



wwPDB X-ray Structure Validation Summary Report

Oct 3, 2023 – 05:13 AM EDT

PDB ID : 6O4B
Title : Structure of ALDH7A1 mutant W175G complexed with NAD
Authors : Tanner, J.J.; Korasick, D.A.; Laciak, A.R.
Deposited on : 2019-02-28
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  symbol.

The types of validation reports are described at

<https://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 33057 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
			Total	C	N	O	S			
1	A	509	3848	2445	665	720	18	0	2	0
1	B	509	3862	2454	670	720	18	0	2	0
1	C	509	3852	2445	670	719	18	0	1	0
1	D	509	3857	2451	668	720	18	0	3	0
1	E	509	3859	2455	670	717	17	0	3	0
1	F	509	3873	2457	676	723	17	0	1	0
1	G	509	3854	2449	665	723	17	0	3	0
1	H	509	3849	2444	668	719	18	0	1	0

There are 24 discrepancies between the modelled and reference sequences:

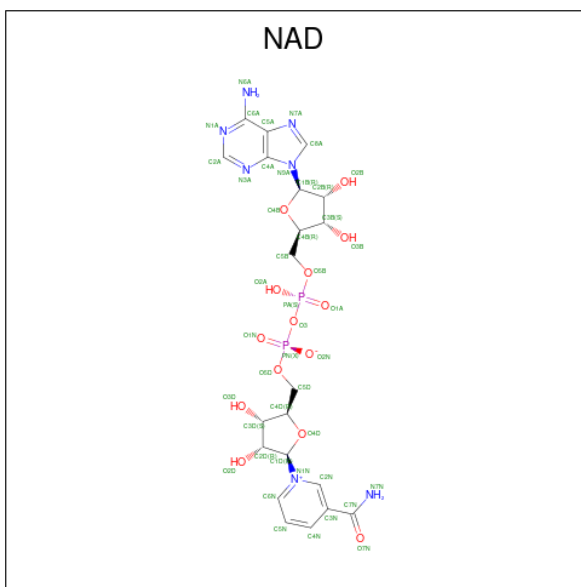
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P49419
A	0	HIS	-	expression tag	UNP P49419
A	175	GLY	TRP	engineered mutation	UNP P49419
B	-1	GLY	-	expression tag	UNP P49419
B	0	HIS	-	expression tag	UNP P49419
B	175	GLY	TRP	engineered mutation	UNP P49419
C	-1	GLY	-	expression tag	UNP P49419
C	0	HIS	-	expression tag	UNP P49419
C	175	GLY	TRP	engineered mutation	UNP P49419
D	-1	GLY	-	expression tag	UNP P49419
D	0	HIS	-	expression tag	UNP P49419
D	175	GLY	TRP	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	175	GLY	TRP	engineered mutation	UNP P49419
F	-1	GLY	-	expression tag	UNP P49419
F	0	HIS	-	expression tag	UNP P49419
F	175	GLY	TRP	engineered mutation	UNP P49419
G	-1	GLY	-	expression tag	UNP P49419
G	0	HIS	-	expression tag	UNP P49419
G	175	GLY	TRP	engineered mutation	UNP P49419
H	-1	GLY	-	expression tag	UNP P49419
H	0	HIS	-	expression tag	UNP P49419
H	175	GLY	TRP	engineered mutation	UNP P49419

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



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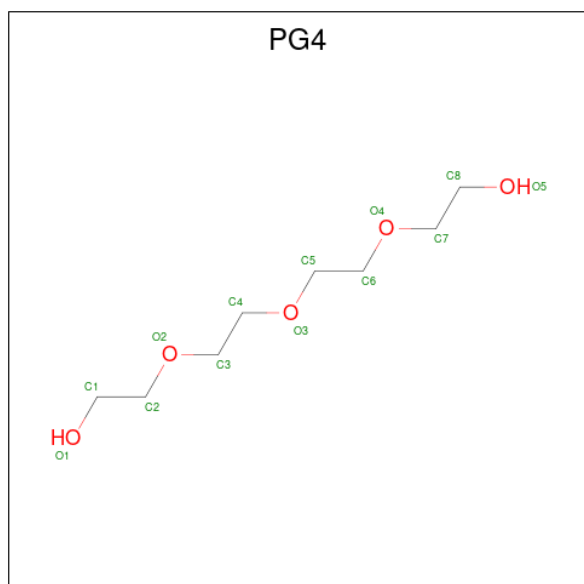
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		
3	C	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	E	2	Total	Cl	0	0
			2	2		
3	G	2	Total	Cl	0	0
			2	2		

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



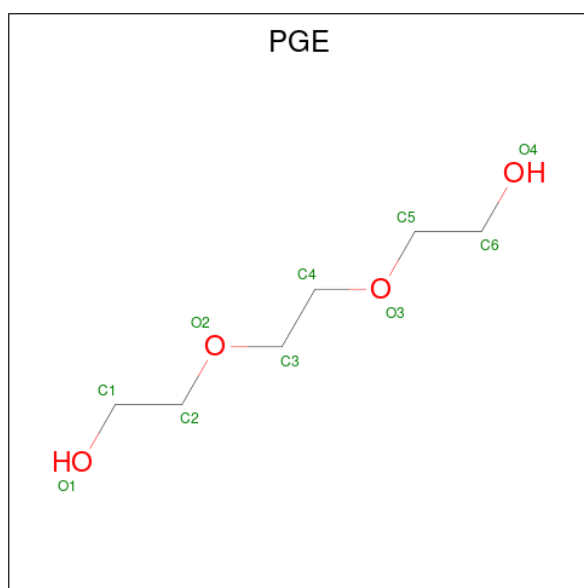
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	8	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			13	8	5		
4	D	1	Total	C	O	0	0
			13	8	5		
4	E	1	Total	C	O	0	0
			13	8	5		
4	F	1	Total	C	O	0	0
			13	8	5		
4	H	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



