



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 05:59 pm BST

PDB ID : 6U2X  
Title : Structure of ALDH7A1 mutant E399G complexed with NAD  
Authors : Tanner, J.J.; Korasick, D.A.; Laciak, A.R.  
Deposited on : 2019-08-20  
Resolution : 2.15 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

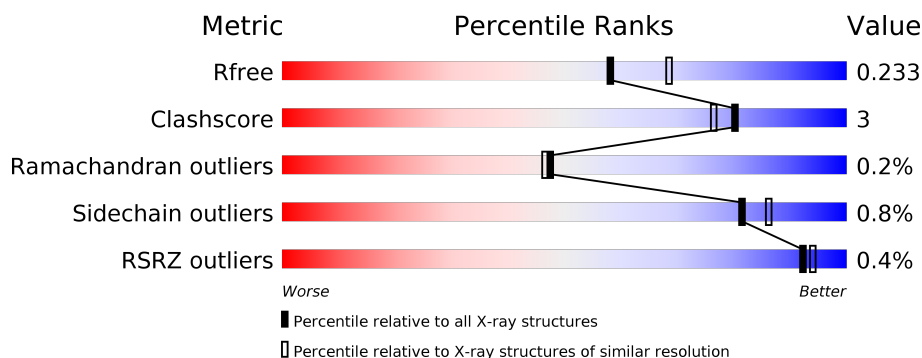
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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>94%</div> <div>5%</div> </div>
1	B	513	<div> <div>91%</div> <div>9%</div> </div>
1	C	513	<div> <div>92%</div> <div>7%</div> </div>
1	D	513	<div> <div>%</div> <div>93%</div> <div>6%</div> </div>
1	E	513	<div> <div>90%</div> <div>9%</div> </div>
1	F	513	<div> <div>92%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	513	<div><div></div><div>89%</div><div>8%</div><div></div></div>
1	H	513	<div>%<div><div></div><div>91%</div><div>8%</div><div></div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32254 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	509	Total	C	N	O	S	0	0	0
			3817	2427	663	710	17			
1	B	509	Total	C	N	O	S	0	0	0
			3832	2436	666	713	17			
1	C	509	Total	C	N	O	S	0	0	0
			3813	2422	663	711	17			
1	D	509	Total	C	N	O	S	0	0	0
			3811	2421	663	710	17			
1	E	509	Total	C	N	O	S	0	0	0
			3823	2430	665	711	17			
1	F	509	Total	C	N	O	S	0	0	0
			3822	2426	668	711	17			
1	G	499	Total	C	N	O	S	0	0	0
			3758	2384	653	704	17			
1	H	509	Total	C	N	O	S	0	0	0
			3816	2425	665	709	17			

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	399	GLY	GLU	engineered mutation	UNP P49419
B	-1	GLY	-	expression tag	UNP P49419
B	0	HIS	-	expression tag	UNP P49419
B	399	GLY	GLU	engineered mutation	UNP P49419
C	-1	GLY	-	expression tag	UNP P49419
C	0	HIS	-	expression tag	UNP P49419
C	399	GLY	GLU	engineered mutation	UNP P49419
D	-1	GLY	-	expression tag	UNP P49419
D	0	HIS	-	expression tag	UNP P49419
D	399	GLY	GLU	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	399	GLY	GLU	engineered mutation	UNP P49419
F	-1	GLY	-	expression tag	UNP P49419
F	0	HIS	-	expression tag	UNP P49419
F	399	GLY	GLU	engineered mutation	UNP P49419
G	-1	GLY	-	expression tag	UNP P49419
G	0	HIS	-	expression tag	UNP P49419
G	399	GLY	GLU	engineered mutation	UNP P49419
H	-1	GLY	-	expression tag	UNP P49419
H	0	HIS	-	expression tag	UNP P49419
H	399	GLY	GLU	engineered mutation	UNP P49419

- # NAD
- 
- The image displays the chemical structure of Nicotinamide Adenine Dinucleotide (NAD), a crucial coenzyme. The molecule is composed of two nucleotides linked by a pyrophosphate bridge. The first nucleotide consists of a nicotinamide ring (a pyridine ring with a nitrogen atom at the bottom) attached to a ribose sugar. The second nucleotide consists of an adenine ring (a purine ring with an amino group at the top) attached to a ribose sugar. The two ribose sugars are linked by a pyrophosphate bridge, which is shown as two phosphate groups connected by an oxygen atom. The structure is color-coded: the nicotinamide ring is blue, the adenine ring is red, and the ribose sugars are green. The pyrophosphate bridge is shown in yellow and orange. The overall structure is a complex, branched molecule with various functional groups and a high degree of symmetry.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	B	1	Total 54	C 20	N 10	O 20	P 4	0	1
2	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	D	1	Total 54	C 20	N 10	O 20	P 4	0	1
2	E	1	Total 27	C 10	N 5	O 10	P 2	0	0



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	H	1	Total	C	N	O	P	0	1
			54	20	10	20	4		

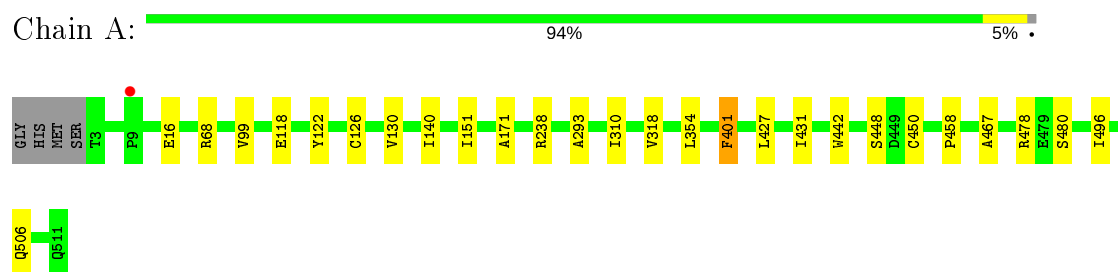
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	187	Total	O	0	0
			187	187		
3	B	182	Total	O	0	0
			182	182		
3	C	201	Total	O	0	0
			201	201		
3	D	156	Total	O	0	0
			156	156		
3	E	200	Total	O	0	0
			200	200		
3	F	189	Total	O	0	0
			189	189		
3	G	179	Total	O	0	0
			179	179		
3	H	171	Total	O	0	0
			171	171		

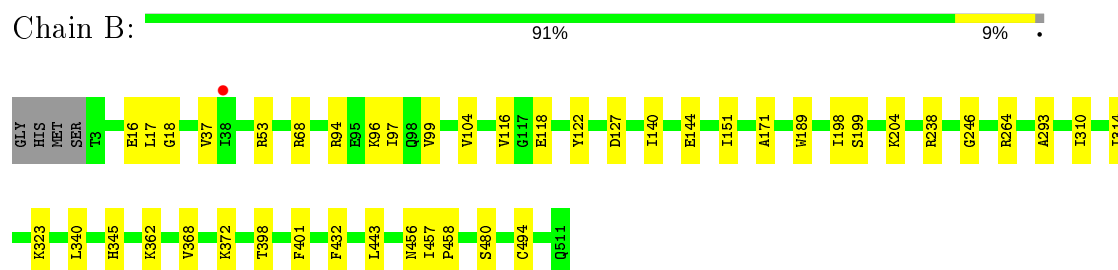
### 3 Residue-property plots [i](#)

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.

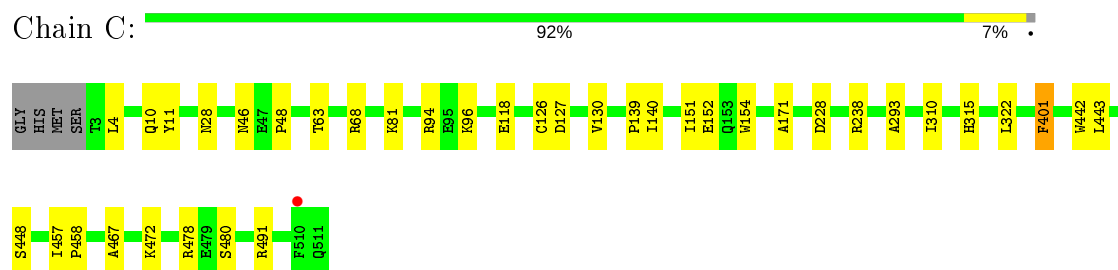
- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase



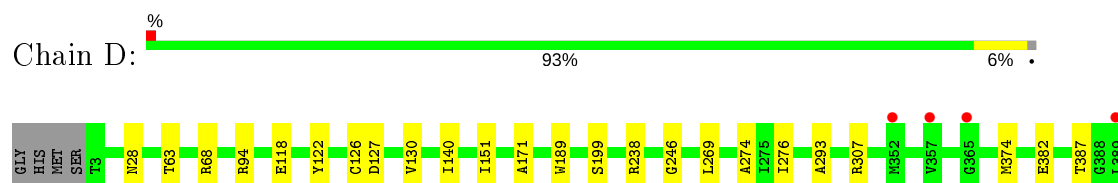
- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase



- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase



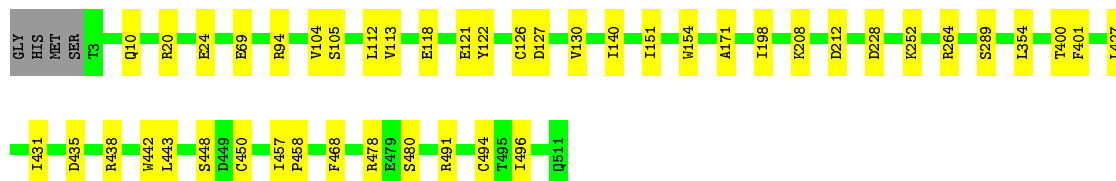
- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase





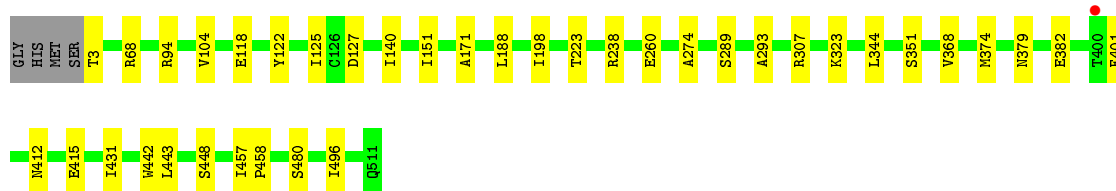
- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain E: 90% 9%



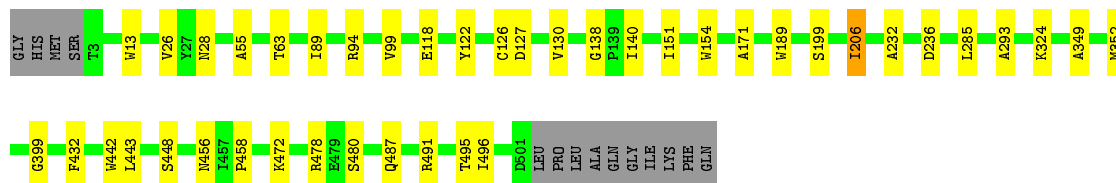
- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain F: 92% 7%



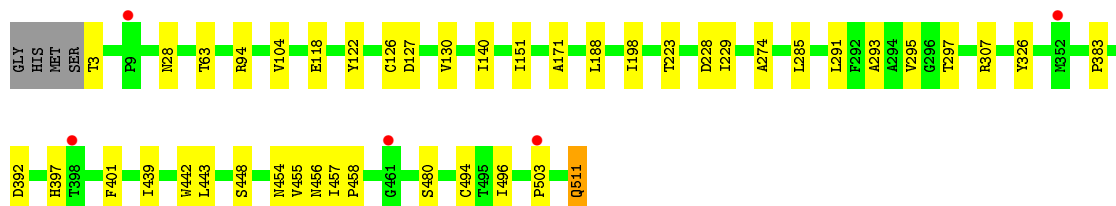
- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain G: 89% 8%



- Molecule 1: Alpha-aminoadipic semialdehyde dehydrogenase

Chain H: 91% 8%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.27Å 161.65Å 158.80Å 90.00° 94.41° 90.00°	Depositor
Resolution (Å)	49.16 – 2.15 49.16 – 2.15	Depositor EDS
% Data completeness (in resolution range)	95.0 (49.16-2.15) 95.3 (49.16-2.15)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.93 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.14 _3260: ???	Depositor
R, $R_{free}$	0.174 , 0.233 0.175 , 0.233	Depositor DCC
$R_{free}$ test set	10066 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.5	Xtriage
Anisotropy	0.606	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	32254	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.60% 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: 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	0.41	1/3896 (0.0%)	0.57	0/5293
1	B	0.38	0/3911	0.56	0/5310
1	C	0.39	0/3892	0.57	2/5289 (0.0%)
1	D	0.37	0/3890	0.54	0/5286
1	E	0.39	0/3902	0.55	0/5300
1	F	0.39	0/3901	0.56	0/5300
1	G	0.40	0/3835	0.56	0/5208
1	H	0.39	0/3895	0.55	0/5293
All	All	0.39	1/31122 (0.0%)	0.56	2/42279 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	401	PHE	C-N	-5.71	1.21	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	401	PHE	C-N-CA	5.23	134.78	121.70
1	C	228	ASP	CB-CG-OD1	5.04	122.84	118.30

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	3817	0	3769	16	0
1	B	3832	0	3800	26	0
1	C	3813	0	3754	22	0
1	D	3811	0	3749	17	0
1	E	3823	0	3783	26	0
1	F	3822	0	3771	24	0
1	G	3758	0	3712	25	0
1	H	3816	0	3769	28	0
2	A	27	0	11	1	0
2	B	54	0	22	1	0
2	C	27	0	11	1	0
2	D	54	0	22	2	0
2	E	27	0	11	0	0
2	F	27	0	11	1	0
2	G	27	0	12	0	0
2	H	54	0	22	2	0
3	A	187	0	0	0	0
3	B	182	0	0	3	0
3	C	201	0	0	4	0
3	D	156	0	0	0	0
3	E	200	0	0	3	0
3	F	189	0	0	1	0
3	G	179	0	0	0	0
3	H	171	0	0	0	0
All	All	32254	0	30229	167	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 167 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:E:94:ARG:NH2	1:E:127:ASP:OD2	2.15	0.79
1:A:151:ILE:HB	1:D:140:ILE:HD11	1.66	0.78
1:B:140:ILE:HD11	1:C:151:ILE:HB	1.65	0.76
1:E:289:SER:HB3	1:E:458:PRO:HG3	1.71	0.72
1:H:94:ARG:NH2	1:H:127:ASP:OD2	2.25	0.69

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	507/513 (99%)	490 (97%)	16 (3%)	1 (0%)	47	46
1	B	507/513 (99%)	490 (97%)	16 (3%)	1 (0%)	47	46
1	C	507/513 (99%)	490 (97%)	16 (3%)	1 (0%)	47	46
1	D	507/513 (99%)	490 (97%)	16 (3%)	1 (0%)	47	46
1	E	507/513 (99%)	488 (96%)	18 (4%)	1 (0%)	47	46
1	F	507/513 (99%)	490 (97%)	16 (3%)	1 (0%)	47	46
1	G	497/513 (97%)	479 (96%)	16 (3%)	2 (0%)	34	29
1	H	507/513 (99%)	492 (97%)	14 (3%)	1 (0%)	47	46
All	All	4046/4104 (99%)	3909 (97%)	128 (3%)	9 (0%)	47	46

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	SER
1	B	480	SER
1	C	480	SER
1	D	480	SER
1	E	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	390/409 (95%)	388 (100%)	2 (0%)	88	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	394/409 (96%)	390 (99%)	4 (1%)	76	81
1	C	389/409 (95%)	387 (100%)	2 (0%)	88	92
1	D	388/409 (95%)	386 (100%)	2 (0%)	88	92
1	E	392/409 (96%)	386 (98%)	6 (2%)	65	69
1	F	391/409 (96%)	390 (100%)	1 (0%)	92	95
1	G	387/409 (95%)	384 (99%)	3 (1%)	81	86
1	H	390/409 (95%)	385 (99%)	5 (1%)	69	74
All	All	3121/3272 (95%)	3096 (99%)	25 (1%)	81	86

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	121	GLU
1	E	354	LEU
1	H	401	PHE
1	E	122	TYR
1	E	400	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

11 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[B]	-	24,29,48	4.91	9 (37%)	29,45,73	1.53	4 (13%)
2	NAD	F	601	-	24,29,48	4.68	9 (37%)	29,45,73	1.30	2 (6%)
2	NAD	B	601[A]	-	24,29,48	4.89	9 (37%)	29,45,73	1.51	3 (10%)
2	NAD	D	601[A]	-	24,29,48	4.89	9 (37%)	29,45,73	1.48	3 (10%)
2	NAD	B	601[B]	-	24,29,48	4.90	9 (37%)	29,45,73	1.56	4 (13%)
2	NAD	G	601	-	24,29,48	4.79	9 (37%)	29,45,73	1.47	3 (10%)
2	NAD	E	601	-	24,29,48	4.89	8 (33%)	29,45,73	1.47	4 (13%)
2	NAD	C	601	-	24,29,48	4.84	9 (37%)	29,45,73	1.51	4 (13%)
2	NAD	A	601	-	24,29,48	4.79	8 (33%)	29,45,73	1.50	3 (10%)
2	NAD	H	601[B]	-	24,29,48	4.86	7 (29%)	29,45,73	1.44	3 (10%)
2	NAD	H	601[A]	-	24,29,48	4.82	7 (29%)	29,45,73	1.45	3 (10%)

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[B]	-	-	3/12/32/62	0/3/3/5
2	NAD	F	601	-	-	5/12/32/62	0/3/3/5
2	NAD	B	601[A]	-	-	3/12/32/62	0/3/3/5
2	NAD	D	601[A]	-	-	1/12/32/62	0/3/3/5
2	NAD	B	601[B]	-	-	2/12/32/62	0/3/3/5
2	NAD	G	601	-	-	2/12/32/62	0/3/3/5
2	NAD	E	601	-	-	1/12/32/62	0/3/3/5
2	NAD	C	601	-	-	3/12/32/62	0/3/3/5
2	NAD	A	601	-	-	0/12/32/62	0/3/3/5
2	NAD	H	601[B]	-	-	3/12/32/62	0/3/3/5
2	NAD	H	601[A]	-	-	1/12/32/62	0/3/3/5

