



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 11:20 am BST

PDB ID : 1DO8
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 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
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) : 2.11

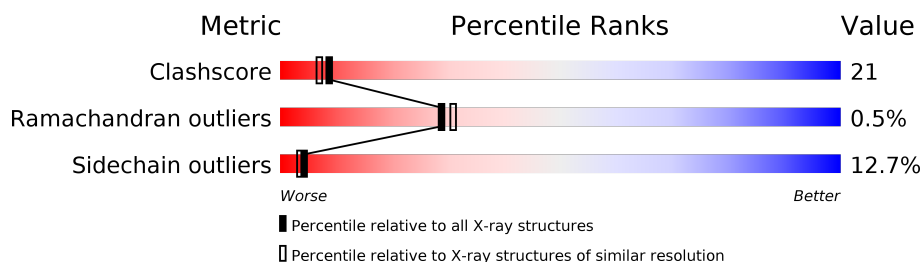
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	564	
1	B	564	
1	C	564	
1	D	564	

2 Entry composition [i](#)

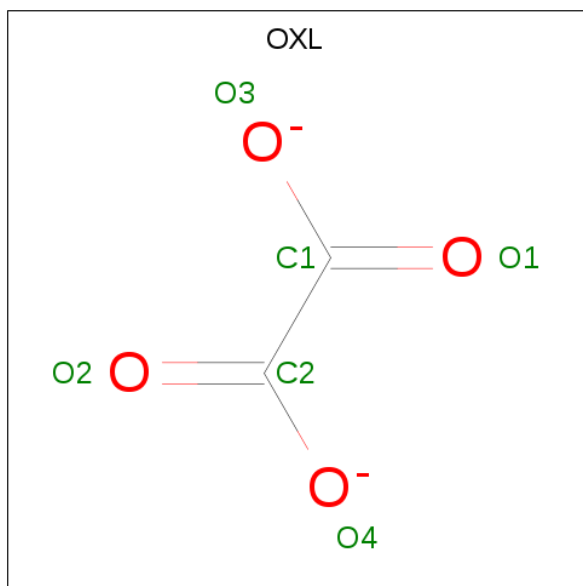
There are 5 unique types of molecules in this entry. The entry contains 18807 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: OXL) (formula: C₂O₄).



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		

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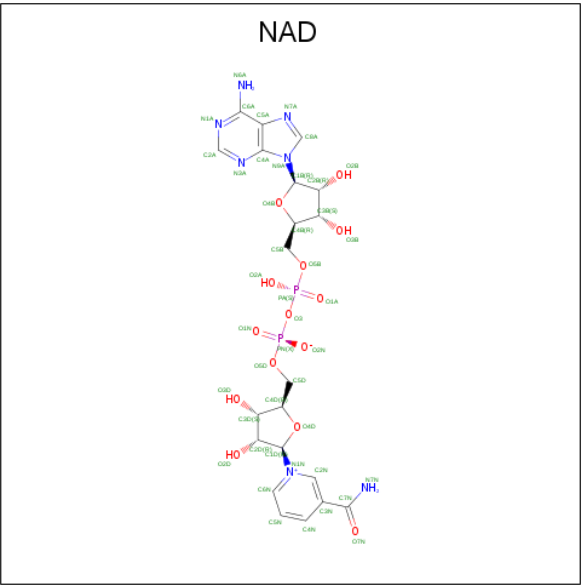
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			6	2	4		
2	D	1	Total	C	O	0	0
			6	2	4		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



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

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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.

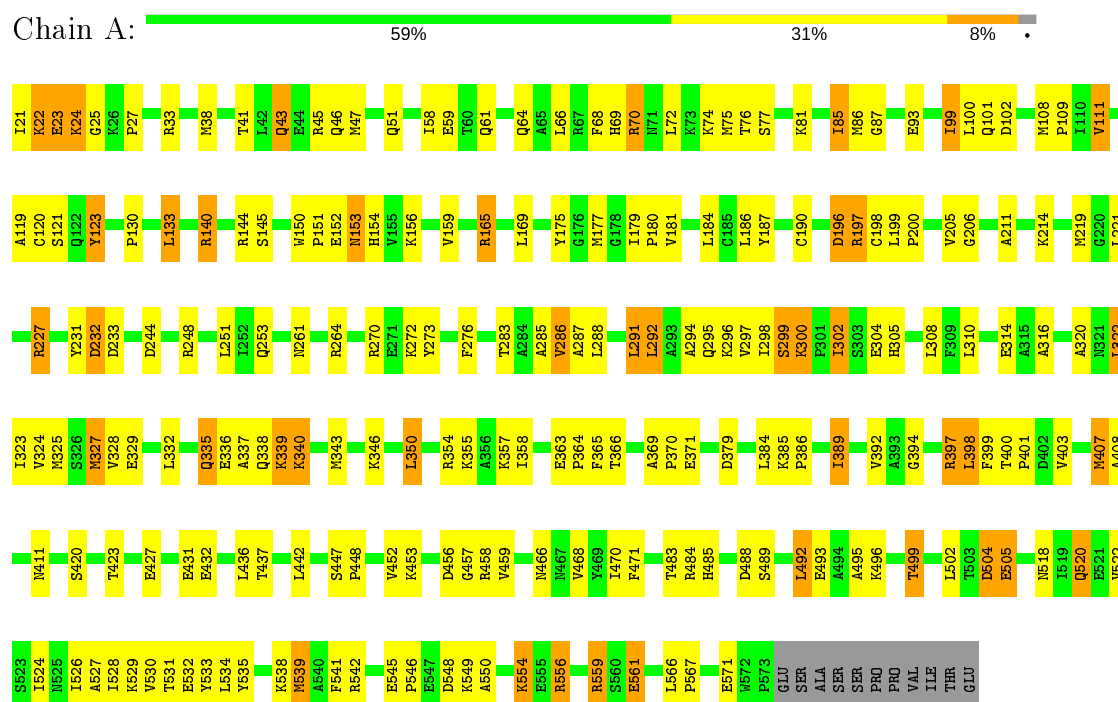
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	239	Total 239	O 239	0	0
5	B	199	Total 199	O 199	0	0
5	C	275	Total 275	O 275	0	0
5	D	246	Total 246	O 246	0	0

