



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 04:28 AM UTC

PDB ID : 1DO8 / pdb_00001do8
Title : CRYSTAL STRUCTURE OF A CLOSED FORM OF HUMAN MITOCHONDRIAL NAD(P)⁺-DEPENDENT MALIC ENZYME
Authors : Yang, Z.; Floyd, D.L.; Loeber, G.; Tong, L.
Deposited on : 1999-12-19
Resolution : 2.20 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

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

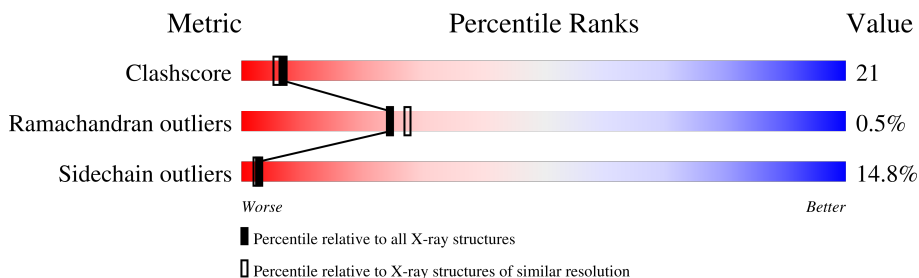
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	564	 57% 32% 9% .
1	B	564	 53% 37% 7% .
1	C	564	 60% 31% 7% .
1	D	564	 60% 30% 8% .

2 Entry composition [i](#)

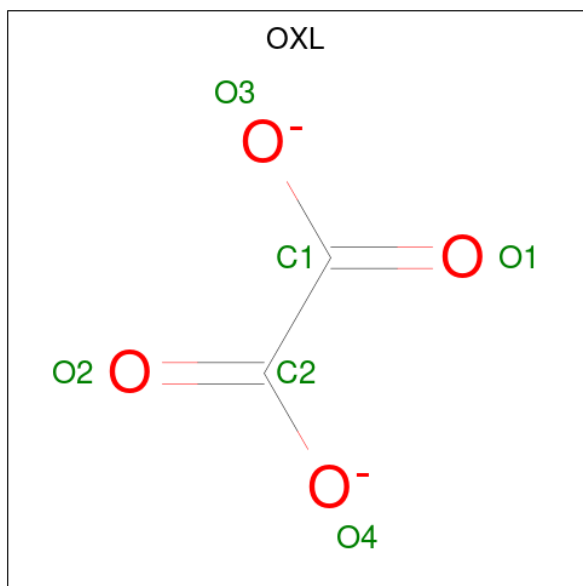
There are 5 unique types of molecules in this entry. The entry contains 18807 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MALIC ENZYME.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			
1	B	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			
1	C	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			
1	D	553	Total	C	N	O	S	Se	0	0	0
			4367	2796	744	804	9	14			

- Molecule 2 is OXALATE ION (CCD ID: OXL) (formula: C_2O_4).



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

Continued on next page...

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

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3 | A | 1 | Total Mn
1 1 | 0 | 0 |
| 3 | B | 1 | Total Mn
1 1 | 0 | 0 |
| 3 | C | 1 | Total Mn
1 1 | 0 | 0 |
| 3 | D | 1 | Total Mn
1 1 | 0 | 0 |

- # NAD

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
4	A	1	Total 44	C 21	N 7	O 14	P 2	9	0
4	B	1	Total 44	C 21	N 7	O 14	P 2	0	0



WORLD WIDE
PDB
PROTEIN DATA BANK

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total 44	C 21	N 7	O 14	P 2	9	0
4	C	1	Total 44	C 21	N 7	O 14	P 2	0	0
4	C	1	Total 44	C 21	N 7	O 14	P 2	9	0
4	D	1	Total 44	C 21	N 7	O 14	P 2	0	0
4	D	1	Total 44	C 21	N 7	O 14	P 2	9	0

- Molecule 5 is water.

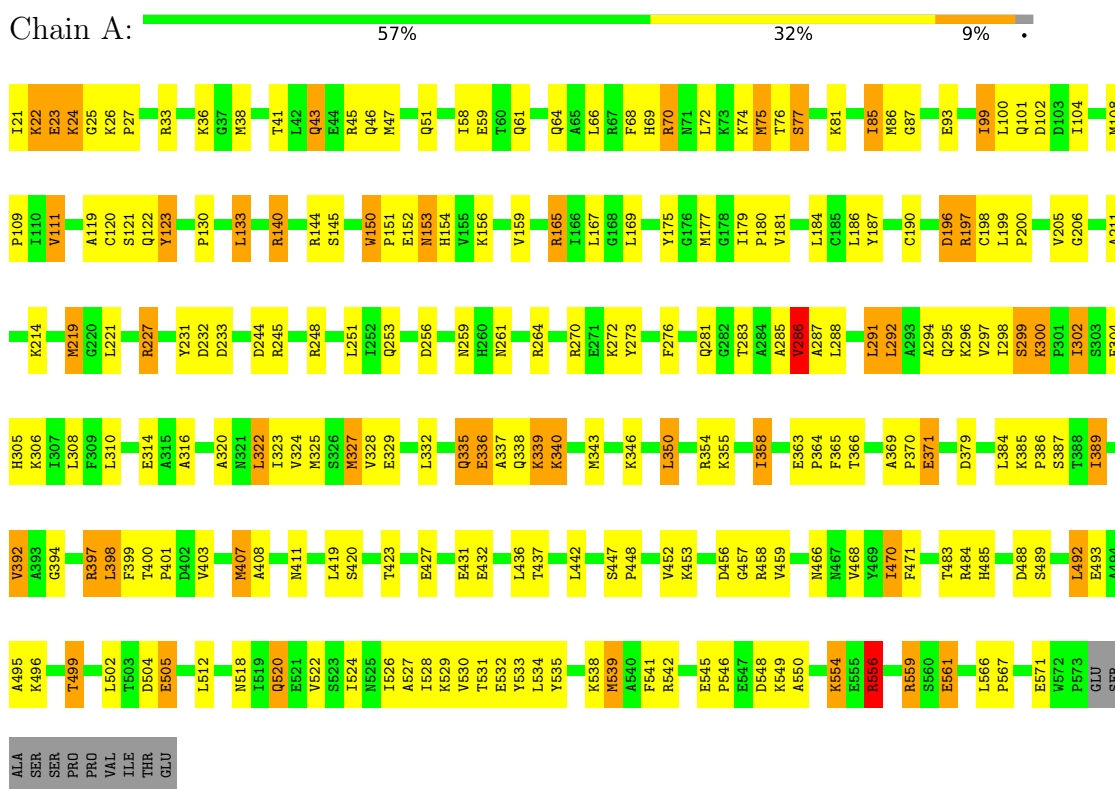
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	239	Total 239	O 239	0	0
5	B	199	Total 199	O 199	0	0
5	C	275	Total 275	O 275	0	0
5	D	246	Total 246	O 246	0	0

3 Residue-property plots

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. 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. 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.