The worst 5 of 93 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	NAD	C2B-C1B	-16.19	1.29	1.53
2	H	601[B]	NAD	C2B-C1B	-16.14	1.29	1.53
2	D	601[B]	NAD	C2B-C1B	-16.09	1.29	1.53
2	E	601	NAD	C2B-C1B	-16.03	1.29	1.53
2	D	601[A]	NAD	C2B-C1B	-16.01	1.29	1.53

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	601	NAD	N3A-C2A-N1A	-5.85	119.53	128.68
2	D	601[A]	NAD	N3A-C2A-N1A	-5.42	120.21	128.68
2	D	601[B]	NAD	N3A-C2A-N1A	-5.40	120.23	128.68
2	B	601[B]	NAD	N3A-C2A-N1A	-5.34	120.33	128.68
2	B	601[A]	NAD	N3A-C2A-N1A	-5.30	120.39	128.68

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	601[B]	NAD	C5B-O5B-PA-O1A
2	D	601[B]	NAD	C5B-O5B-PA-O3
2	D	601[B]	NAD	PN-O3-PA-O5B
2	F	601	NAD	PA-O3-PN-O5D
2	B	601[A]	NAD	PA-O3-PN-O5D

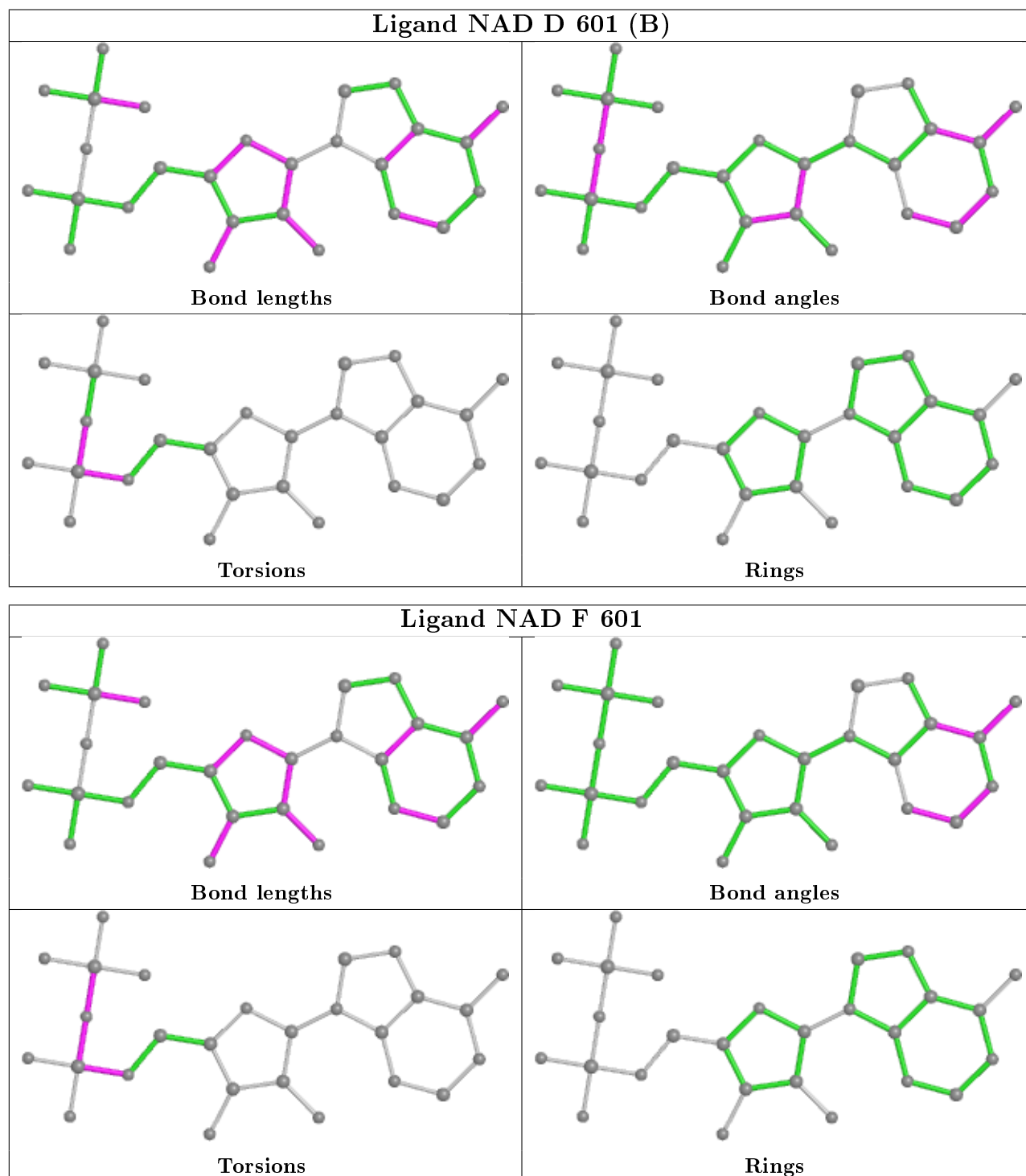
There are no ring outliers.

8 monomers are involved in 8 short contacts:

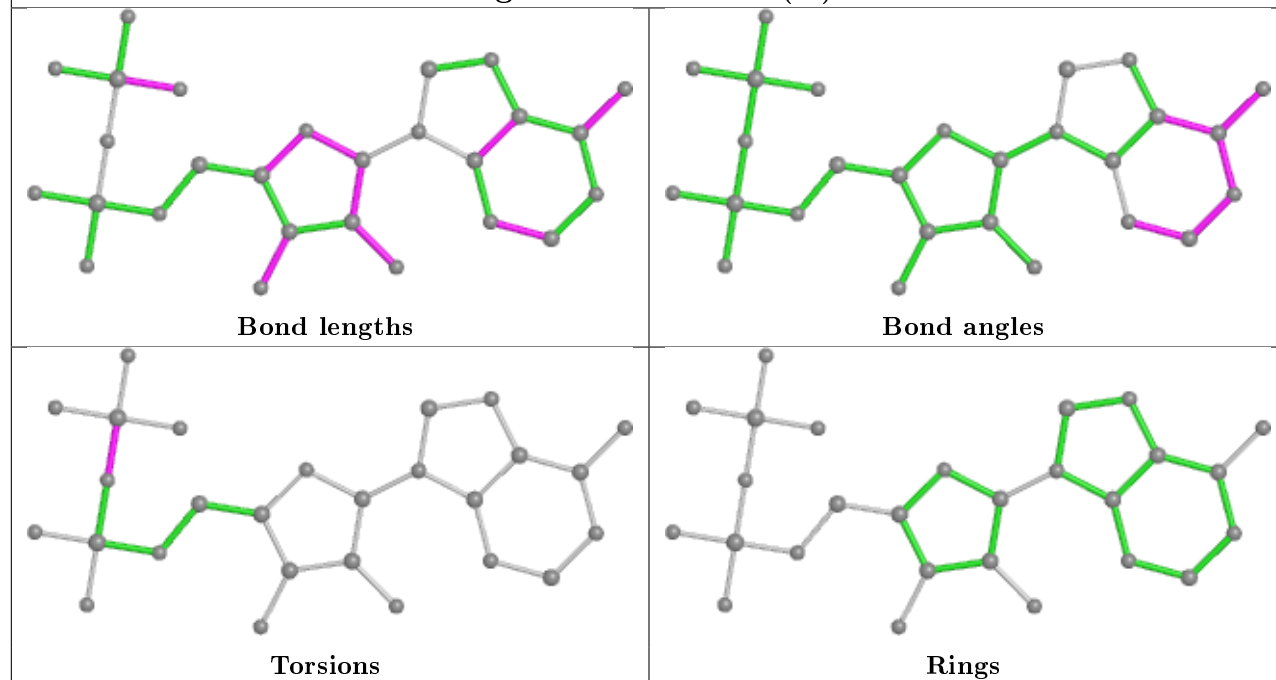
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601[B]	NAD	1	0
2	F	601	NAD	1	0
2	B	601[A]	NAD	1	0
2	D	601[A]	NAD	1	0
2	C	601	NAD	1	0
2	A	601	NAD	1	0
2	H	601[B]	NAD	1	0
2	H	601[A]	NAD	1	0