3 Residue-property plots

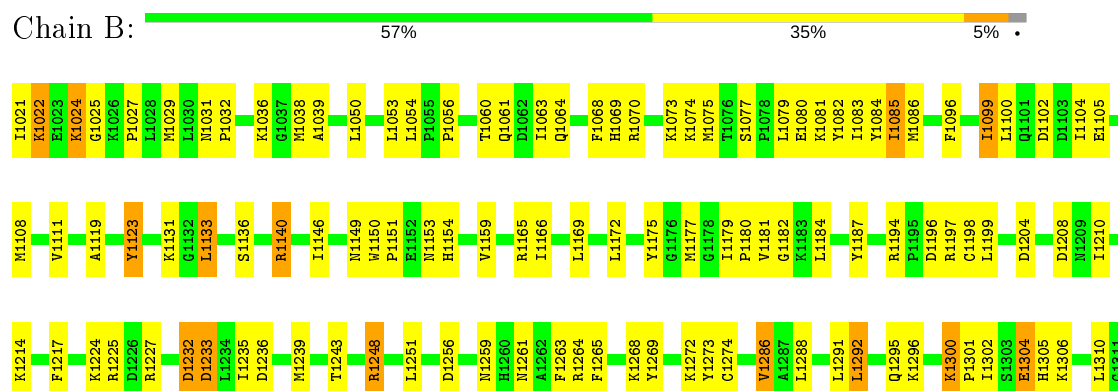
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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.

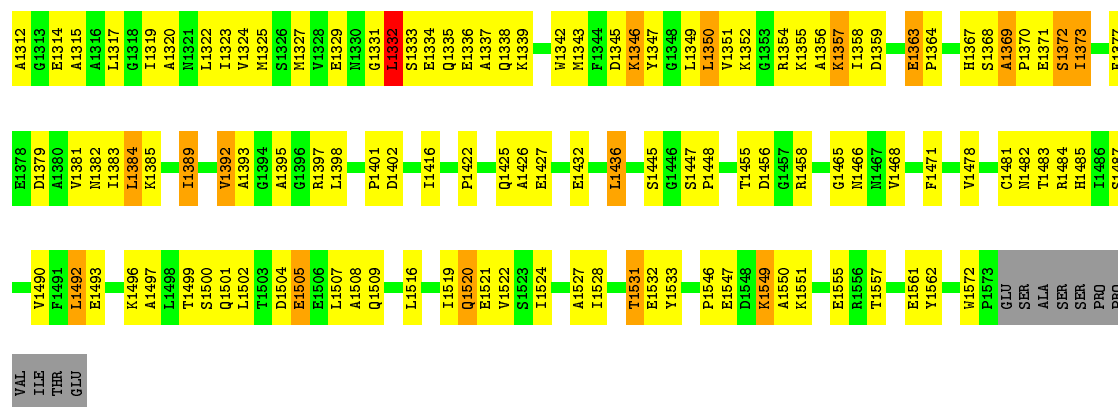
Note EDS was not executed.