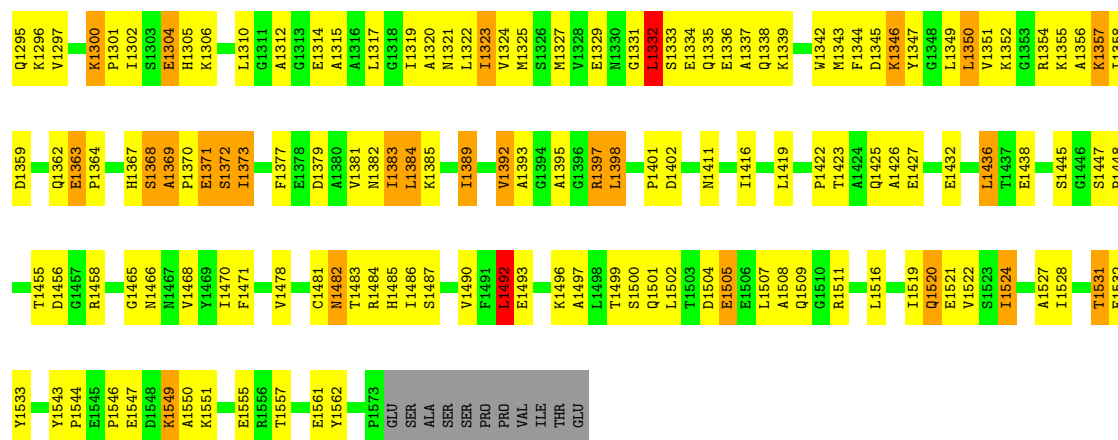
Note EDS was not executed.

• Molecule 1: MALIC ENZYME

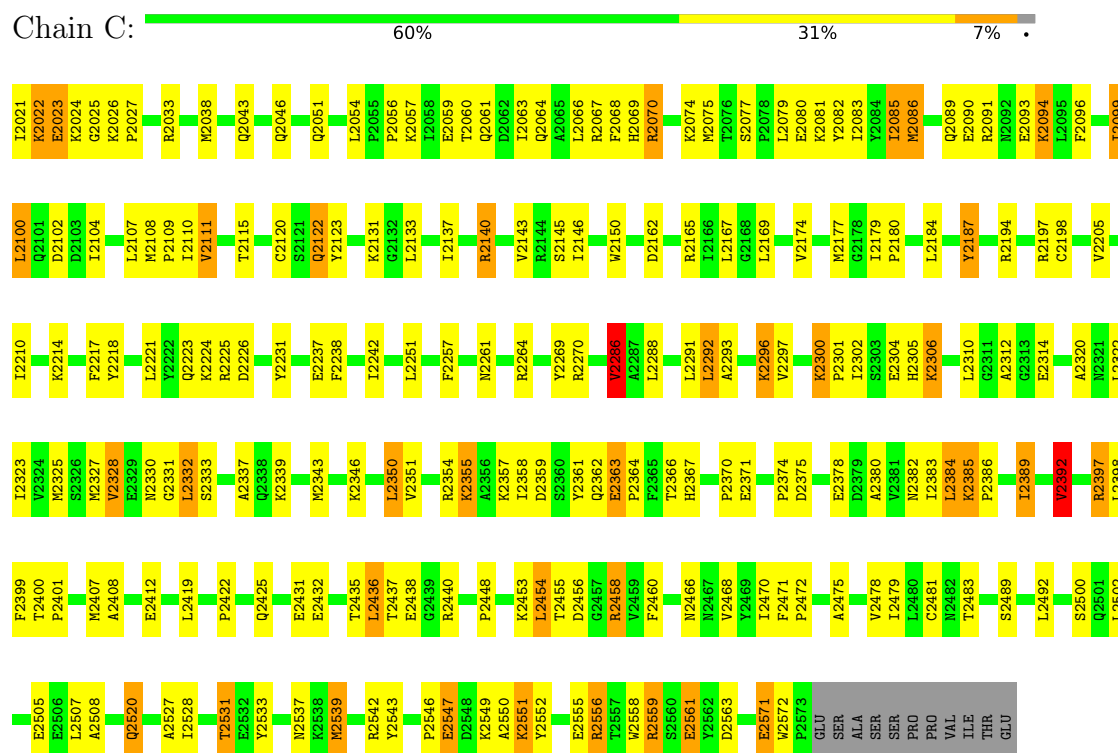


• Molecule 1: MALIC ENZYME





• Molecule 1: MALIC ENZYME



• Molecule 1: MALIC ENZYME



K3496	R3397	F3309	L3221
L3502	L3398	L3310	K3224
L3507	F3399	A3315	K3227
R3511	T3400	A3320	R3228
L3512	P3401	M3321	Q3229
Y3513	V3402	L3322	Q3230
P3514	V3403	I3323	Y3231
P3515	M3407	V3324	D3232
L3516	E3412	M3327	D3233
A3517	R3413	V3328	R3245
N3518	P3414	E3329	Y3246
I3519	F3417	L3332	G3247
Q3520	A3418	S3333	R3248
E3521	L3419	E3334	L3251
I3526	E3427	Q3335	D3256
A3527	E3431	E3336	N3259
I3528	L3436	A3337	R3260
K3529	T3437	Q3338	K3261
V3530	E3438	K3339	A3262
T3531	G3439	K3340	F3263
E3532	R3440	M3343	R3264
N3537	C3441	K3346	F3265
K3538	L3442	L3350	L3266
M3539	P3448	V3351	Y3269
A3540	V3452	K3352	K3272
E3545	K3453	G3353	Q3281
P3546	R3458	R3354	A3284
E3547	T3461	K3355	A3285
D3548	N3467	F3365	V3286
K3549	V3468	T3366	A3287
A3550	T3469	T3366	L3288
K3551	F3470	A3369	L3291
E3555	F3471	P3370	L3292
R3556	P3472	E3371	A3293
T3557	G3473	S3372	A3294
K3558	V3474	I3373	Q3295
R3559	V3478	A3380	K3296
E3571	C3481	L3384	V3297
W3572	N3482	S3299	I3298
P3573	T3483	K3385	K3300
GLU	R3484	P3301	P3301
SER	H3485	S3387	I3302
ALA	S3489	T3388	S3303
SER	L3492	I3389	K3306
SER		I3390	L3308
PRO		G3391	
PRO		V3392	
VAL			
ILE			
THR			
GLU			