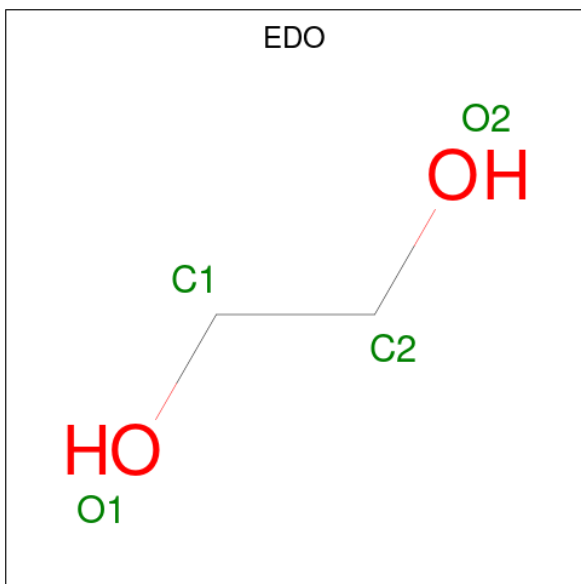
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	A	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		
5	C	1	Total	C	O	0	0
			10	6	4		
5	D	1	Total	C	O	0	0
			10	6	4		
5	E	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C O 10 6 4	0	0
5	F	1	Total C O 10 6 4	0	0
5	F	1	Total C O 10 6 4	0	0
5	G	1	Total C O 10 6 4	0	0
5	G	1	Total C O 7 4 3	0	0
5	G	1	Total C O 10 6 4	0	0
5	H	1	Total C O 10 6 4	0	0
5	H	1	Total C O 10 6 4	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



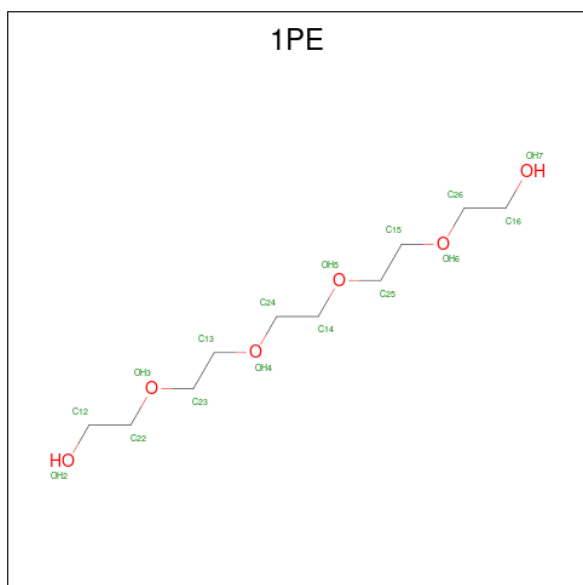
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			16	10	6		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	211	Total	O	0	0
			211	211		
8	B	188	Total	O	0	0
			188	188		
8	C	216	Total	O	0	0
			216	216		
8	D	169	Total	O	0	0
			169	169		
8	E	215	Total	O	0	0
			215	215		
8	F	195	Total	O	0	0
			195	195		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	189	Total 189	O 189	0	0
8	H	208	Total 209	O 209	0	1

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	155.15Å 161.49Å 158.59Å 90.00° 94.72° 90.00°	Depositor
Resolution (Å)	62.78 – 1.85	Depositor
% Data completeness (in resolution range)	89.6 (62.78-1.85)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 1.86Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.170 , 0.212	Depositor
Wilson B-factor (Å ²)	22.4	Xtrriage
Anisotropy	0.457	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	33057	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 8 are monoatomic - leaving 34 for Mogul analysis.