• Molecule 1: MALIC ENZYME

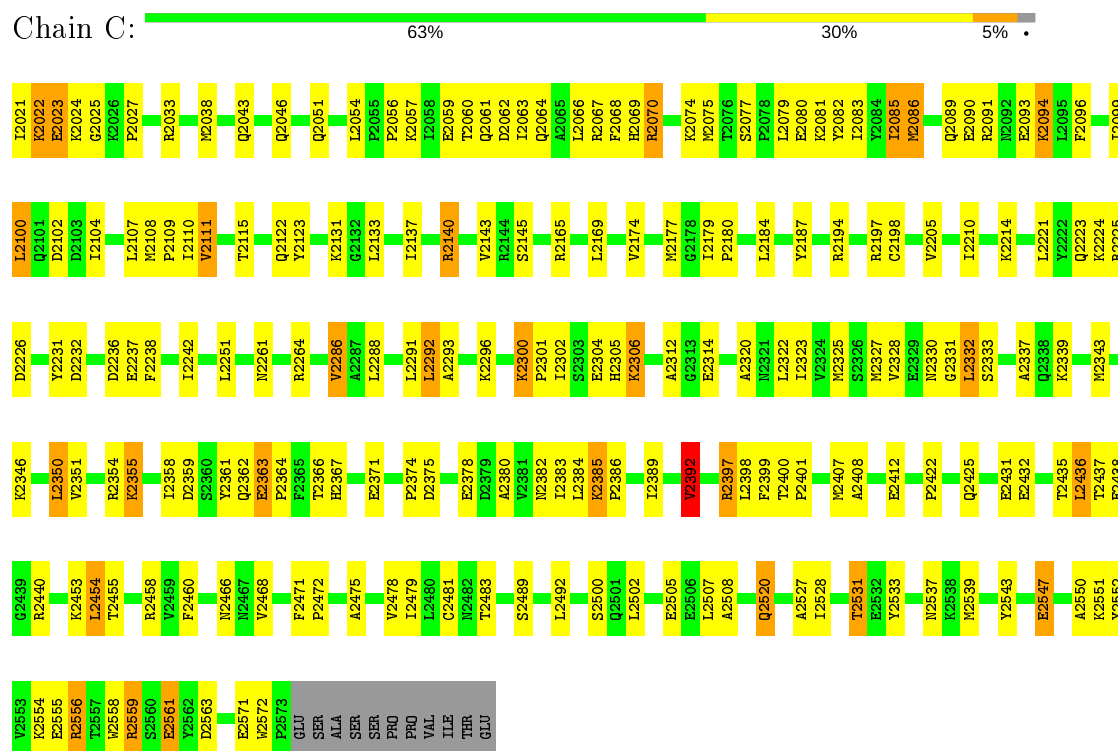


• Molecule 1: MALIC ENZYME

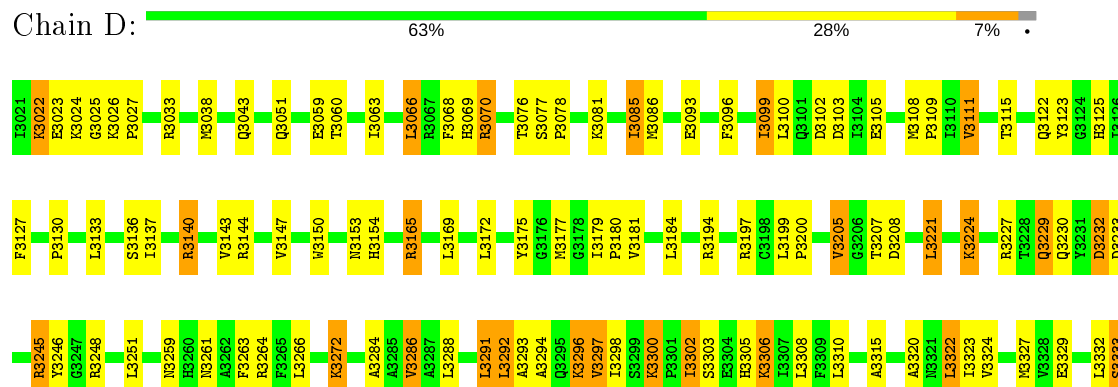




• Molecule 1: MALIC ENZYME



• Molecule 1: MALIC ENZYME



T3531	E3426	E3334
E3532	E3427	Q3335
		E3336
N3537	E3431	A3337
K3538		Q3338
K3539	L3436	K3339
A3540		I3340
	R3440	
E3545	C3441	M3343
P3546	L3442	
E3547		K3346
D3548		
K3549	V3452	L3350
A3550	K3453	T3351
K3551		R3352
	R3458	K3353
		R3354
E3555	T3461	K3355
R3556		
T3557	N3467	T3358
N3558	V3468	
R3559	V3469	E3363
	I3470	P3364
E3571	F3471	F3365
K3572	P3472	T3366
P3573	G3473	
GLU	V3474	
SER		A3369
ALA	V3478	P3370
SER		E3371
SER	G3481	S3372
PRO	N3482	I3373
PRO	T3483	
VAL	R3484	A3380
ILE	H3485	
THR		L3384
GLU	S3489	K3385
		P3386
	L3492	
		T3389
	K3496	T3390
		Q3391
	L3502	V3392
	L3507	R3397
		L3398
	R3511	F3399
	L3512	T3400
		P3401
	L3516	D3402
	A3517	V3403
	N3518	
	I3519	M3407
	Q3520	
	E3521	E3412
		R3413
		P3414
	I3526	
	A3527	
	I3528	
	K3529	F3417
	V3530	Q3425

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: OXL, MN, 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	0.37	0/4447	0.61	0/5998
1	B	0.37	0/4447	0.61	0/5998
1	C	0.38	0/4447	0.61	0/5998
1	D	0.38	0/4447	0.60	0/5998
All	All	0.37	0/17788	0.61	0/23992

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	4367	0	4407	203	0
1	B	4367	0	4407	229	0
1	C	4367	0	4407	141	0
1	D	4367	0	4407	179	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	14	0
5	B	199	0	0	30	0
5	C	275	0	0	18	0
5	D	246	0	0	12	0
All	All	18807	0	17836	731	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 731 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 [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	551/564 (98%)	530 (96%)	19 (3%)	2 (0%)	34 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	551/564 (98%)	522 (95%)	26 (5%)	3 (0%)	29	31
1	C	551/564 (98%)	530 (96%)	17 (3%)	4 (1%)	22	22
1	D	551/564 (98%)	528 (96%)	20 (4%)	3 (0%)	29	31
All	All	2204/2256 (98%)	2110 (96%)	82 (4%)	12 (0%)	29	31

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%)	406 (87%)	63 (13%)	4	3
1	B	469/465 (101%)	412 (88%)	57 (12%)	5	4
1	C	469/465 (101%)	409 (87%)	60 (13%)	4	3
1	D	469/465 (101%)	410 (87%)	59 (13%)	4	3
All	All	1876/1860 (101%)	1637 (87%)	239 (13%)	4	3

5 of 239 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1502	LEU
1	C	2122	GLN
1	D	3358	ILE
1	B	1507	LEU
1	C	2022	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1425	GLN
1	C	2064	GLN
1	D	3482	ASN
1	B	1520	GLN
1	C	2069	HIS

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](#)