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	229.00Å 118.70Å 113.00Å 90.00° 109.60° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.20)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.204 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18807	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

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, OXL, MN

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	0.45	0/4447	0.95	14/5998 (0.2%)
1	B	0.45	0/4447	0.94	16/5998 (0.3%)
1	C	0.47	0/4447	0.92	13/5998 (0.2%)
1	D	0.48	1/4447 (0.0%)	0.94	15/5998 (0.3%)
All	All	0.47	1/17788 (0.0%)	0.94	58/23992 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	3514	PRO	CA-C	6.08	1.55	1.51

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3470	ILE	N-CA-C	10.53	119.94	111.62
1	B	1470	ILE	N-CA-C	9.42	119.06	111.62
1	C	2470	ILE	N-CA-C	8.97	119.27	111.56
1	A	470	ILE	N-CA-C	8.81	118.58	111.62
1	A	387	SER	N-CA-C	-7.30	104.53	113.50

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	4367	0	4407	208	0
1	B	4367	0	4407	235	0
1	C	4367	0	4407	149	0
1	D	4367	0	4407	182	0
2	A	6	0	0	0	0
2	B	6	0	0	0	0
2	C	6	0	0	0	0
2	D	6	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	88	0	52	2	0
4	B	88	0	52	3	0
4	C	88	0	52	2	0
4	D	88	0	52	1	0
5	A	239	0	0	15	0
5	B	199	0	0	30	0
5	C	275	0	0	18	0
5	D	246	0	0	11	0
All	All	18807	0	17836	753	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 21.

The worst 5 of 753 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:177:MSE:HE2	1:A:181:VAL:HG23	1.29	1.14
1:D:3177:MSE:HE2	1:D:3181:VAL:HG23	1.35	1.08
1:A:123:TYR:HD2	1:A:219:MSE:HE1	1.18	1.06
1:B:1358:ILE:HG22	5:B:4650:HOH:O	1.54	1.06
1:A:140:ARG:HH22	1:A:233:ASP:HB3	1.14	1.05

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	551/564 (98%)	530 (96%)	19 (3%)	2 (0%)	30	34
1	B	551/564 (98%)	522 (95%)	26 (5%)	3 (0%)	24	27
1	C	551/564 (98%)	530 (96%)	17 (3%)	4 (1%)	18	19
1	D	551/564 (98%)	528 (96%)	20 (4%)	3 (0%)	24	27
All	All	2204/2256 (98%)	2110 (96%)	82 (4%)	12 (0%)	24	27

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1332	LEU
1	C	2332	LEU
1	A	397	ARG
1	C	2392	VAL
1	D	3302	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	469/465 (101%)	400 (85%)	69 (15%)	3	2
1	B	469/465 (101%)	395 (84%)	74 (16%)	2	2
1	C	469/465 (101%)	400 (85%)	69 (15%)	3	2
1	D	469/465 (101%)	404 (86%)	65 (14%)	3	3
All	All	1876/1860 (101%)	1599 (85%)	277 (15%)	3	2

5 of 277 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	3193	ILE
1	D	3266	LEU
1	D	3384	LEU
1	B	1267	ARG
1	B	1243	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2261	ASN
1	D	3125	HIS
1	C	2425	GLN
1	D	3064	GLN
1	D	3229	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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
4	NAD	C	2601	-	46,48,48	1.83	9 (19%)	64,73,73	1.85	12 (18%)
4	NAD	C	2602	-	46,48,48	2.67	13 (28%)	64,73,73	1.86	11 (17%)
4	NAD	A	601	-	46,48,48	2.01	12 (26%)	64,73,73	1.84	10 (15%)
4	NAD	D	3601	-	46,48,48	2.01	13 (28%)	64,73,73	1.85	11 (17%)
2	OXL	B	1603	3	5,5,5	1.68	2 (40%)	6,6,6	2.46	2 (33%)
4	NAD	B	1602	-	46,48,48	2.31	13 (28%)	64,73,73	1.84	11 (17%)
2	OXL	A	603	3	5,5,5	1.93	2 (40%)	6,6,6	2.27	2 (33%)
4	NAD	D	3602	-	46,48,48	2.23	9 (19%)	64,73,73	1.86	11 (17%)
2	OXL	C	2603	3	5,5,5	1.68	2 (40%)	6,6,6	2.41	2 (33%)
4	NAD	B	1601	-	46,48,48	1.93	12 (26%)	64,73,73	1.86	11 (17%)
2	OXL	D	3603	3	5,5,5	1.74	2 (40%)	6,6,6	2.34	2 (33%)
4	NAD	A	602	-	46,48,48	2.26	13 (28%)	64,73,73	1.86	11 (17%)

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
4	NAD	C	2601	-	-	3/30/62/62	0/5/5/5
4	NAD	C	2602	-	-	7/30/62/62	0/5/5/5
4	NAD	A	601	-	-	2/30/62/62	0/5/5/5
4	NAD	D	3601	-	-	2/30/62/62	0/5/5/5
2	OXL	B	1603	3	-	0/4/4/4	-
4	NAD	B	1602	-	-	7/30/62/62	0/5/5/5
2	OXL	A	603	3	-	0/4/4/4	-
4	NAD	D	3602	-	-	7/30/62/62	0/5/5/5
2	OXL	C	2603	3	-	0/4/4/4	-
4	NAD	B	1601	-	-	2/30/62/62	0/5/5/5
2	OXL	D	3603	3	-	0/4/4/4	-
4	NAD	A	602	-	-	8/30/62/62	0/5/5/5

