



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 12:09 pm BST

PDB ID : 6O4H  
Title : Structure of ALDH7A1 mutant A171V complexed with NAD  
Authors : Tanner, J.J.; Korasick, D.A.; Laciak, A.R.  
Deposited on : 2019-02-28  
Resolution : 2.05 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.11  
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) : 2.11

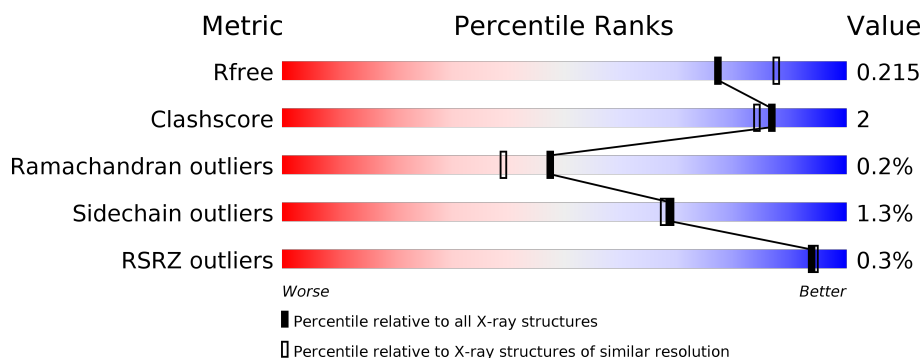
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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  $\geq 3$ , 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	513	<div> <div>91%</div> <div>6% •</div> </div>
1	B	513	<div> <div>91%</div> <div>6% •</div> </div>
1	C	513	<div> <div>%</div> <div>90%</div> <div>7% •</div> </div>
1	D	513	<div> <div>90%</div> <div>7% •</div> </div>
1	E	513	<div> <div>91%</div> <div>6% •</div> </div>
1	F	513	<div> <div>91%</div> <div>5% • •</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	513	 92% 5% •
1	H	513	 93% • •

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31649 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 Alpha-aminoadipic semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	1	0
			3745	2376	651	701	17			
1	B	497	Total	C	N	O	S	0	1	0
			3721	2360	645	699	17			
1	C	497	Total	C	N	O	S	0	1	0
			3696	2349	639	691	17			
1	D	497	Total	C	N	O	S	0	1	0
			3725	2368	644	696	17			
1	E	498	Total	C	N	O	S	0	2	0
			3767	2392	652	705	18			
1	F	497	Total	C	N	O	S	0	1	0
			3762	2389	653	703	17			
1	G	497	Total	C	N	O	S	0	0	0
			3763	2389	654	703	17			
1	H	497	Total	C	N	O	S	0	2	0
			3767	2393	653	703	18			

There are 24 discrepancies between the modelled and reference sequences:

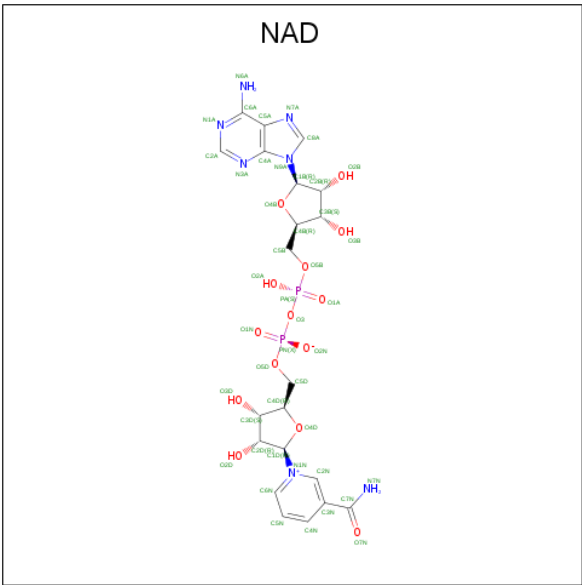
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P49419
A	0	HIS	-	expression tag	UNP P49419
A	171	VAL	ALA	engineered mutation	UNP P49419
B	-1	GLY	-	expression tag	UNP P49419
B	0	HIS	-	expression tag	UNP P49419
B	171	VAL	ALA	engineered mutation	UNP P49419
C	-1	GLY	-	expression tag	UNP P49419
C	0	HIS	-	expression tag	UNP P49419
C	171	VAL	ALA	engineered mutation	UNP P49419
D	-1	GLY	-	expression tag	UNP P49419
D	0	HIS	-	expression tag	UNP P49419
D	171	VAL	ALA	engineered mutation	UNP P49419
E	-1	GLY	-	expression tag	UNP P49419

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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	HIS	-	expression tag	UNP P49419
E	171	VAL	ALA	engineered mutation	UNP P49419
F	-1	GLY	-	expression tag	UNP P49419
F	0	HIS	-	expression tag	UNP P49419
F	171	VAL	ALA	engineered mutation	UNP P49419
G	-1	GLY	-	expression tag	UNP P49419
G	0	HIS	-	expression tag	UNP P49419
G	171	VAL	ALA	engineered mutation	UNP P49419
H	-1	GLY	-	expression tag	UNP P49419
H	0	HIS	-	expression tag	UNP P49419
H	171	VAL	ALA	engineered mutation	UNP P49419

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by author).



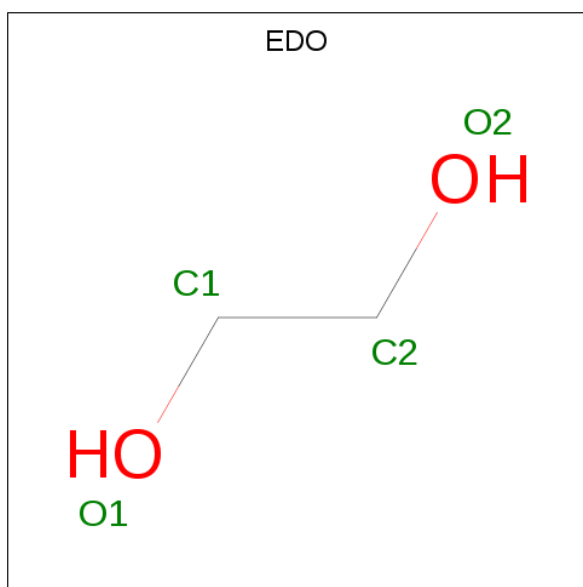
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	206	Total	O	0	0
			206	206		
4	B	157	Total	O	0	0
			157	157		
4	C	134	Total	O	0	0
			134	134		
4	D	133	Total	O	0	0
			133	133		

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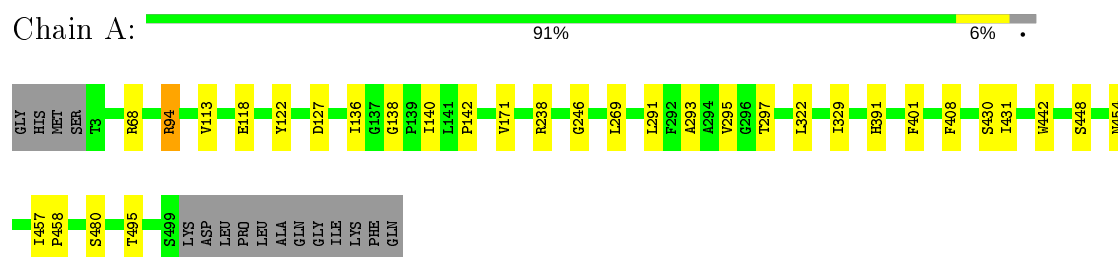
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	188	Total 188	O 188	0	0
4	F	175	Total 175	O 175	0	0
4	G	177	Total 177	O 177	0	0
4	H	173	Total 173	O 173	0	0

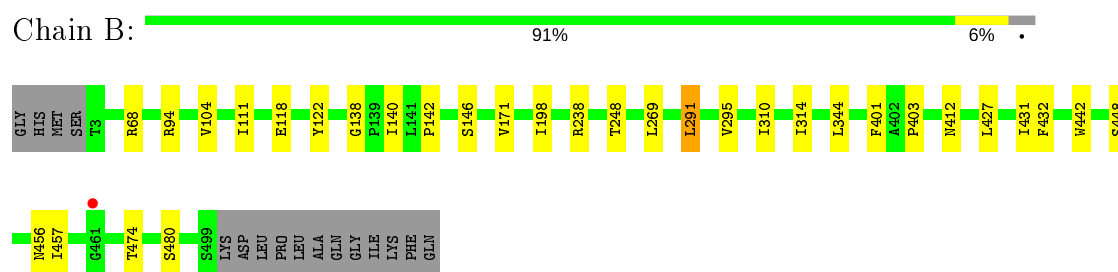
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