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	B	1602	-	42,48,48	2.18	11 (26%)	50,73,73	1.42	6 (12%)
4	NAD	D	3602	-	42,48,48	2.08	9 (21%)	50,73,73	1.51	6 (12%)
2	OXL	D	3603	3	0,5,5	0.00	-	0,6,6	0.00	-
2	OXL	B	1603	3	0,5,5	0.00	-	0,6,6	0.00	-
4	NAD	C	2602	-	42,48,48	2.79	12 (28%)	50,73,73	1.56	7 (14%)
2	OXL	C	2603	3	0,5,5	0.00	-	0,6,6	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OXL	A	603	3	0,5,5	0.00	-	0,6,6	0.00	-
4	NAD	D	3601	-	42,48,48	2.04	11 (26%)	50,73,73	1.29	4 (8%)
4	NAD	A	602	-	42,48,48	2.19	13 (30%)	50,73,73	1.48	6 (12%)
4	NAD	C	2601	-	42,48,48	1.87	9 (21%)	50,73,73	1.29	4 (8%)
4	NAD	A	601	-	42,48,48	2.04	12 (28%)	50,73,73	1.26	3 (6%)
4	NAD	B	1601	-	42,48,48	1.94	13 (30%)	50,73,73	1.36	5 (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
4	NAD	B	1602	-	-	6/26/62/62	0/5/5/5
4	NAD	D	3602	-	-	6/26/62/62	0/5/5/5
2	OXL	D	3603	3	-	0/0/4/4	-
2	OXL	B	1603	3	-	0/0/4/4	-
4	NAD	C	2602	-	-	7/26/62/62	0/5/5/5
2	OXL	C	2603	3	-	0/0/4/4	-
2	OXL	A	603	3	-	0/0/4/4	-
4	NAD	D	3601	-	-	2/26/62/62	0/5/5/5
4	NAD	A	602	-	-	7/26/62/62	0/5/5/5
4	NAD	C	2601	-	-	2/26/62/62	0/5/5/5
4	NAD	A	601	-	-	2/26/62/62	0/5/5/5
4	NAD	B	1601	-	-	2/26/62/62	0/5/5/5

The worst 5 of 90 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2602	NAD	C2N-N1N	9.85	1.47	1.35
4	A	602	NAD	C2N-N1N	7.88	1.44	1.35
4	B	1602	NAD	C2N-N1N	7.15	1.43	1.35
4	B	1602	NAD	O4D-C1D	7.15	1.51	1.41
4	A	601	NAD	C2N-N1N	6.55	1.42	1.35

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3602	NAD	N3A-C2A-N1A	-5.10	120.70	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	NAD	N3A-C2A-N1A	-5.06	120.76	128.68
4	B	1601	NAD	N3A-C2A-N1A	-5.06	120.77	128.68
4	C	2601	NAD	N3A-C2A-N1A	-5.05	120.79	128.68
4	B	1602	NAD	N3A-C2A-N1A	-5.02	120.83	128.68

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

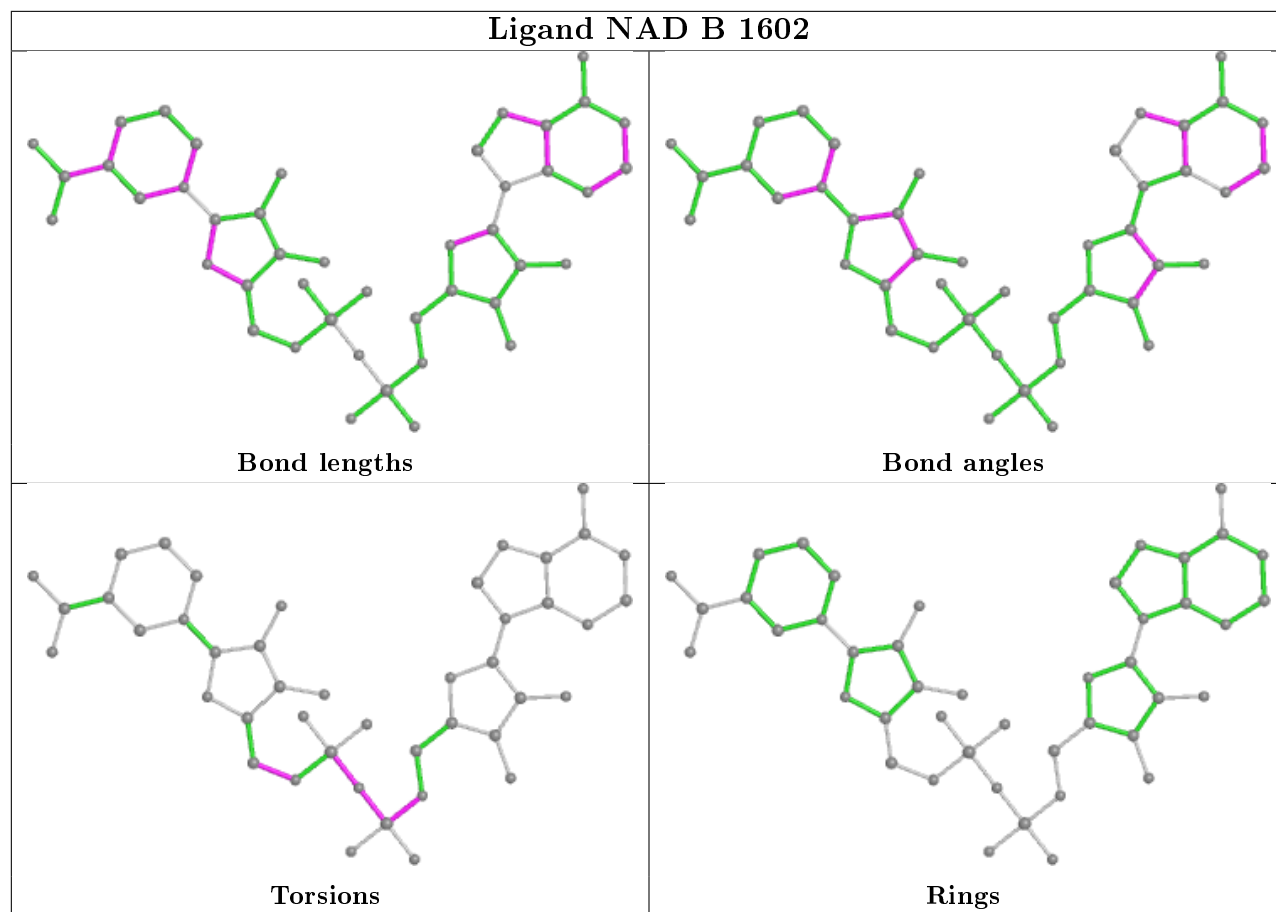
Mol	Chain	Res	Type	Atoms
4	B	1602	NAD	C5B-O5B-PA-O2A
4	B	1602	NAD	C5B-O5B-PA-O3
4	D	3602	NAD	C5B-O5B-PA-O1A
4	D	3602	NAD	C5B-O5B-PA-O2A
4	C	2602	NAD	C5B-O5B-PA-O2A