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

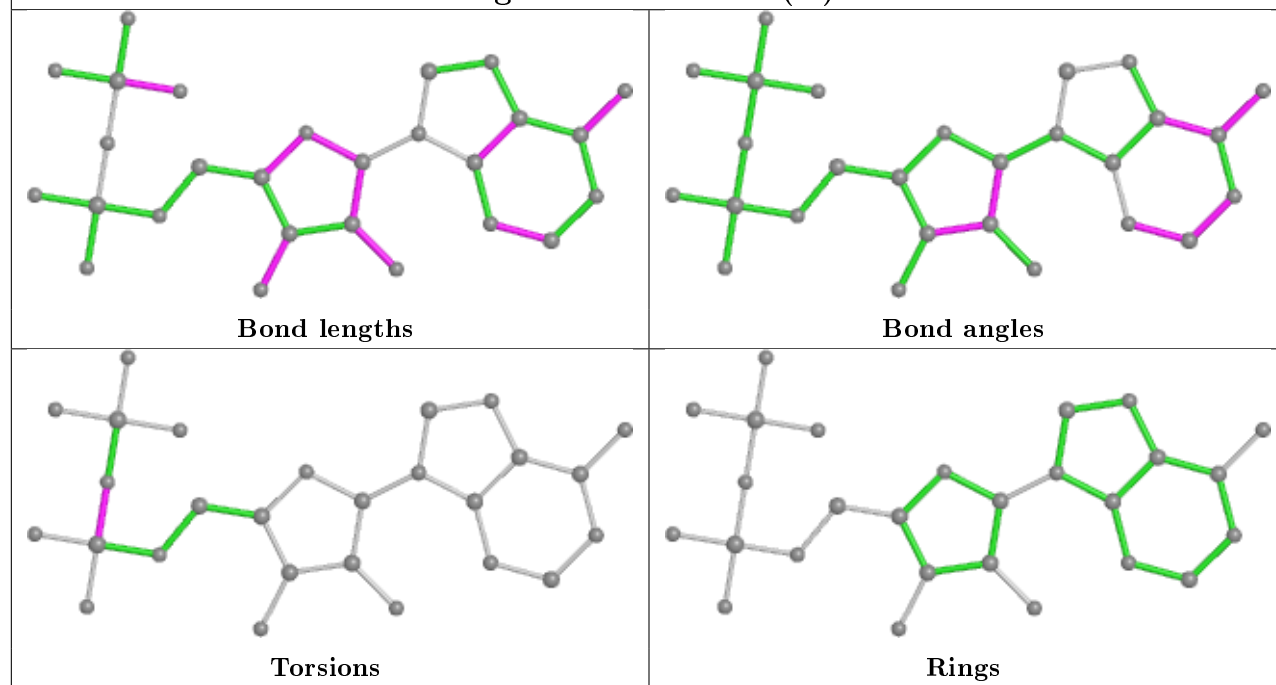
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.



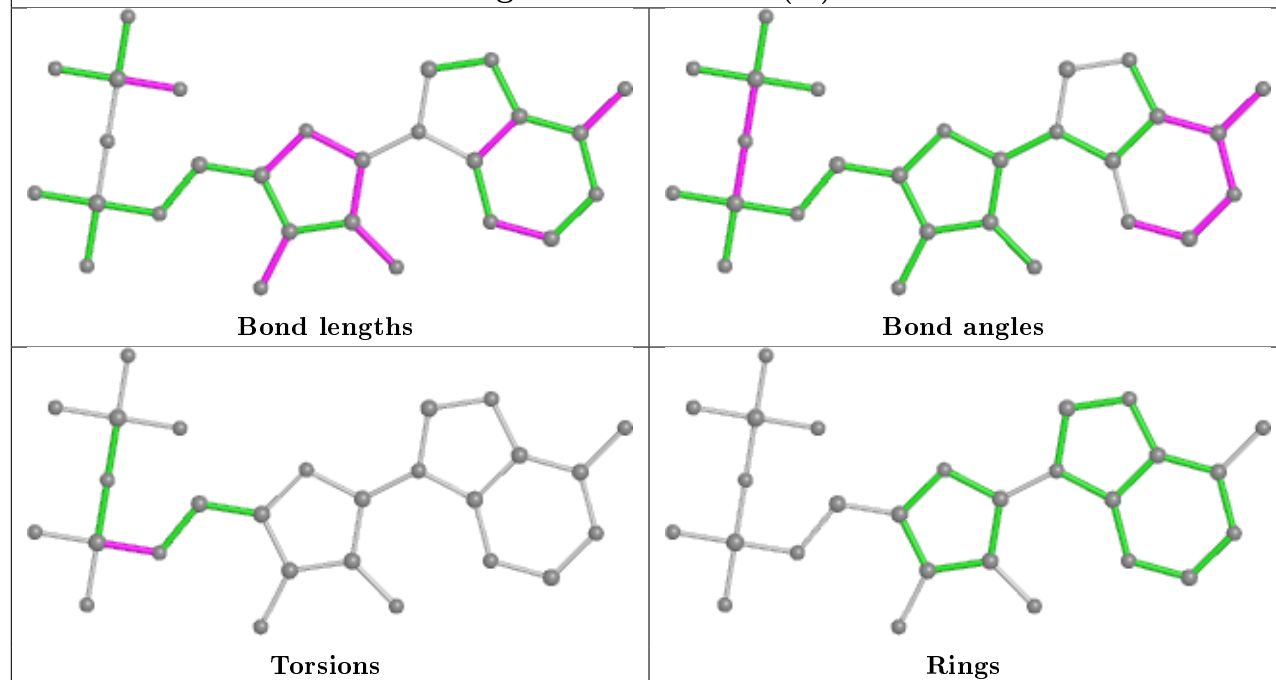
## Ligand NAD B 601 (A)



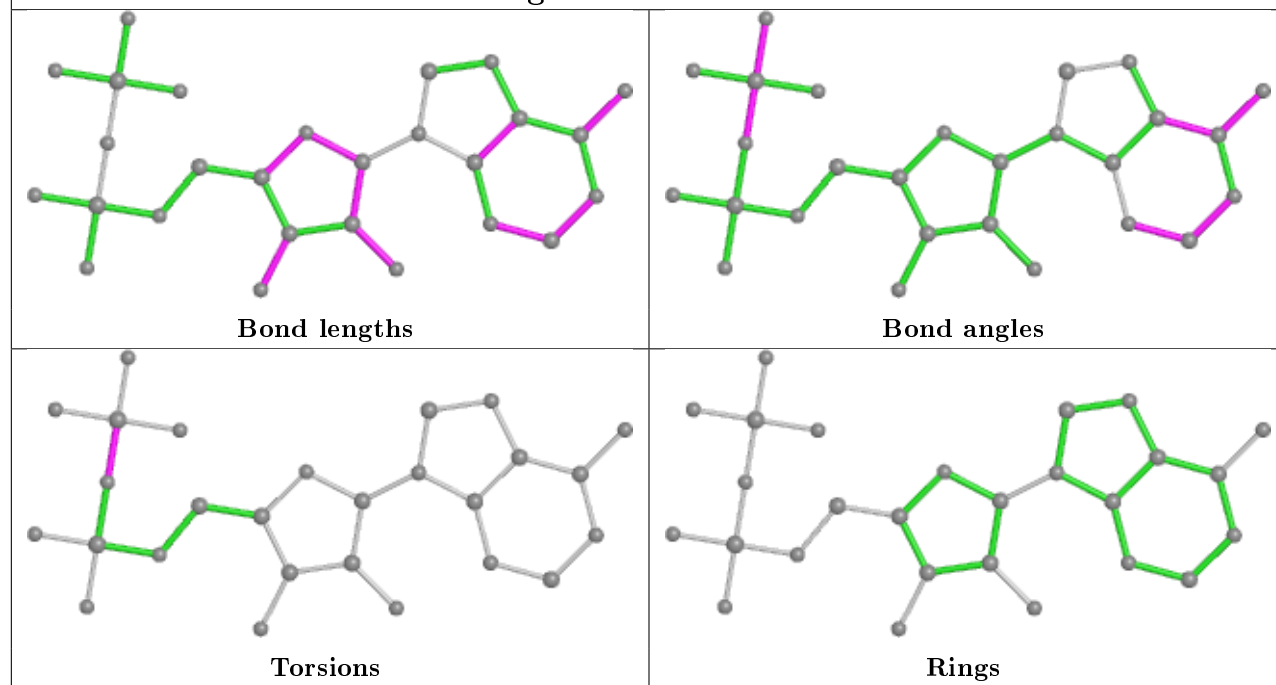
## Ligand NAD D 601 (A)