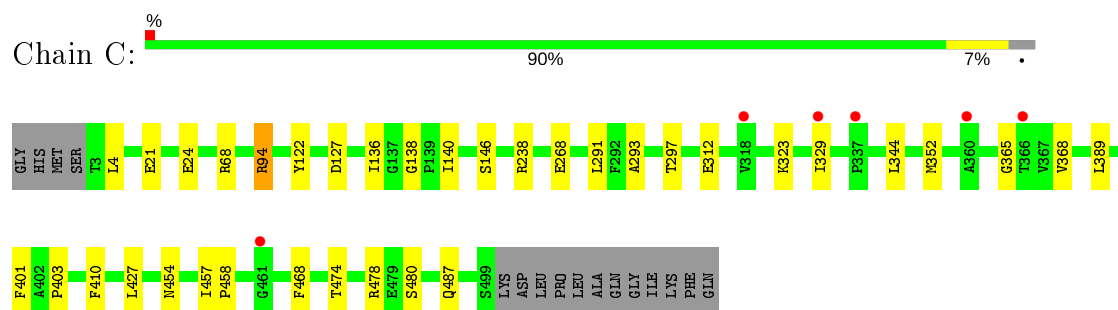
- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase



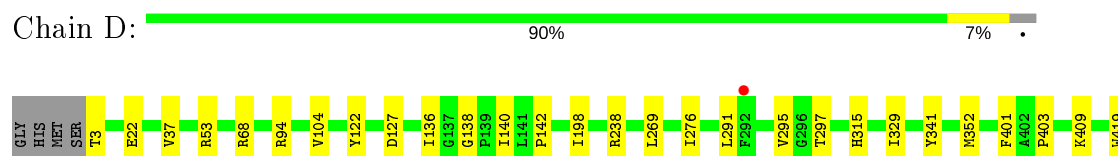
- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase



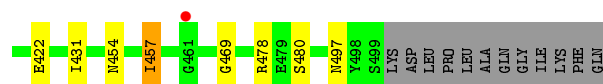
- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase



- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

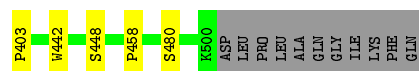






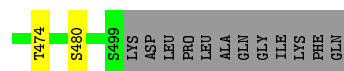
- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain E: 91% 6% .



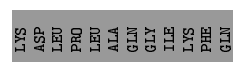
- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain F: 91% 5% . .



- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain G: 92% 5% .



- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain H: 93% . .



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.98Å 161.36Å 159.16Å 90.00° 95.00° 90.00°	Depositor
Resolution (Å)	56.55 – 2.05 56.55 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.7 (56.55-2.05) 99.7 (56.55-2.05)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 2.05Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.174 , 0.219 0.168 , 0.215	Depositor DCC
$R_{free}$ test set	12115 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.8	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	31649	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: EDO, 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	0.40	0/3825	0.54	0/5199
1	B	0.39	0/3800	0.54	0/5170
1	C	0.38	0/3775	0.53	0/5139
1	D	0.36	0/3805	0.52	0/5175
1	E	0.38	0/3850	0.54	0/5229
1	F	0.38	0/3842	0.54	0/5218
1	G	0.38	0/3840	0.54	0/5213
1	H	0.38	0/3850	0.54	0/5228
All	All	0.38	0/30587	0.54	0/41571

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	3745	0	3699	23	0
1	B	3721	0	3653	16	0
1	C	3696	0	3617	19	0
1	D	3725	0	3665	20	0
1	E	3767	0	3735	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3762	0	3738	18	0
1	G	3763	0	3746	14	0
1	H	3767	0	3747	12	0
2	A	44	0	24	2	0
2	B	44	0	24	0	0
2	C	44	0	25	2	0
2	D	44	0	24	1	0
2	E	44	0	24	0	0
2	F	44	0	24	2	0
2	G	44	0	24	1	0
2	H	44	0	24	2	0
3	B	4	0	6	0	0
3	F	4	0	6	0	0
4	A	206	0	0	2	0
4	B	157	0	0	1	0
4	C	134	0	0	0	0
4	D	133	0	0	1	0
4	E	188	0	0	2	0
4	F	175	0	0	1	0
4	G	177	0	0	0	0
4	H	173	0	0	1	0
All	All	31649	0	29805	127	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 2.

The worst 5 of 127 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:LEU:HD11	1:D:329:ILE:HD11	1.77	0.66
1:E:295:VAL:HG11	1:E:329:ILE:HD13	1.78	0.65
1:E:94:ARG:NH1	1:E:127:ASP:OD2	2.30	0.64
1:A:68:ARG:HD2	1:A:238:ARG:HB3	1.81	0.63
1:H:228:ASP:HB2	4:H:854:HOH:O	2.00	0.61

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	496/513 (97%)	481 (97%)	14 (3%)	1 (0%)	47	39
1	B	496/513 (97%)	481 (97%)	14 (3%)	1 (0%)	47	39
1	C	496/513 (97%)	480 (97%)	15 (3%)	1 (0%)	47	39
1	D	496/513 (97%)	480 (97%)	15 (3%)	1 (0%)	47	39
1	E	498/513 (97%)	482 (97%)	15 (3%)	1 (0%)	47	39
1	F	496/513 (97%)	482 (97%)	13 (3%)	1 (0%)	47	39
1	G	495/513 (96%)	480 (97%)	14 (3%)	1 (0%)	47	39
1	H	497/513 (97%)	482 (97%)	14 (3%)	1 (0%)	47	39
All	All	3970/4104 (97%)	3848 (97%)	114 (3%)	8 (0%)	47	39

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	SER
1	E	480	SER
1	F	480	SER
1	G	480	SER
1	H	480	SER

### 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	387/411 (94%)	383 (99%)	4 (1%)	76	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	381/411 (93%)	375 (98%)	6 (2%)	62	59
1	C	374/411 (91%)	367 (98%)	7 (2%)	57	53
1	D	381/411 (93%)	376 (99%)	5 (1%)	69	67
1	E	391/411 (95%)	388 (99%)	3 (1%)	81	82
1	F	391/411 (95%)	385 (98%)	6 (2%)	65	63
1	G	392/411 (95%)	387 (99%)	5 (1%)	69	67
1	H	392/411 (95%)	389 (99%)	3 (1%)	81	82
All	All	3089/3288 (94%)	3050 (99%)	39 (1%)	69	67

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	122	TYR
1	D	457	ILE
1	H	122	TYR
1	D	297	THR
1	D	352	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	155	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

10 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	D	601	-	42,48,48	5.24	16 (38%)	50,73,73	1.30	7 (14%)
2	NAD	H	601	-	42,48,48	5.22	16 (38%)	50,73,73	1.27	6 (12%)
2	NAD	C	601	-	42,48,48	5.25	16 (38%)	50,73,73	1.28	5 (10%)
2	NAD	A	601	-	42,48,48	5.17	15 (35%)	50,73,73	1.32	7 (14%)
2	NAD	G	601	-	42,48,48	5.20	16 (38%)	50,73,73	1.34	6 (12%)
2	NAD	E	601	-	42,48,48	5.13	16 (38%)	50,73,73	1.29	8 (16%)
2	NAD	B	602	-	42,48,48	5.16	16 (38%)	50,73,73	1.39	8 (16%)
3	EDO	B	601	-	3,3,3	0.48	0	2,2,2	0.14	0
2	NAD	F	602	-	42,48,48	5.15	16 (38%)	50,73,73	1.36	5 (10%)
3	EDO	F	601	-	3,3,3	0.44	0	2,2,2	0.31	0

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	D	601	-	-	4/26/62/62	0/5/5/5
2	NAD	H	601	-	-	5/26/62/62	0/5/5/5
2	NAD	C	601	-	-	3/26/62/62	0/5/5/5
2	NAD	A	601	-	-	3/26/62/62	0/5/5/5
2	NAD	G	601	-	-	3/26/62/62	0/5/5/5
2	NAD	E	601	-	-	4/26/62/62	0/5/5/5
2	NAD	B	602	-	-	4/26/62/62	0/5/5/5
3	EDO	B	601	-	-	0/1/1/1	-
2	NAD	F	602	-	-	3/26/62/62	0/5/5/5
3	EDO	F	601	-	-	0/1/1/1	-

The worst 5 of 127 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	NAD	C2D-C1D	-16.61	1.28	1.53
2	D	601	NAD	C2B-C1B	-16.52	1.28	1.53
2	G	601	NAD	C2D-C1D	-16.47	1.28	1.53
2	B	602	NAD	C2D-C1D	-16.34	1.29	1.53
2	F	602	NAD	C2D-C1D	-16.25	1.29	1.53

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	601	NAD	N3A-C2A-N1A	-5.32	120.36	128.68
2	F	602	NAD	N3A-C2A-N1A	-5.25	120.47	128.68
2	C	601	NAD	N3A-C2A-N1A	-4.94	120.95	128.68
2	E	601	NAD	N3A-C2A-N1A	-4.86	121.09	128.68
2	D	601	NAD	N3A-C2A-N1A	-4.84	121.12	128.68

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	601	NAD	O4D-C4D-C5D-O5D
2	H	601	NAD	O4D-C1D-N1N-C6N
2	D	601	NAD	O4D-C4D-C5D-O5D
2	D	601	NAD	C3D-C4D-C5D-O5D
2	H	601	NAD	C3D-C4D-C5D-O5D

There are no ring outliers.