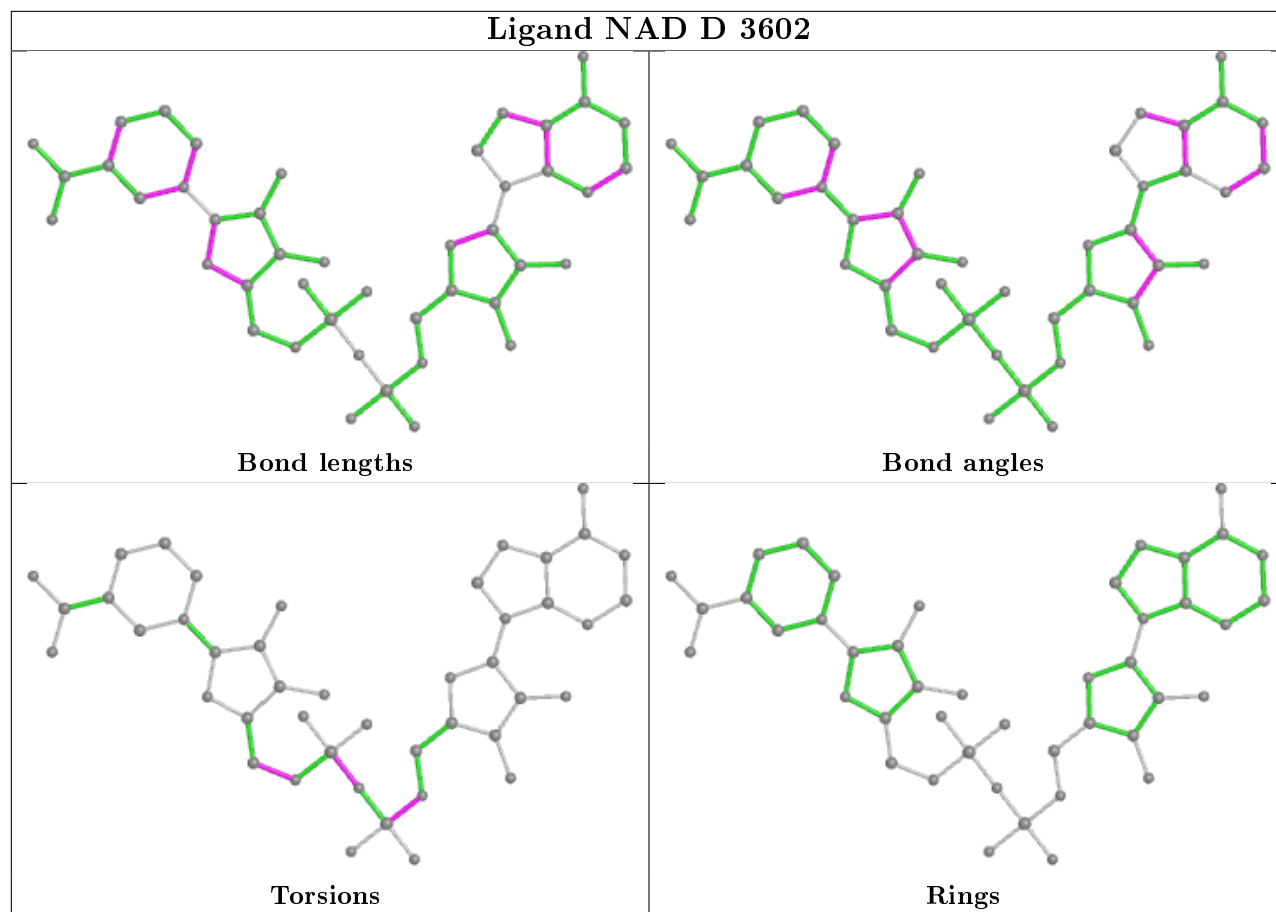
There are no ring outliers.