The worst 5 of 102 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2602	NAD	C2N-N1N	10.90	1.47	1.35
4	A	602	NAD	C2N-N1N	8.72	1.44	1.35
4	B	1602	NAD	C2N-N1N	7.91	1.43	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1602	NAD	O4D-C1D	7.74	1.51	1.40
4	A	601	NAD	C2N-N1N	7.25	1.42	1.35

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2602	NAD	C5A-C4A-N3A	-6.20	118.18	126.72
4	A	602	NAD	C5A-C4A-N3A	-6.08	118.35	126.72
4	D	3602	NAD	C5A-C4A-N3A	-6.07	118.36	126.72
4	B	1601	NAD	C5A-C4A-N3A	-5.97	118.50	126.72
4	B	1602	NAD	C5A-C4A-N3A	-5.96	118.52	126.72

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	NAD	O4D-C1D-N1N-C6N
4	A	602	NAD	C5B-O5B-PA-O1A
4	A	602	NAD	C5B-O5B-PA-O2A
4	A	602	NAD	C5B-O5B-PA-O3
4	B	1601	NAD	O4D-C1D-N1N-C6N

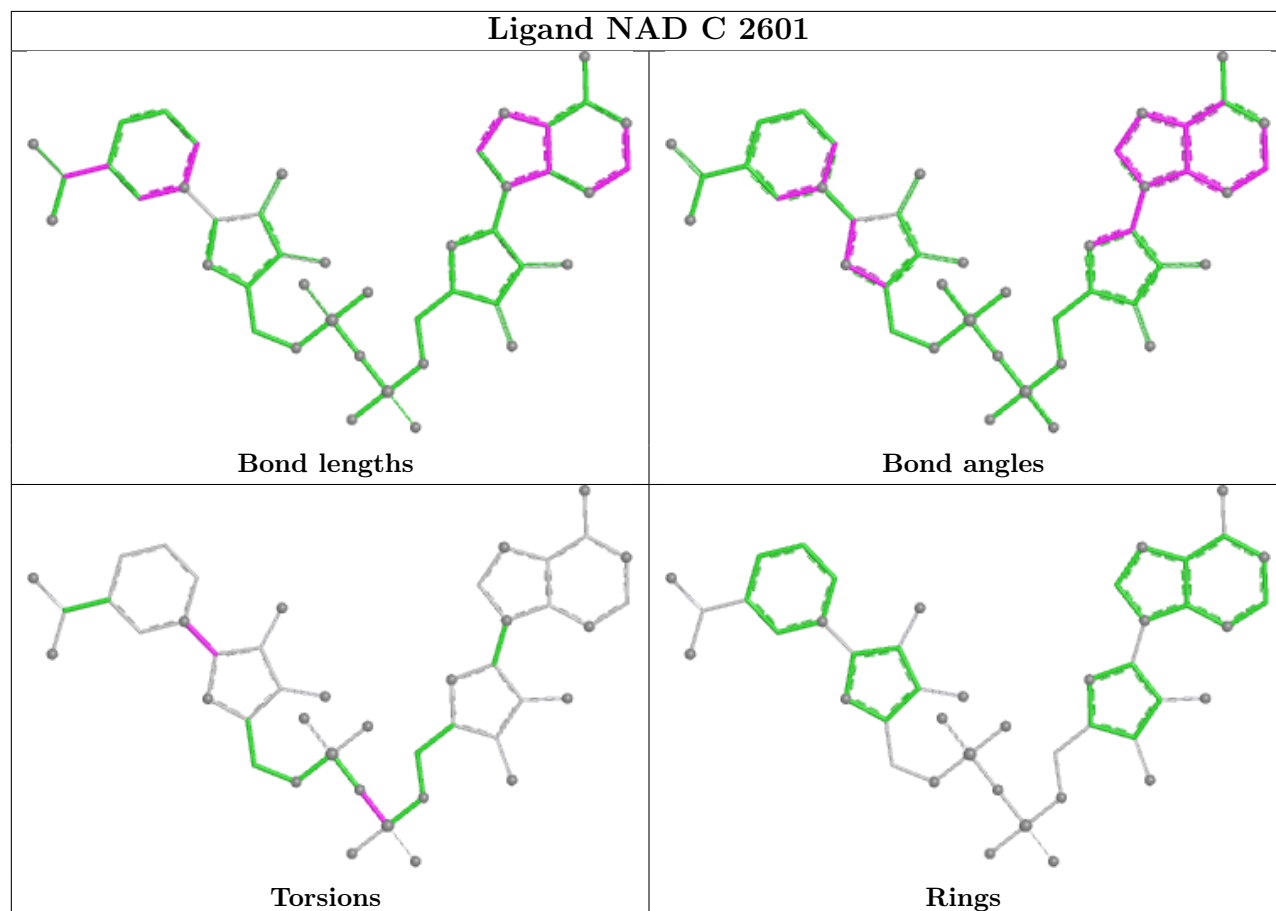
There are no ring outliers.