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	B	601	-	42,48,48	5.15	16 (38%)	50,73,73	1.46	7 (14%)
5	PGE	C	603	-	9,9,9	0.55	0	8,8,8	0.31	0
6	EDO	E	607	-	3,3,3	0.53	0	2,2,2	0.47	0
6	EDO	D	606	-	3,3,3	0.50	0	2,2,2	0.26	0
5	PGE	E	605	-	9,9,9	0.55	0	8,8,8	0.31	0
5	PGE	A	606	-	9,9,9	0.46	0	8,8,8	0.32	0
6	EDO	C	604	-	3,3,3	0.48	0	2,2,2	0.21	0
4	PG4	D	603	-	12,12,12	0.67	0	11,11,11	0.27	0
4	PG4	F	602	-	12,12,12	0.65	0	11,11,11	0.32	0
2	NAD	F	601	-	42,48,48	5.04	16 (38%)	50,73,73	1.38	4 (8%)
5	PGE	E	606	-	9,9,9	0.56	0	8,8,8	0.26	0
2	NAD	D	601	-	42,48,48	5.16	16 (38%)	50,73,73	1.33	7 (14%)
4	PG4	E	604	-	12,12,12	0.70	0	11,11,11	0.40	0
2	NAD	E	601	-	42,48,48	5.09	16 (38%)	50,73,73	1.45	7 (14%)
6	EDO	A	607	-	3,3,3	0.48	0	2,2,2	0.24	0
5	PGE	F	604	-	9,9,9	0.53	0	8,8,8	0.27	0
5	PGE	G	605	-	6,6,9	0.56	0	5,5,8	0.27	0
5	PGE	G	606	-	9,9,9	0.52	0	8,8,8	0.39	0
4	PG4	A	604	-	12,12,12	0.63	0	11,11,11	0.35	0
5	PGE	D	604	-	9,9,9	0.57	0	8,8,8	0.30	0
2	NAD	A	601	-	42,48,48	5.07	16 (38%)	50,73,73	1.42	6 (12%)
5	PGE	H	604	-	9,9,9	0.55	0	8,8,8	0.25	0
4	PG4	B	602	-	12,12,12	0.62	0	11,11,11	0.29	0
2	NAD	H	601	-	42,48,48	5.16	15 (35%)	50,73,73	1.22	4 (8%)
2	NAD	G	601	-	42,48,48	5.18	16 (38%)	50,73,73	1.37	4 (8%)
4	PG4	H	602	-	12,12,12	0.64	0	11,11,11	0.23	0
5	PGE	F	603	-	9,9,9	0.51	0	8,8,8	0.35	0
7	1PE	C	605	-	15,15,15	0.52	0	14,14,14	0.35	0
6	EDO	D	605	-	3,3,3	0.47	0	2,2,2	0.37	0
2	NAD	C	601	-	42,48,48	5.19	16 (38%)	50,73,73	1.29	4 (8%)
5	PGE	H	603	-	9,9,9	0.50	0	8,8,8	0.29	0
5	PGE	B	603	-	9,9,9	0.52	0	8,8,8	0.31	0
5	PGE	A	605	-	9,9,9	0.54	0	8,8,8	0.22	0
5	PGE	G	604	-	9,9,9	0.52	0	8,8,8	0.41	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	B	601	-	-	1/26/62/62	0/5/5/5
5	PGE	C	603	-	-	2/7/7/7	-
6	EDO	E	607	-	-	1/1/1/1	-
6	EDO	D	606	-	-	0/1/1/1	-
5	PGE	E	605	-	-	5/7/7/7	-
5	PGE	A	606	-	-	7/7/7/7	-
6	EDO	C	604	-	-	1/1/1/1	-
4	PG4	D	603	-	-	5/10/10/10	-
4	PG4	F	602	-	-	2/10/10/10	-
2	NAD	F	601	-	-	2/26/62/62	0/5/5/5
5	PGE	E	606	-	-	4/7/7/7	-
2	NAD	D	601	-	-	1/26/62/62	0/5/5/5
4	PG4	E	604	-	-	6/10/10/10	-
2	NAD	E	601	-	-	3/26/62/62	0/5/5/5
6	EDO	A	607	-	-	1/1/1/1	-
5	PGE	F	604	-	-	5/7/7/7	-
5	PGE	G	605	-	-	2/4/4/7	-
5	PGE	G	606	-	-	2/7/7/7	-
4	PG4	A	604	-	-	6/10/10/10	-
5	PGE	D	604	-	-	4/7/7/7	-
2	NAD	A	601	-	-	2/26/62/62	0/5/5/5
5	PGE	H	604	-	-	0/7/7/7	-
4	PG4	B	602	-	-	1/10/10/10	-
2	NAD	H	601	-	-	2/26/62/62	0/5/5/5
2	NAD	G	601	-	-	2/26/62/62	0/5/5/5
4	PG4	H	602	-	-	5/10/10/10	-
5	PGE	F	603	-	-	5/7/7/7	-
7	1PE	C	605	-	-	4/13/13/13	-
6	EDO	D	605	-	-	0/1/1/1	-
2	NAD	C	601	-	-	1/26/62/62	0/5/5/5
5	PGE	H	603	-	-	5/7/7/7	-
5	PGE	B	603	-	-	4/7/7/7	-
5	PGE	A	605	-	-	1/7/7/7	-
5	PGE	G	604	-	-	4/7/7/7	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	601	NAD	C2D-C1D	-16.23	1.29	1.53
2	C	601	NAD	C2D-C1D	-16.21	1.29	1.53
2	C	601	NAD	C2B-C1B	-15.98	1.29	1.53
2	H	601	NAD	C2B-C1B	-15.93	1.29	1.53
2	A	601	NAD	C2D-C1D	-15.92	1.29	1.53

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	601	NAD	N3A-C2A-N1A	-5.81	119.60	128.68
2	F	601	NAD	N3A-C2A-N1A	-5.55	120.01	128.68
2	A	601	NAD	N3A-C2A-N1A	-5.52	120.05	128.68
2	B	601	NAD	N3A-C2A-N1A	-5.38	120.27	128.68
2	D	601	NAD	N3A-C2A-N1A	-5.31	120.38	128.68

There are no chirality outliers.