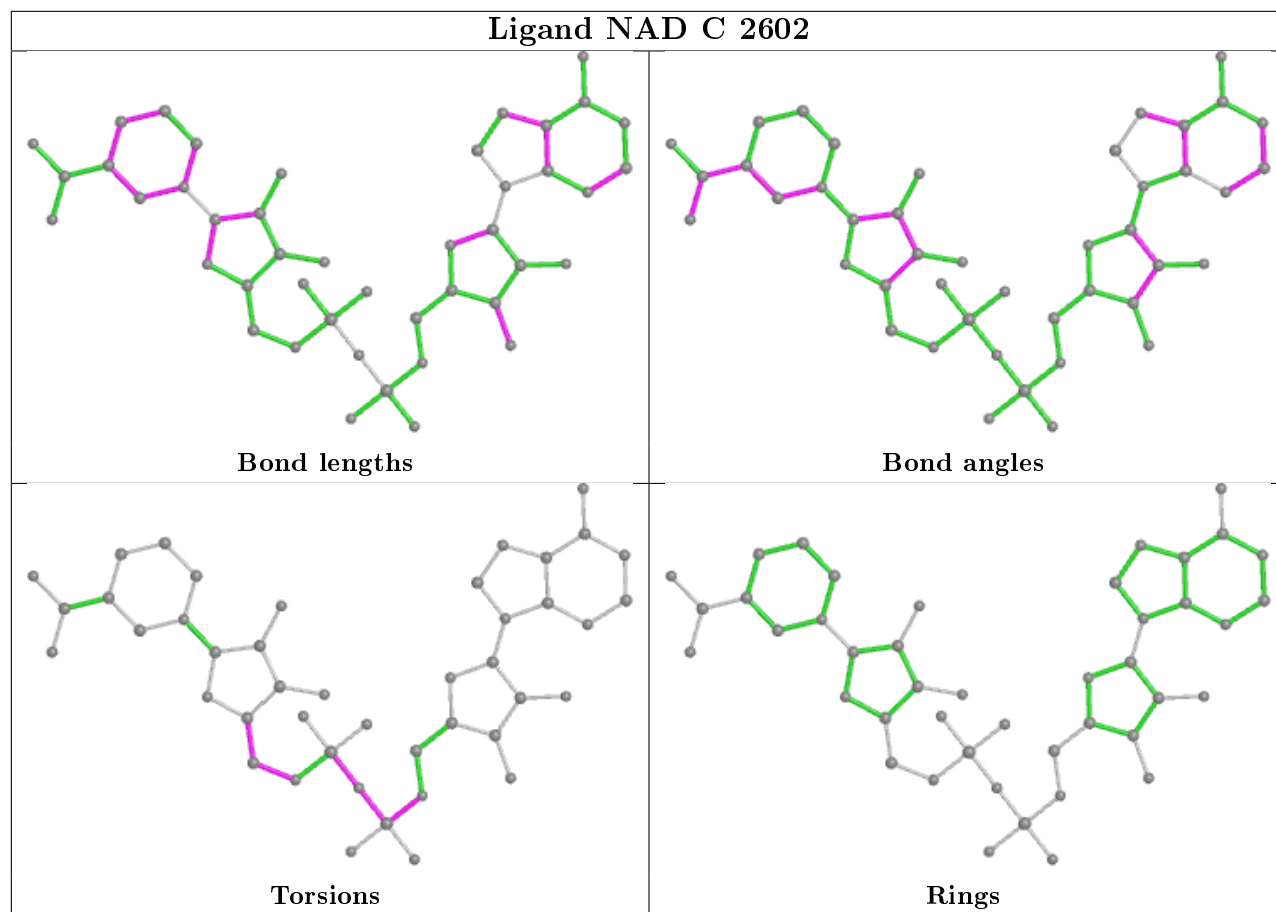
6 monomers are involved in 9 short contacts:

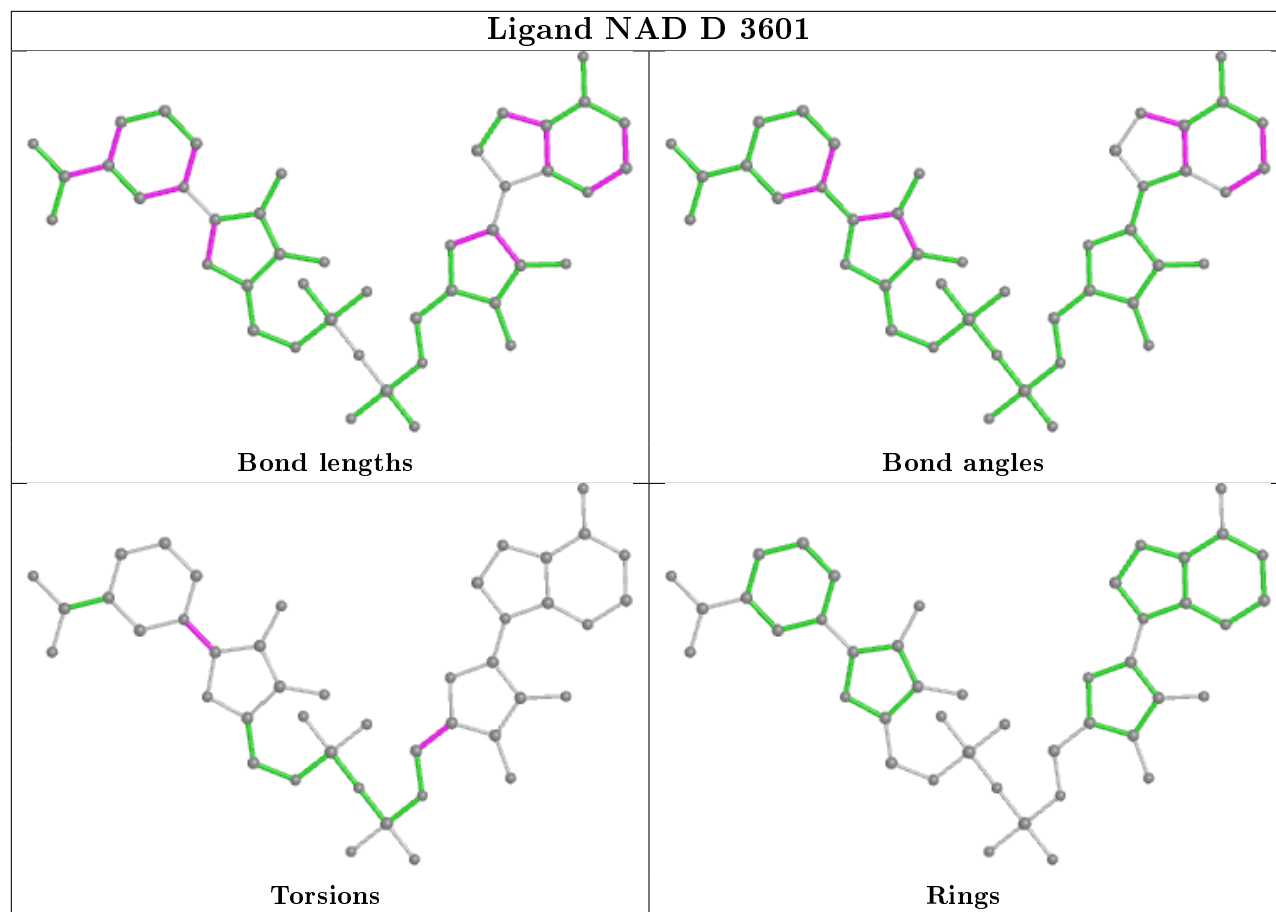
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	3602	NAD	1	0
2	D	3603	OXL	1	0
4	C	2602	NAD	1	0
4	C	2601	NAD	1	0
4	A	601	NAD	2	0
4	B	1601	NAD	3	0