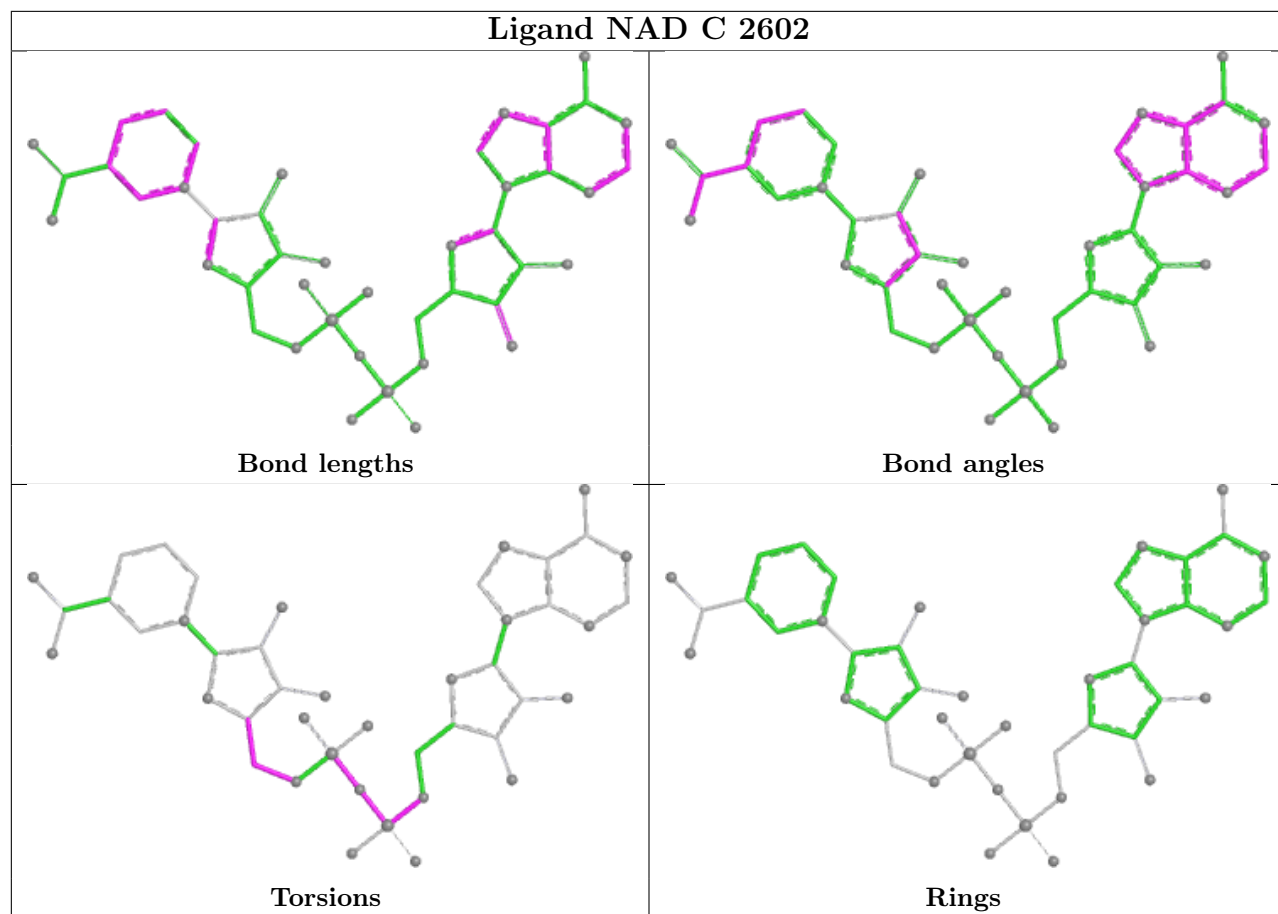
6 monomers are involved in 9 short contacts:

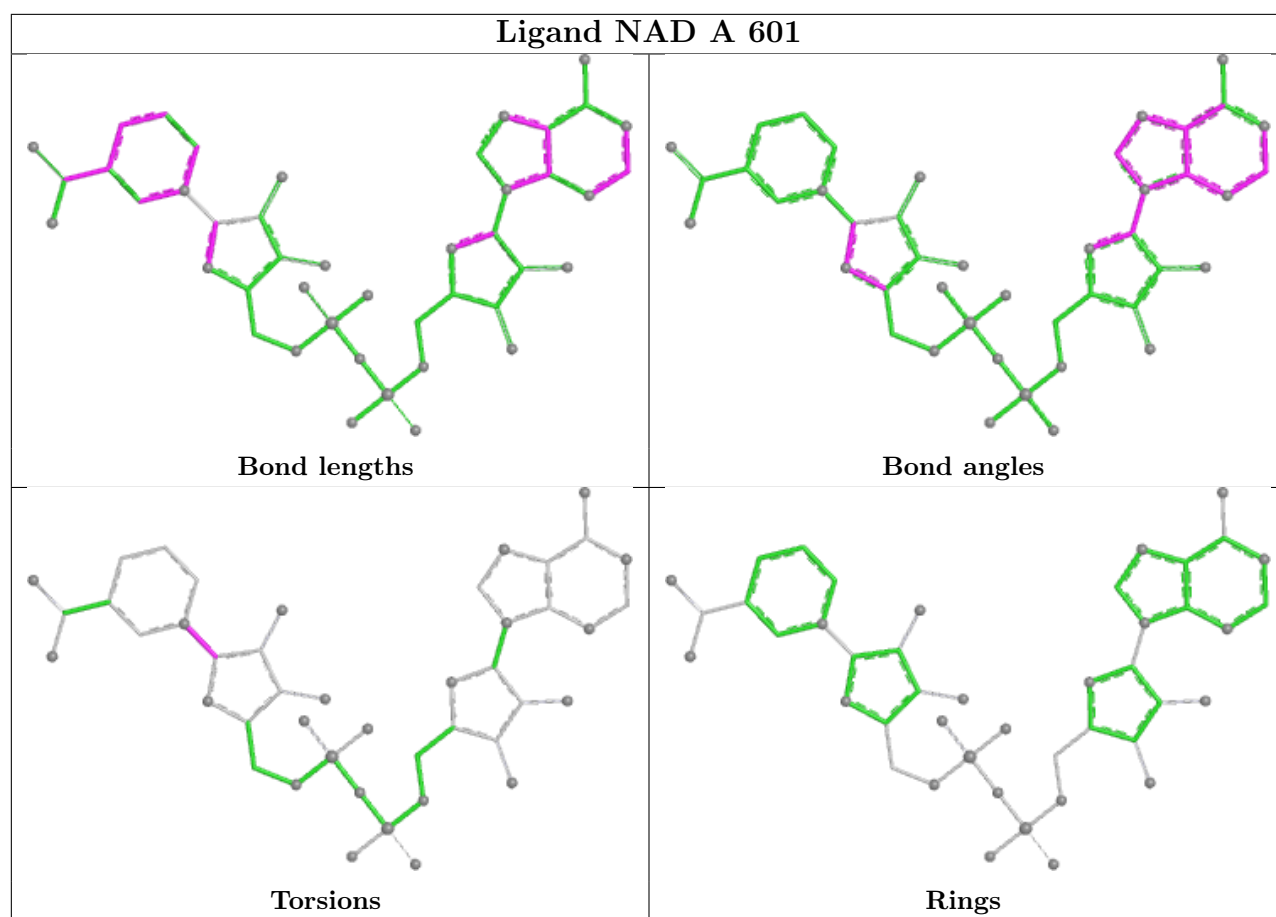
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2601	NAD	1	0
4	C	2602	NAD	1	0
4	A	601	NAD	2	0
4	D	3602	NAD	1	0
4	B	1601	NAD	3	0
2	D	3603	OXL	1	0