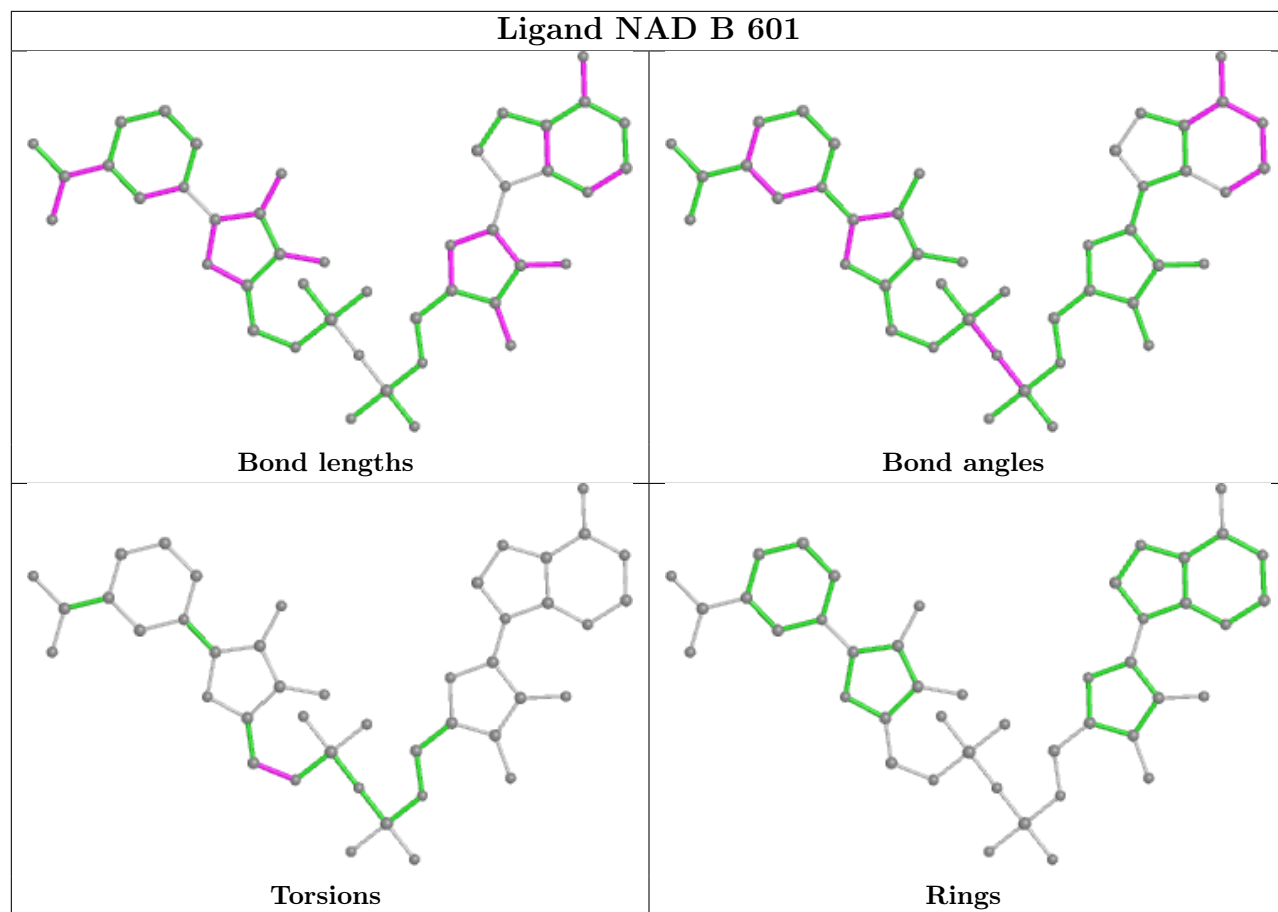
5 of 96 torsion outliers are listed below:

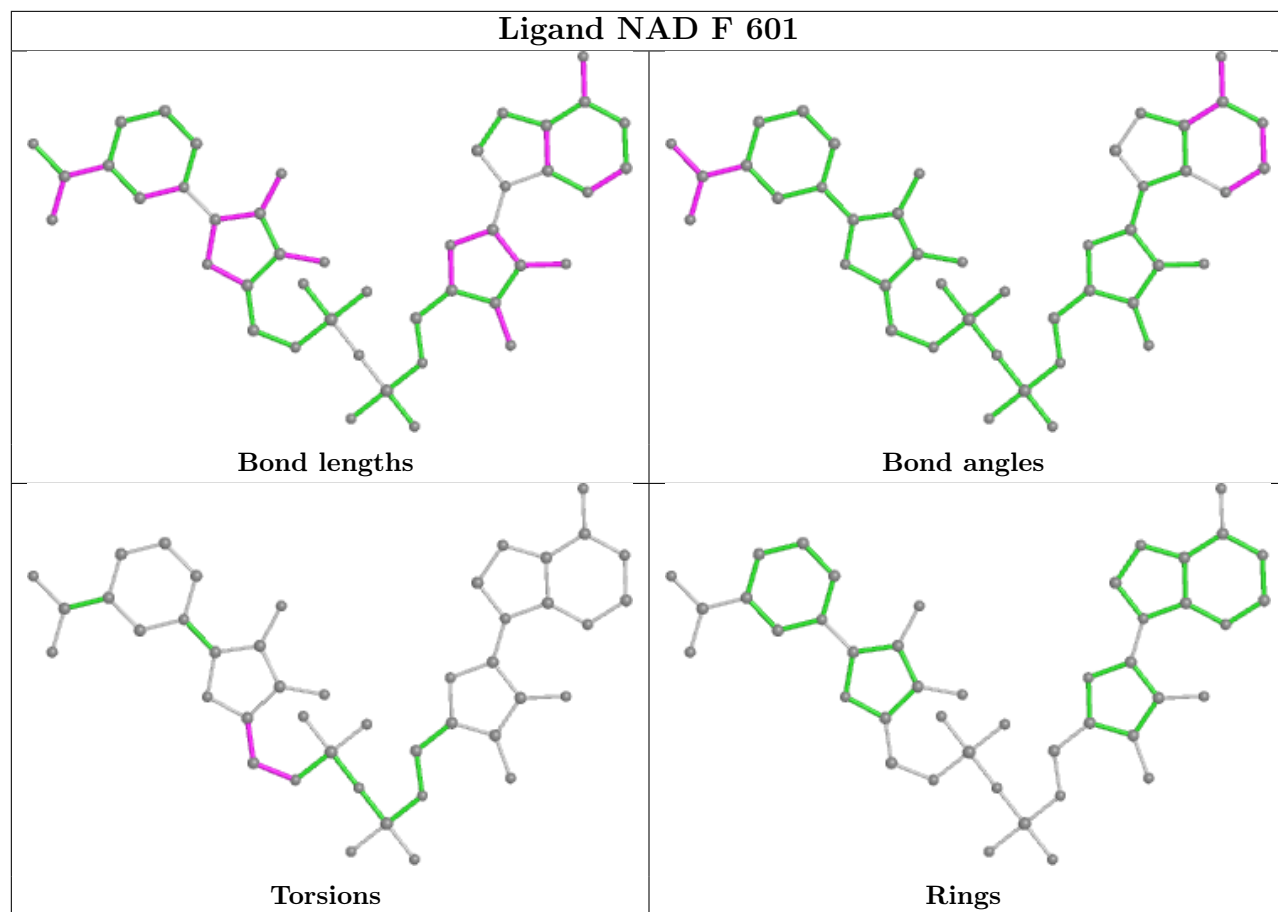
Mol	Chain	Res	Type	Atoms
5	F	603	PGE	C3-C4-O3-C5
5	D	604	PGE	C4-C3-O2-C2
5	F	603	PGE	O3-C5-C6-O4
4	A	604	PG4	C3-C4-O3-C5
4	H	602	PG4	C6-C5-O3-C4