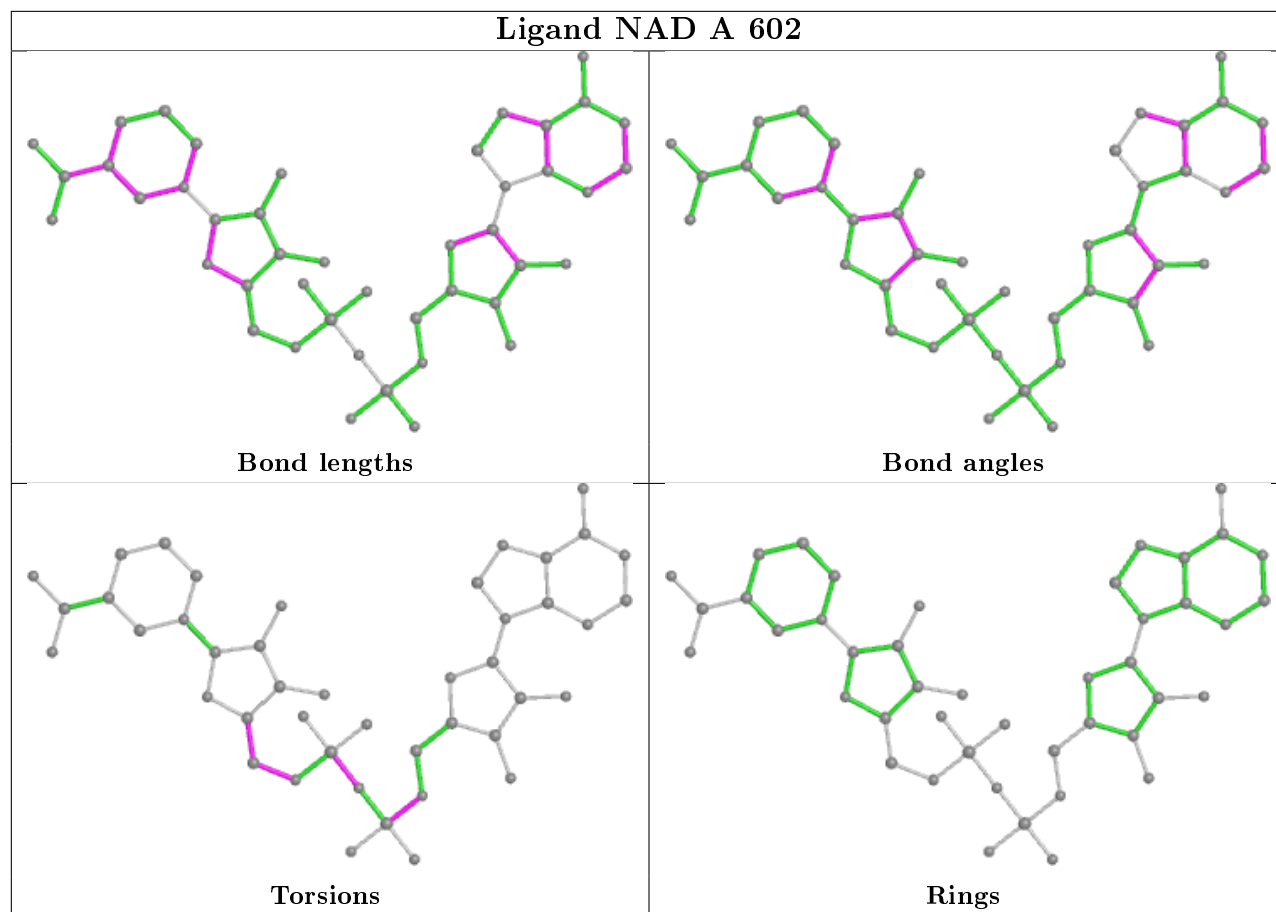
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