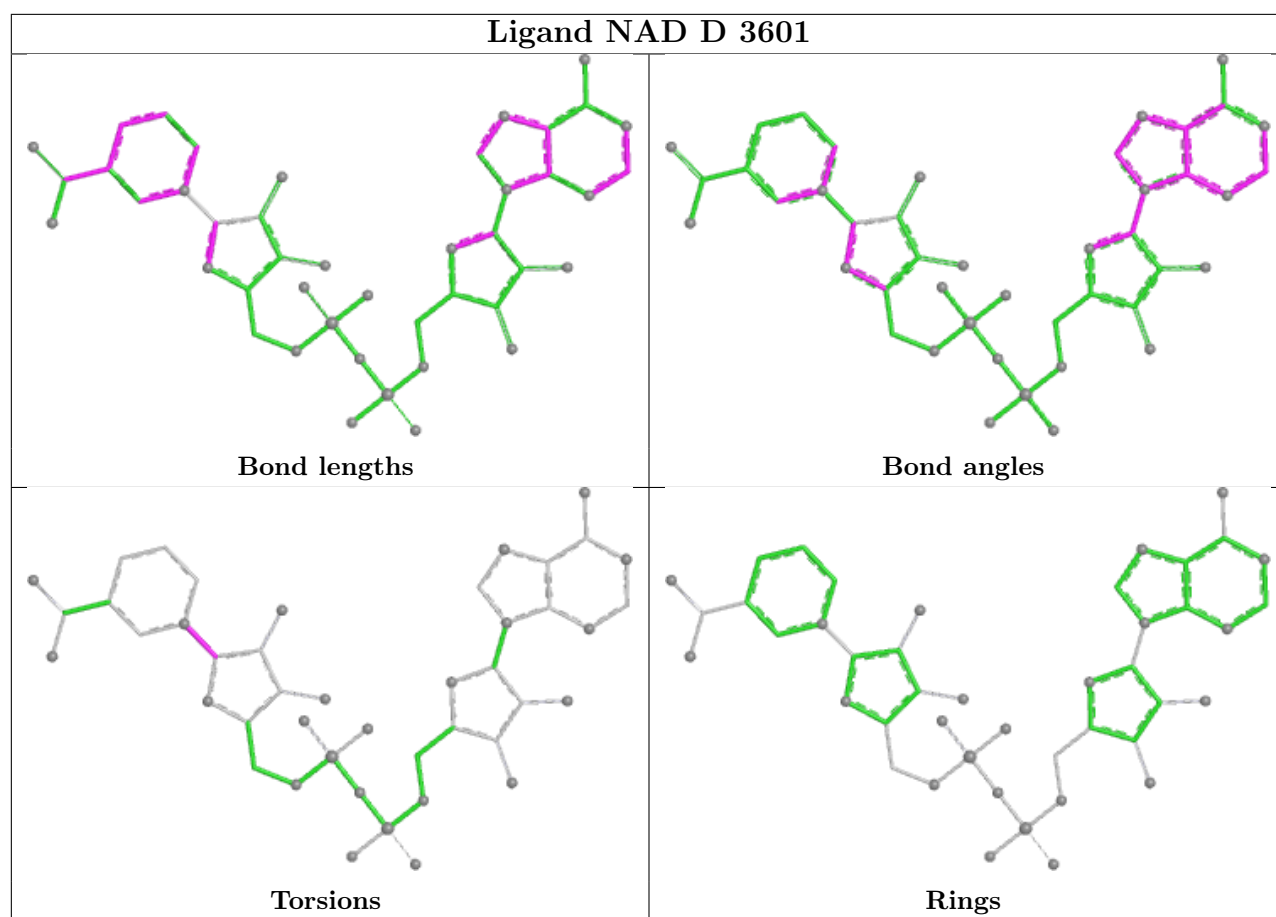
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

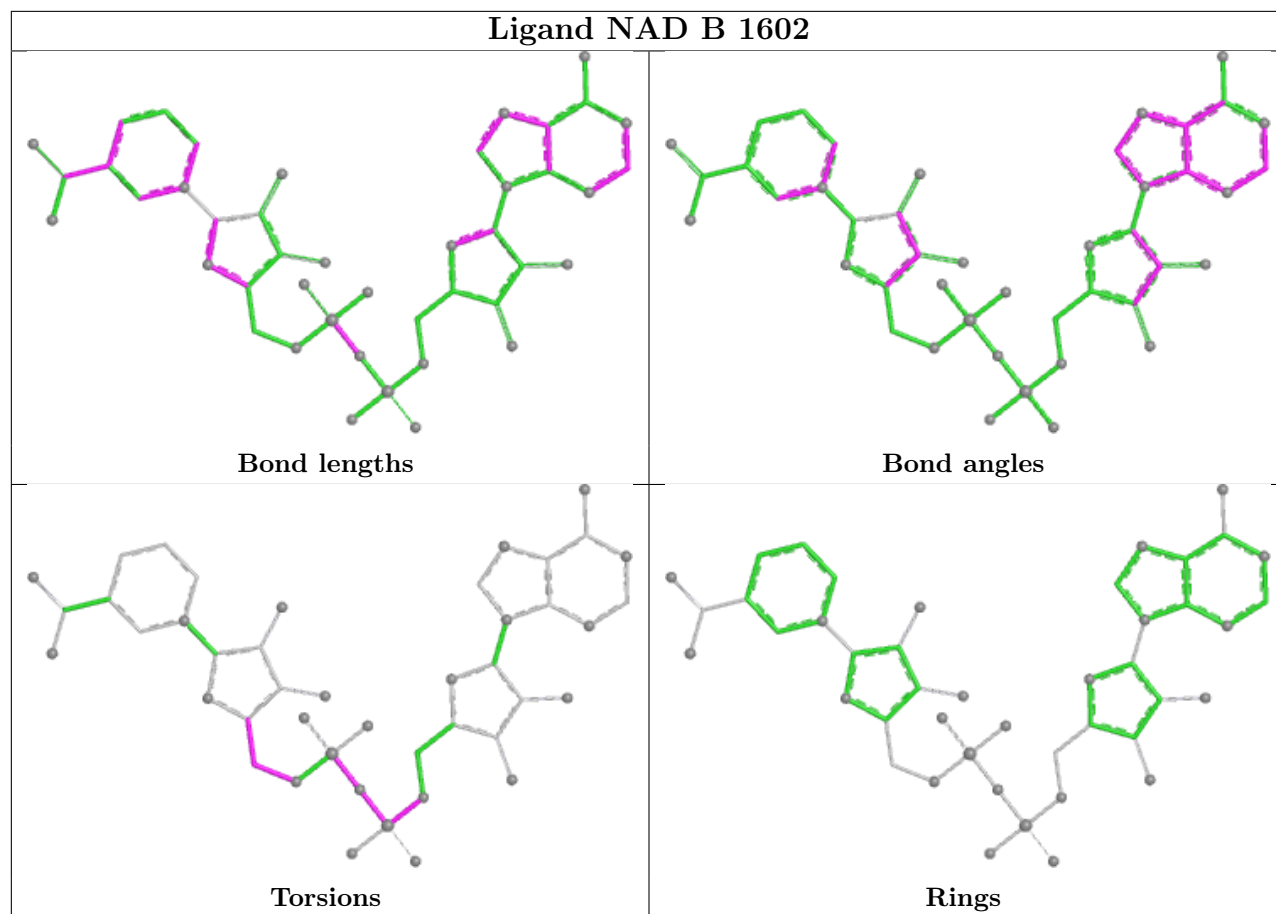
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

