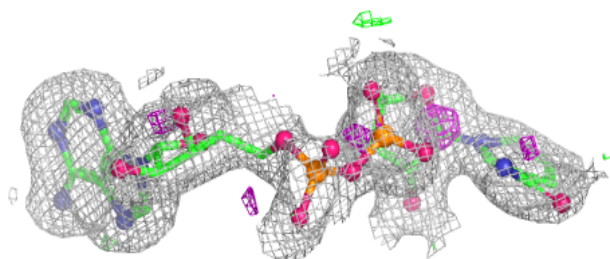
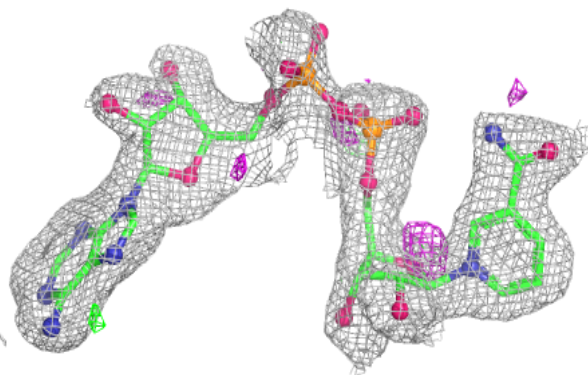
**Electron density around NAD E 301 (B):**

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and green (positive)

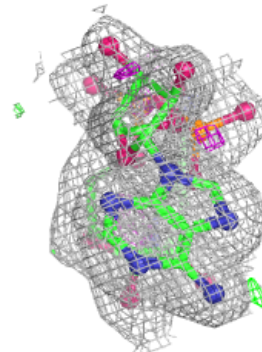
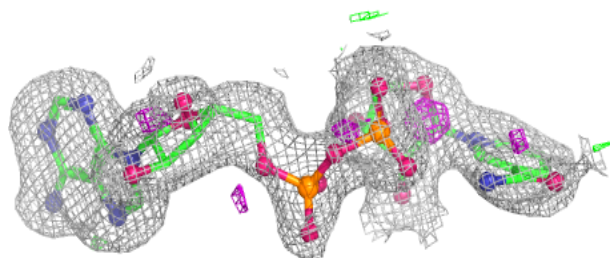
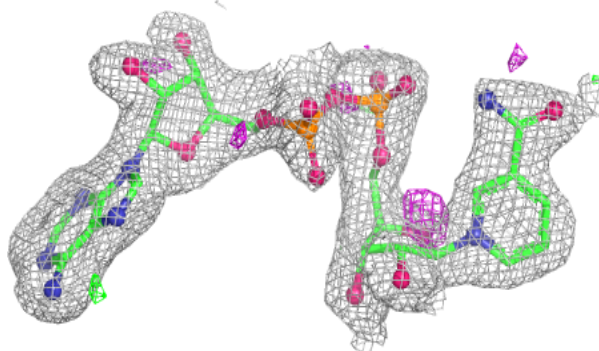


Electron density around NAD A 301 (A):

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and green (positive)

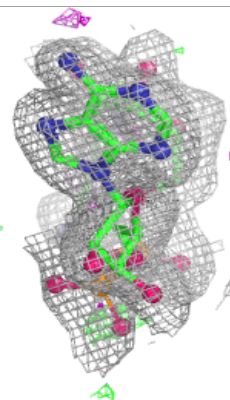
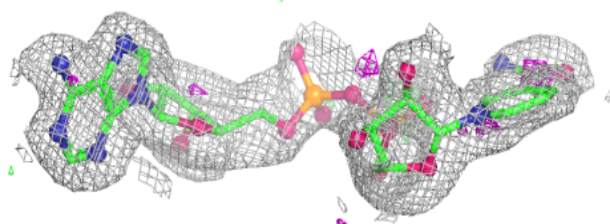
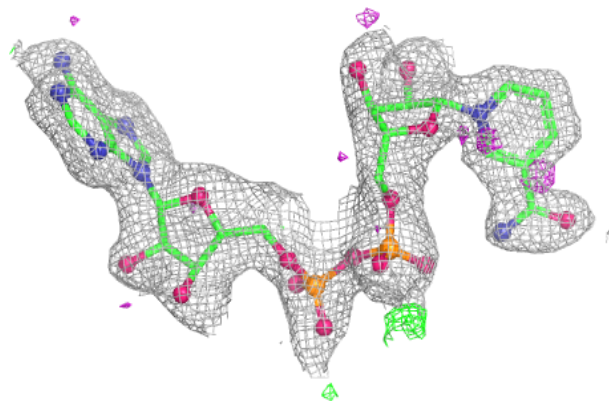
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and green (positive)

