wwPDB X-ray Structure Validation Summary Report (i)

Sep 29, 2020 – 05:24 PM BST

PDB ID	:	6ZZS
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 wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

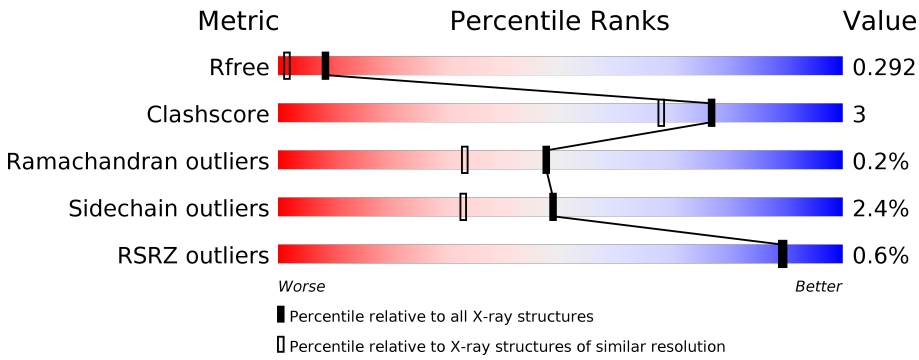
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 1.85 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}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (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 on 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 <=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	% 90% 9%
1	B	261	92% 8%
1	C	261	93% 7%
1	D	261	92% 8%
1	E	261	% 91% 6% •
1	F	261	2% 85% 11% •

2 Entry composition (i)

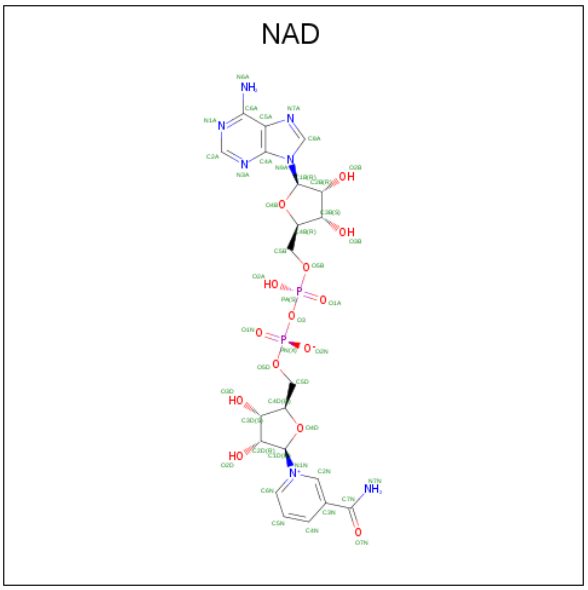
There are 4 unique types of molecules in this entry. The entry contains 12429 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

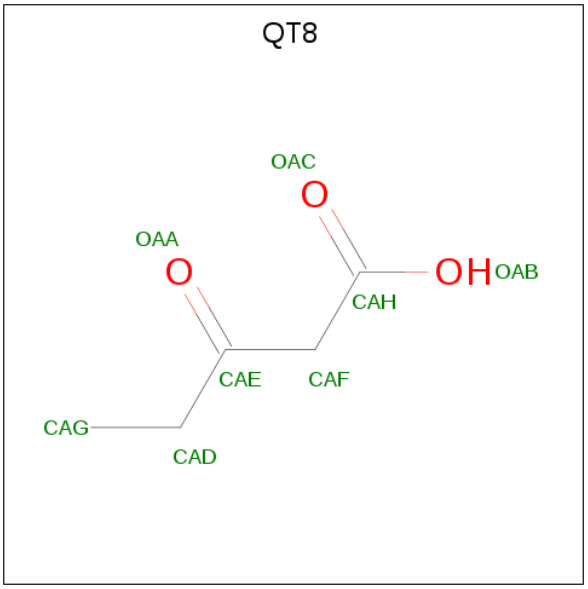
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	260	1900	1208	314	366	12	0	4	0
1	B	260	1906	1214	314	366	12	0	5	0
1	C	260	1905	1212	317	365	11	0	2	0
1	D	261	1906	1210	320	364	12	0	3	0
1	E	254	1832	1168	302	350	12	0	2	0
1	F	252	1823	1161	304	348	10	0	2	0

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



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

- Molecule 3 is 3-oxidanylidenepentanoic acid (three-letter code: QT8) (formula: $C_5H_8O_3$) (labeled as "Ligand of Interest" by author).



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

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

- Molecule 4 is water.

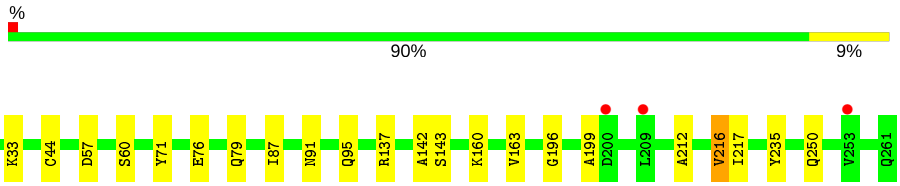
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	122	124	124	0	2
			Total	O		
4	B	123	129	129	0	6
			Total	O		
4	C	108	113	113	0	5
			Total	O		
4	D	118	125	125	0	7
			Total	O		
4	E	75	76	76	0	1
			Total	O		
4	F	57	58	58	0	1

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

Chain A:

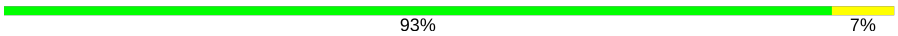


- Molecule 1: 3-hydroxybutyrate dehydrogenase

Chain B:

- Molecule 1: 3-hydroxybutyrate dehydrogenase

Chain C:

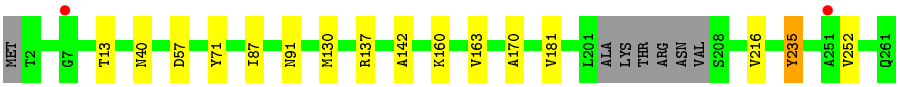


- Molecule 1: 3-hydroxybutyrate dehydrogenase

Chain D:

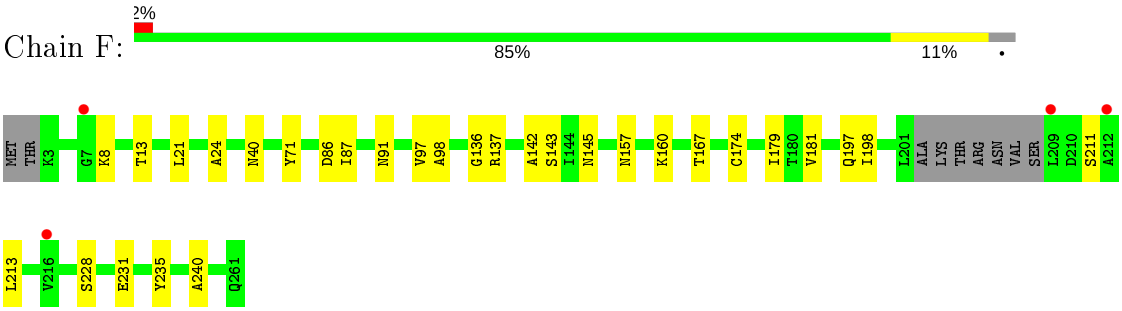
- Molecule 1: 3-hydroxybutyrate dehydrogenase

Chain E:



- Molecule 1: 3-hydroxybutyrate dehydrogenase

Chain F:


2%
85%
11%
MET
THR
K3
G7
K8
T13
L21
A24
N40
Y71
D86
I87
N91
V97
A98
G136
R137
A142
S143
I144
N145
N157
K160
T167
C174
I179
T180
V181
Q197
I198
L201
ALA
LYS
THR
ARG
ASN
VAL
SER
L209
D210
S211
A212
L213
V216
S228
E231
Y235
A240
Q261

4 Data and refinement statistics (i)

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) 99.8 (53.16-1.85)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 , 44.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.71	0/1937	0.82	0/2621
1	B	0.73	0/1946	0.81	0/2632
1	C	0.71	0/1936	0.80	0/2619
1	D	0.72	0/1940	0.82	0/2620
1	E	0.71	0/1862	0.80	0/2519
1	F	0.73	0/1853	0.79	0/2504
All	All	0.72	0/11474	0.81	0/15515

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1900	0	1911	12	0
1	B	1906	0	1929	12	0
1	C	1905	0	1929	15	0
1	D	1906	0	1928	12	0
1	E	1832	0	1829	7	0
1	F	1823	0	1830	13	0
2	A	88	0	52	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	88	0	52	2	0
2	C	88	0	52	2	0
2	D	88	0	52	1	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	2	0
4	B	129	0	0	1	0
4	C	113	0	0	3	0
4	D	125	0	0	2	0
4	E	76	0	0	0	0
4	F	58	0	0	0	0
All	All	12429	0	11642	70	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.

The worst 5 of 70 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250[B]:GLN:NE2	4:A:401:HOH:O	1.60	1.26
2:C:301[B]:NAD:O1A	4:C:402:HOH:O	1.93	0.85
2:D:301[A]:NAD:O1A	4:D:403:HOH:O	2.02	0.78
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

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%)	19	7
1	F	250/261 (96%)	238 (95%)	11 (4%)	1 (0%)	34	19
All	All	1549/1566 (99%)	1495 (96%)	51 (3%)	3 (0%)	47	33

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 (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	193/202 (96%)	187 (97%)	6 (3%)	40	23
1	B	195/202 (96%)	191 (98%)	4 (2%)	53	38
1	C	194/202 (96%)	190 (98%)	4 (2%)	53	38
1	D	193/202 (96%)	189 (98%)	4 (2%)	53	38
1	E	182/202 (90%)	178 (98%)	4 (2%)	52	36
1	F	183/202 (91%)	178 (97%)	5 (3%)	44	29
All	All	1140/1212 (94%)	1113 (98%)	27 (2%)	49	33

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	163	VAL
1	D	163	VAL
1	F	197	GLN
1	C	235	TYR
1	A	217	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	73	GLN
1	D	79	GLN
1	F	96	HIS
1	B	197	GLN
1	D	250	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 monosaccharides 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[A]	-	42,48,48	0.76	2 (4%)	50,73,73	0.84	1 (2%)
3	QT8	B	302	-	4,7,7	1.04	0	3,8,8	0.77	0
3	QT8	D	302	-	4,7,7	0.72	0	3,8,8	1.47	1 (33%)
2	NAD	D	301[B]	-	42,48,48	0.71	1 (2%)	50,73,73	0.75	2 (4%)
3	QT8	F	302	-	4,7,7	0.82	0	3,8,8	0.57	0
2	NAD	F	301	-	42,48,48	0.73	1 (2%)	50,73,73	0.86	2 (4%)
2	NAD	D	301[A]	-	42,48,48	0.78	2 (4%)	50,73,73	0.88	2 (4%)
3	QT8	C	303	-	4,7,7	1.97	1 (25%)	3,8,8	1.40	1 (33%)
2	NAD	B	301[A]	-	42,48,48	0.80	1 (2%)	50,73,73	0.79	2 (4%)
2	NAD	C	301[A]	-	42,48,48	0.77	2 (4%)	50,73,73	0.87	2 (4%)
2	NAD	E	301[B]	-	42,48,48	0.83	2 (4%)	50,73,73	0.91	2 (4%)
3	QT8	A	302	-	4,7,7	0.60	0	3,8,8	1.20	0
2	NAD	C	301[B]	-	42,48,48	0.68	1 (2%)	50,73,73	0.76	3 (6%)
3	QT8	C	302	-	4,7,7	0.84	0	3,8,8	0.59	0
2	NAD	A	301[B]	-	42,48,48	0.87	2 (4%)	50,73,73	0.82	2 (4%)
2	NAD	B	301[B]	-	42,48,48	0.75	2 (4%)	50,73,73	0.85	2 (4%)
2	NAD	E	301[A]	-	42,48,48	0.75	1 (2%)	50,73,73	0.98	3 (6%)

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[A]	-	-	12/26/62/62	0/5/5/5
3	QT8	B	302	-	-	4/4/6/6	-
3	QT8	D	302	-	-	4/4/6/6	-
2	NAD	D	301[B]	-	-	8/26/62/62	0/5/5/5
3	QT8	F	302	-	-	2/4/6/6	-
2	NAD	F	301	-	-	2/26/62/62	0/5/5/5
2	NAD	D	301[A]	-	-	6/26/62/62	0/5/5/5
3	QT8	C	303	-	-	4/4/6/6	-
2	NAD	B	301[A]	-	-	8/26/62/62	0/5/5/5
2	NAD	C	301[A]	-	-	5/26/62/62	0/5/5/5
2	NAD	E	301[B]	-	-	9/26/62/62	0/5/5/5
3	QT8	A	302	-	-	2/4/6/6	-
2	NAD	C	301[B]	-	-	4/26/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	QT8	C	302	-	-	2/4/6/6	-
2	NAD	A	301[B]	-	-	6/26/62/62	0/5/5/5
2	NAD	B	301[B]	-	-	4/26/62/62	0/5/5/5
2	NAD	E	301[A]	-	-	4/26/62/62	0/5/5/5

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301[B]	NAD	C2N-N1N	3.43	1.39	1.35
3	C	303	QT8	CAF-CAE	3.36	1.58	1.52
2	B	301[A]	NAD	C2N-N1N	3.32	1.39	1.35
2	A	301[B]	NAD	C2N-N1N	3.27	1.38	1.35
2	F	301	NAD	C2N-N1N	3.06	1.38	1.35

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	301[A]	NAD	C6N-N1N-C2N	-4.01	118.32	121.97
2	A	301[A]	NAD	C6N-N1N-C2N	-3.48	118.80	121.97
2	E	301[B]	NAD	C6N-N1N-C2N	-3.43	118.84	121.97
2	F	301	NAD	C6N-N1N-C2N	-3.17	119.08	121.97
2	B	301[B]	NAD	C6N-N1N-C2N	-3.08	119.16	121.97

There are no chirality outliers.

5 of 86 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
3	D	302	QT8	CAG-CAD-CAE-CAF

There are no ring outliers.