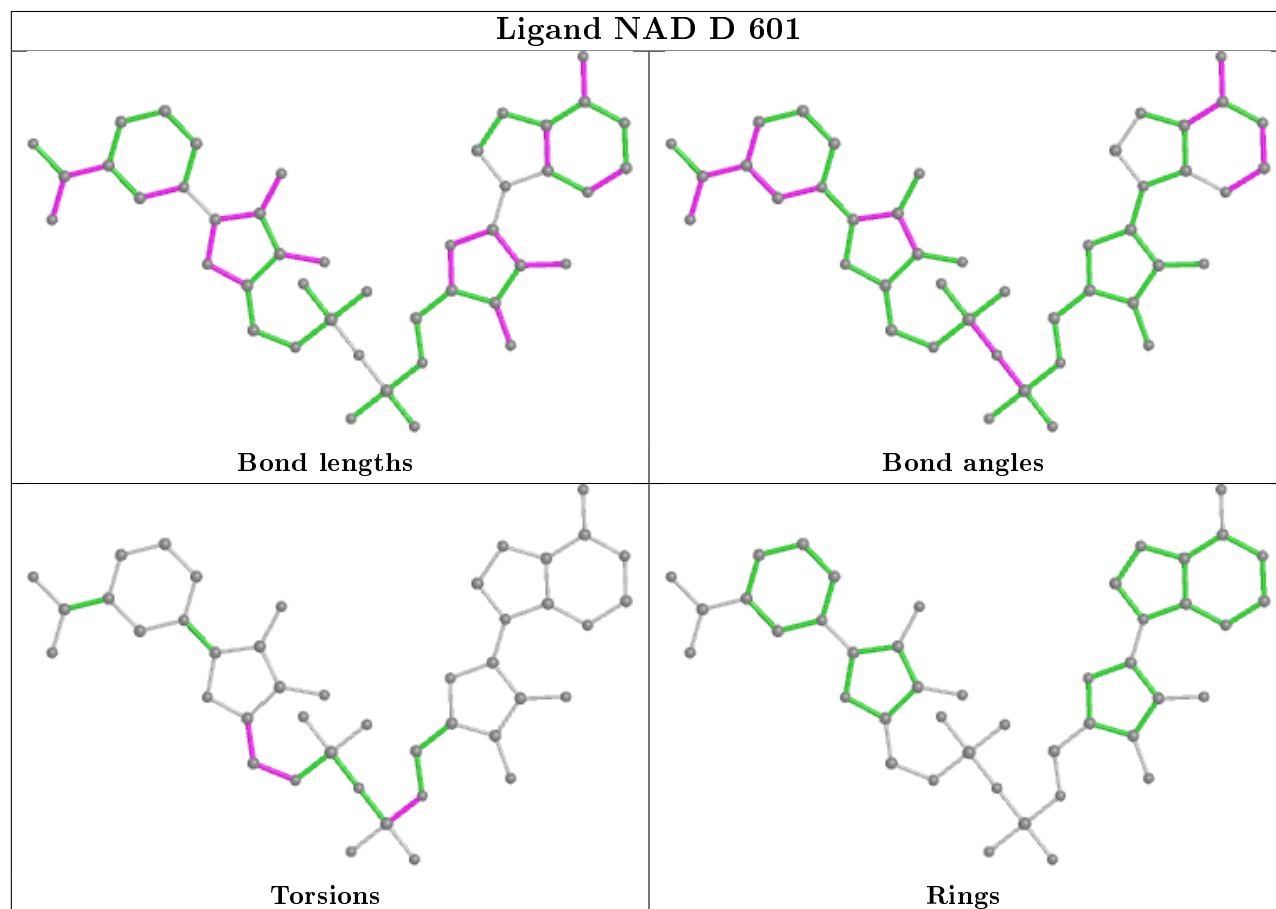
6 monomers are involved in 10 short contacts:

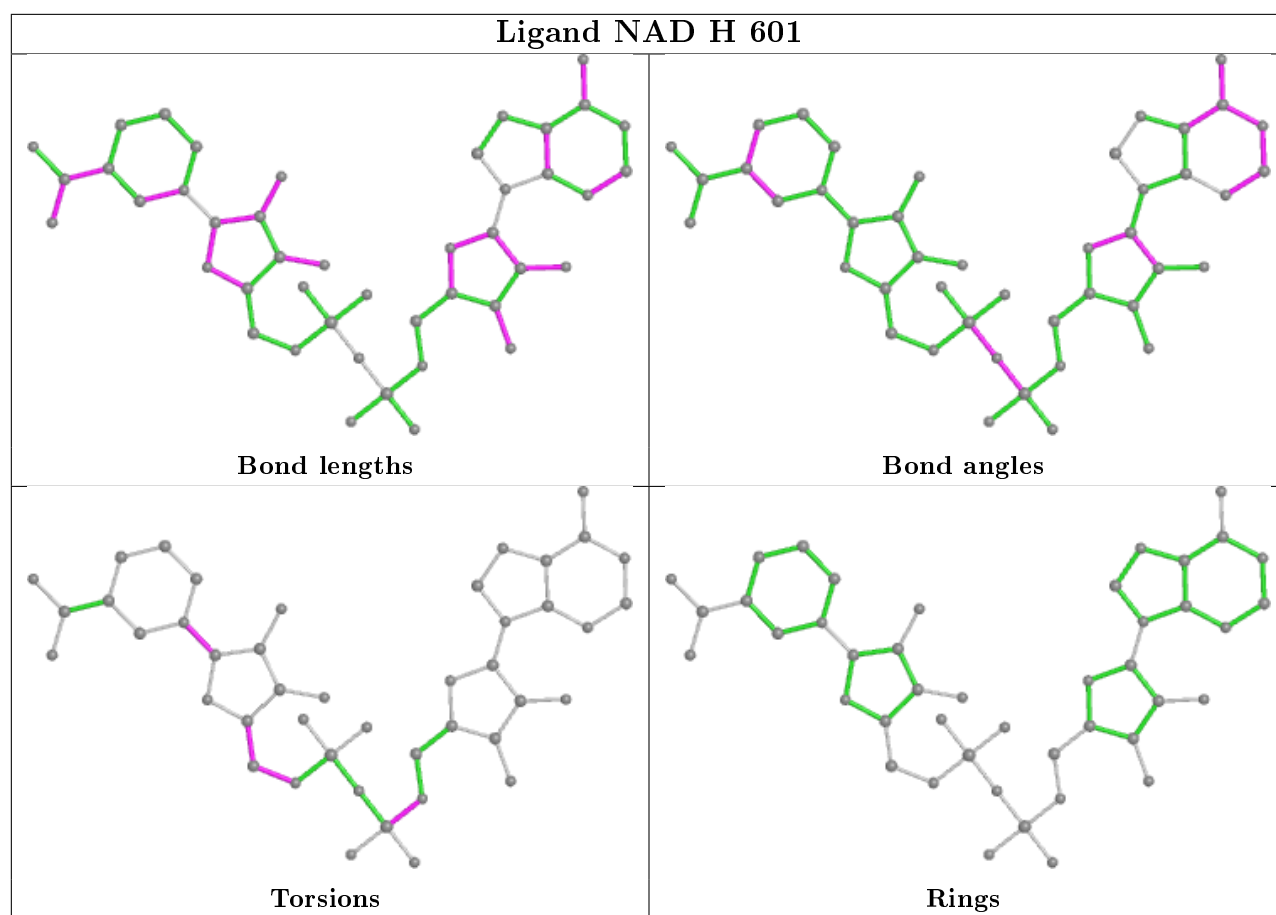
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	NAD	1	0
2	H	601	NAD	2	0
2	C	601	NAD	2	0
2	A	601	NAD	2	0
2	G	601	NAD	1	0
2	F	602	NAD	2	0