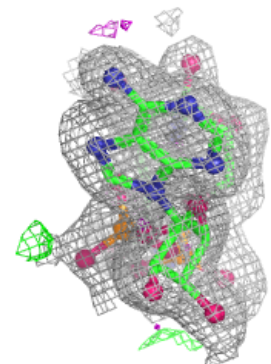
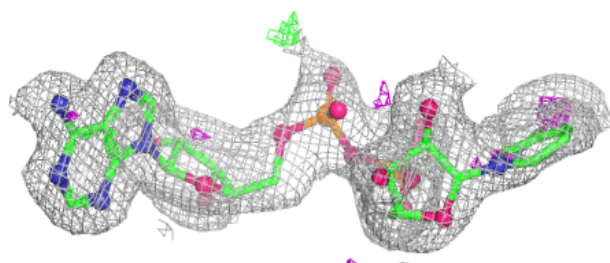
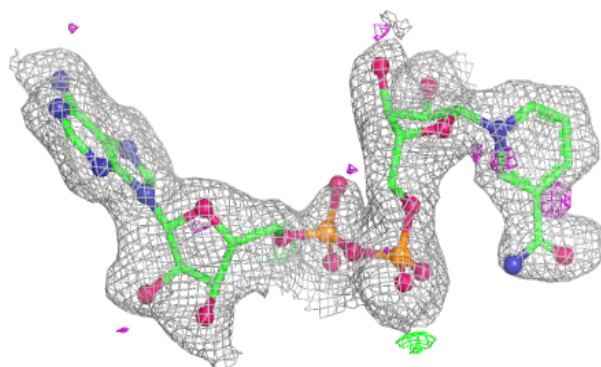


Electron density around NAD B 301 (A):

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

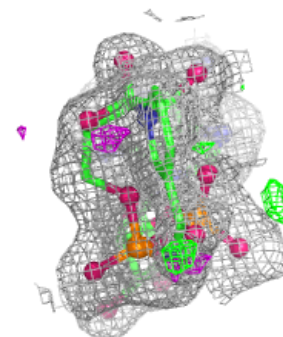
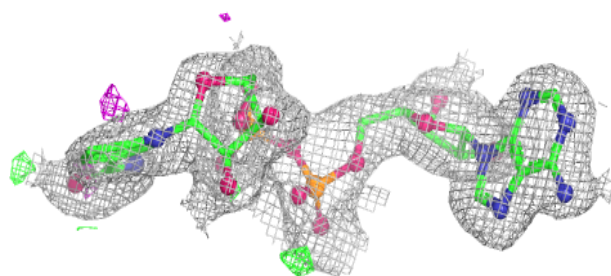
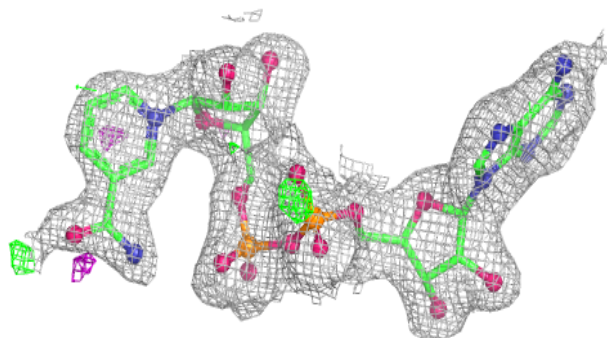
**Electron density around NAD B 301 (B):**