10 monomers are involved in 13 short contacts:

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

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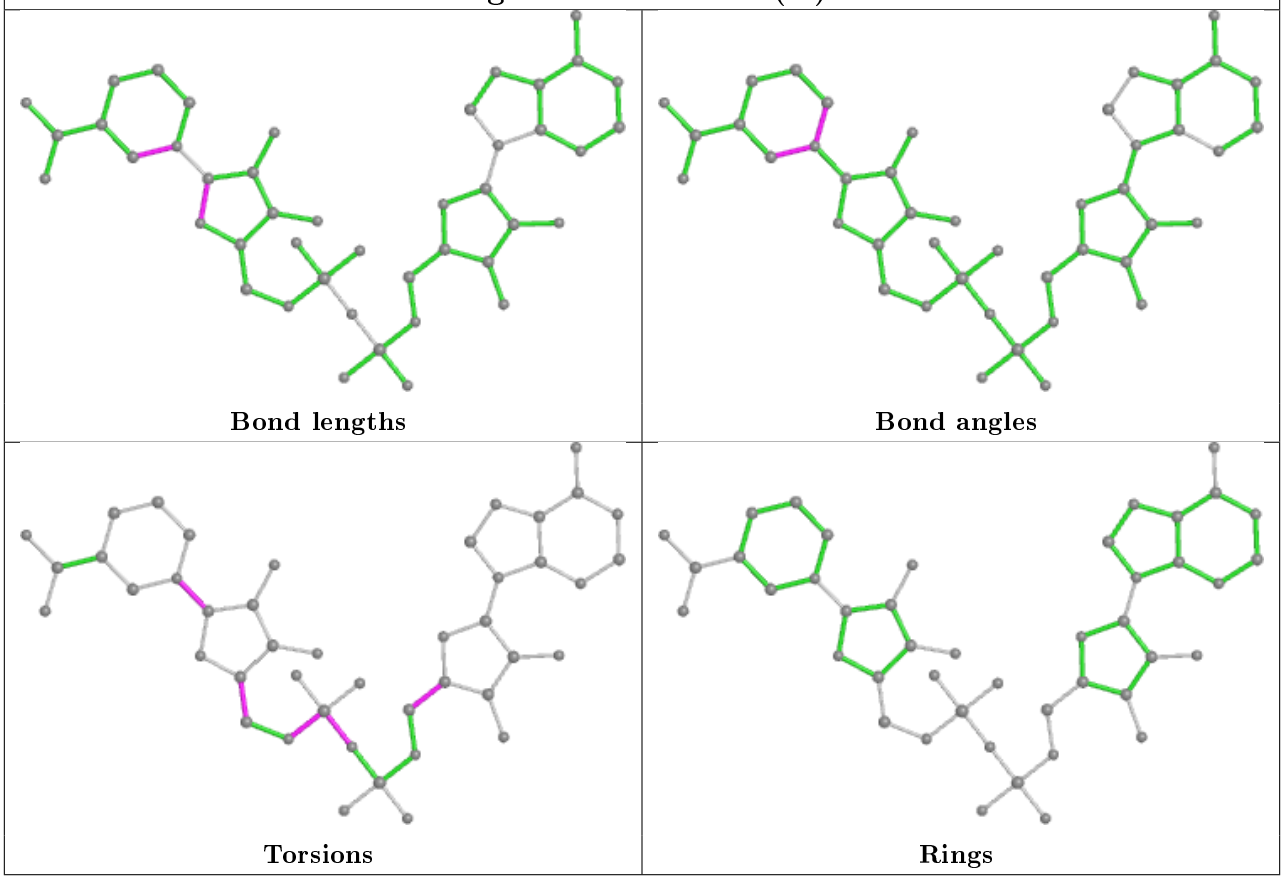
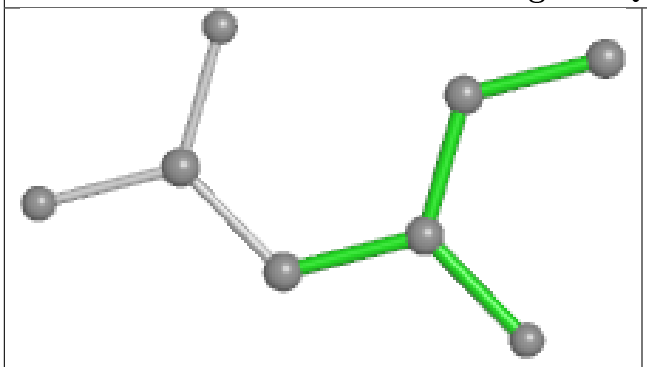
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301[A]	NAD	1	0
2	E	301[B]	NAD	1	0
3	A	302	QT8	2	0
2	C	301[B]	NAD	1	0
3	C	302	QT8	1	0
2	A	301[B]	NAD	2	0
2	B	301[B]	NAD	1	0

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 then 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.

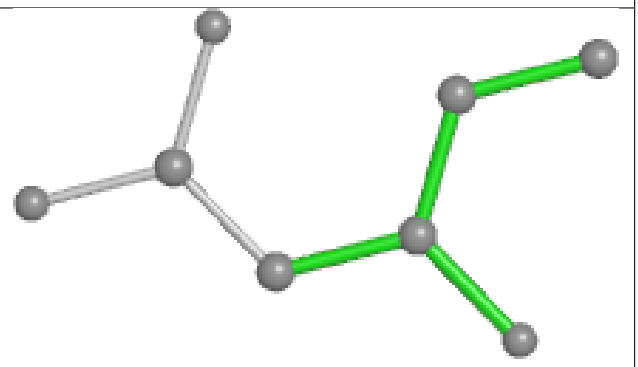
Ligand NAD A 301 (A)