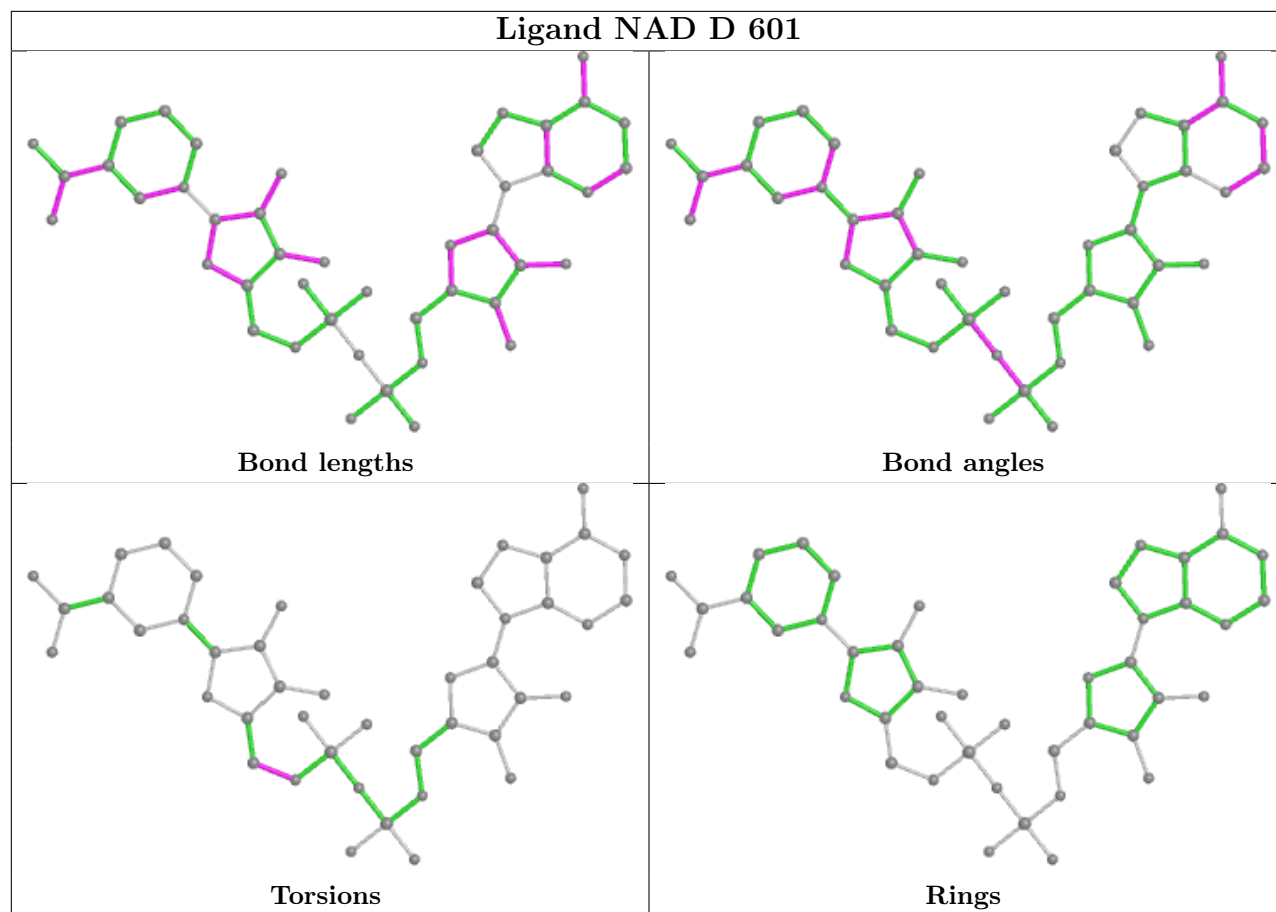
There are no ring outliers.