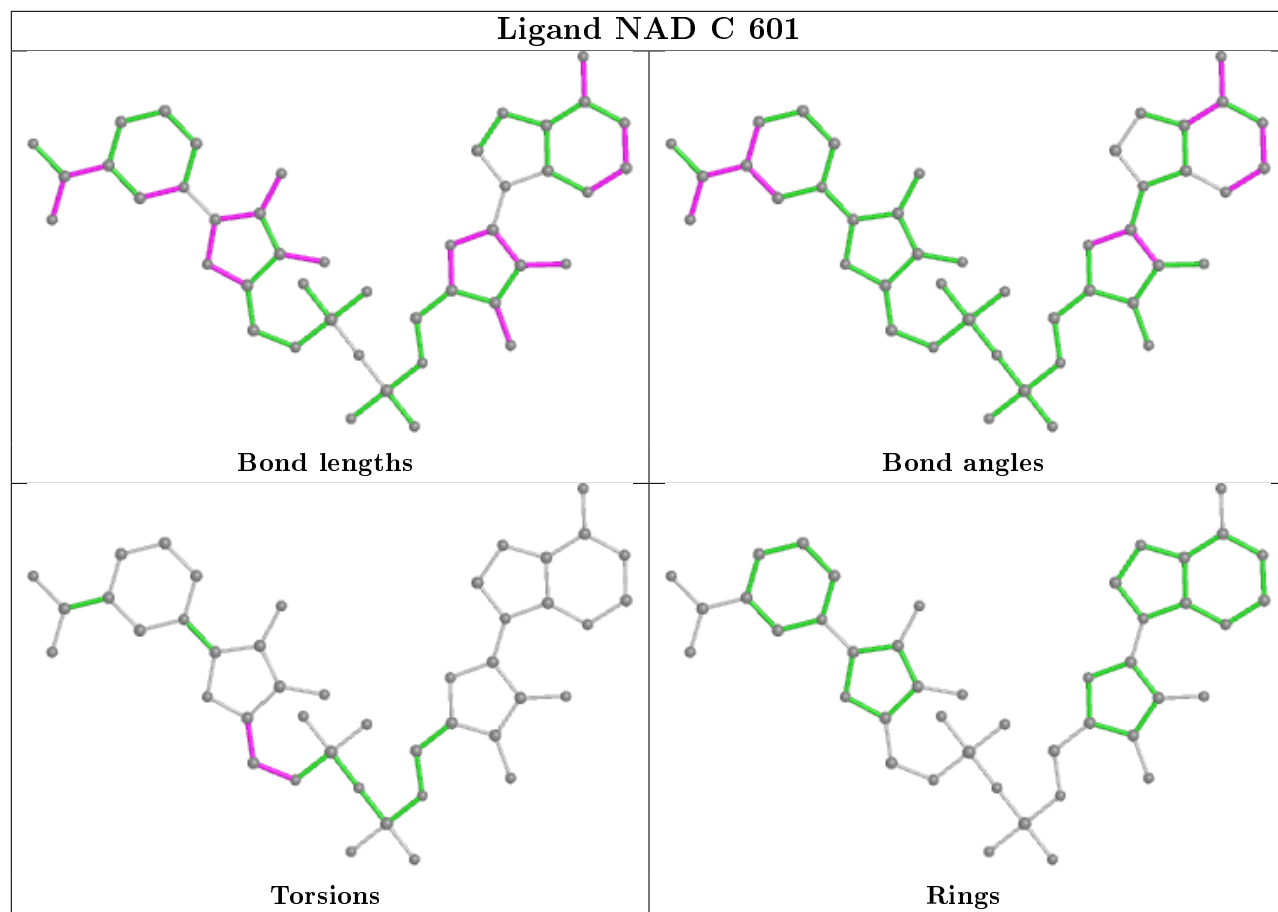
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