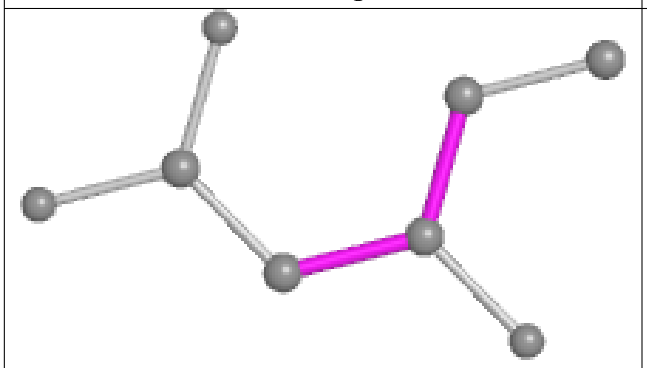
Ligand QT8 B 302



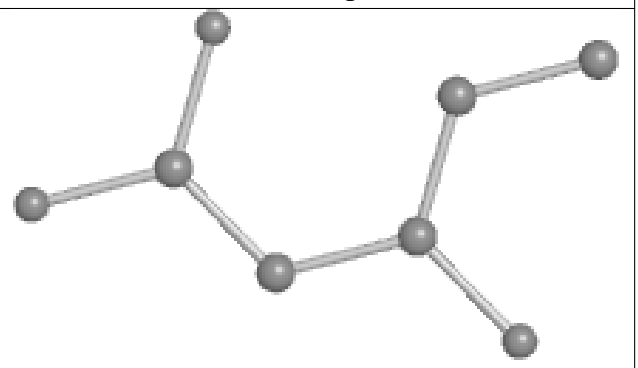
Bond lengths



Bond angles

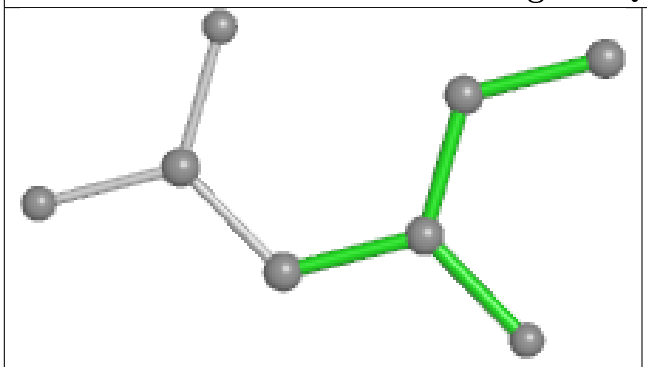


Torsions

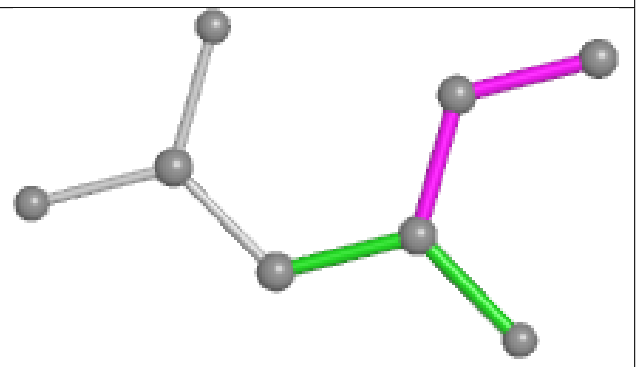


Rings

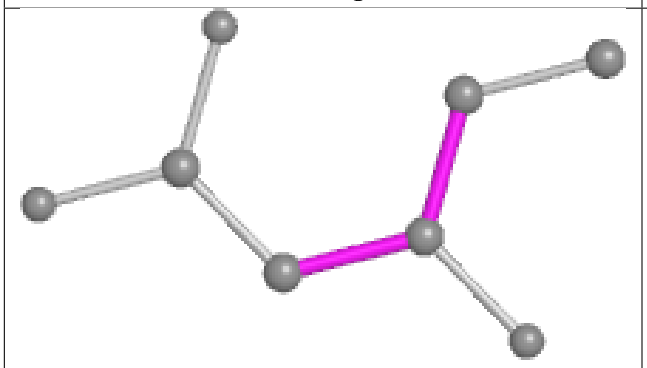
Ligand QT8 D 302



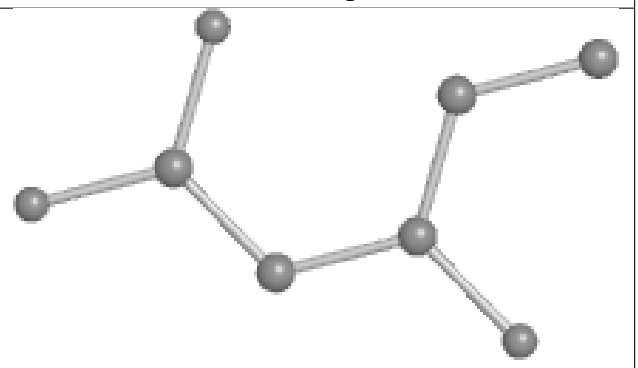
Bond lengths



Bond angles

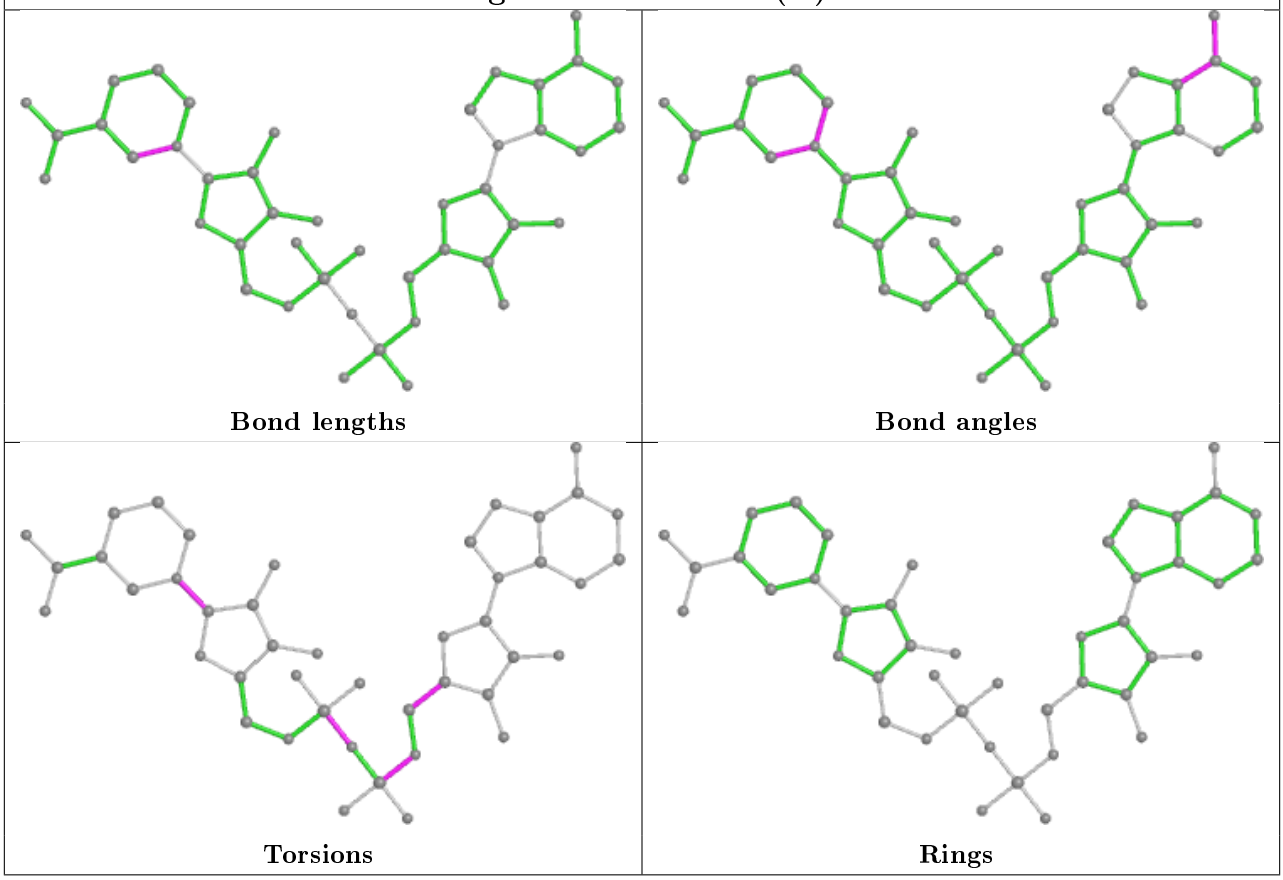


Torsions

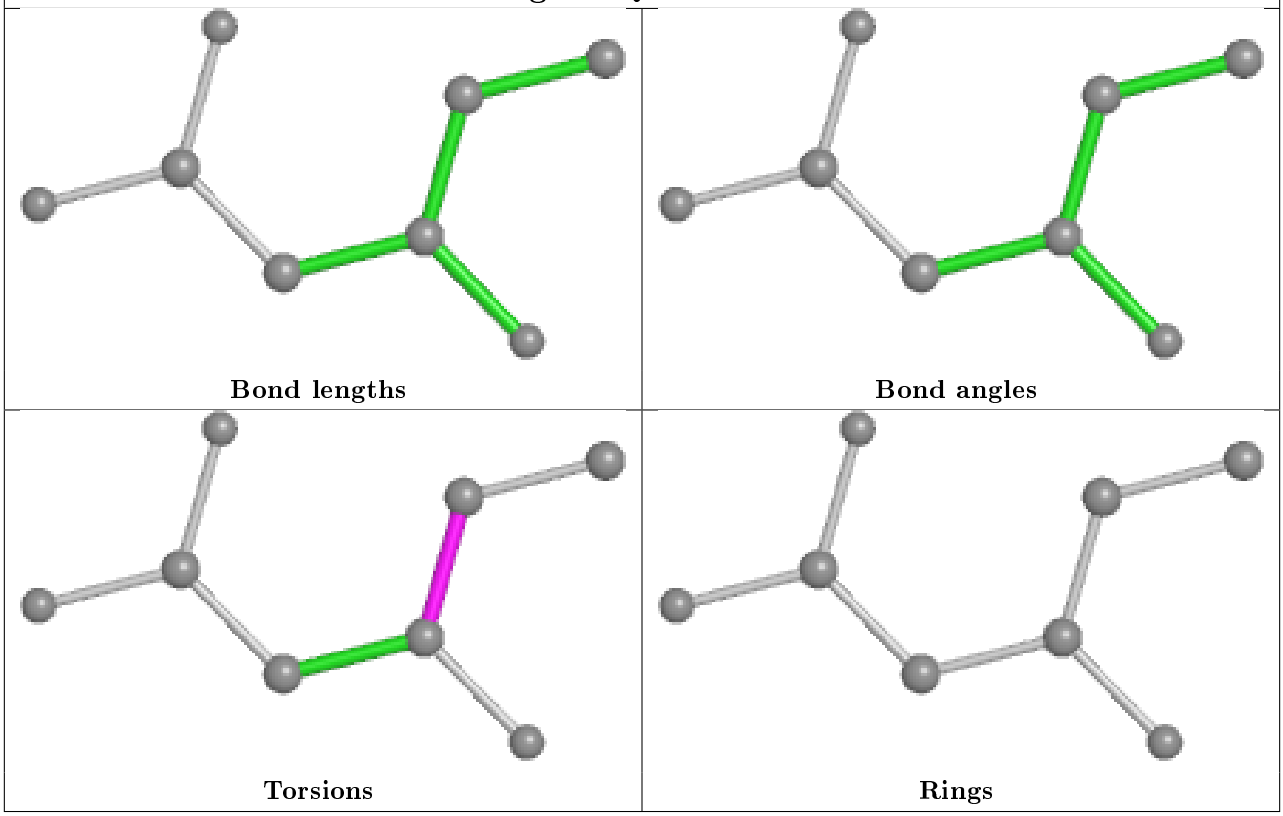


Rings

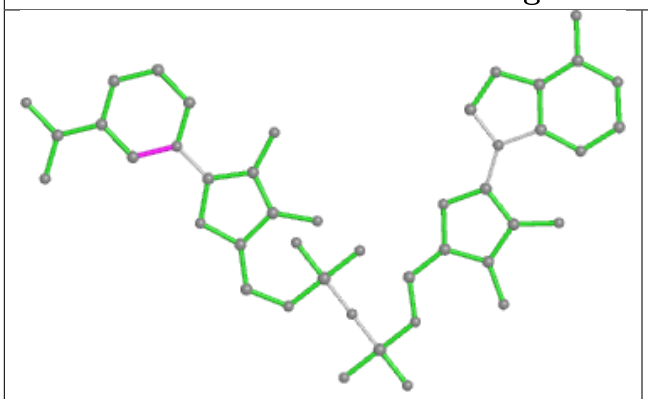
Ligand NAD D 301 (B)



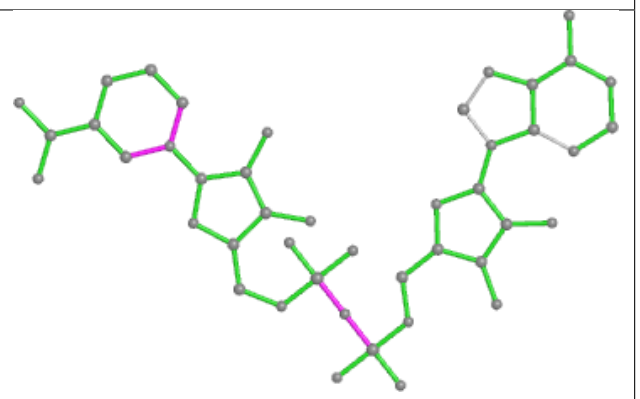
Ligand QT8 F 302



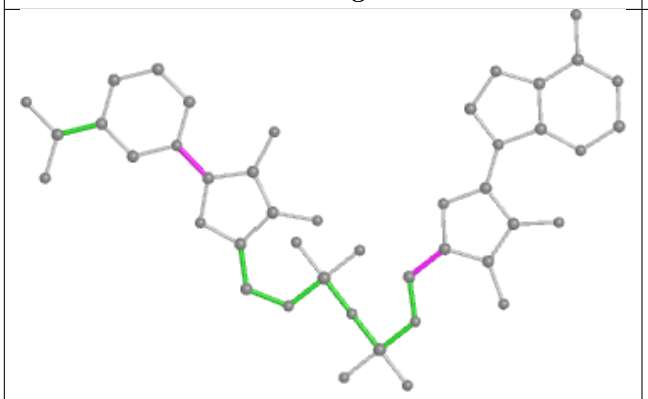
Ligand NAD F 301



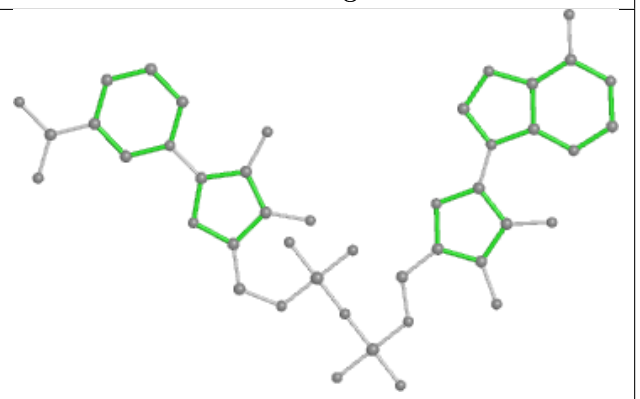
Bond lengths



Bond angles

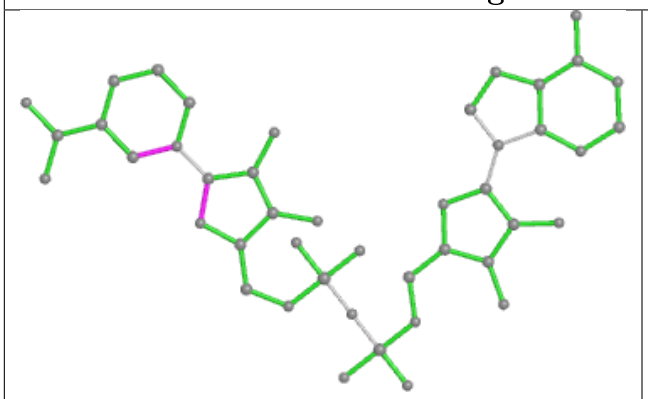


Torsions

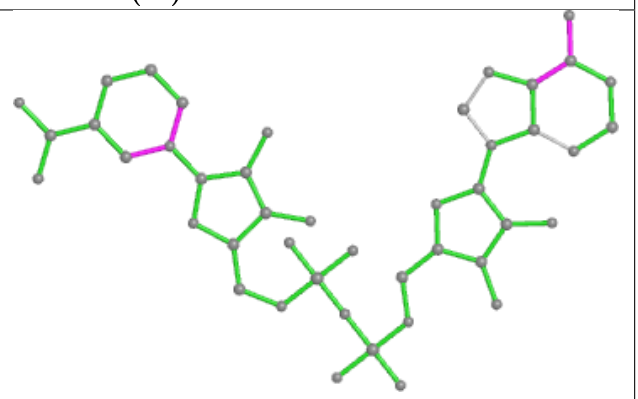


Rings

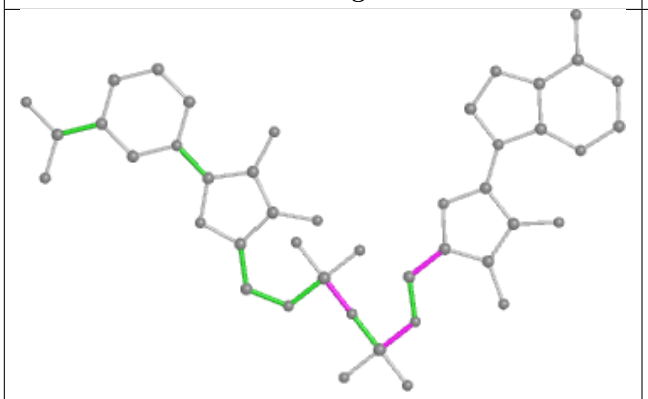
Ligand NAD D 301 (A)



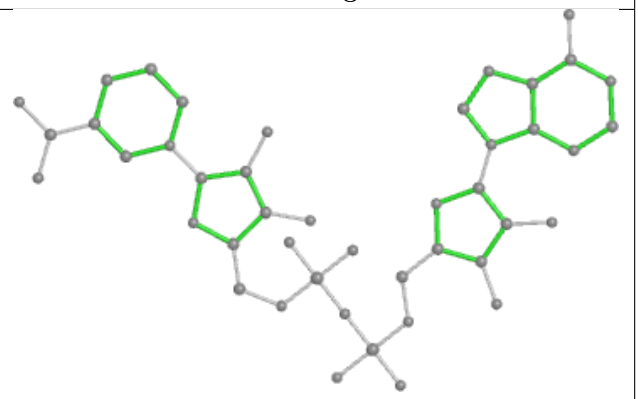
Bond lengths



Bond angles

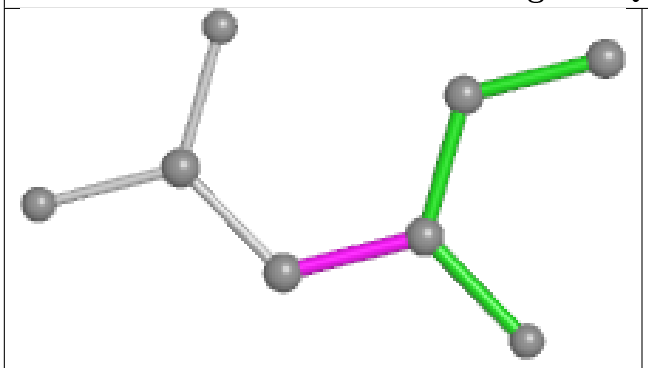


Torsions

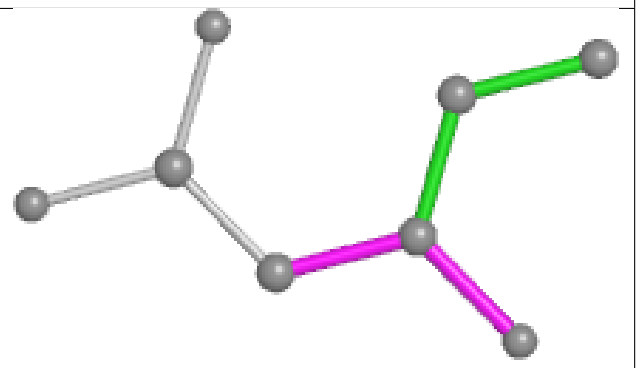


Rings

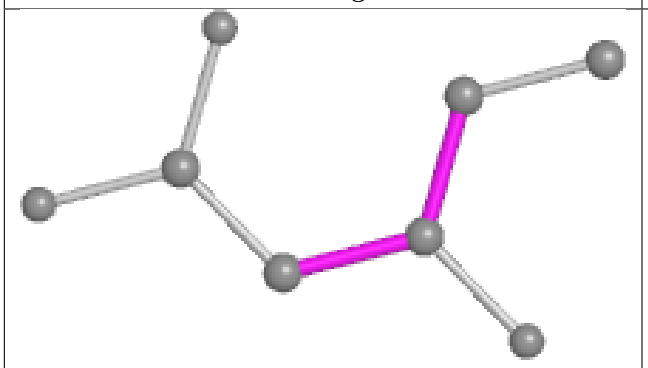
Ligand QT8 C 303



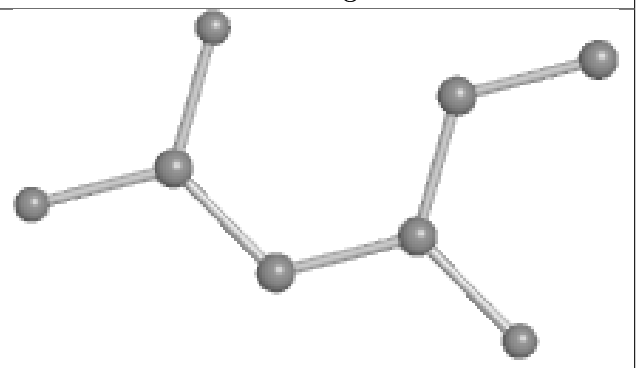
Bond lengths



Bond angles

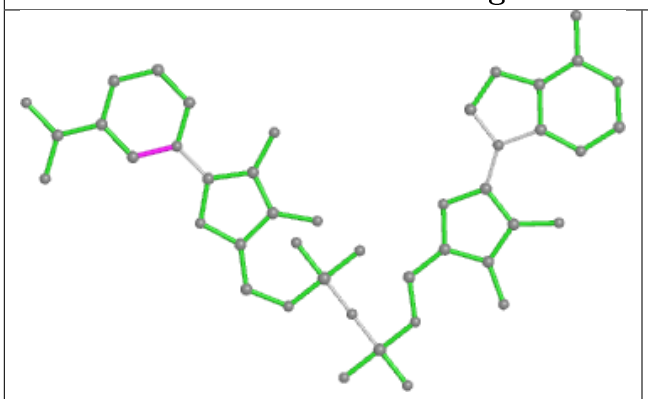


Torsions

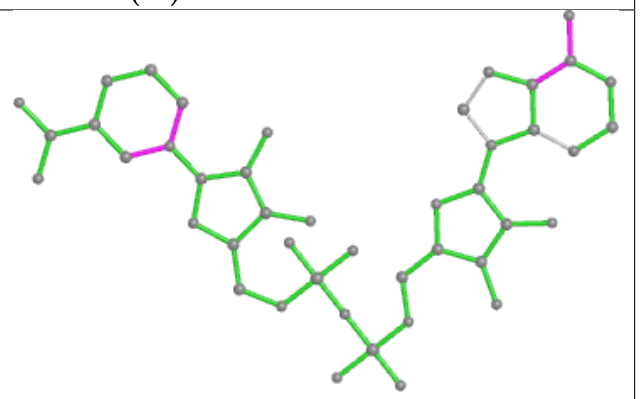


Rings

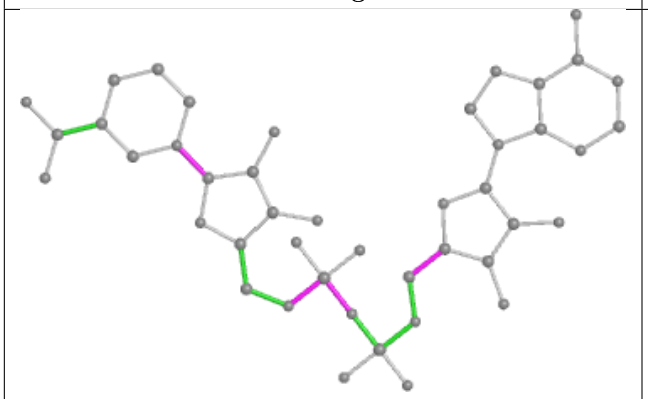
Ligand NAD B 301 (A)