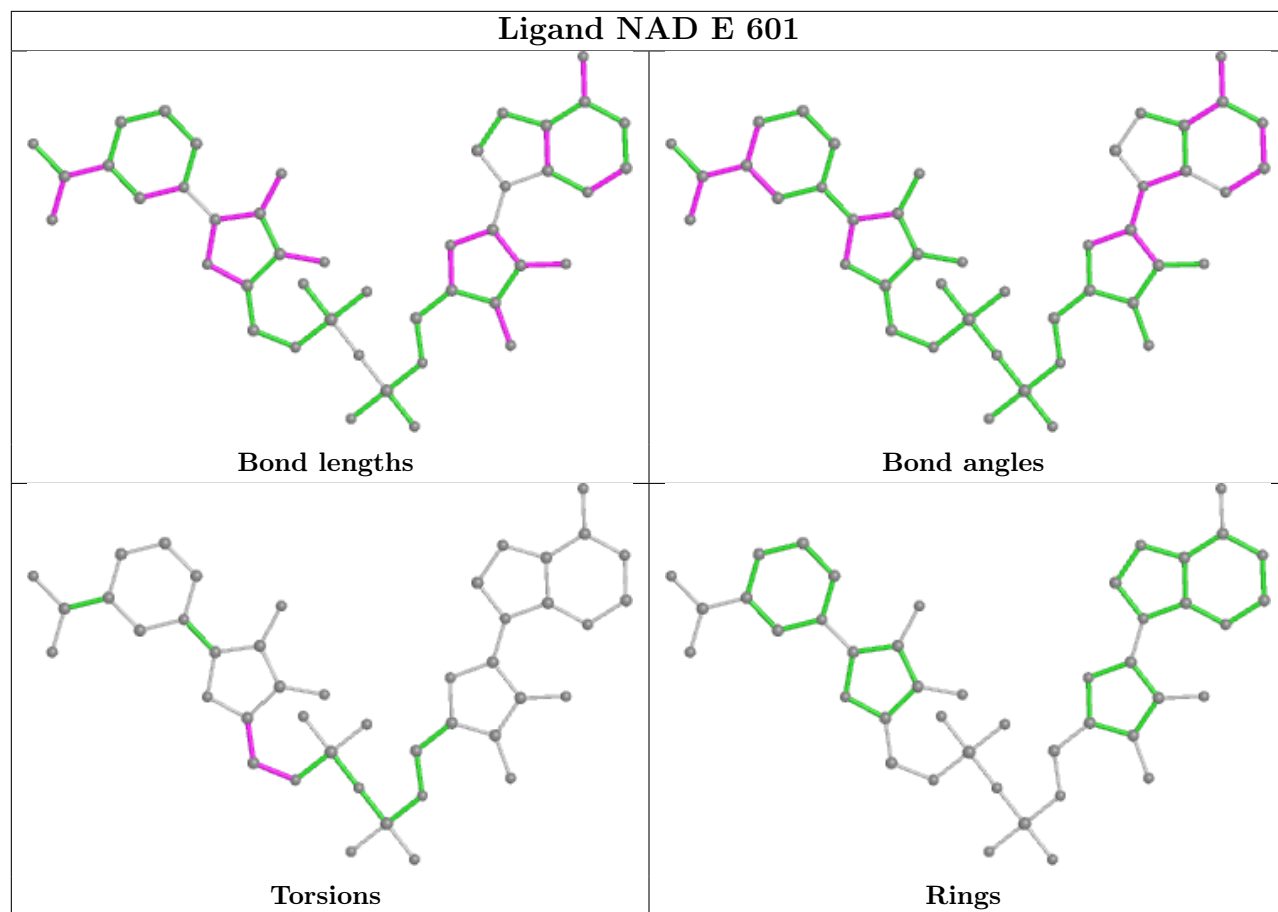
No monomer is involved in short contacts.

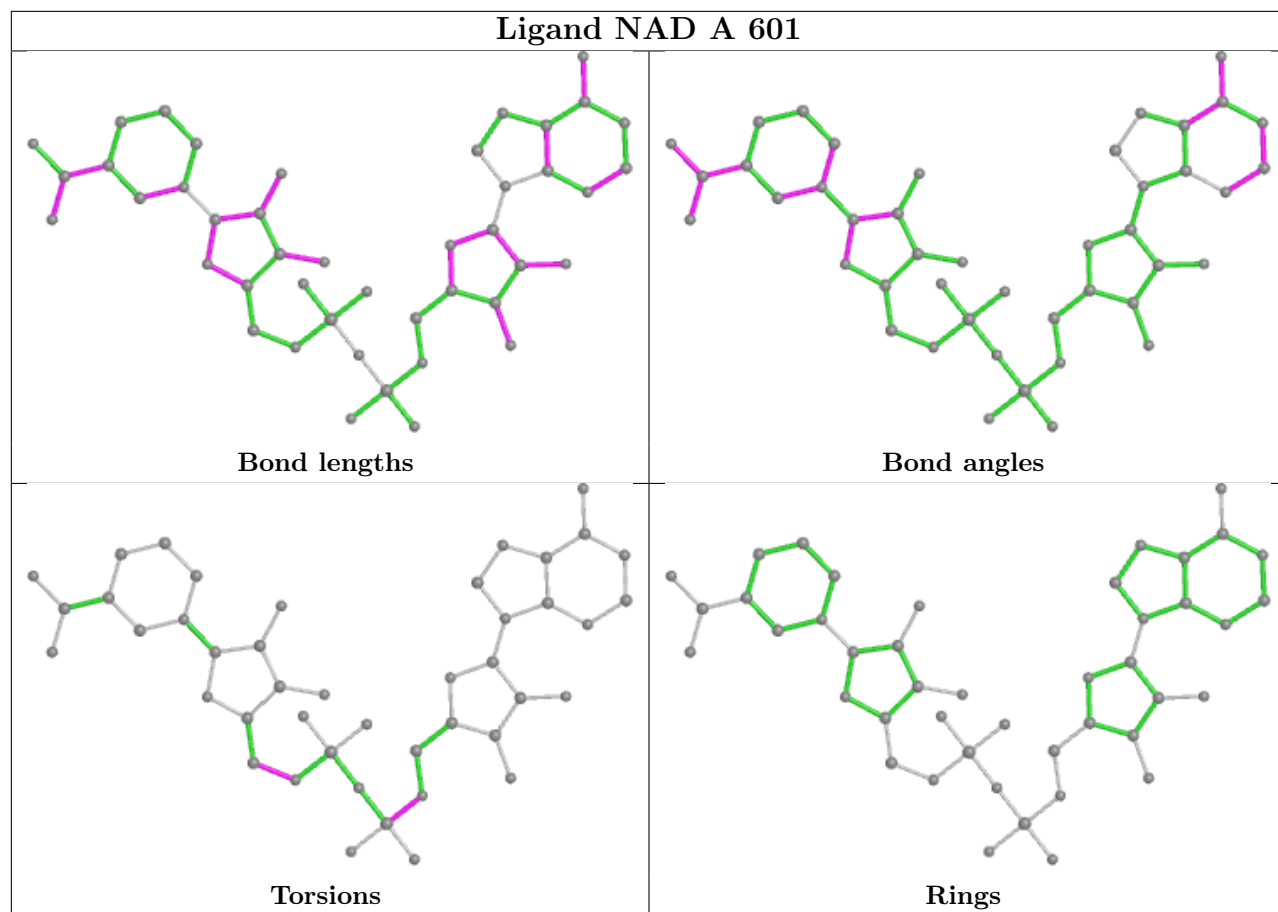
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