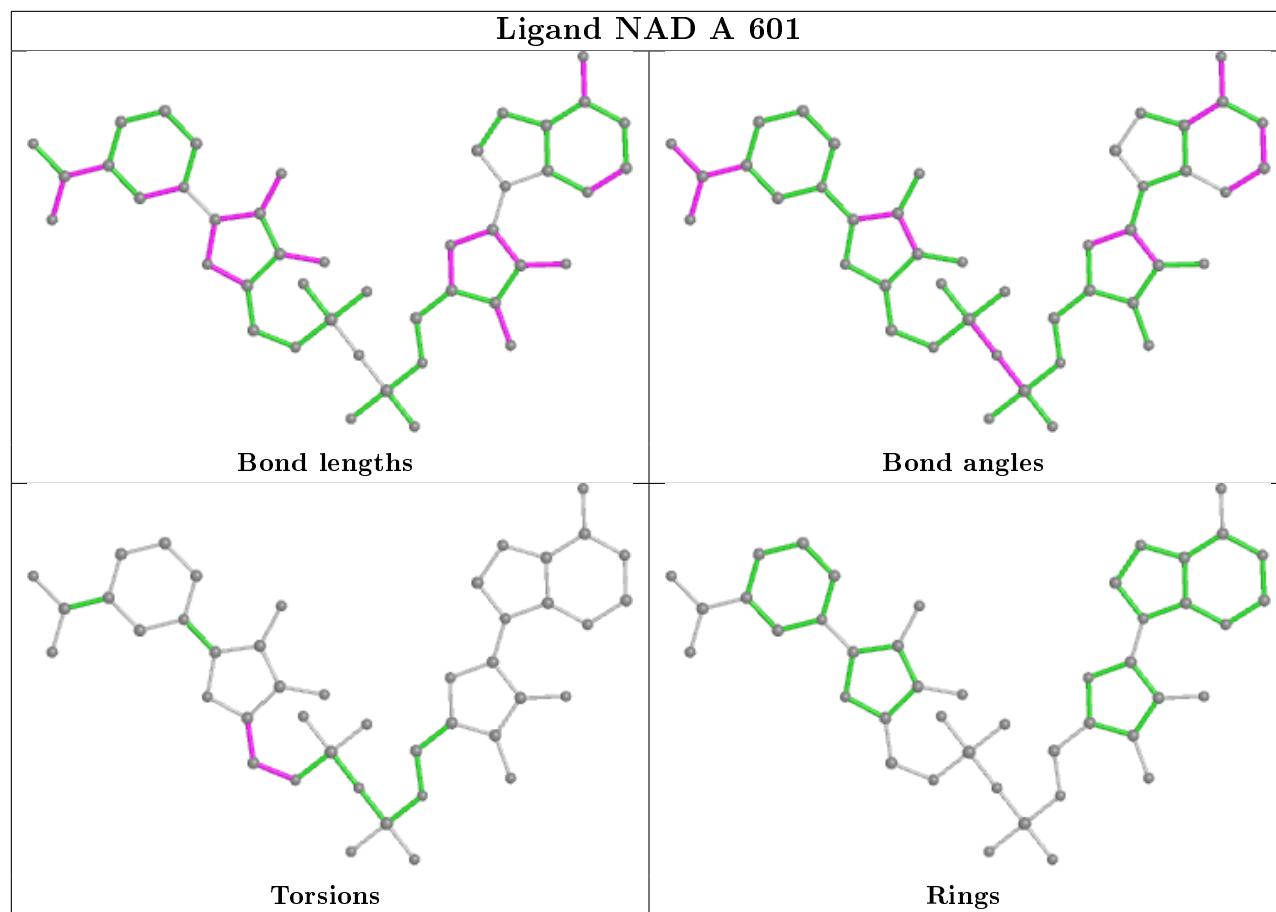


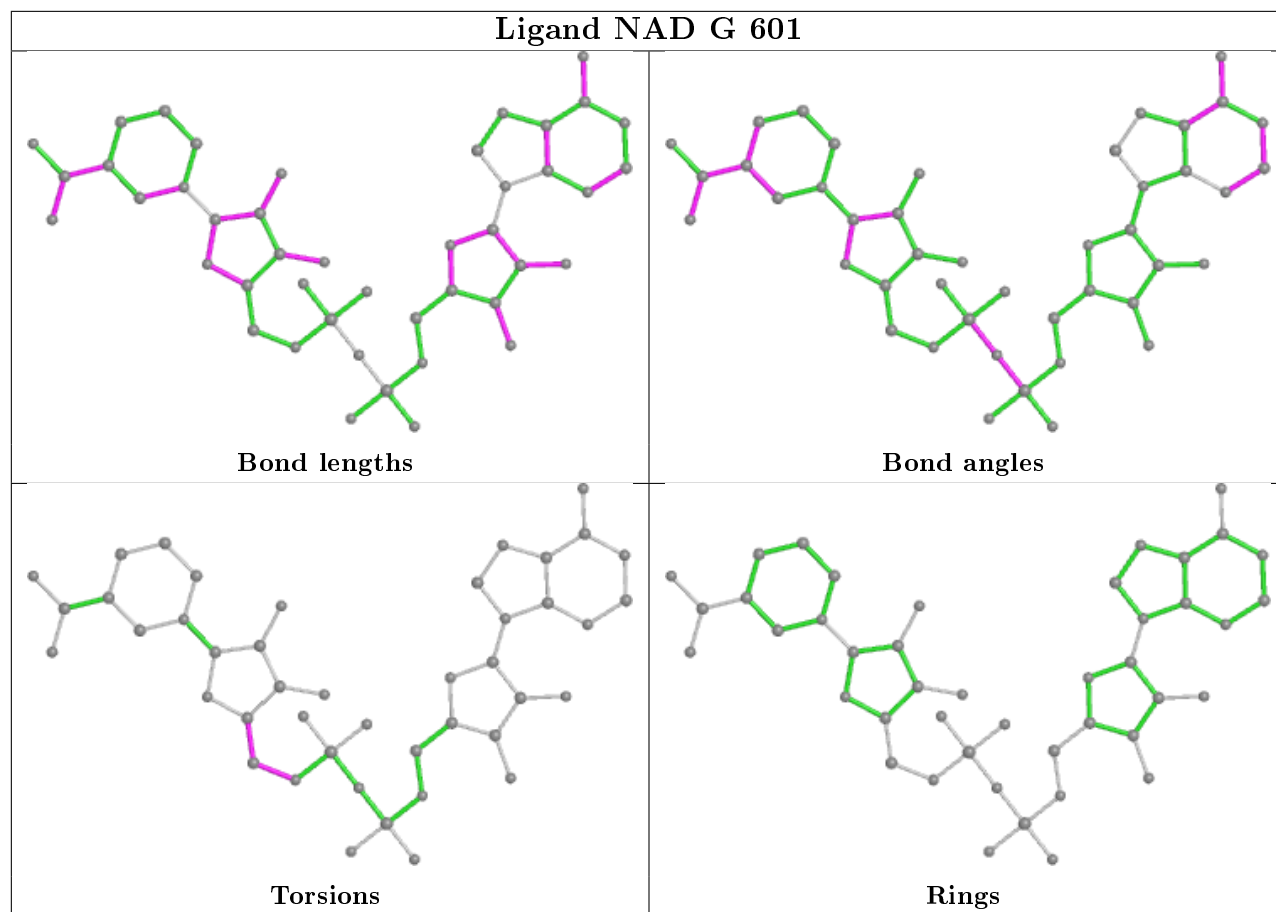
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