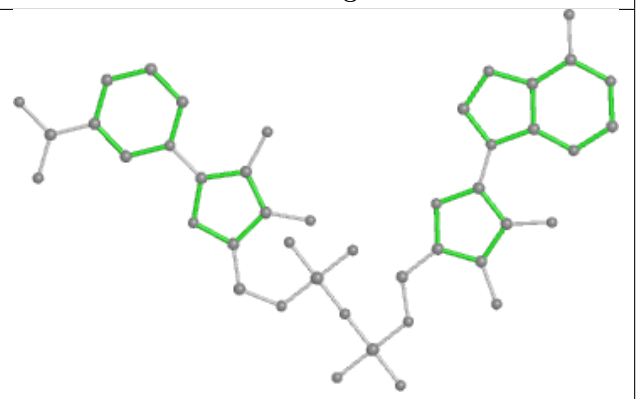
Bond lengths



Bond angles

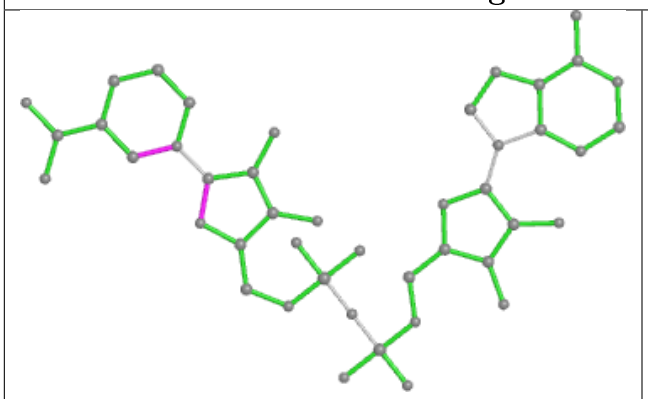


Torsions

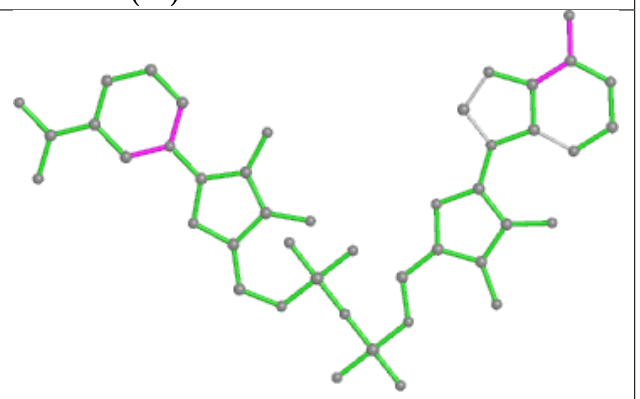


Rings

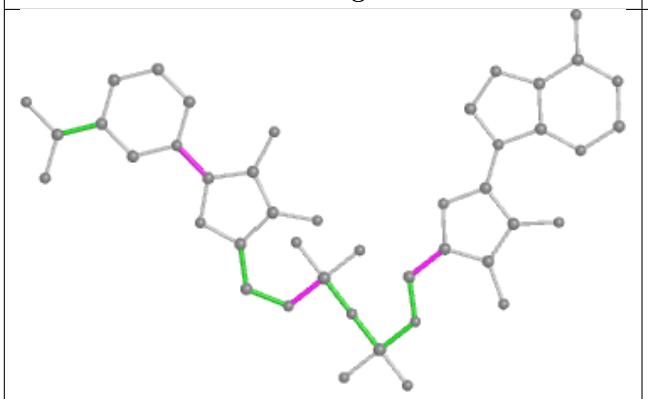
Ligand NAD C 301 (A)