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

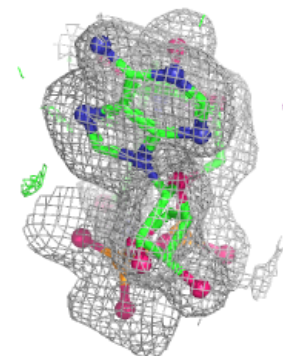
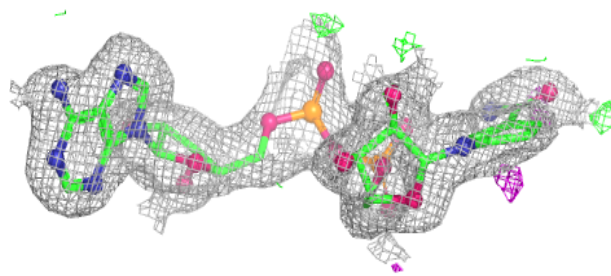
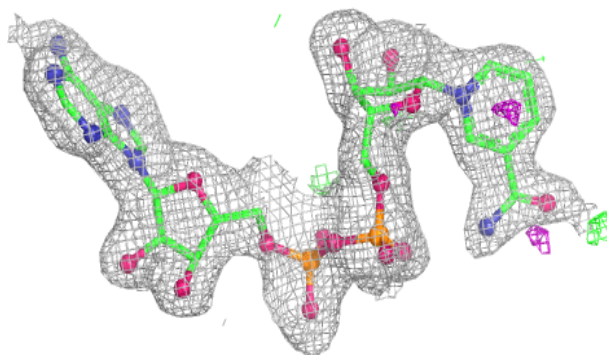


Electron density around NAD D 301 (A):

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

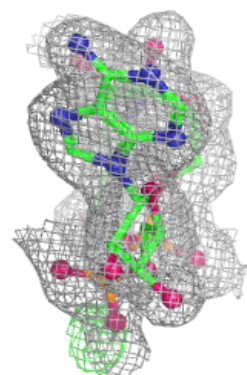
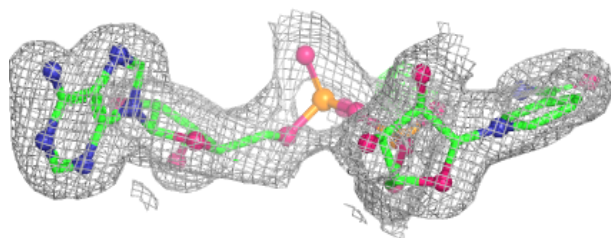
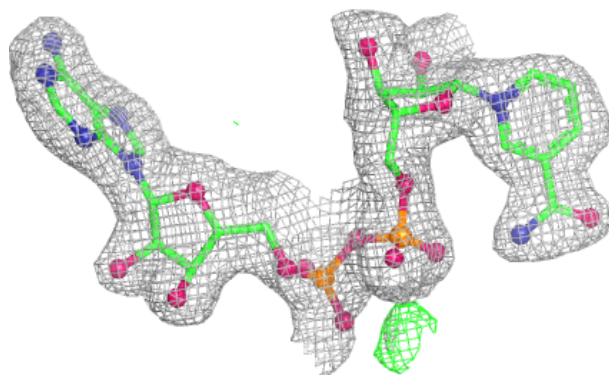
**Electron density around NAD D 301 (B):**

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

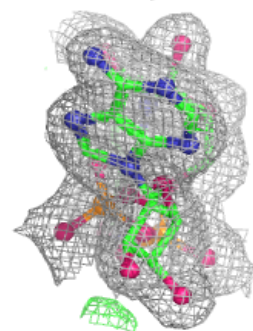
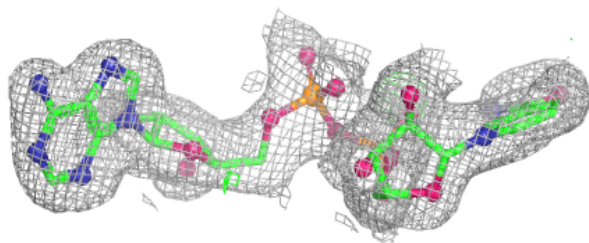
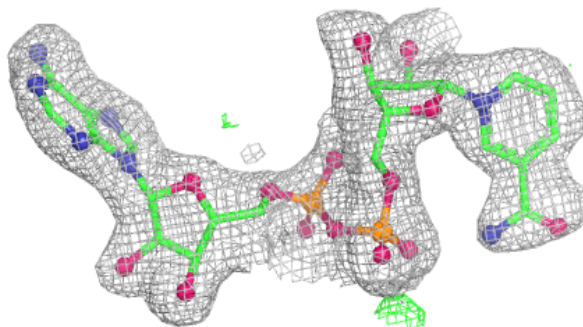