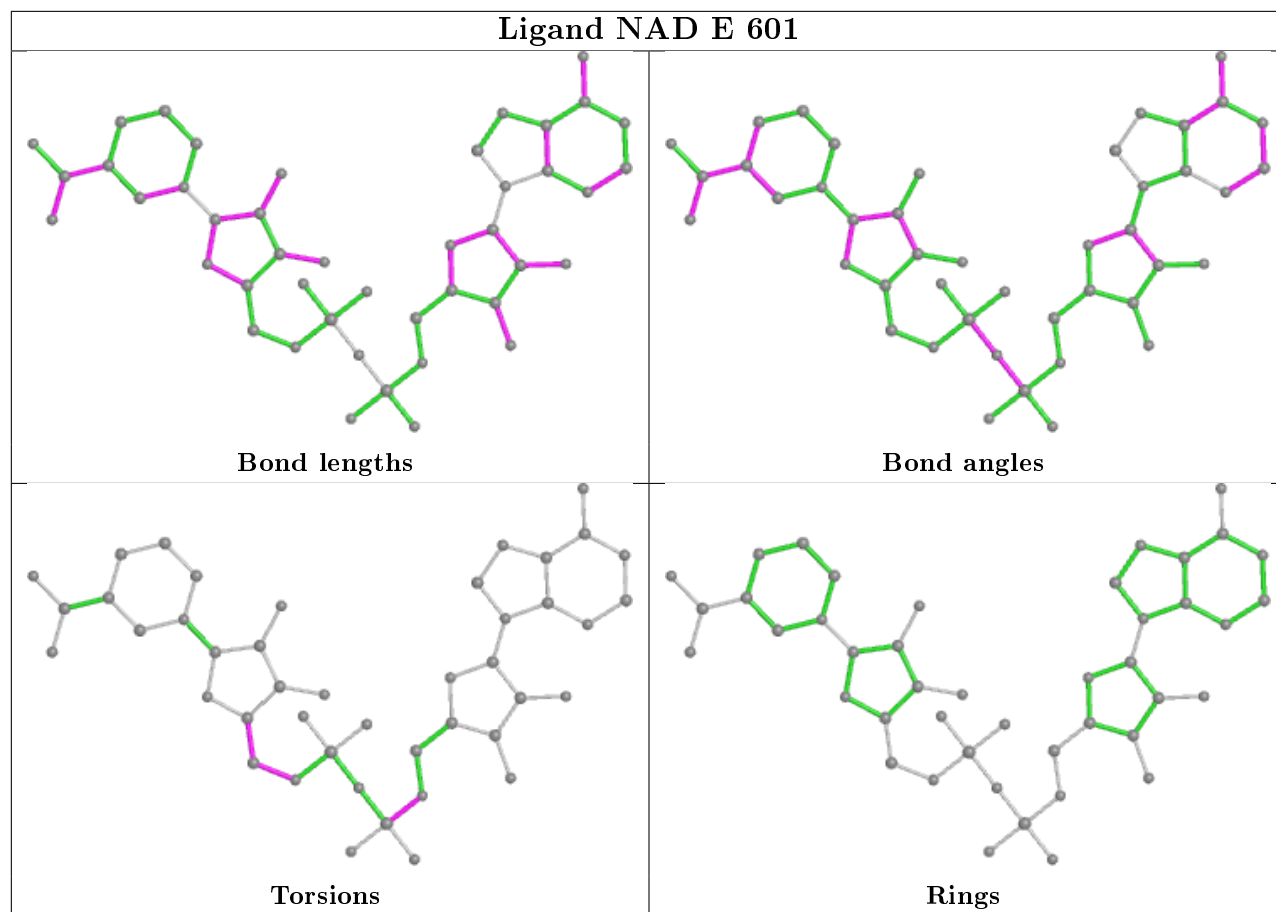


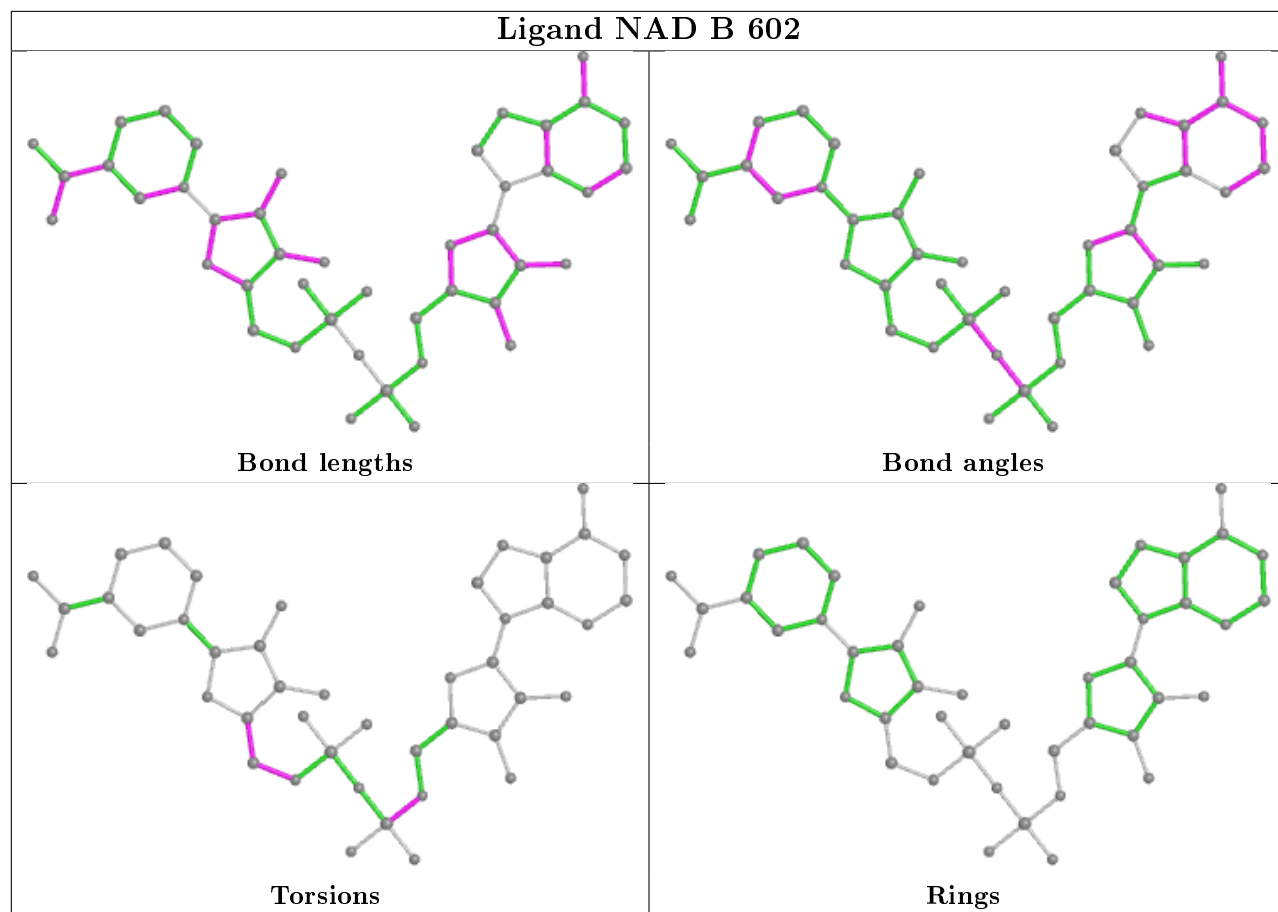


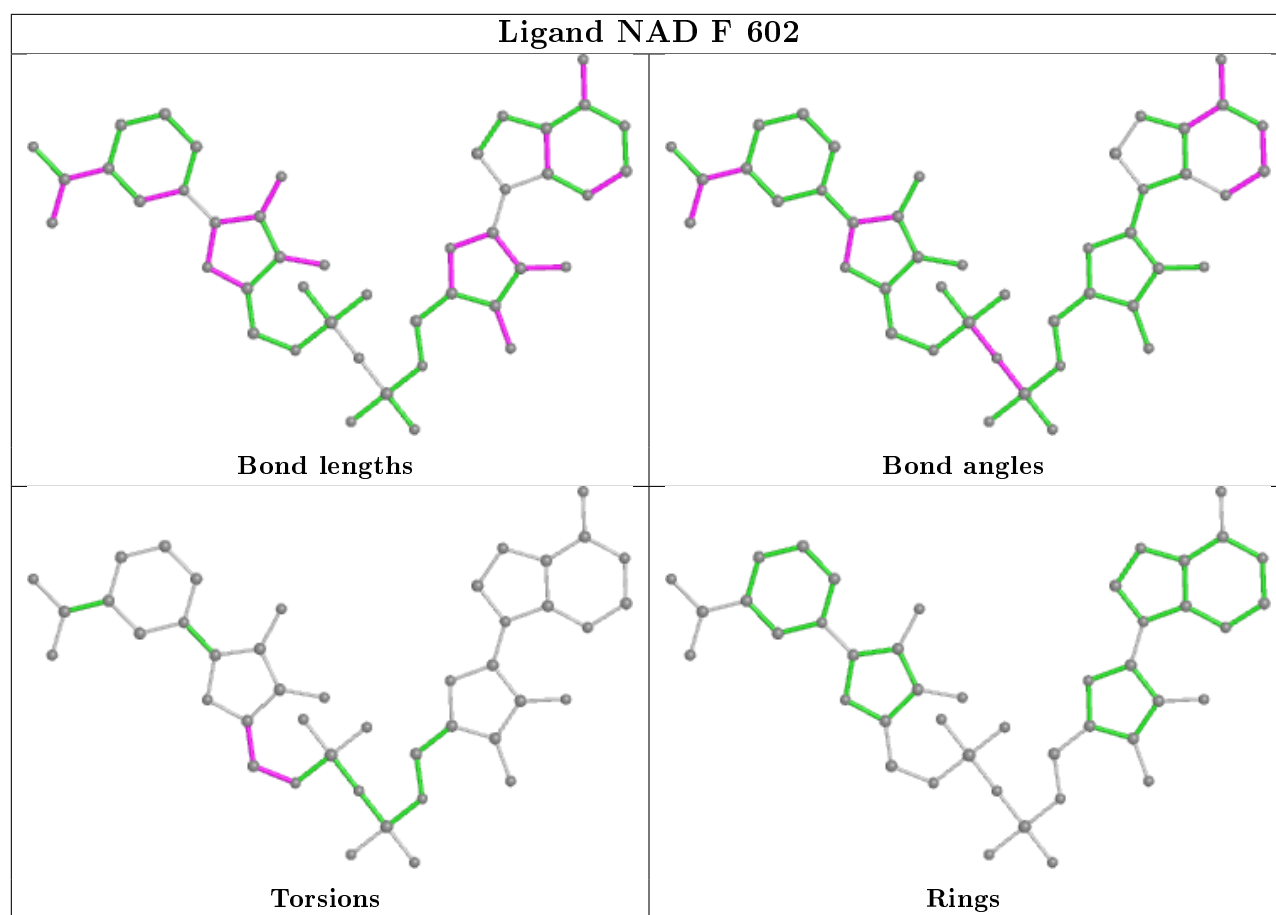












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	497/513 (96%)	-0.42	0 100 100	15, 24, 38, 52	0
1	B	497/513 (96%)	-0.38	1 (0%) 95 95	16, 26, 42, 63	0
1	C	497/513 (96%)	-0.23	6 (1%) 79 81	16, 29, 56, 67	0
1	D	497/513 (96%)	-0.30	2 (0%) 92 93	17, 29, 48, 64	0
1	E	498/513 (97%)	-0.50	0 100 100	17, 25, 38, 54	0
1	F	497/513 (96%)	-0.40	1 (0%) 95 95	17, 25, 42, 72	0
1	G	497/513 (96%)	-0.46	1 (0%) 95 95	18, 26, 40, 58	0
1	H	497/513 (96%)	-0.46	0 100 100	15, 26, 42, 63	0
All	All	3977/4104 (96%)	-0.39	11 (0%) 94 94	15, 26, 44, 72	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	329	ILE	3.8
1	G	337	PRO	2.9
1	F	461	GLY	2.9
1	C	337	PRO	2.8
1	D	292	PHE	2.8