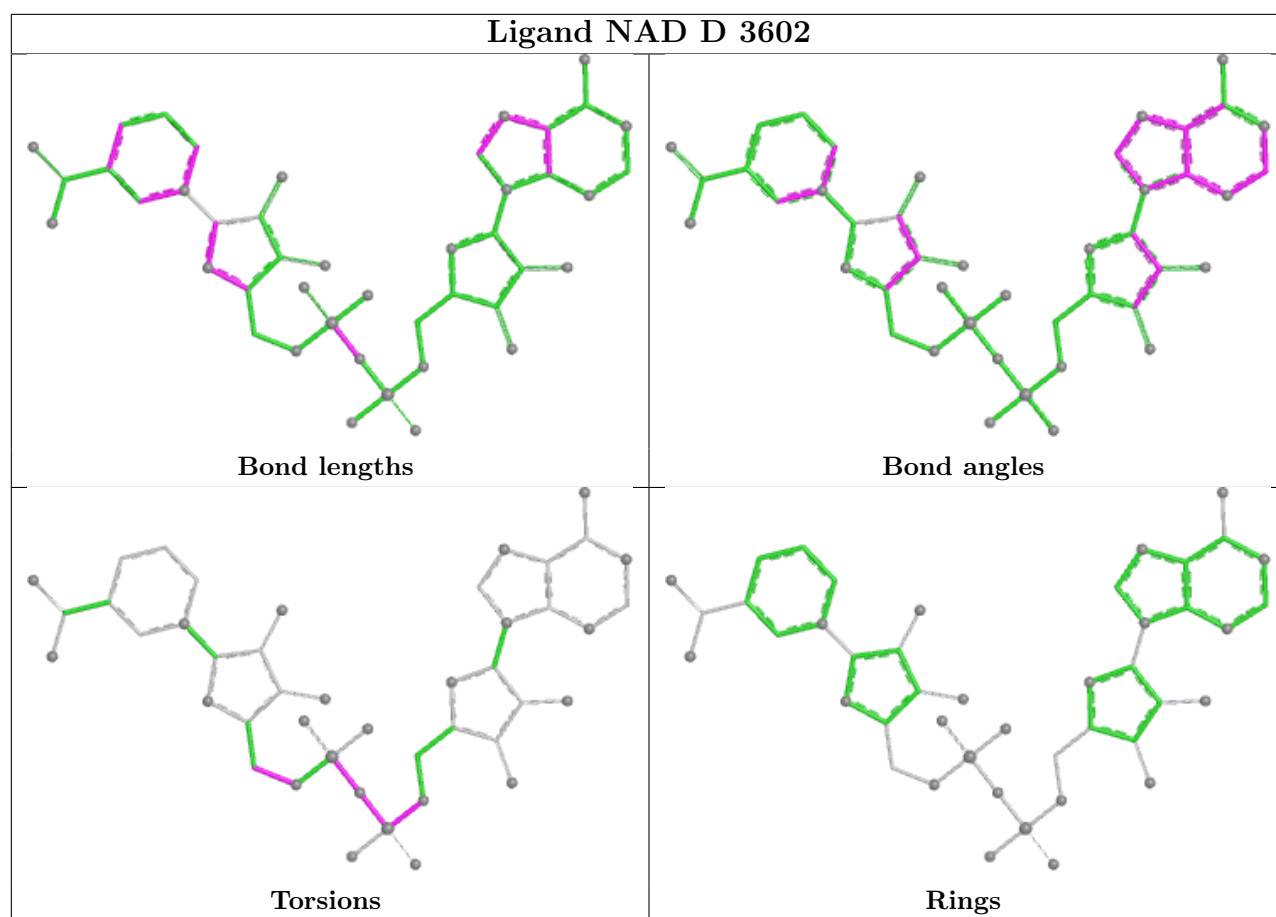


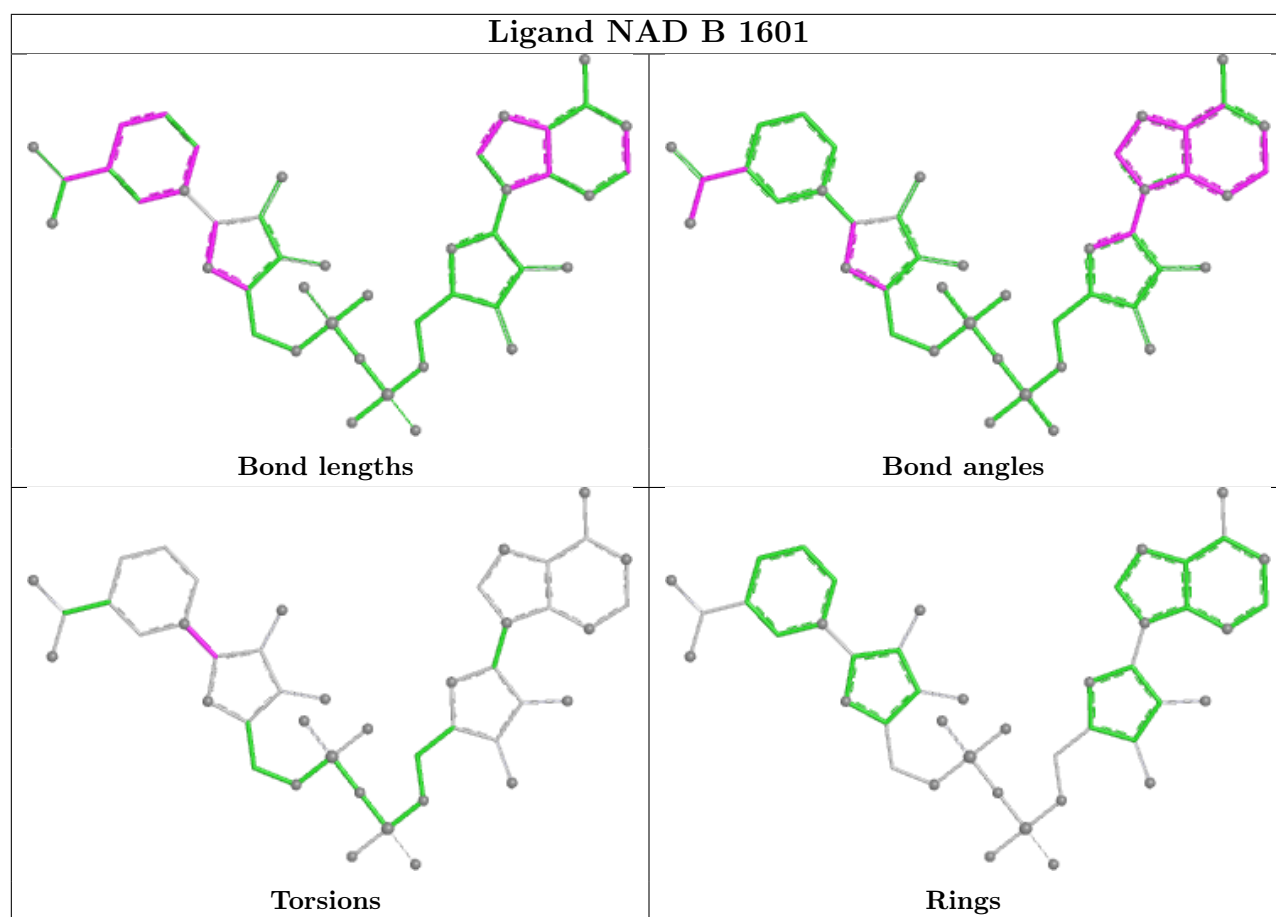