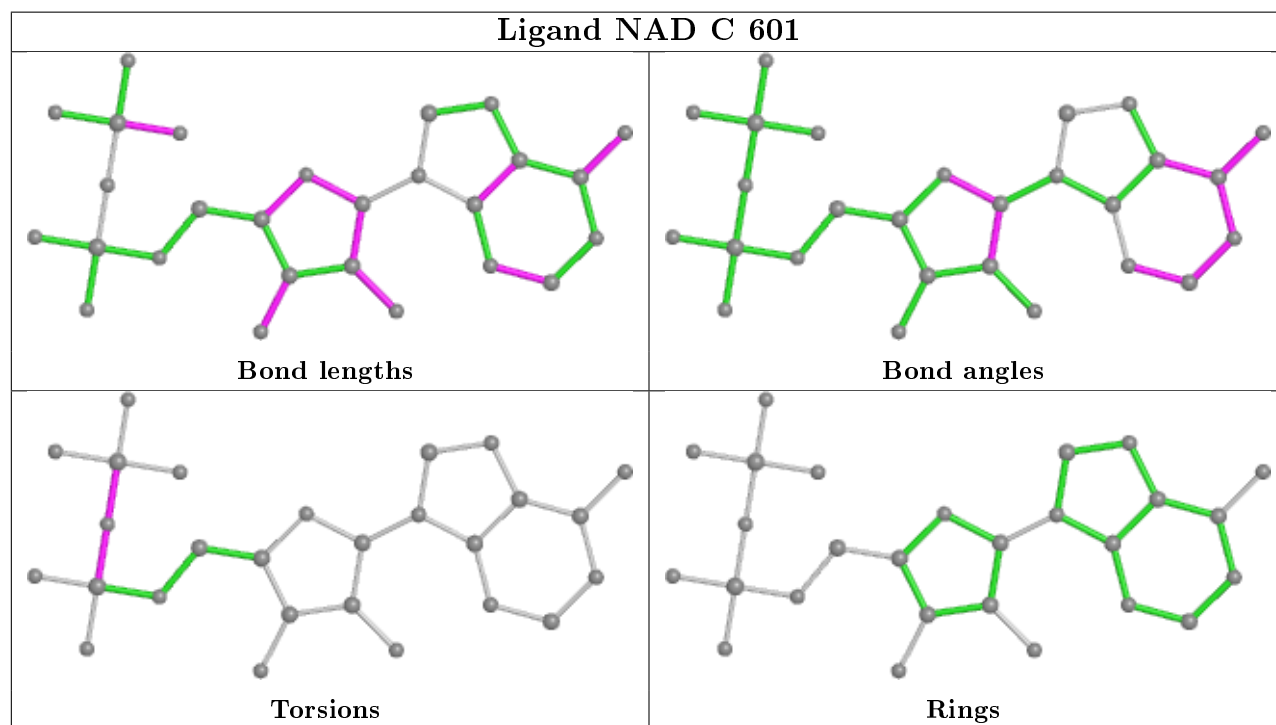
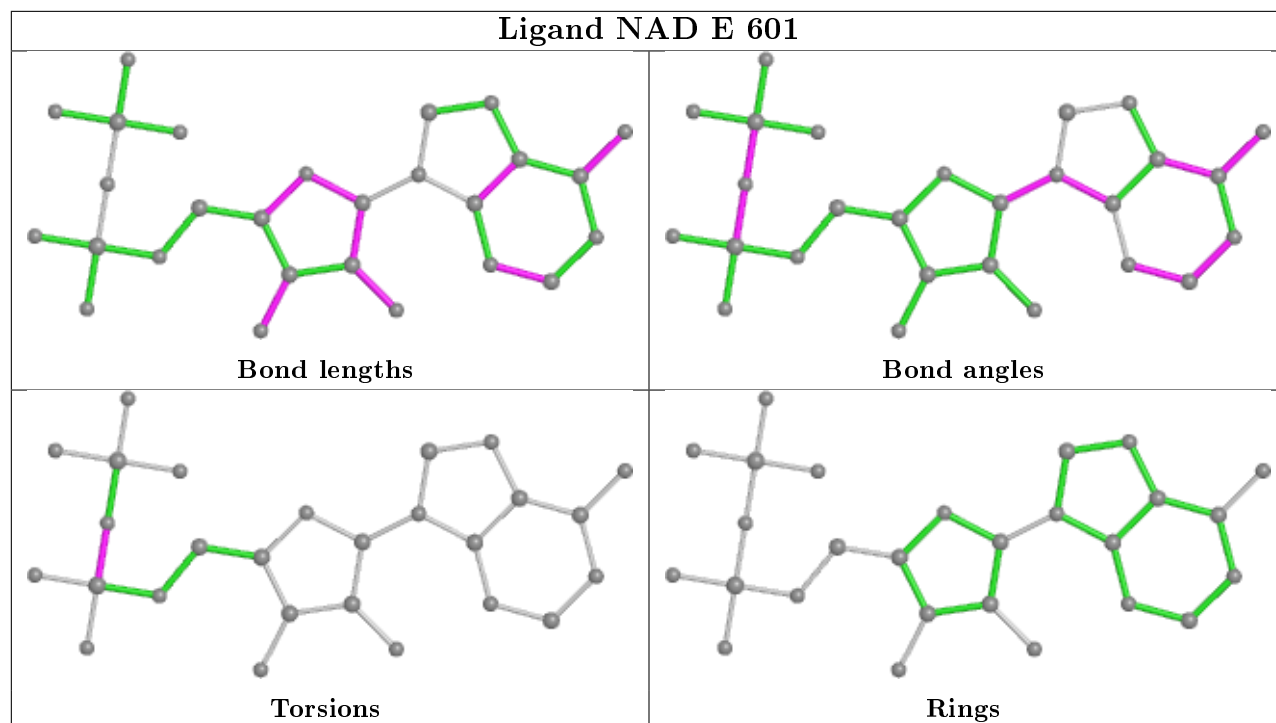


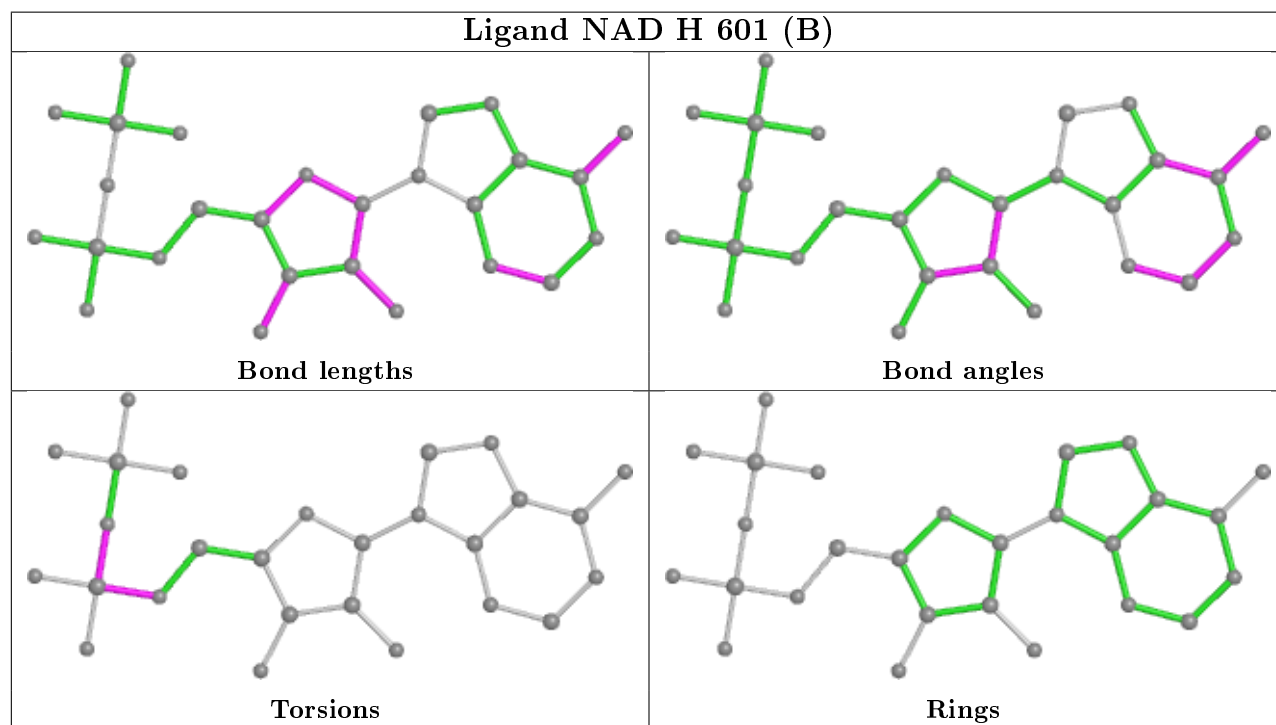
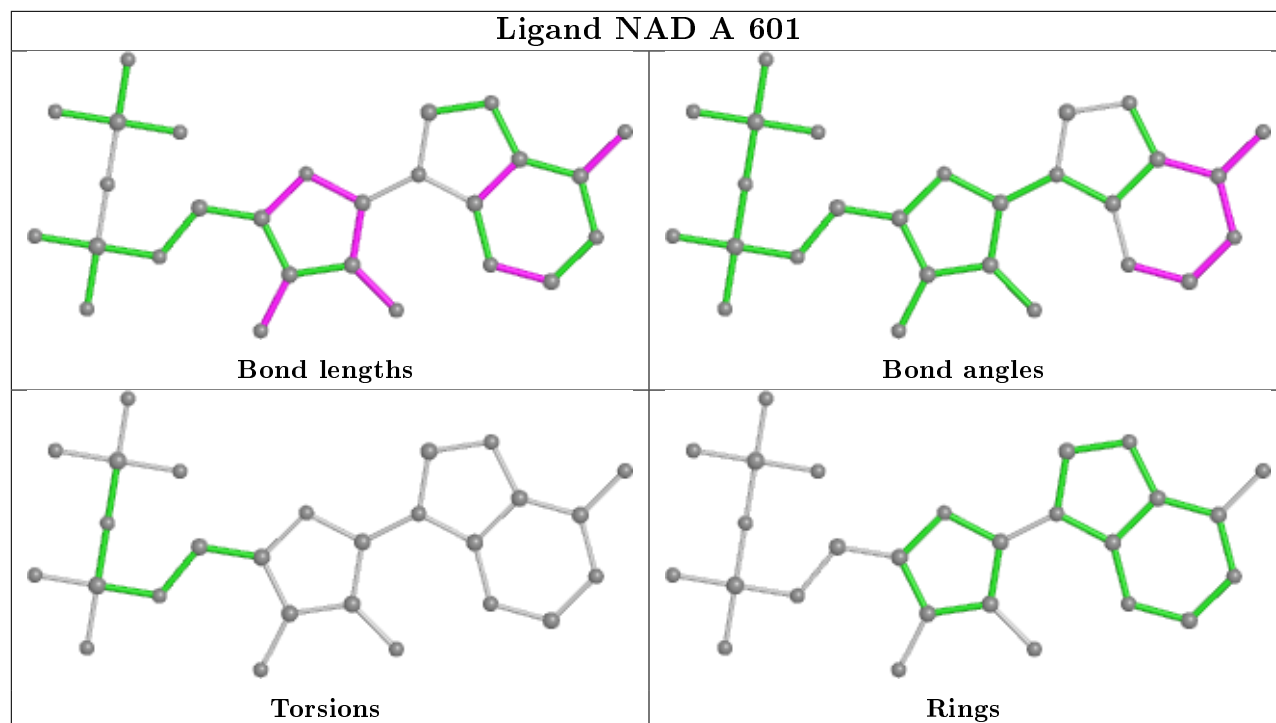
## Ligand NAD B 601 (B)