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

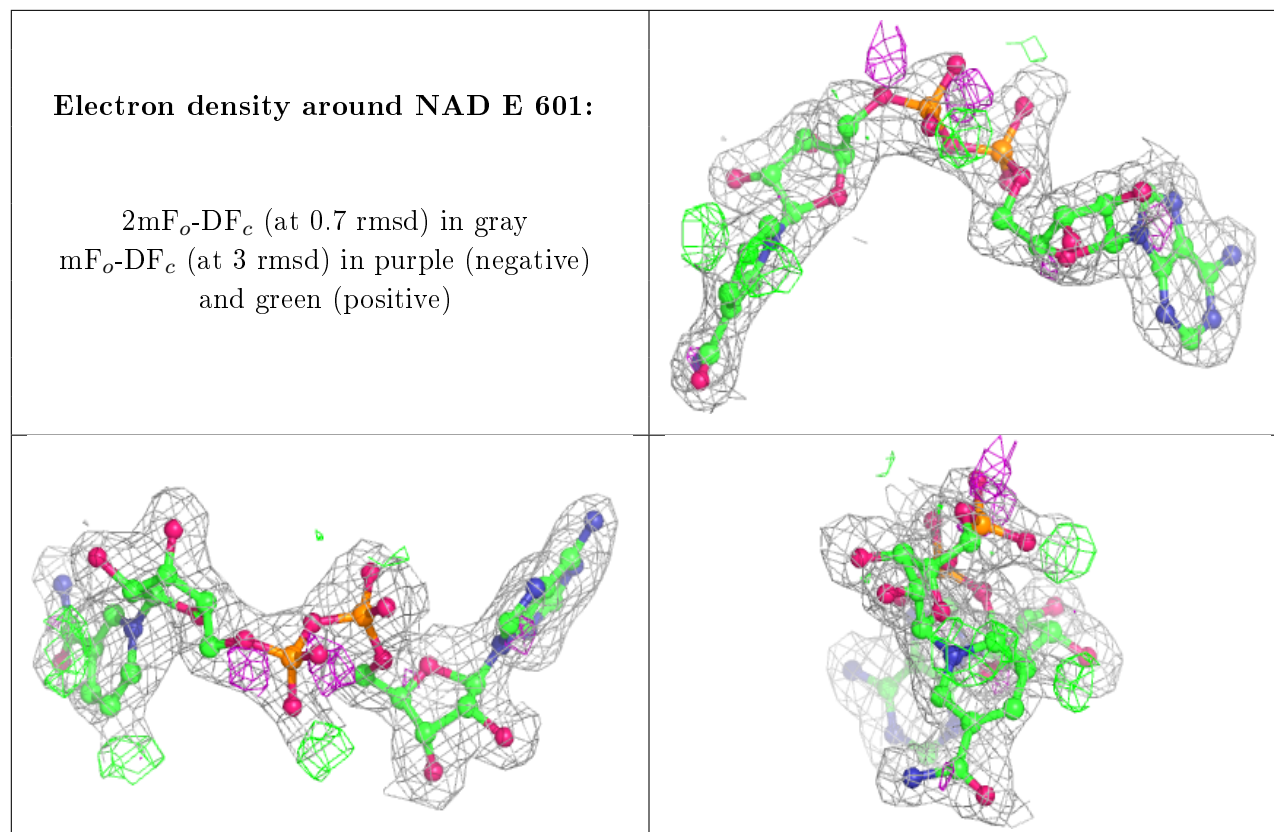
There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

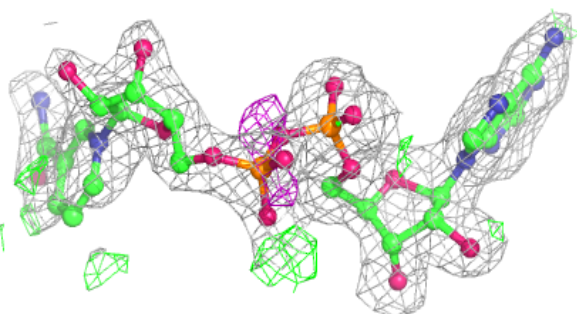
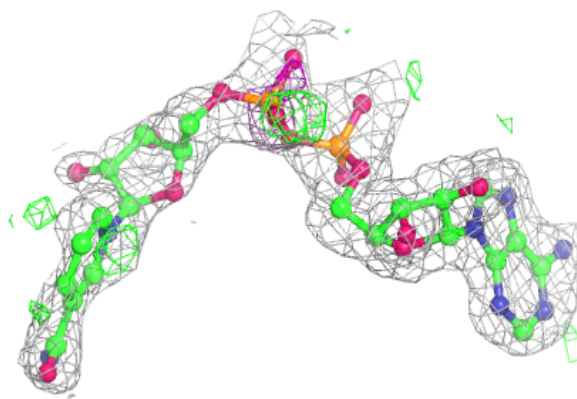
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAD	E	601	44/44	0.89	0.14	18,27,43,48	44
2	NAD	C	601	44/44	0.90	0.16	15,33,54,56	44
2	NAD	A	601	44/44	0.91	0.15	15,28,47,49	44
2	NAD	G	601	44/44	0.91	0.14	20,32,56,58	44
2	NAD	H	601	44/44	0.91	0.14	20,32,46,49	44
2	NAD	B	602	44/44	0.91	0.15	15,33,51,52	44
2	NAD	F	602	44/44	0.91	0.14	15,33,46,52	44
2	NAD	D	601	44/44	0.92	0.15	17,33,46,49	44
3	EDO	B	601	4/4	0.93	0.12	27,33,35,35	0
3	EDO	F	601	4/4	0.94	0.16	27,32,33,37	0

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

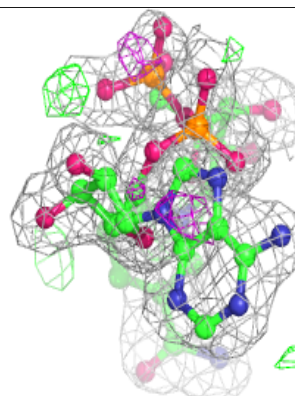
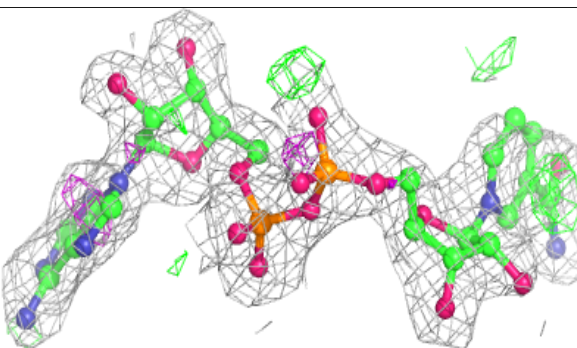
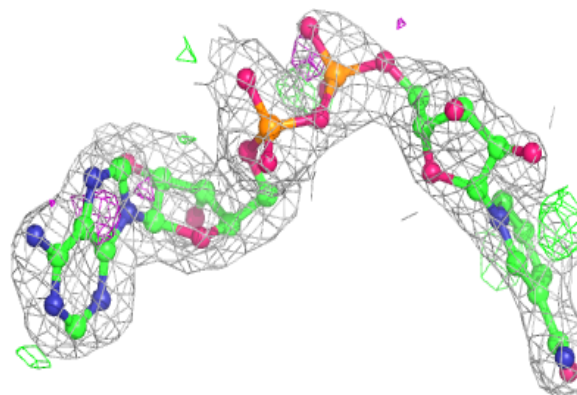


**Electron density around NAD C 601:**

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

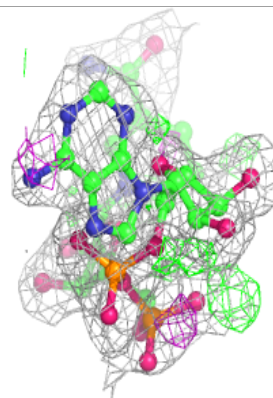
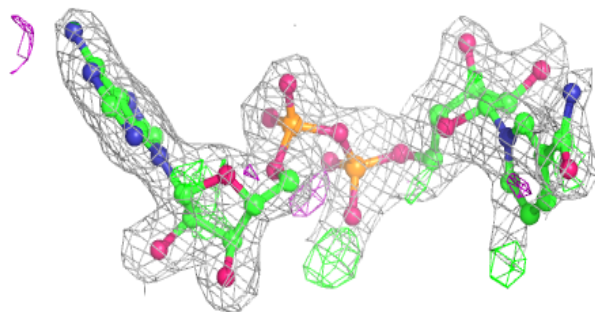
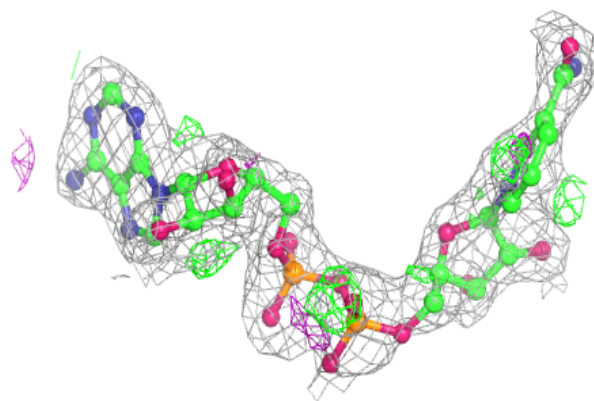
**Electron density around NAD A 601:**