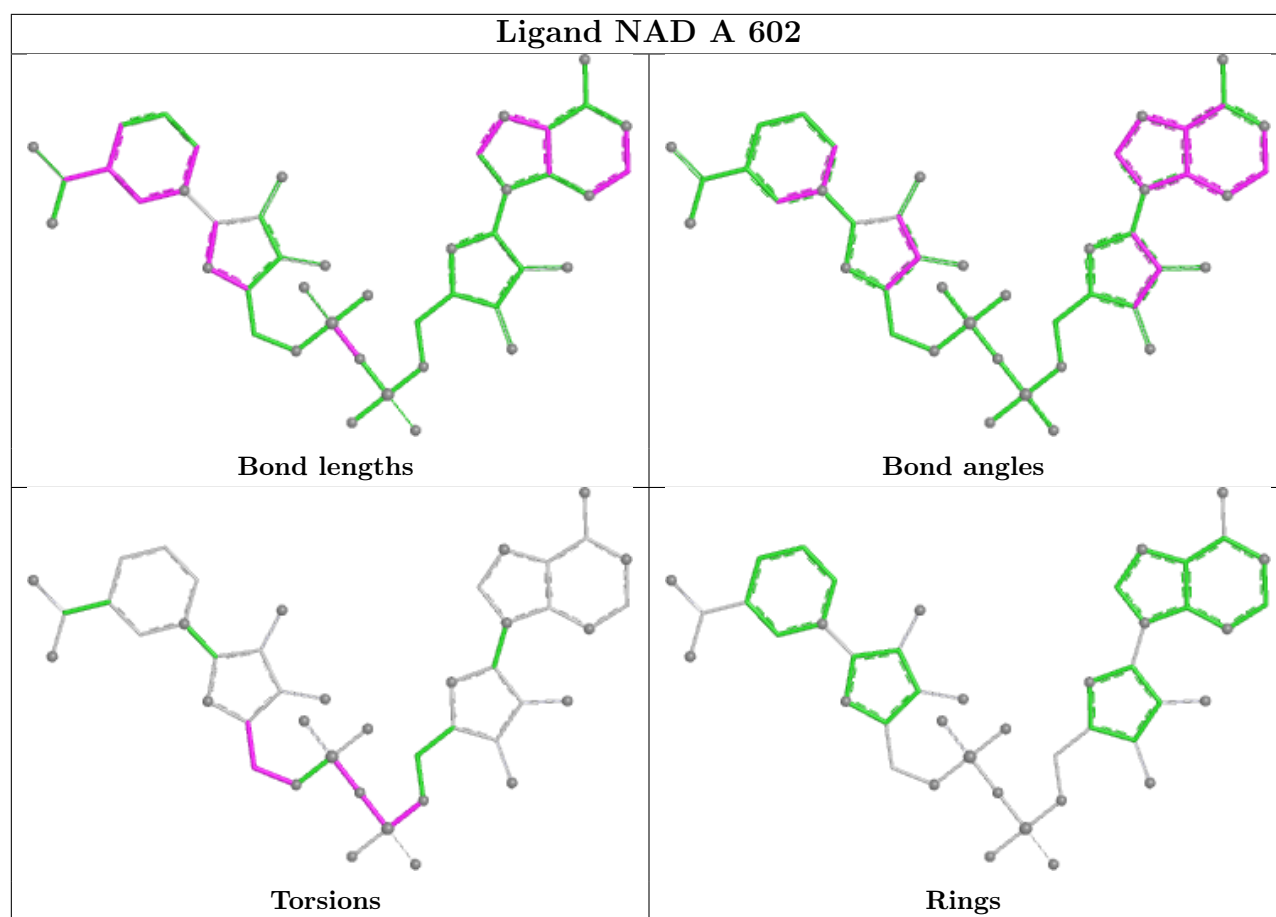












5.7 Other polymers [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.