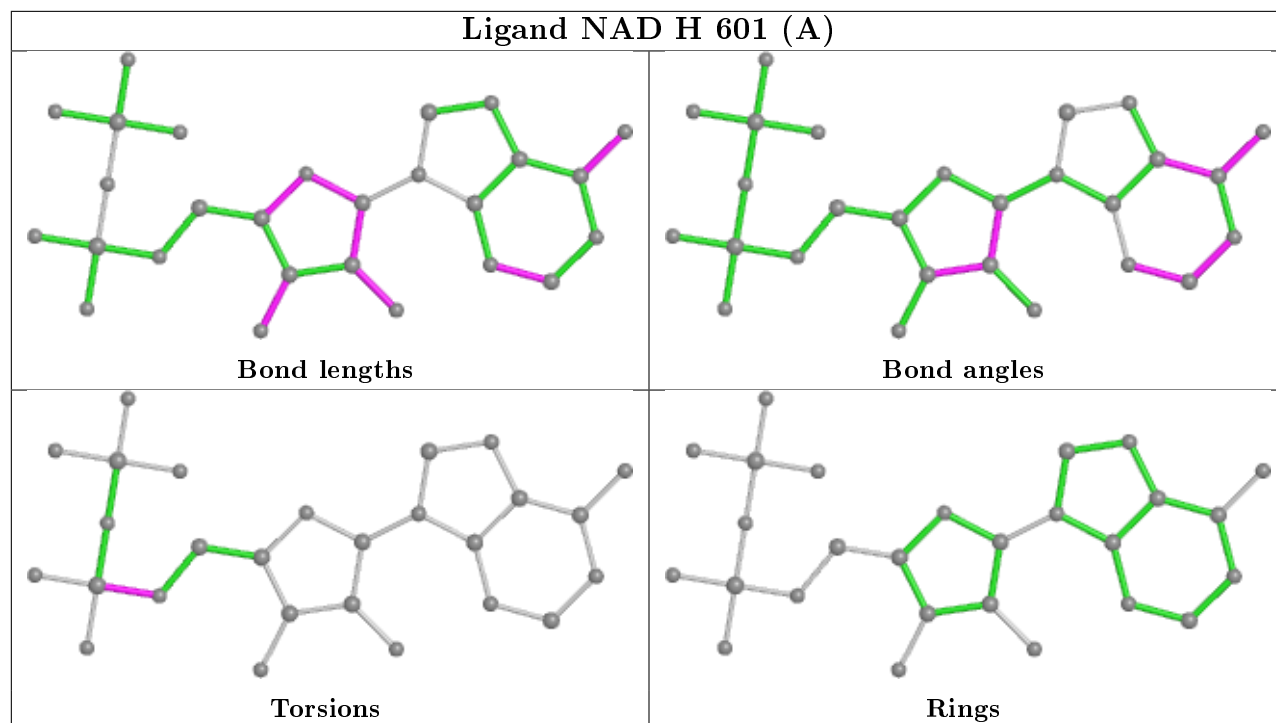


## Ligand NAD G 601









## 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	509/513 (99%)	-0.26	1 (0%) 95 96	17, 28, 46, 72	0
1	B	509/513 (99%)	-0.26	1 (0%) 95 96	17, 28, 47, 82	0
1	C	509/513 (99%)	-0.25	1 (0%) 95 96	18, 28, 49, 73	0
1	D	509/513 (99%)	-0.13	6 (1%) 79 83	18, 32, 55, 78	0
1	E	509/513 (99%)	-0.31	0 100 100	20, 29, 43, 73	0
1	F	509/513 (99%)	-0.22	1 (0%) 95 96	19, 29, 46, 71	0
1	G	499/513 (97%)	-0.30	0 100 100	19, 29, 47, 86	0
1	H	509/513 (99%)	-0.12	5 (0%) 82 86	19, 31, 52, 74	0
All	All	4062/4104 (98%)	-0.23	15 (0%) 92 94	17, 29, 49, 86	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	9	PRO	3.6
1	C	510	PHE	3.4
1	D	389	LEU	2.9
1	H	461	GLY	2.9
1	F	400	THR	2.6

### 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 ⓘ

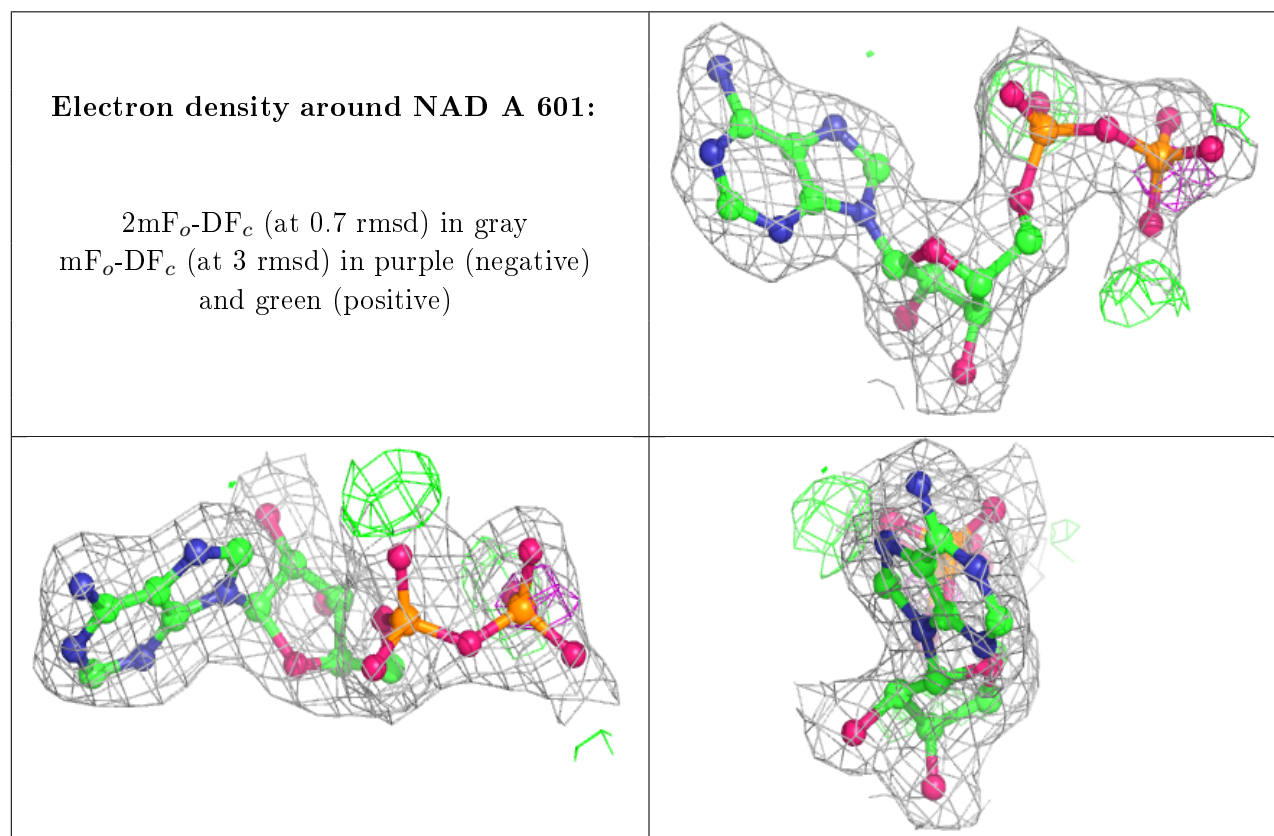
There are no carbohydrates in this entry.