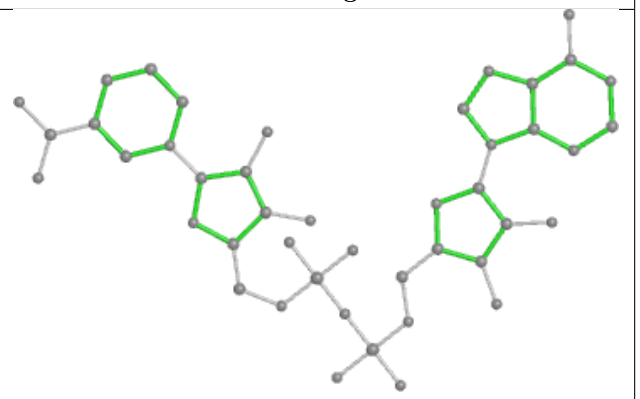
Bond lengths



Bond angles

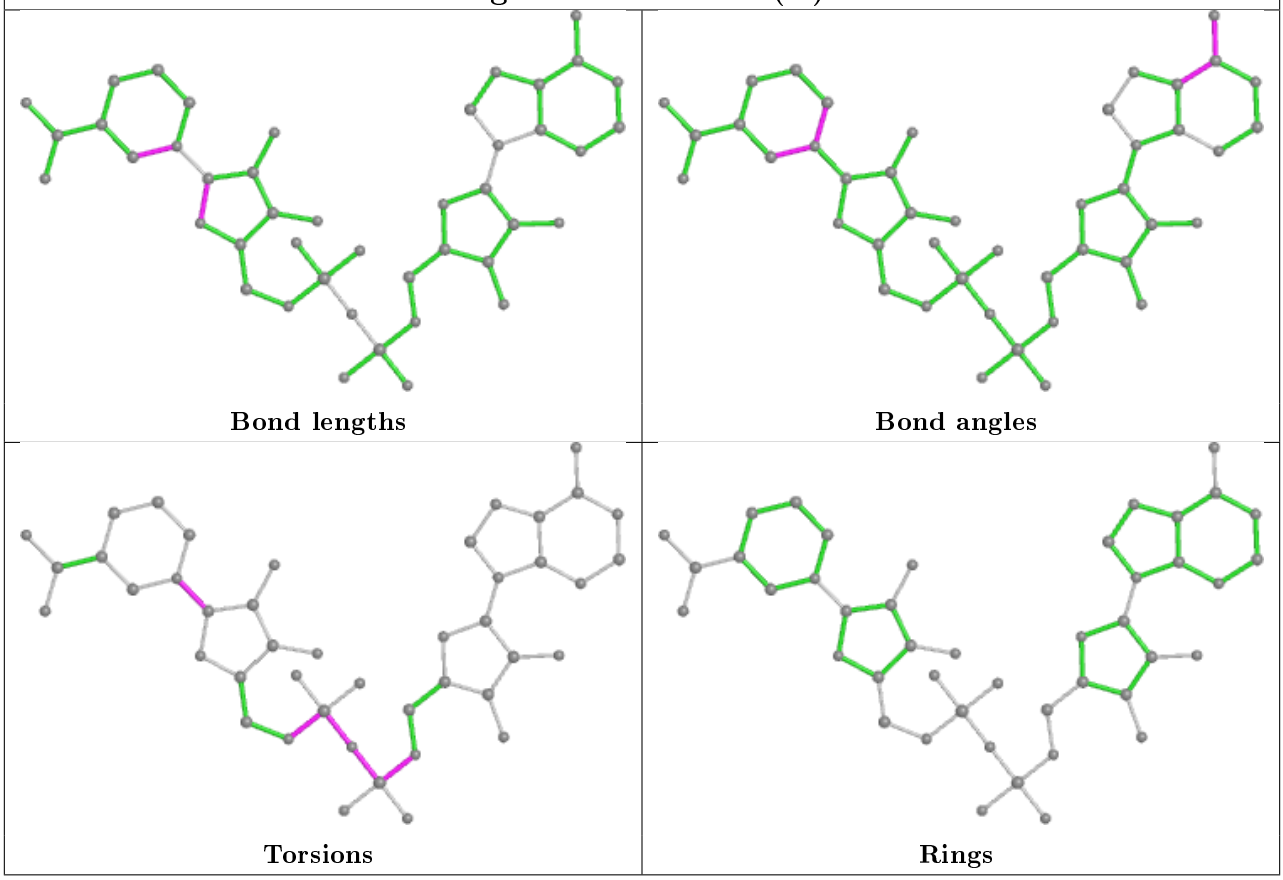


Torsions

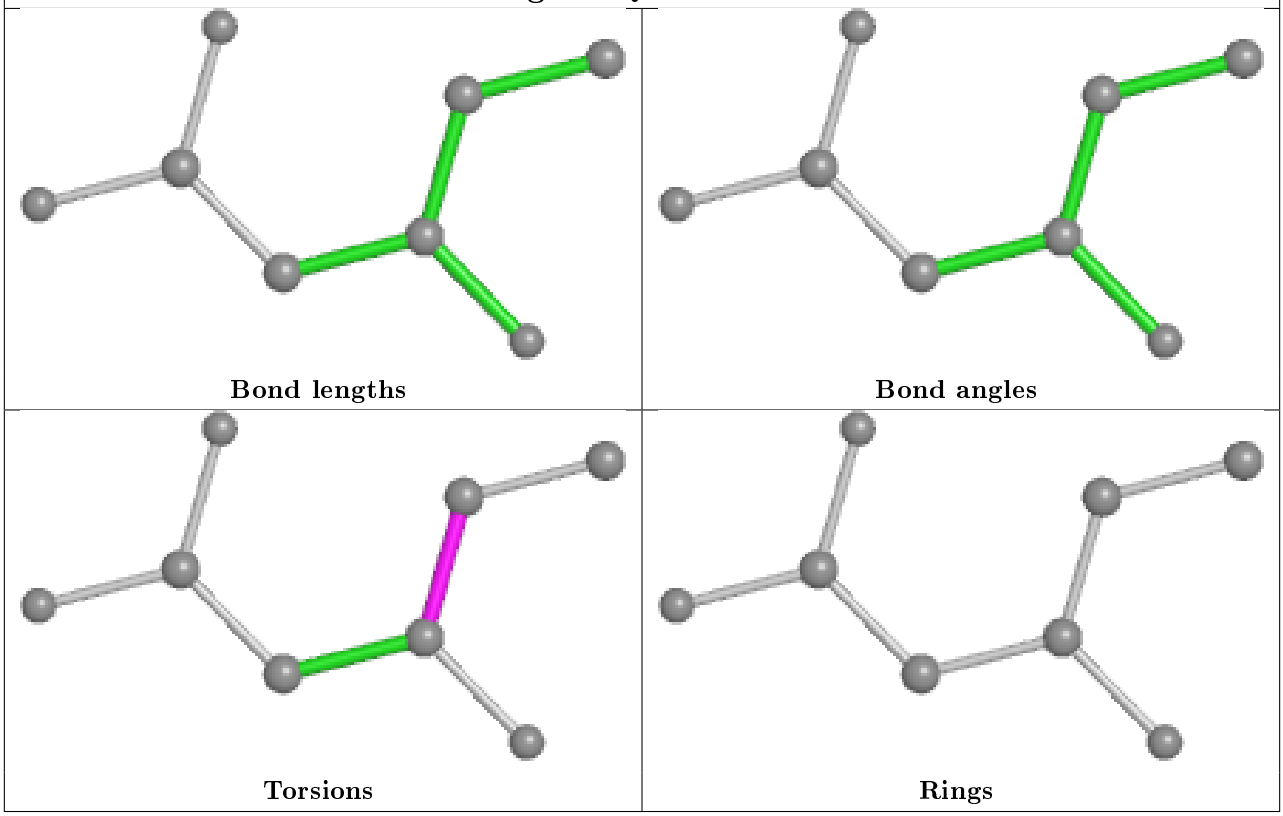


Rings

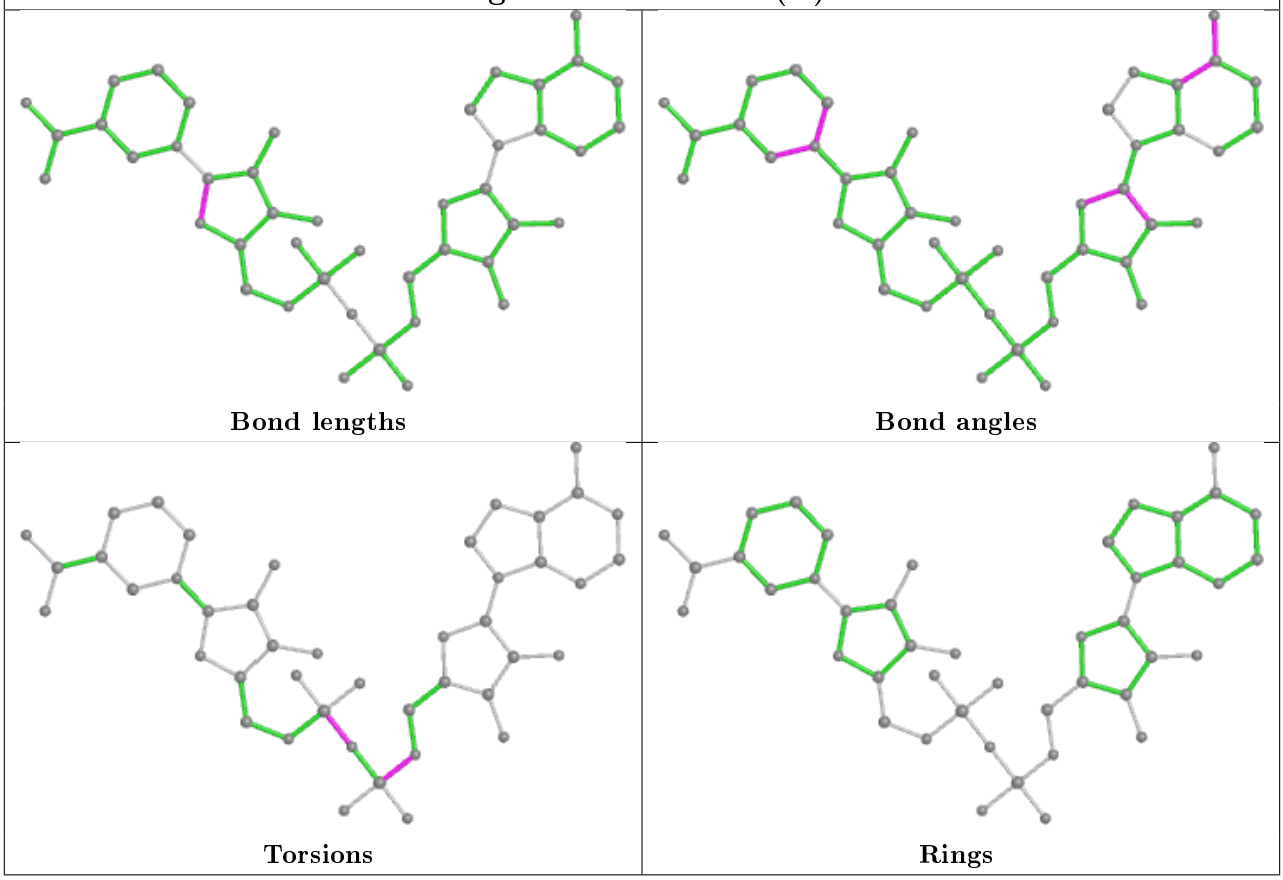
Ligand NAD E 301 (B)



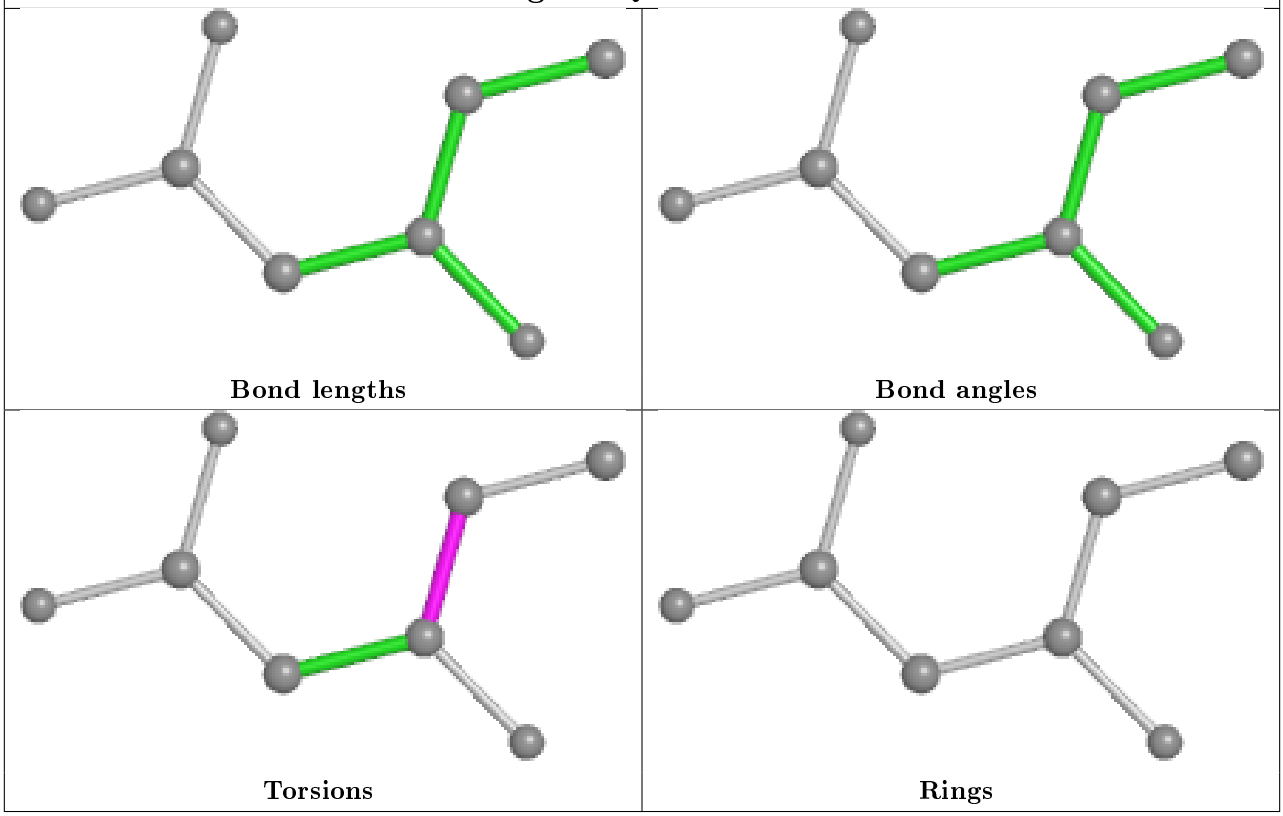
Ligand QT8 A 302



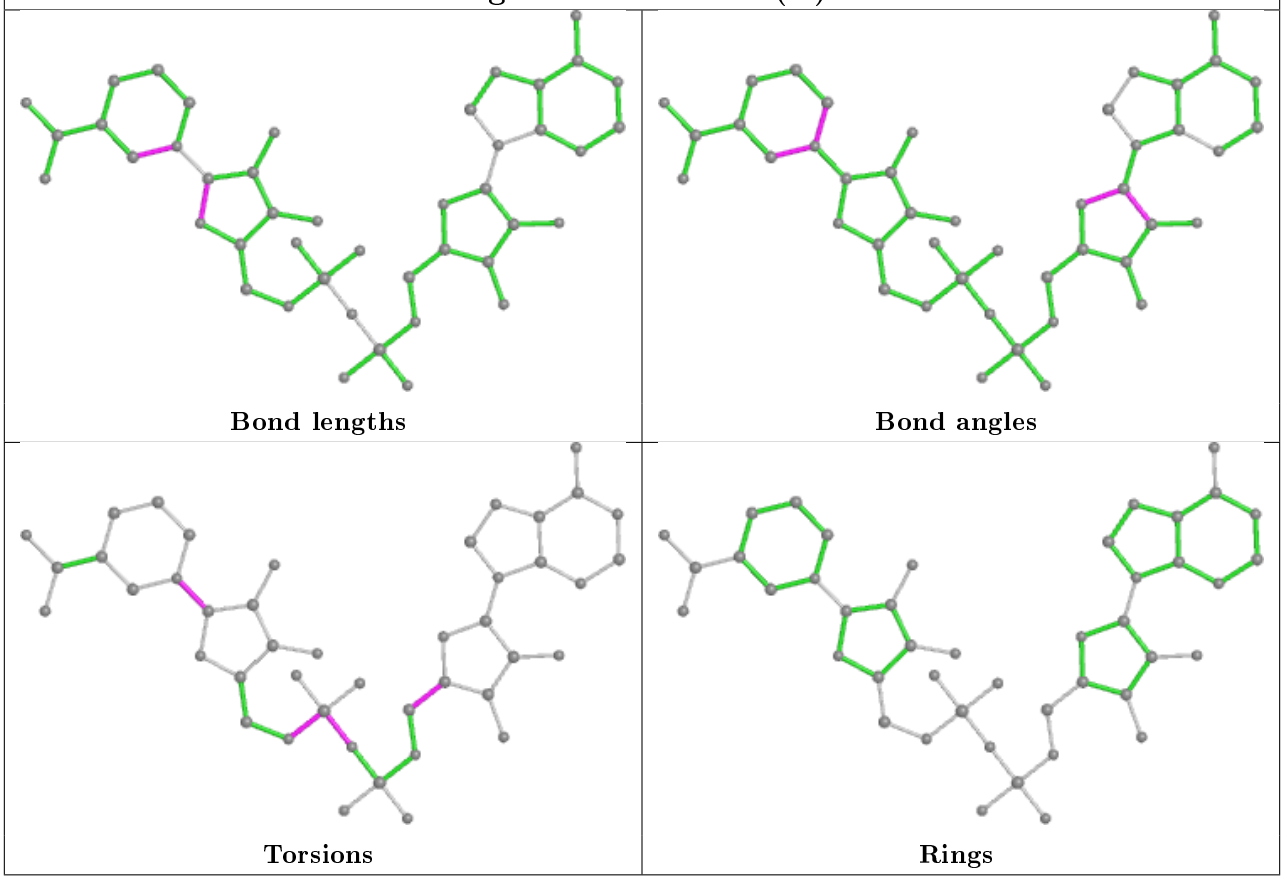
Ligand NAD C 301 (B)



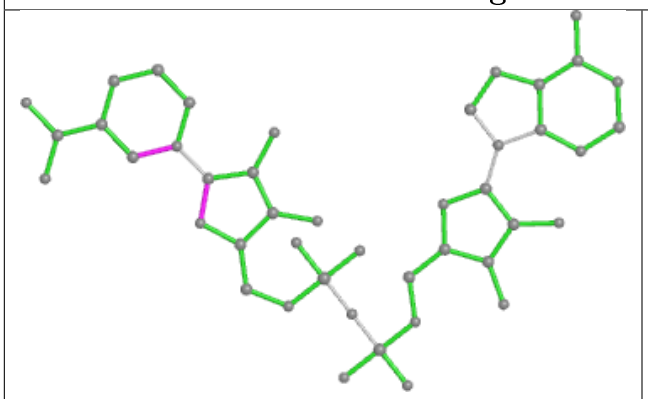
Ligand QT8 C 302



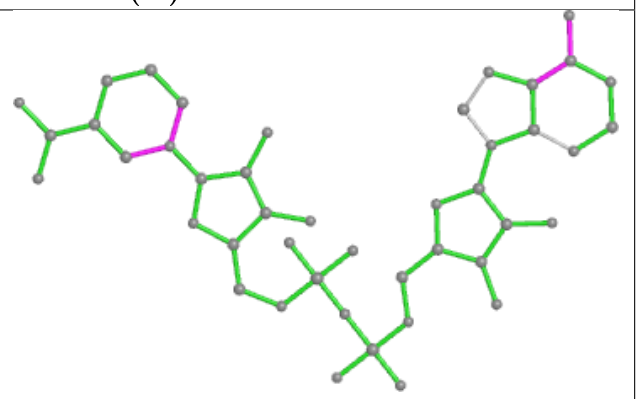
Ligand NAD A 301 (B)



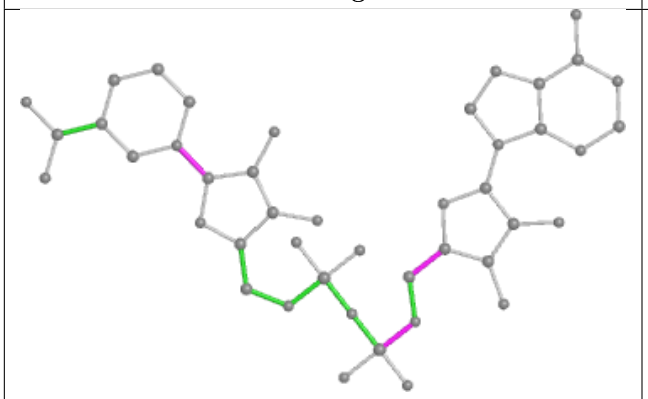
Ligand NAD B 301 (B)