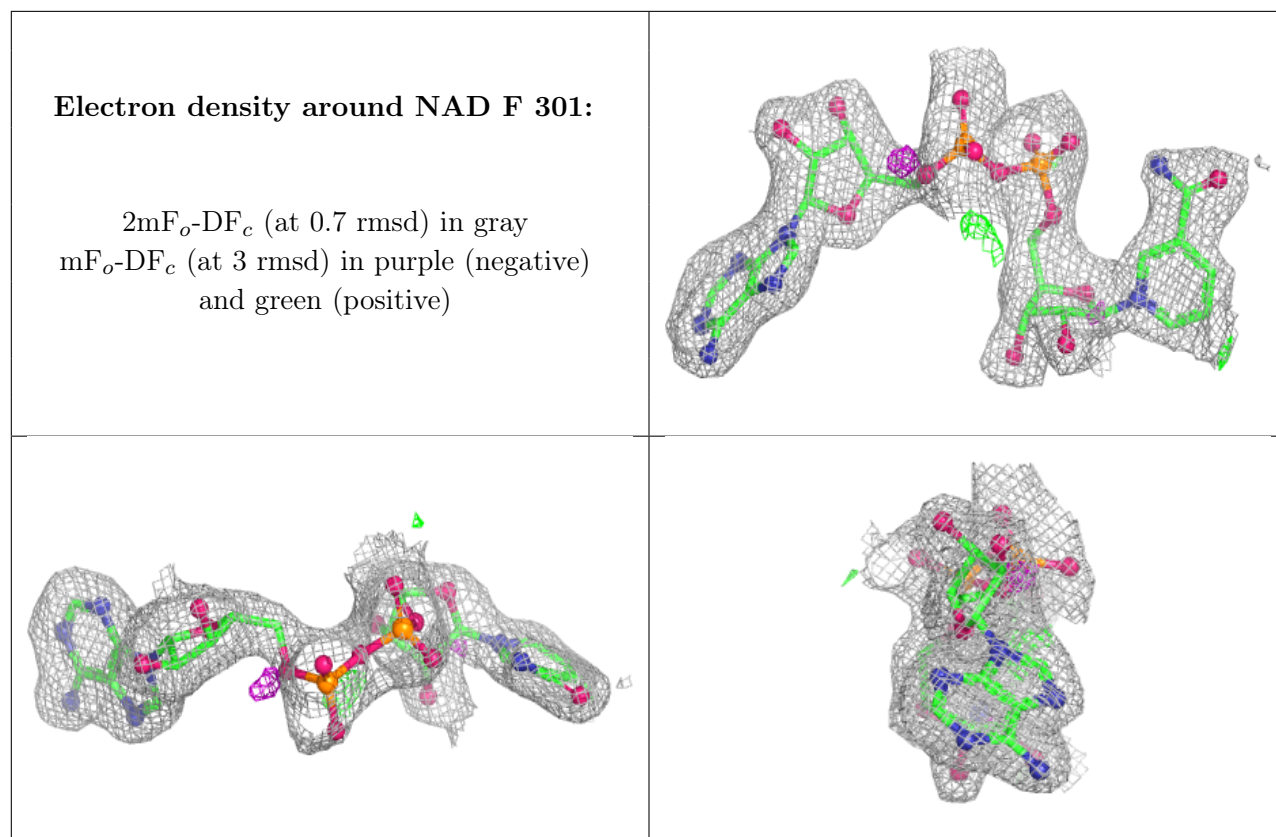
Electron density around NAD C 301 (A):

$2mF_o-DF_c$ (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 (B):**

$2mF_o-DF_c$ (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.