## 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.

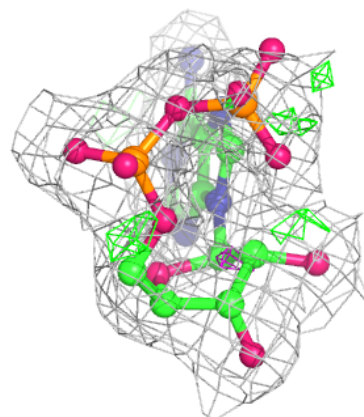
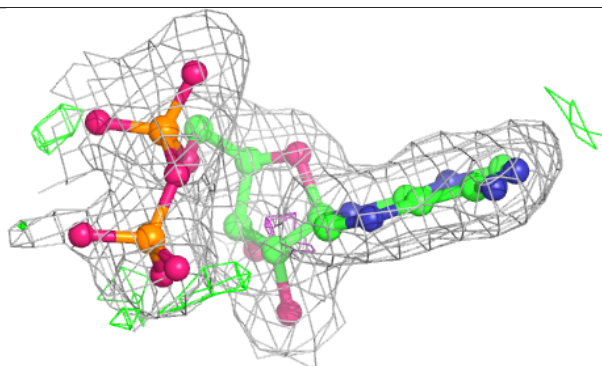
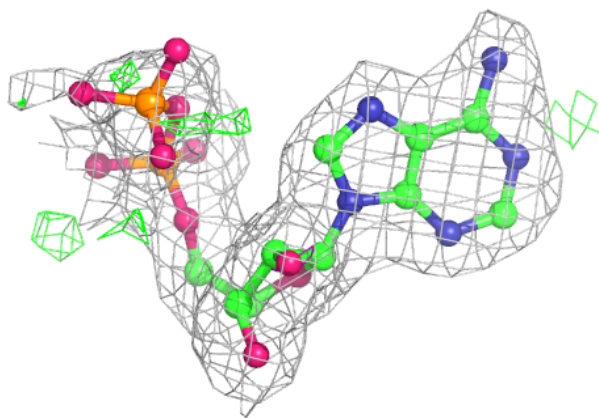
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAD	A	601	27/44	0.92	0.11	20,35,69,69	0
2	NAD	B	601[B]	27/44	0.93	0.12	23,28,38,43	27
2	NAD	B	601[A]	27/44	0.93	0.12	23,27,35,36	27
2	NAD	E	601	27/44	0.94	0.11	21,31,72,78	0
2	NAD	H	601[B]	27/44	0.94	0.12	23,27,40,42	27
2	NAD	H	601[A]	27/44	0.94	0.12	22,27,43,45	27
2	NAD	D	601[B]	27/44	0.95	0.12	26,30,37,40	27
2	NAD	G	601	27/44	0.95	0.10	21,30,64,66	0
2	NAD	D	601[A]	27/44	0.95	0.12	25,30,42,51	27
2	NAD	C	601	27/44	0.96	0.09	18,27,66,71	0
2	NAD	F	601	27/44	0.96	0.09	18,29,60,66	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.

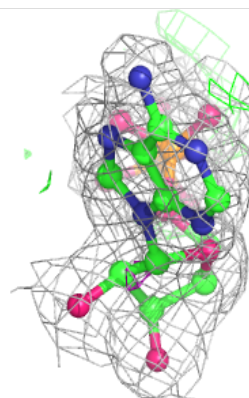
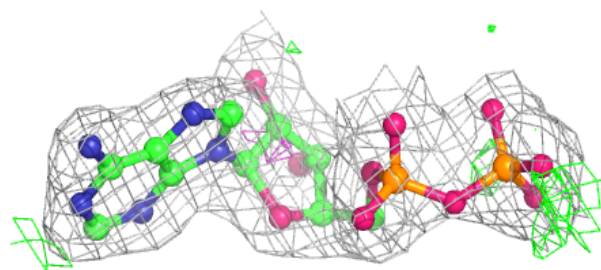
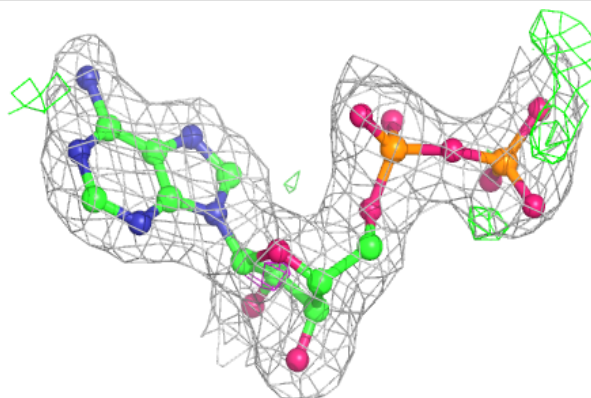


**Electron density around NAD B 601 (B):**

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

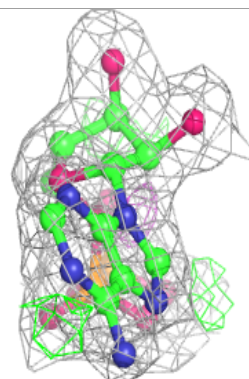
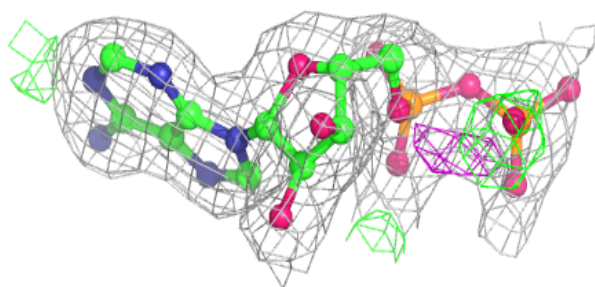
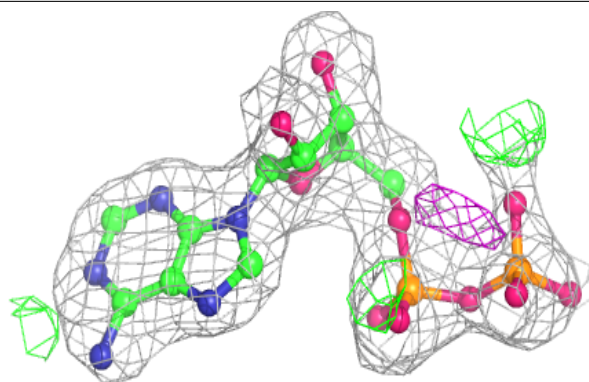
**Electron density around NAD B 601 (A):**

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

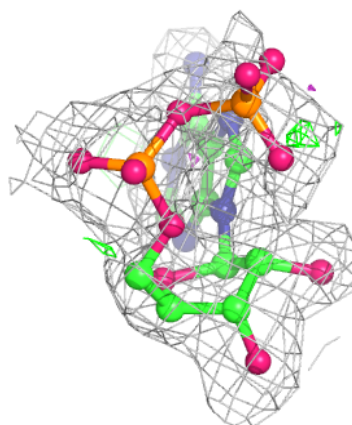
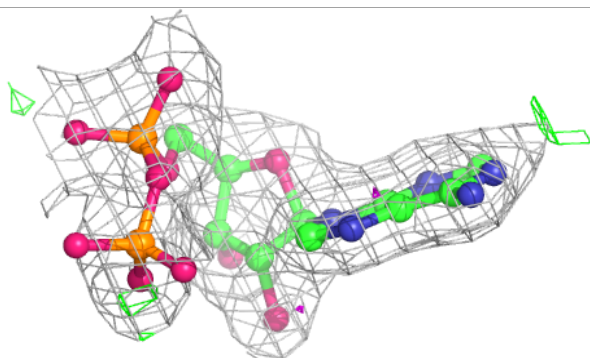
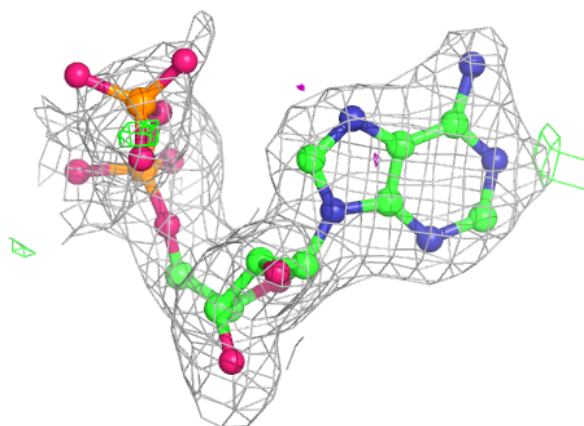


**Electron density around NAD E 601:**

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

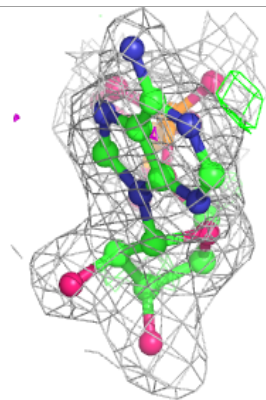
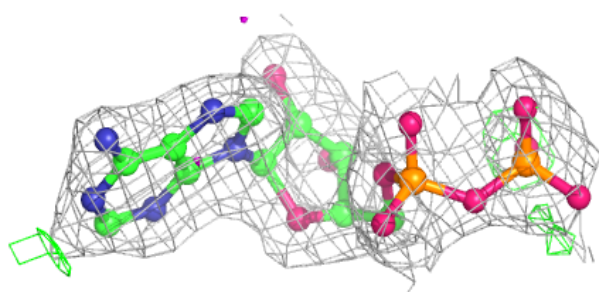
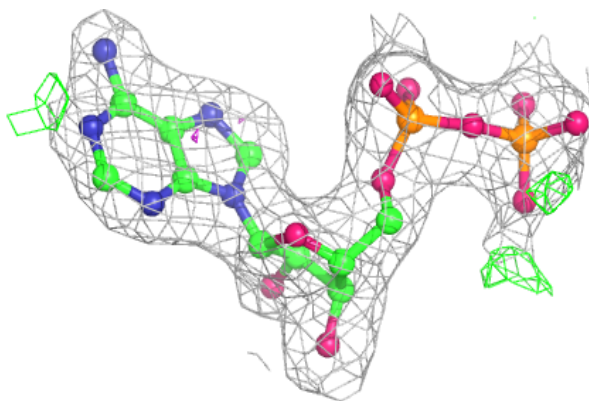
**Electron density around NAD H 601 (B):**