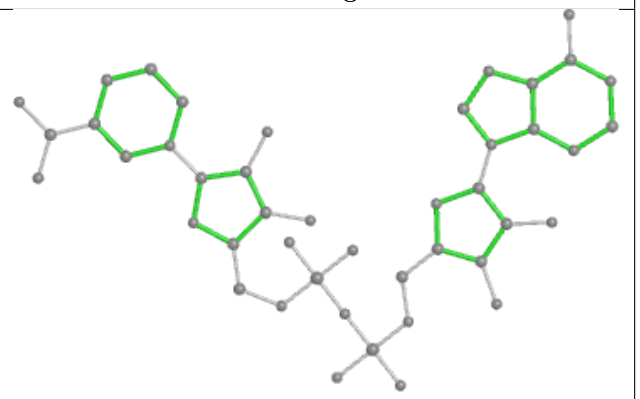
Bond lengths



Bond angles

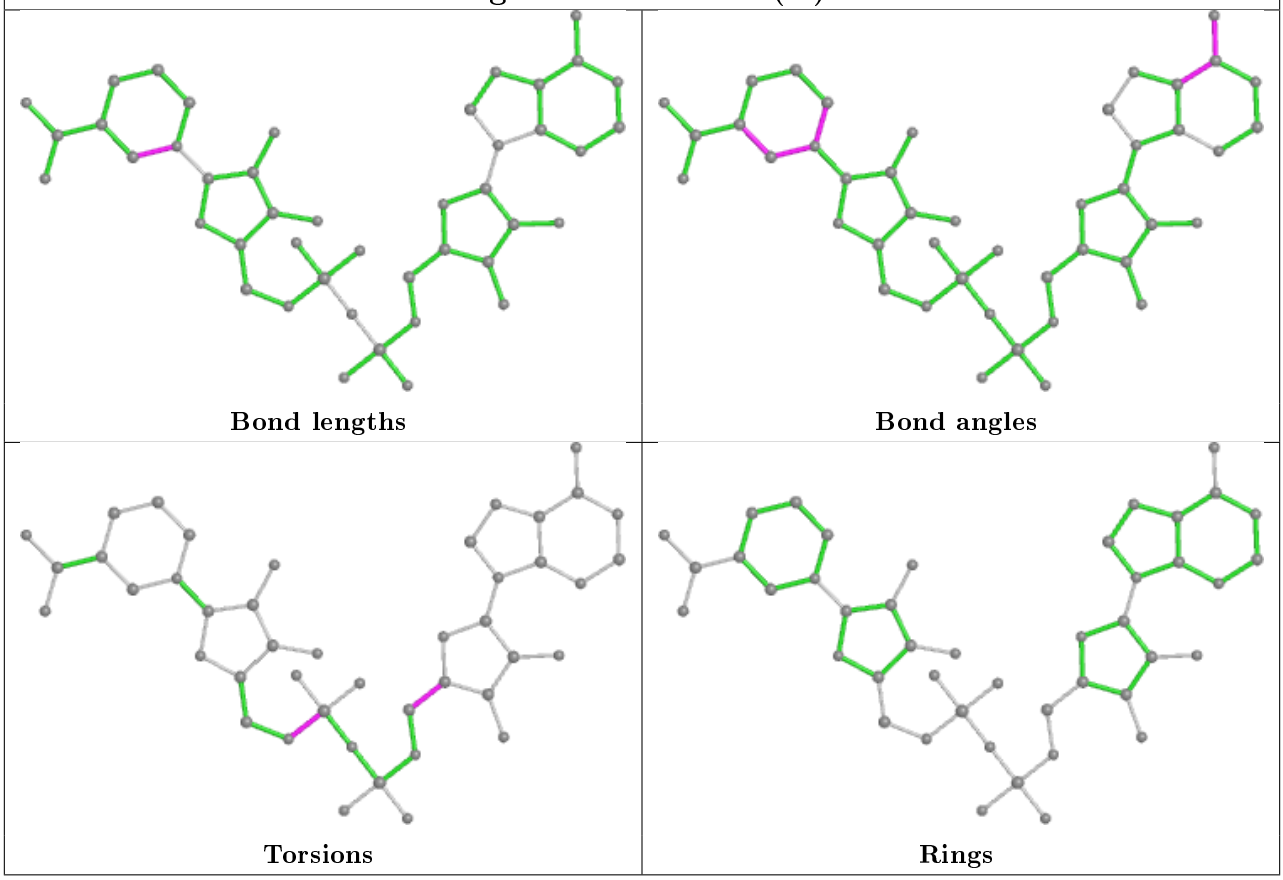


Torsions



Rings

Ligand NAD E 301 (A)



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	260/261 (99%)	-0.01	3 (1%)	79	79	19, 29, 52, 77	0
1	B	260/261 (99%)	-0.01	0	100	100	20, 29, 52, 70	0
1	C	260/261 (99%)	0.02	0	100	100	20, 30, 52, 73	0
1	D	261/261 (100%)	-0.04	0	100	100	19, 30, 52, 70	0
1	E	254/261 (97%)	0.21	2 (0%)	86	86	26, 37, 56, 69	0
1	F	252/261 (96%)	0.22	4 (1%)	72	72	27, 38, 55, 69	0
All	All	1547/1566 (98%)	0.06	9 (0%)	89	89	19, 32, 53, 77	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	209	LEU	3.1
1	F	216	VAL	3.1
1	E	7	GLY	2.9
1	E	251	ALA	2.9
1	F	212	ALA	2.8

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 monosaccharides in this entry.

6.4 Ligands (i)

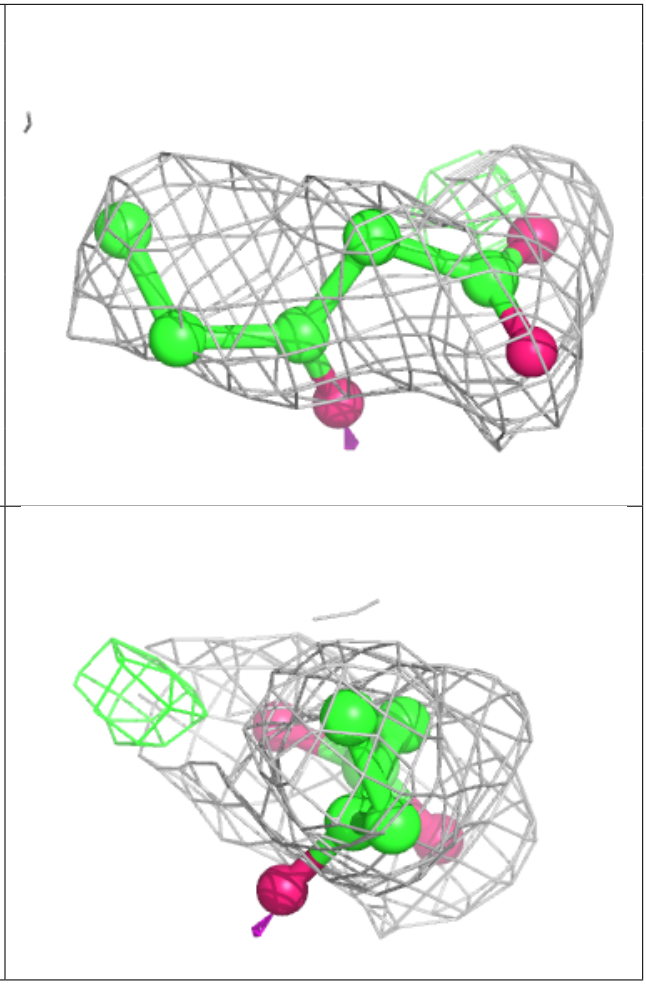
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	QT8	A	302	8/8	0.67	0.23	53,62,66,77	0
3	QT8	D	302	8/8	0.71	0.20	48,58,60,65	0
3	QT8	C	303	8/8	0.73	0.27	55,62,64,73	0
3	QT8	C	302	8/8	0.73	0.21	56,60,66,73	0
3	QT8	F	302	8/8	0.76	0.18	67,70,71,74	0
3	QT8	B	302	8/8	0.81	0.17	64,67,68,73	0
2	NAD	A	301[A]	44/44	0.92	0.13	31,44,55,56	44
2	NAD	E	301[B]	44/44	0.92	0.11	27,32,37,39	44
2	NAD	A	301[B]	44/44	0.92	0.13	20,25,29,31	44
2	NAD	E	301[A]	44/44	0.92	0.11	35,44,59,61	44
2	NAD	D	301[B]	44/44	0.93	0.10	34,40,45,48	44
2	NAD	F	301	44/44	0.93	0.10	33,45,58,73	0
2	NAD	D	301[A]	44/44	0.93	0.10	24,30,34,34	44
2	NAD	B	301[A]	44/44	0.94	0.12	24,32,36,38	44
2	NAD	C	301[A]	44/44	0.94	0.09	25,36,41,43	44
2	NAD	B	301[B]	44/44	0.94	0.12	23,29,34,35	44
2	NAD	C	301[B]	44/44	0.94	0.09	26,33,43,44	44

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.

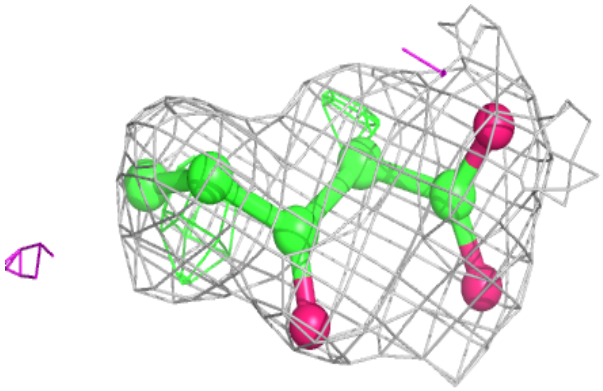
Electron density around QT8 A 302:

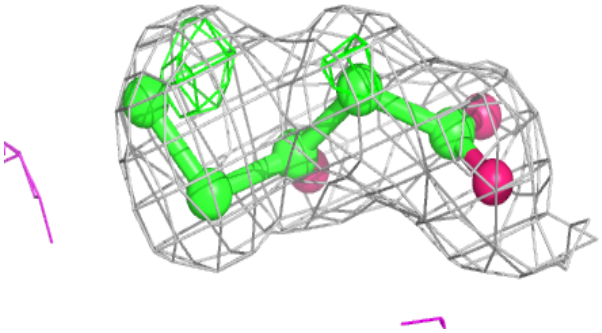
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

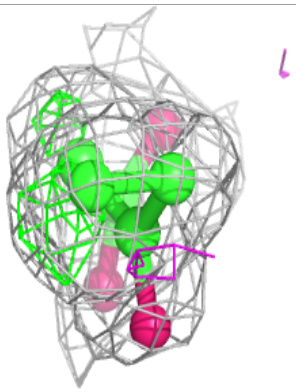


Electron density around QT8 D 302:

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

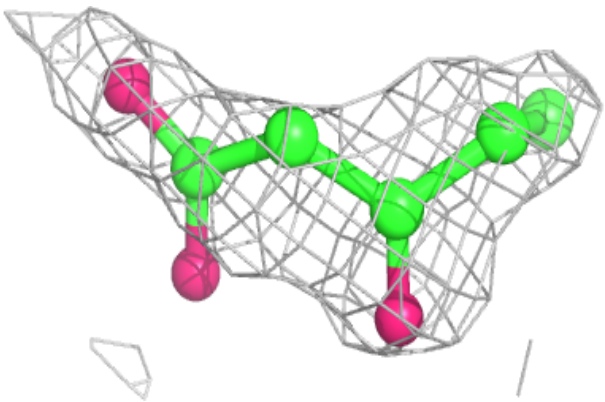


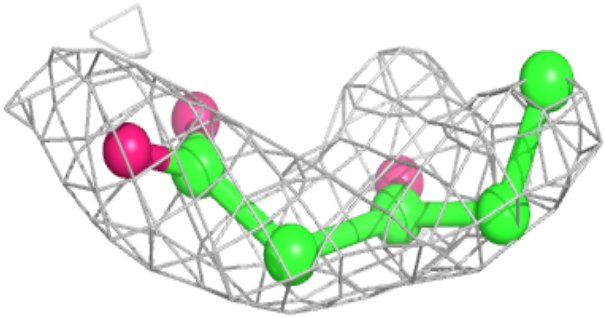


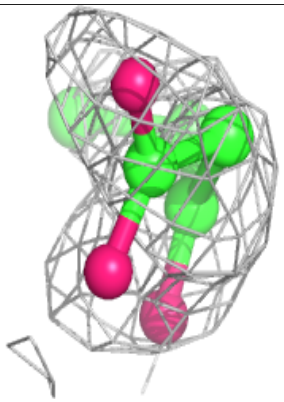


Electron density around QT8 C 303:

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

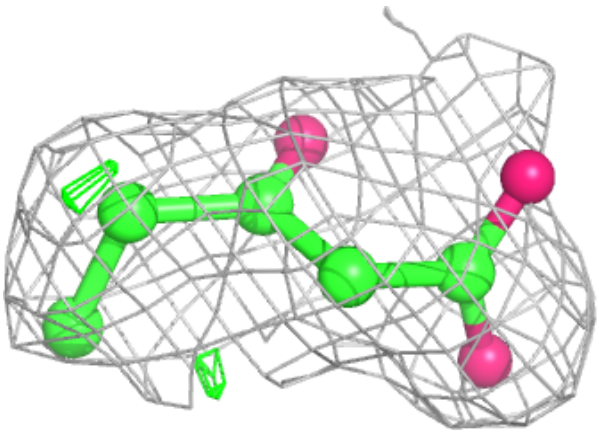


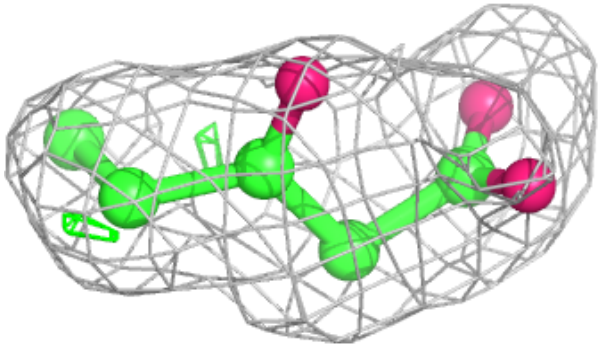


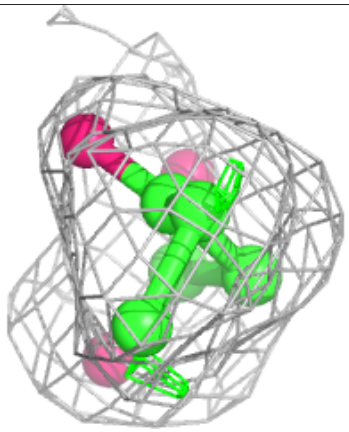


Electron density around QT8 C 302:

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

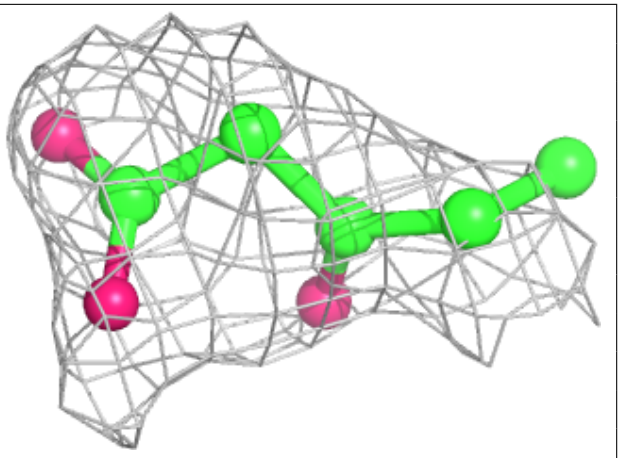


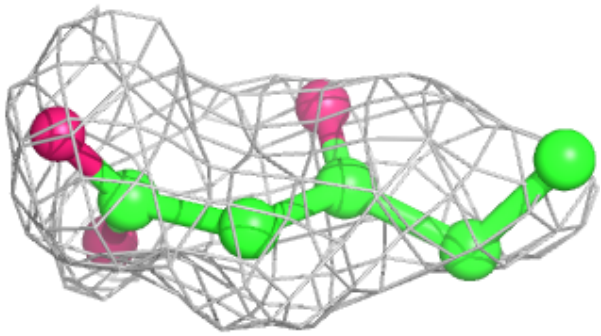


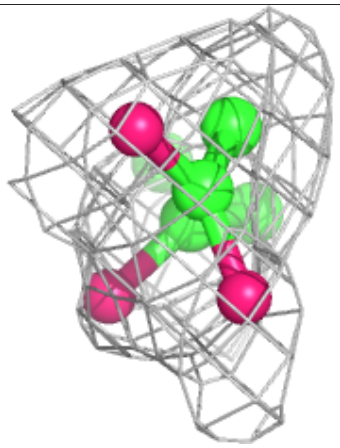


Electron density around QT8 F 302:

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

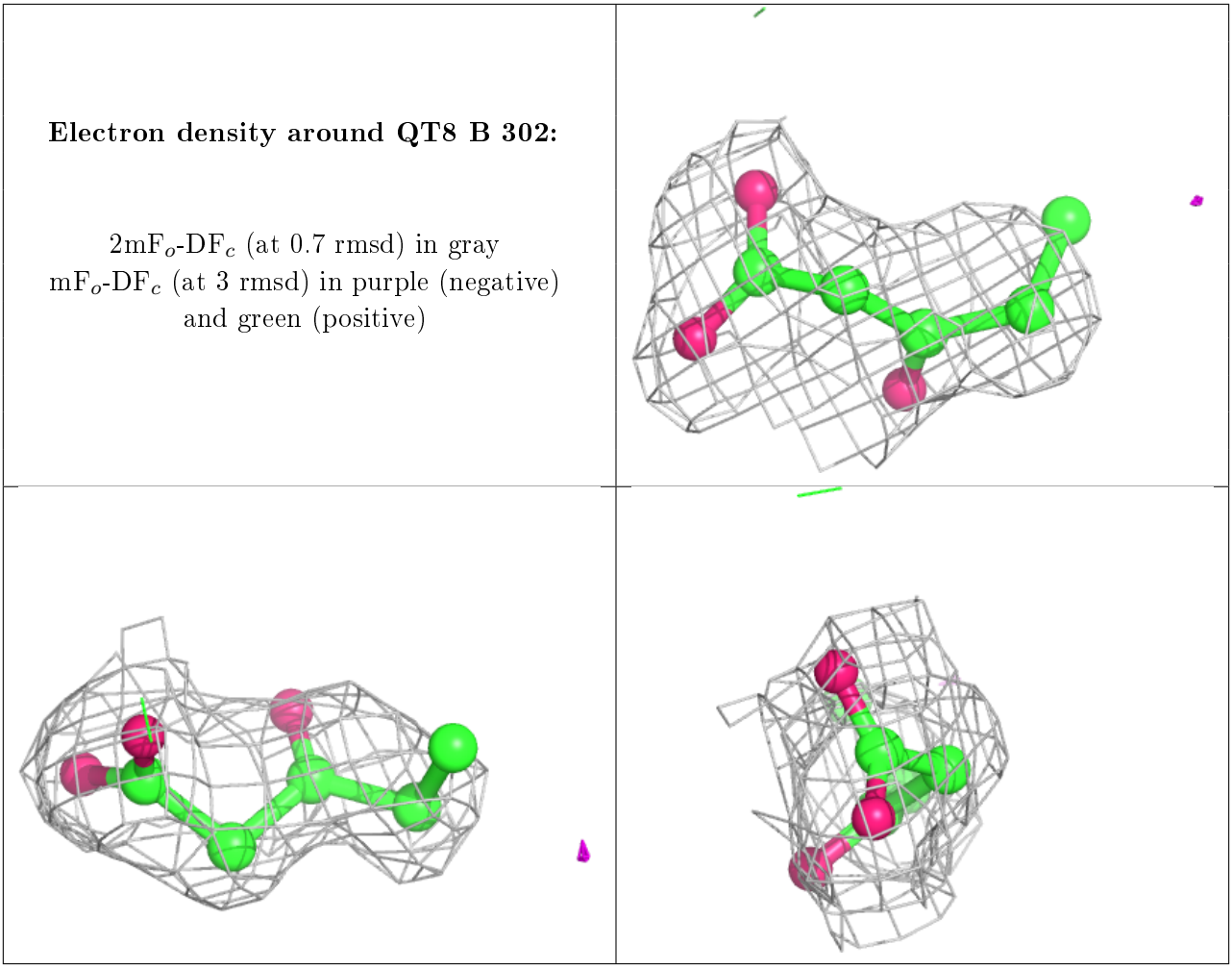






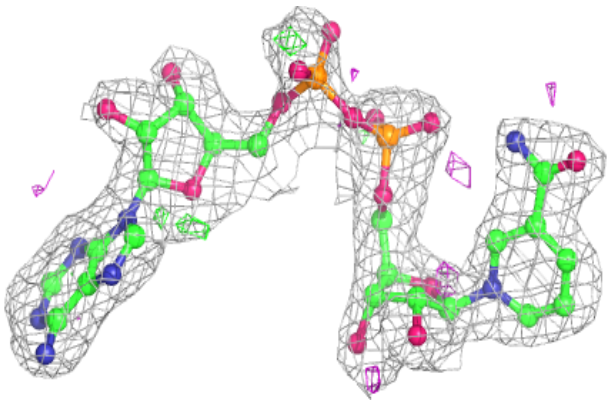
Electron density around QT8 B 302:

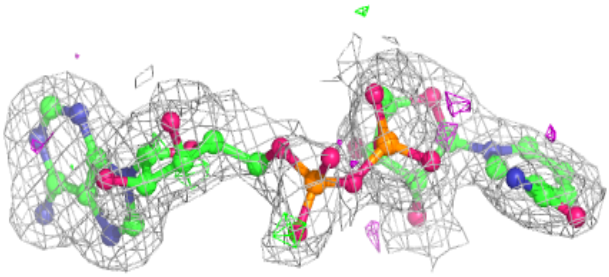
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

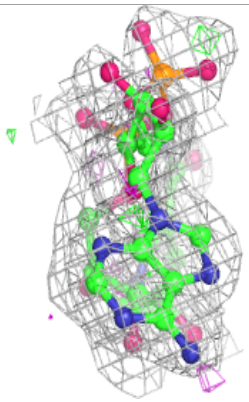


Electron density around NAD A 301 (A):

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

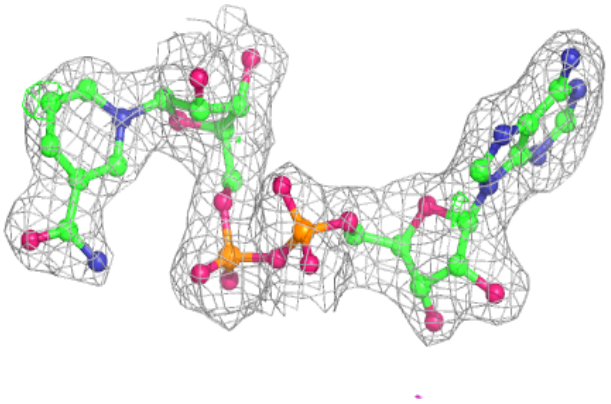


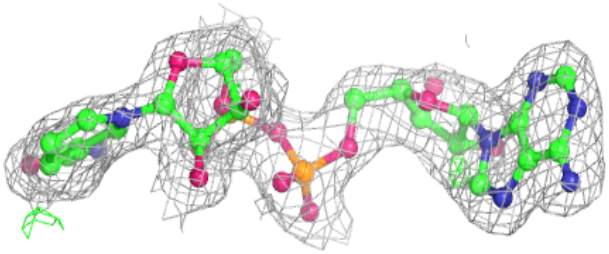


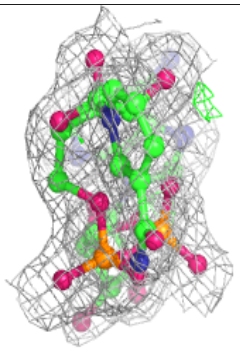


Electron density around NAD E 301 (B):

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

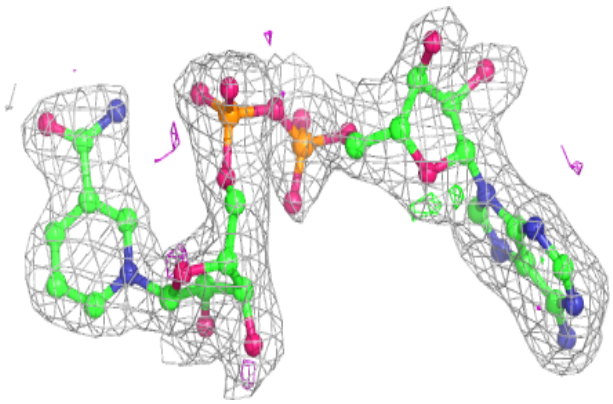


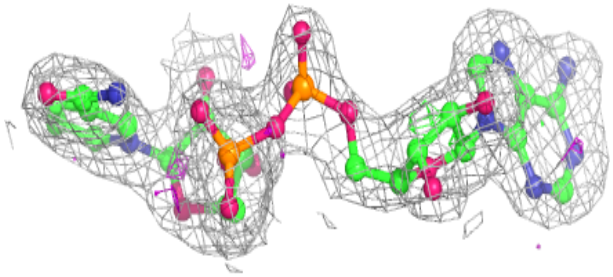


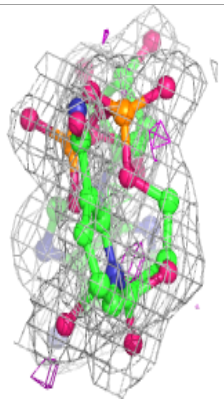


Electron density around NAD A 301 (B):

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

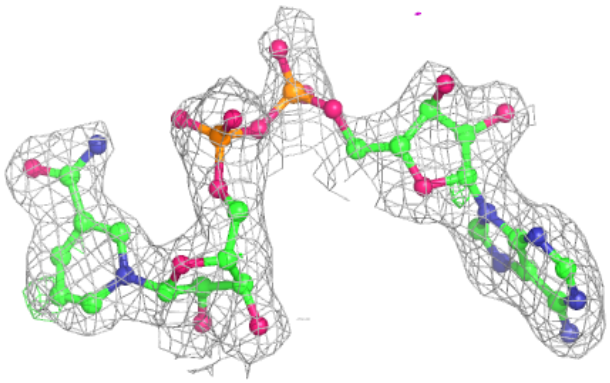


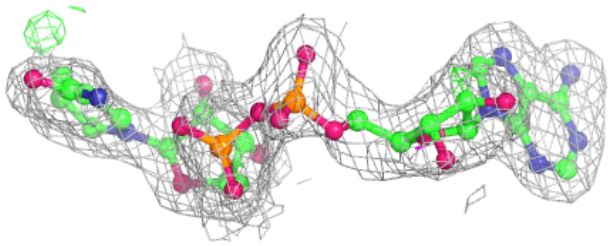


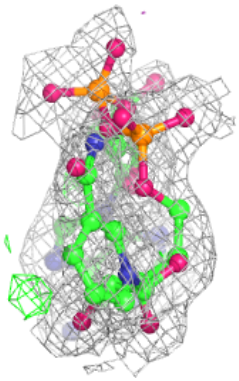


Electron density around NAD E 301 (A):

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

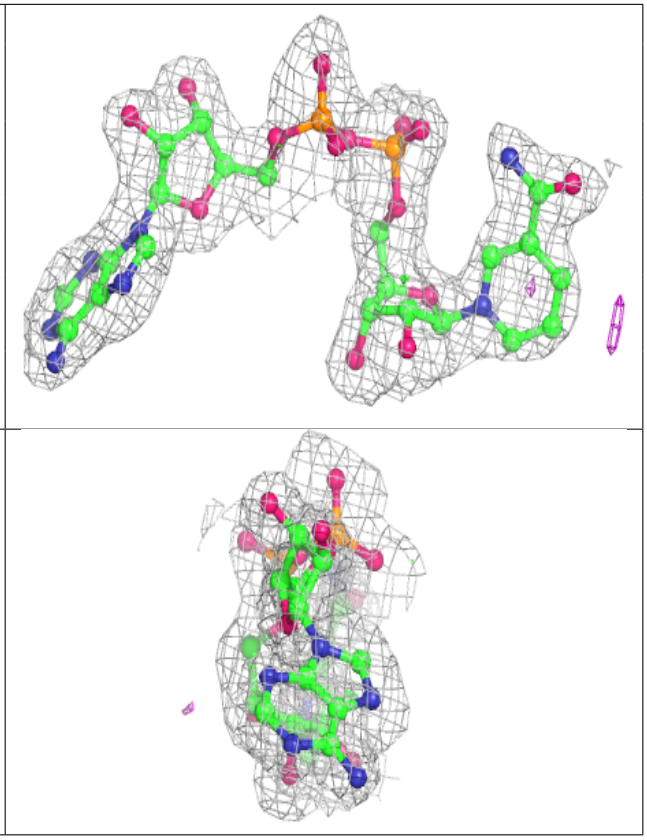


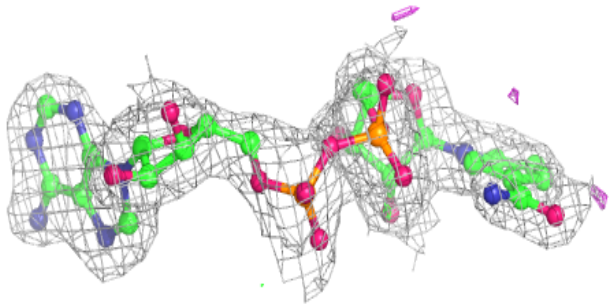




Electron density around NAD D 301 (B):

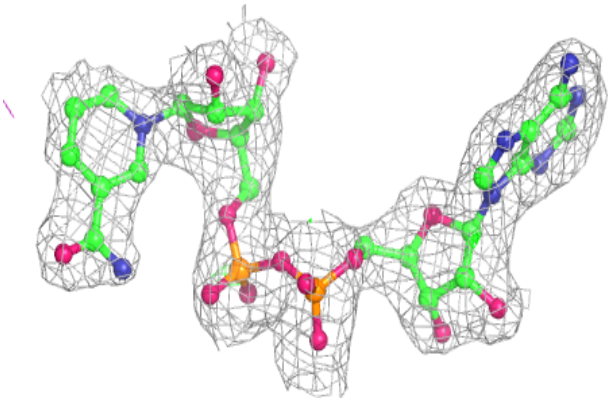
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