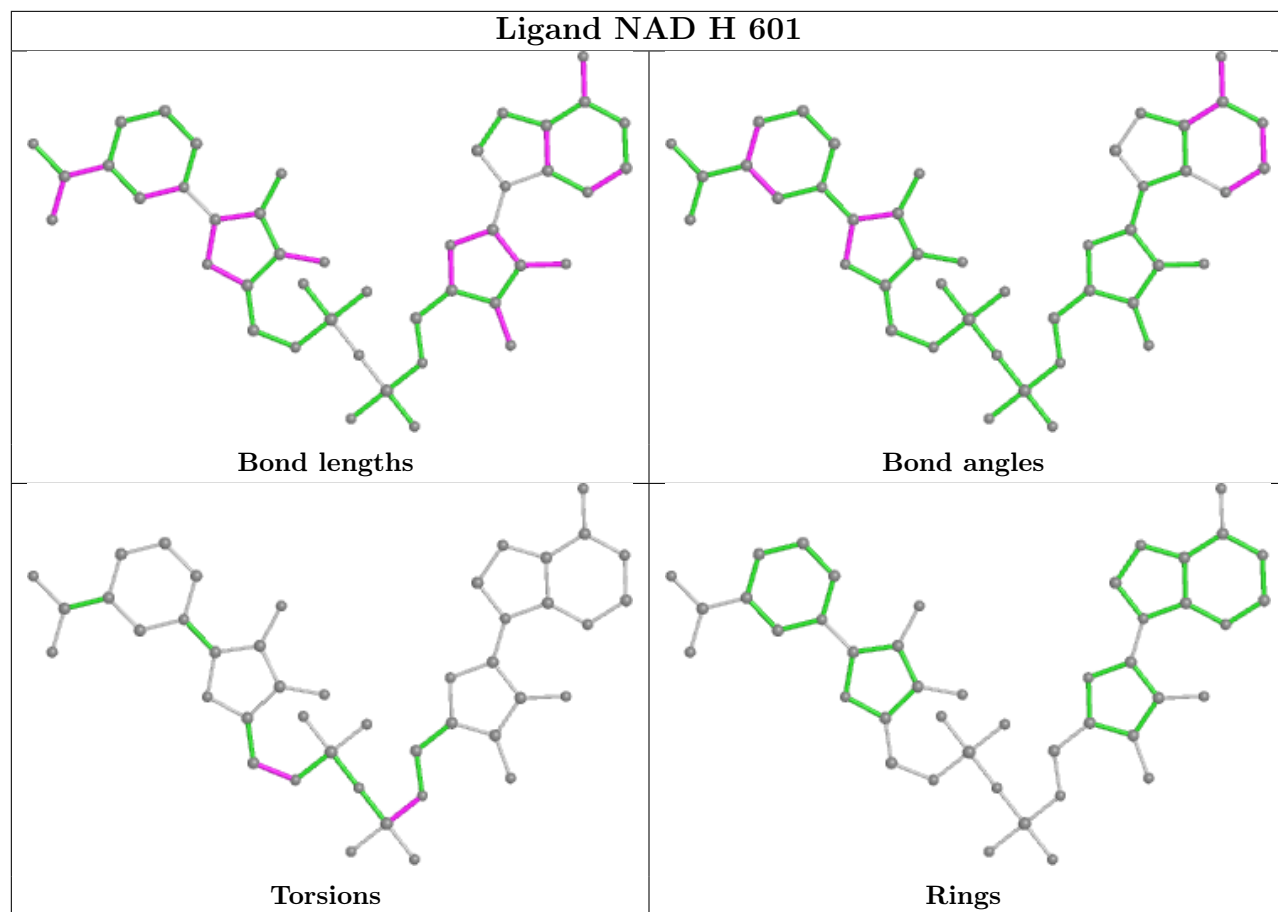


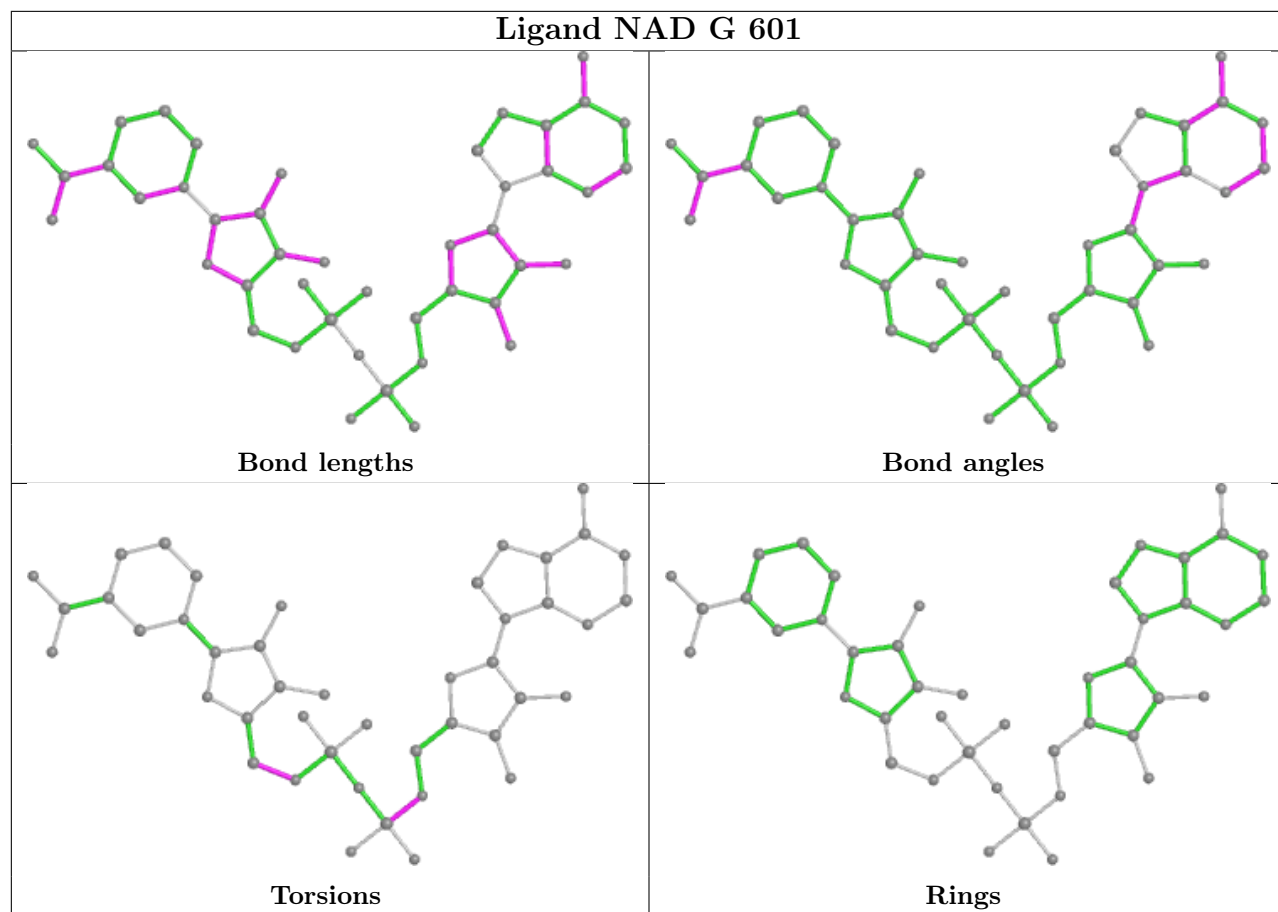