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

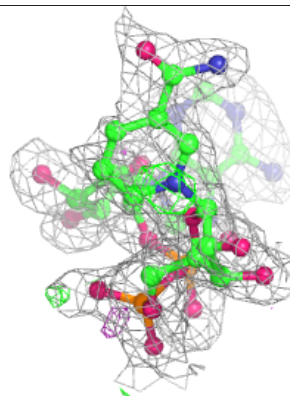
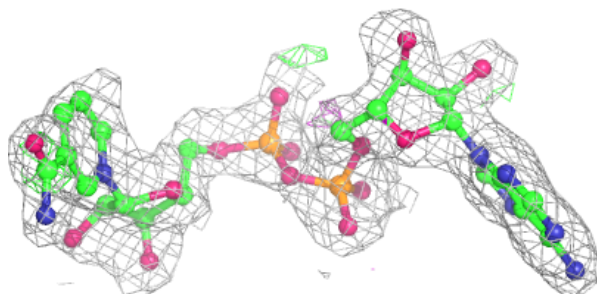
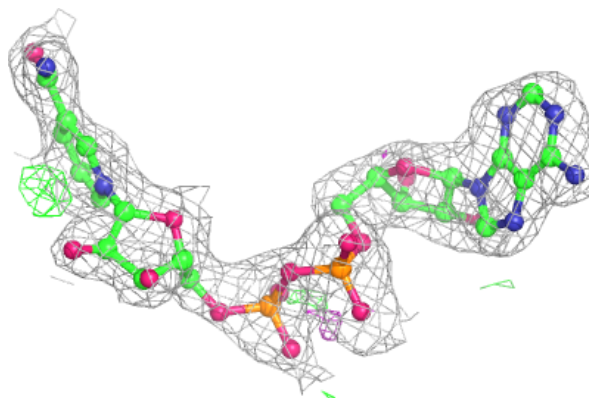


**Electron density around NAD G 601:**

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

**Electron density around NAD H 601:**

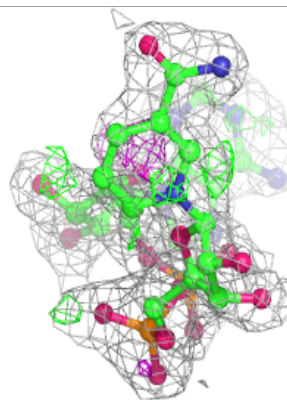
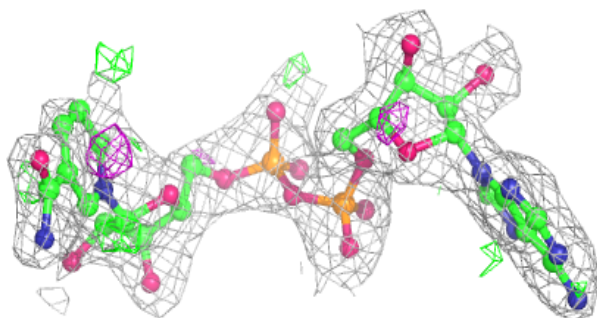
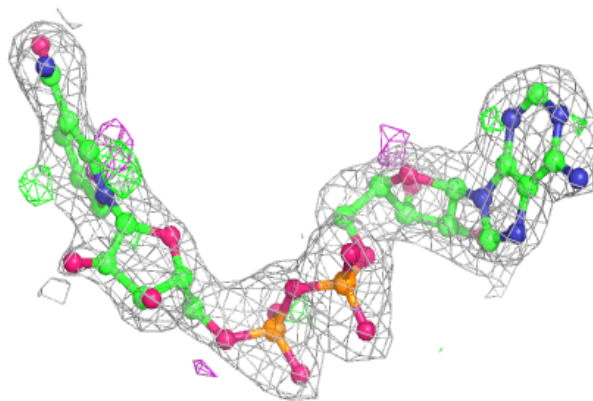
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



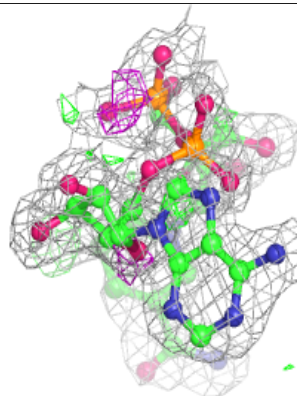
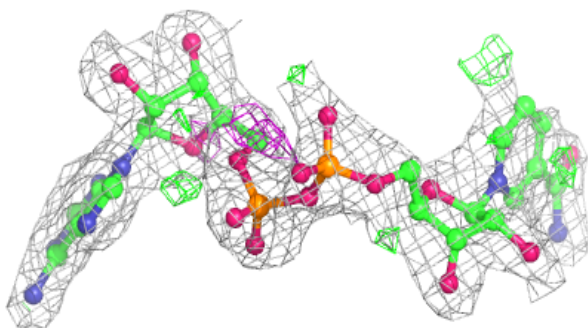
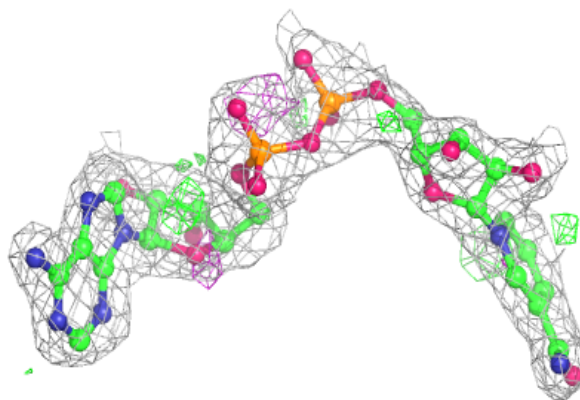


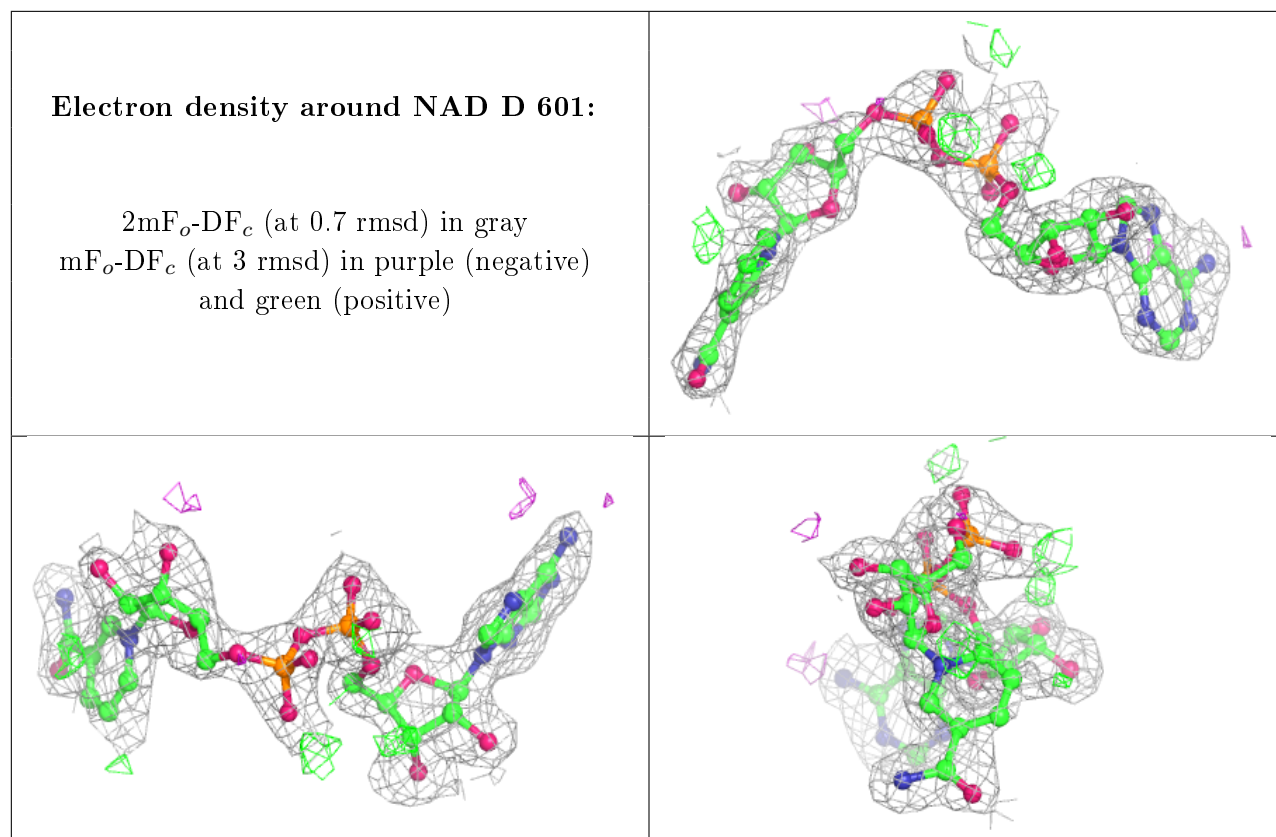
**Electron density around NAD B 602:**

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

**Electron density around NAD F 602:**

$2mF_o-DF_c$  (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.