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



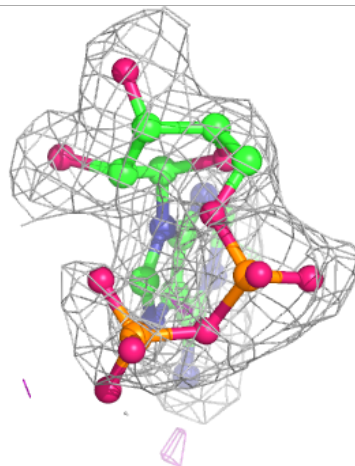
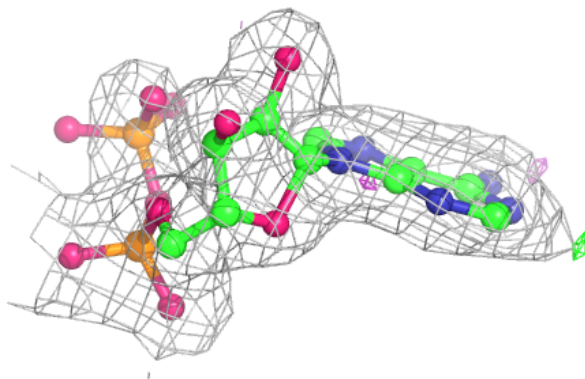
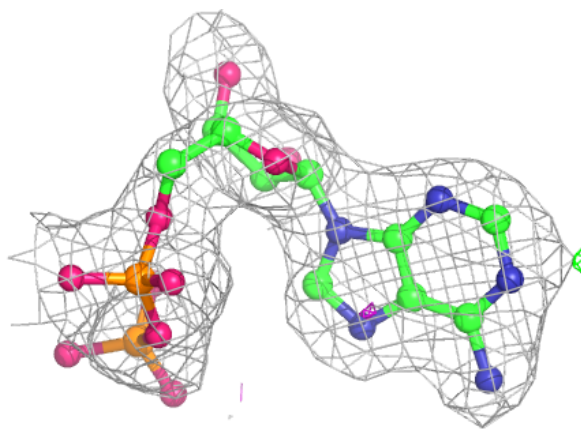
**Electron density around NAD H 601 (A):**

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



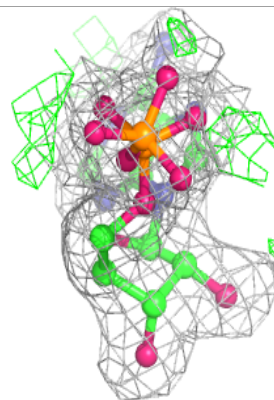
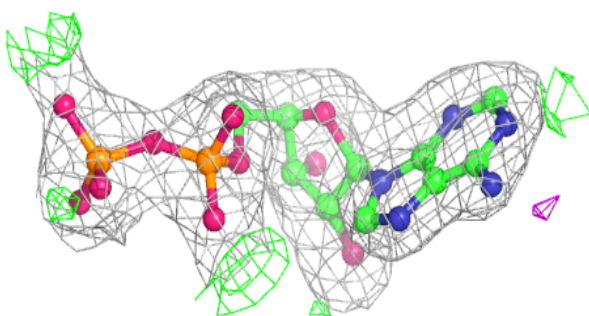
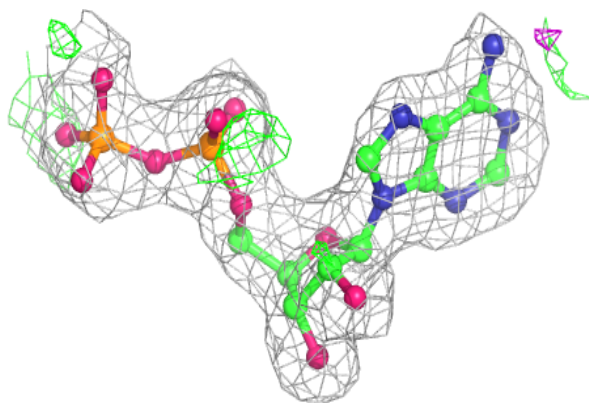
**Electron density around NAD D 601 (B):**

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

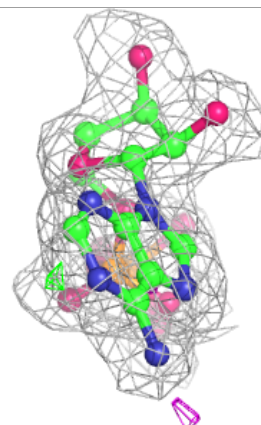
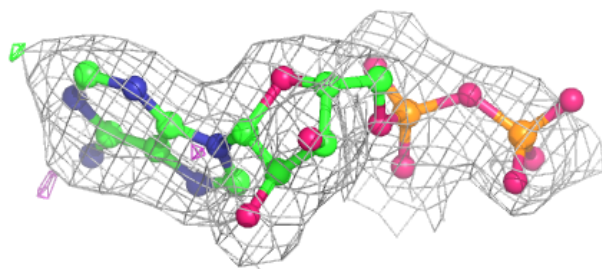
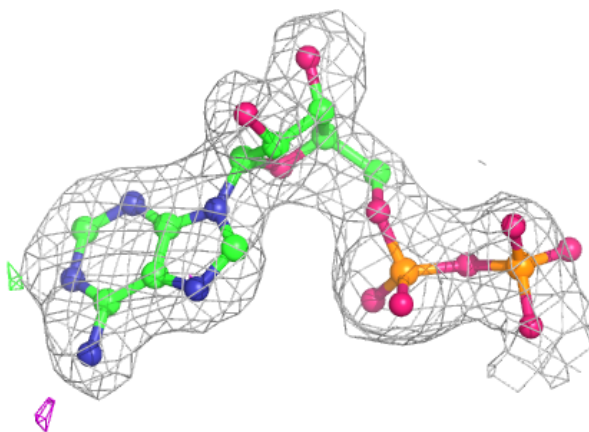


**Electron density around NAD G 601:**

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

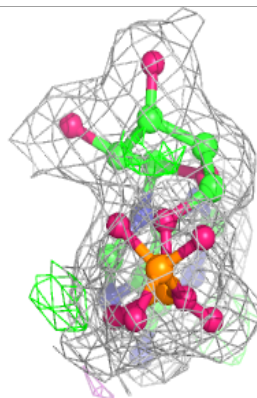
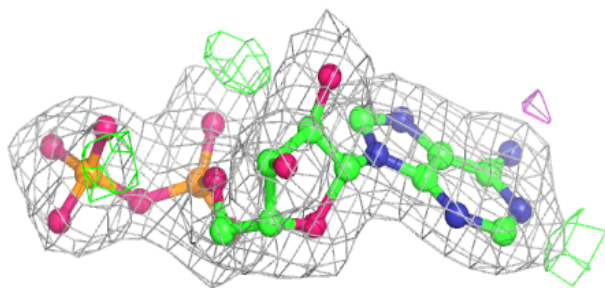
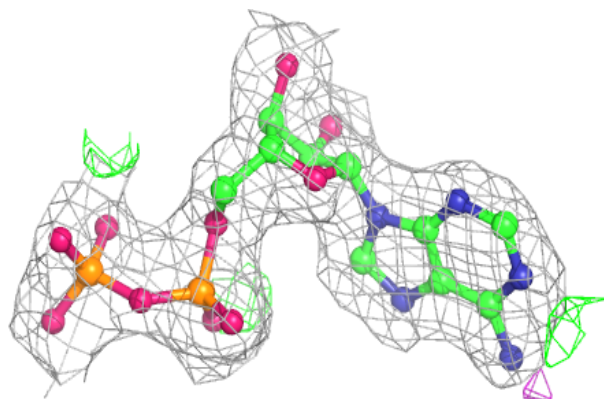
**Electron density around NAD D 601 (A):**

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and green (positive)

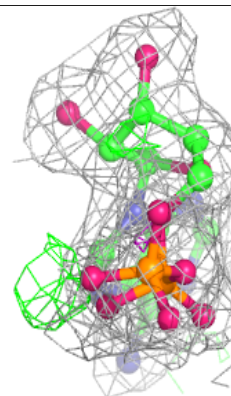
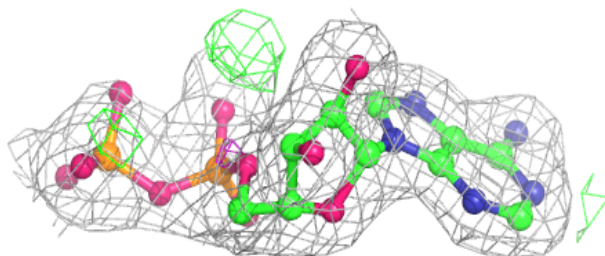
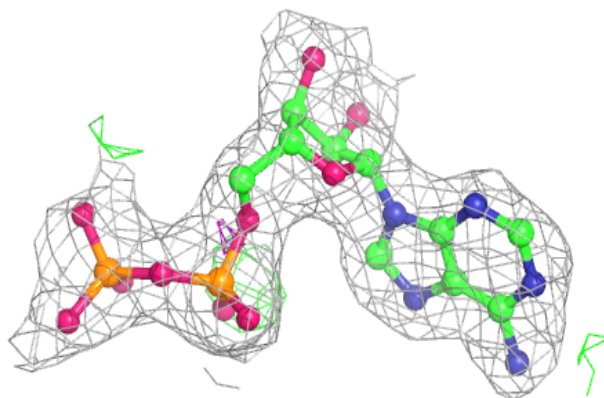


**Electron density around NAD C 601:**

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

**Electron density around NAD F 601:**

$2mF_o-DF_c$  (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.