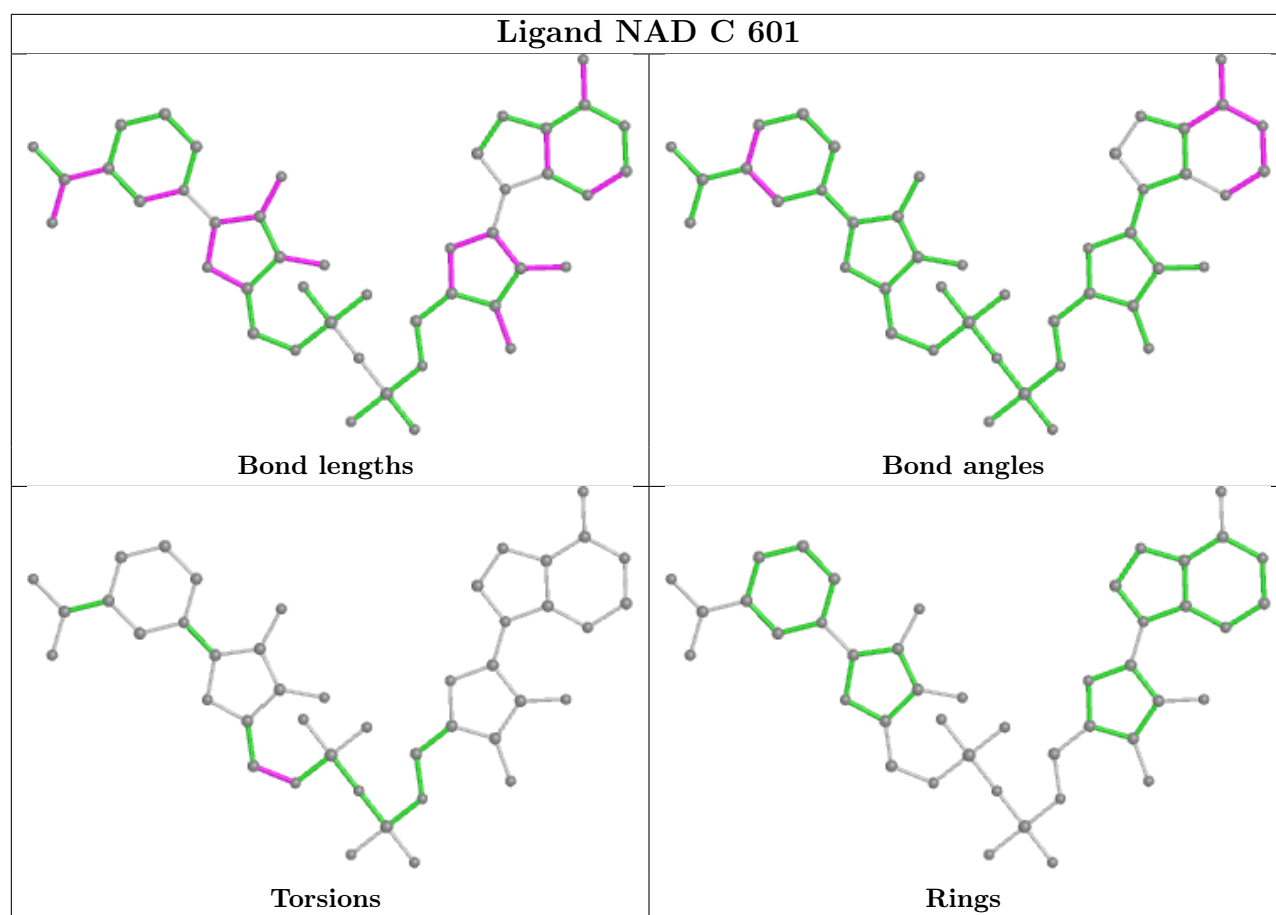












4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.