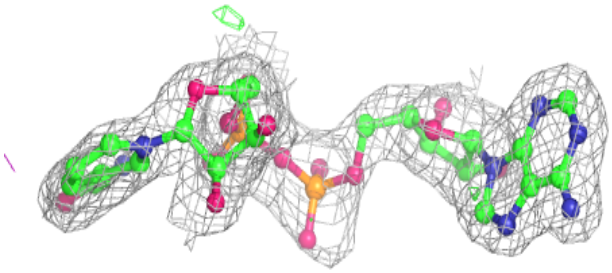


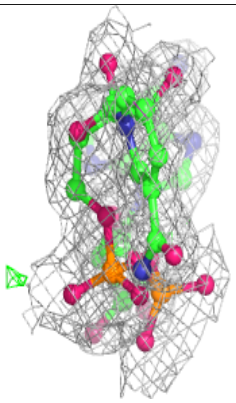


Electron density around NAD F 301:

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

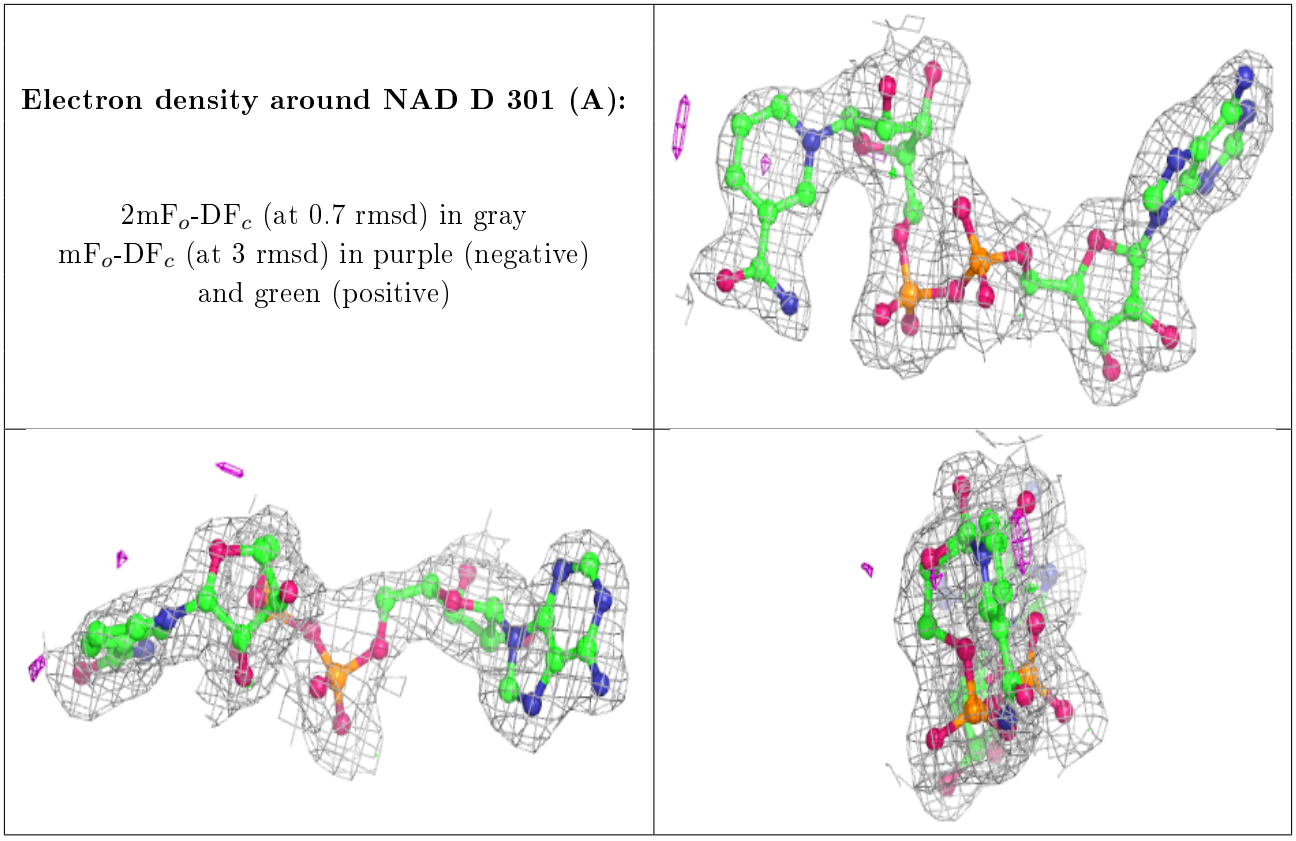






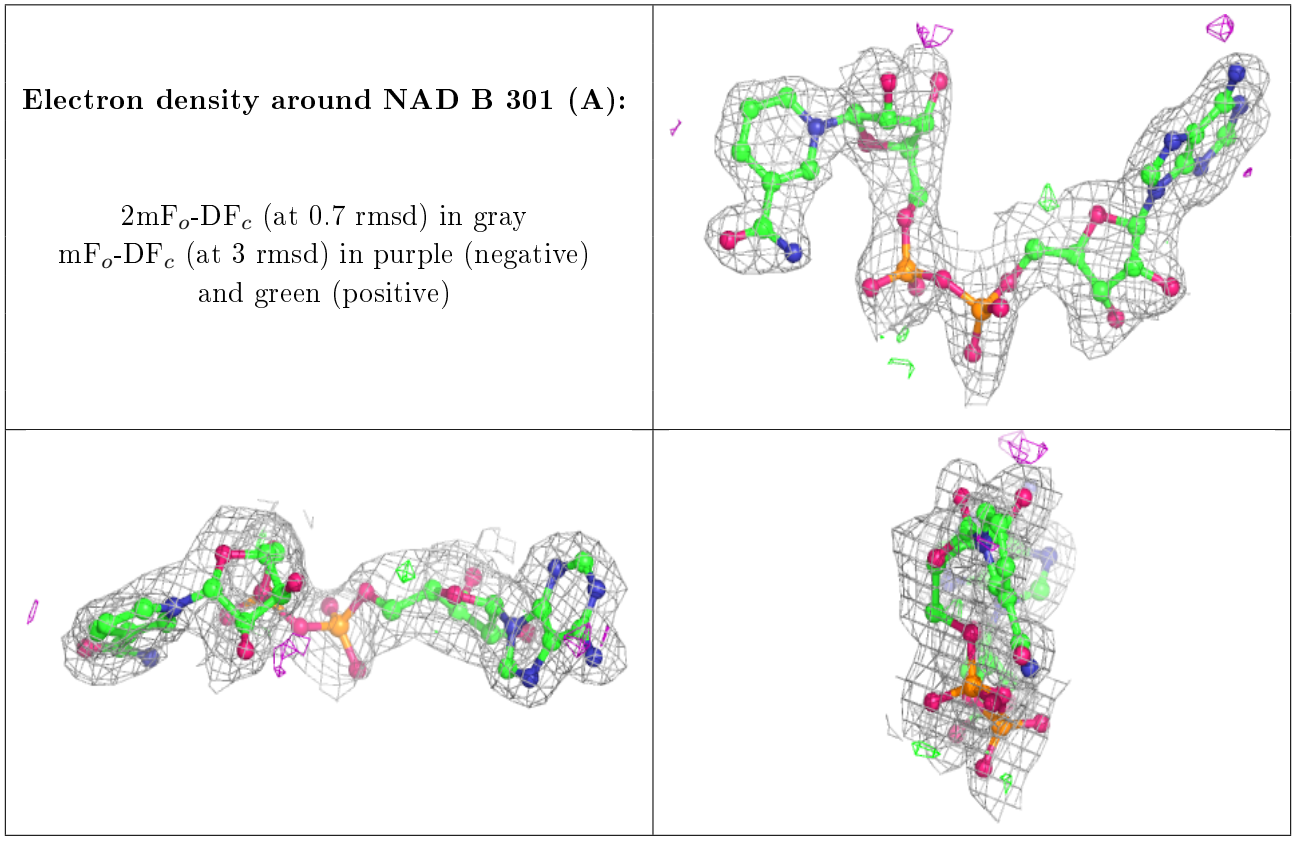
Electron density around NAD D 301 (A):

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



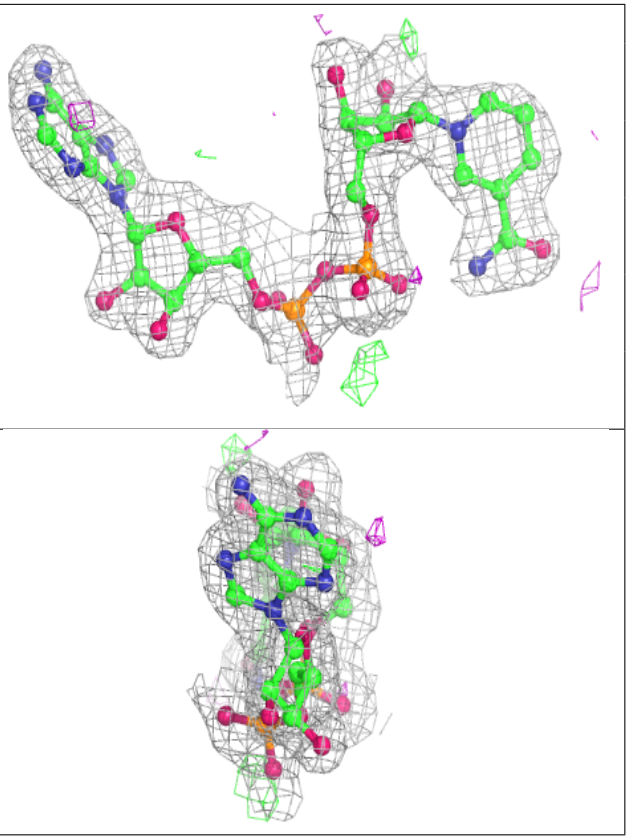
Electron density around NAD B 301 (A):

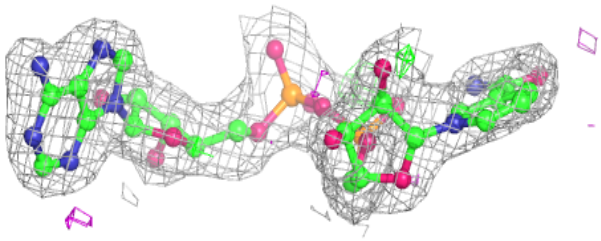
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NAD C 301 (A):

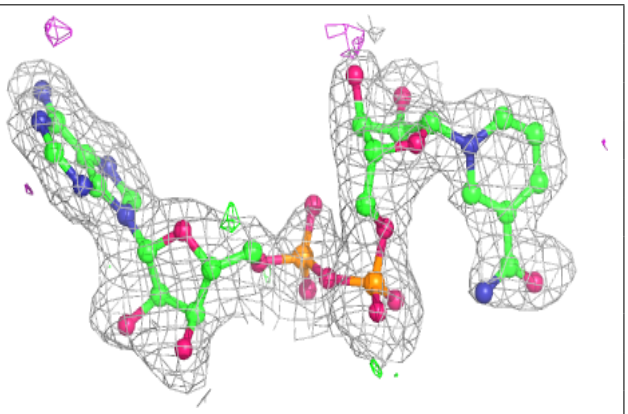
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

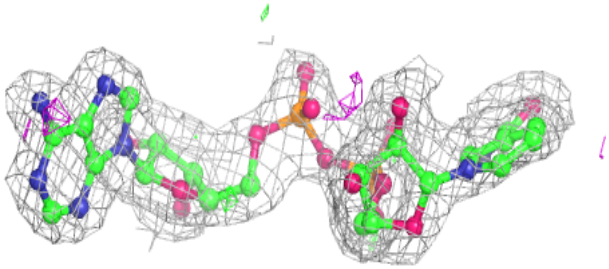


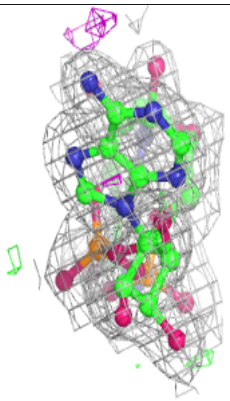


Electron density around NAD B 301 (B):

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

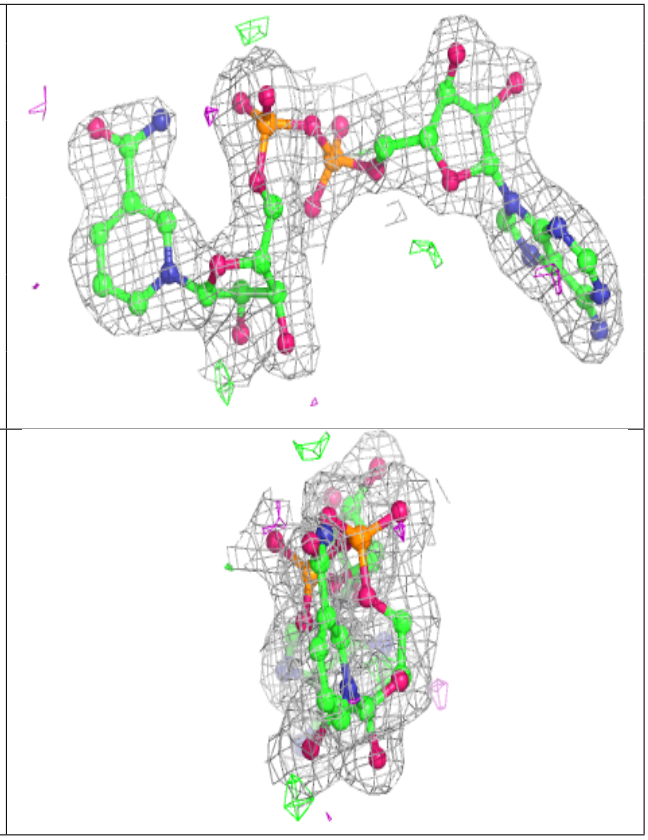






Electron density around NAD C 301 (B):

$2mF_o$-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.