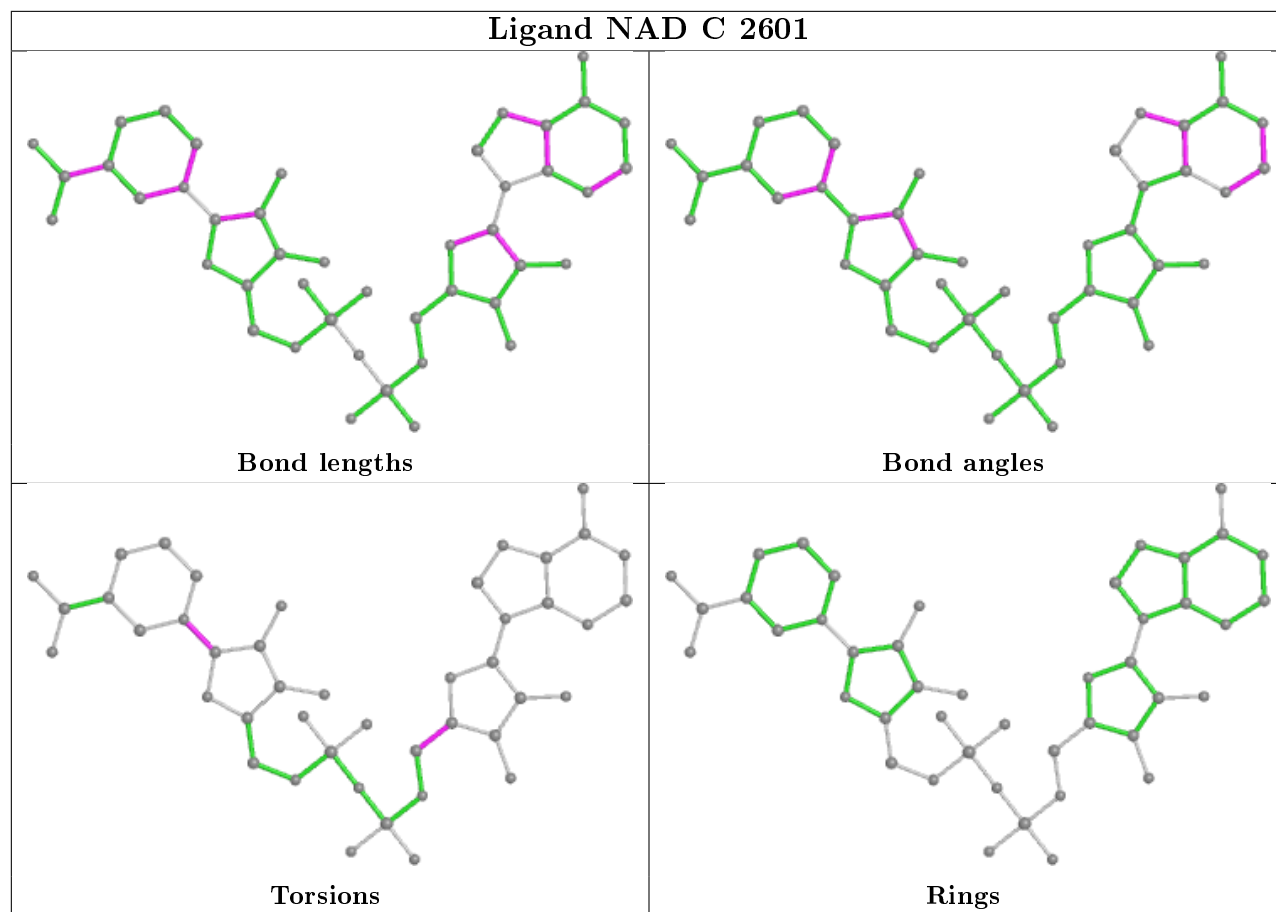


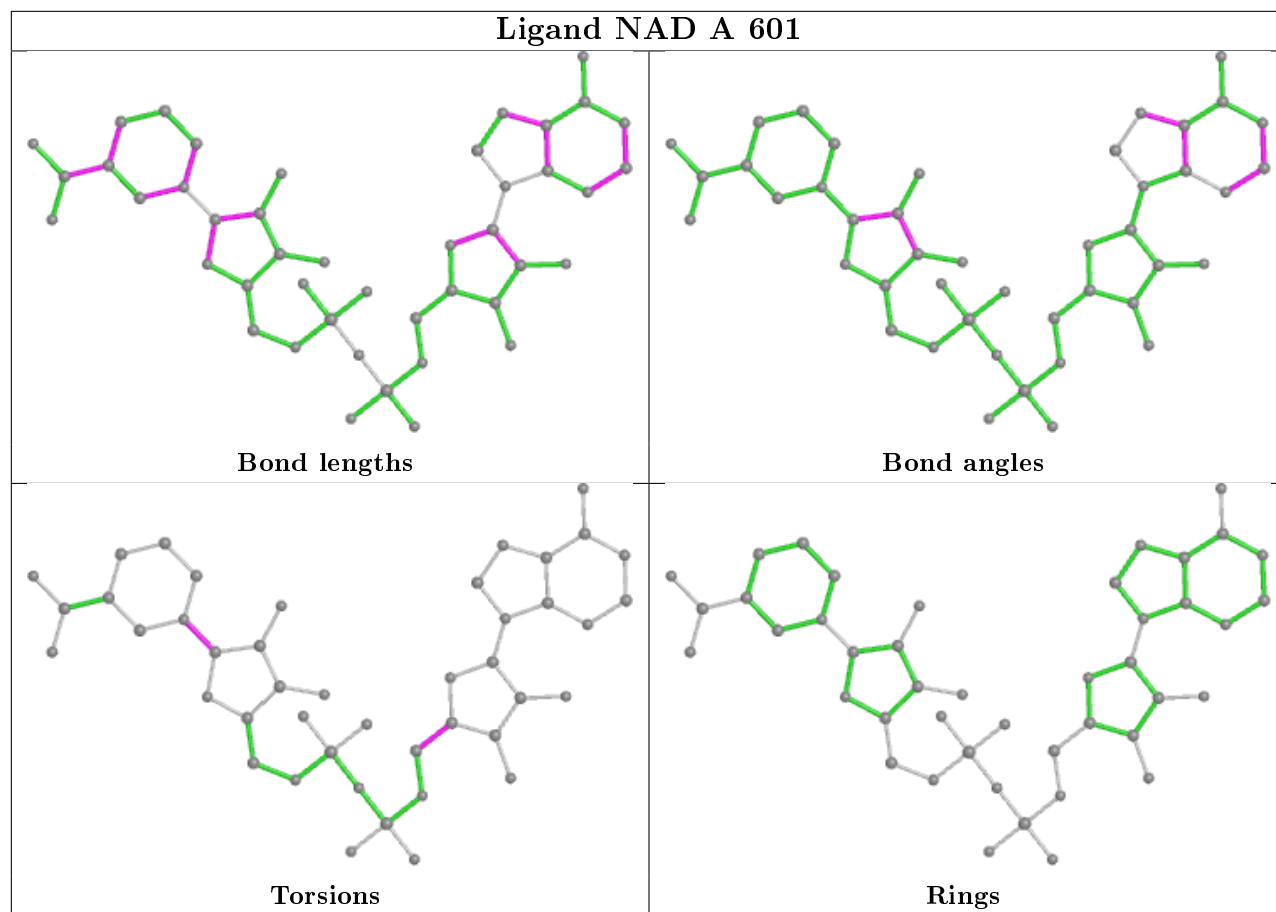


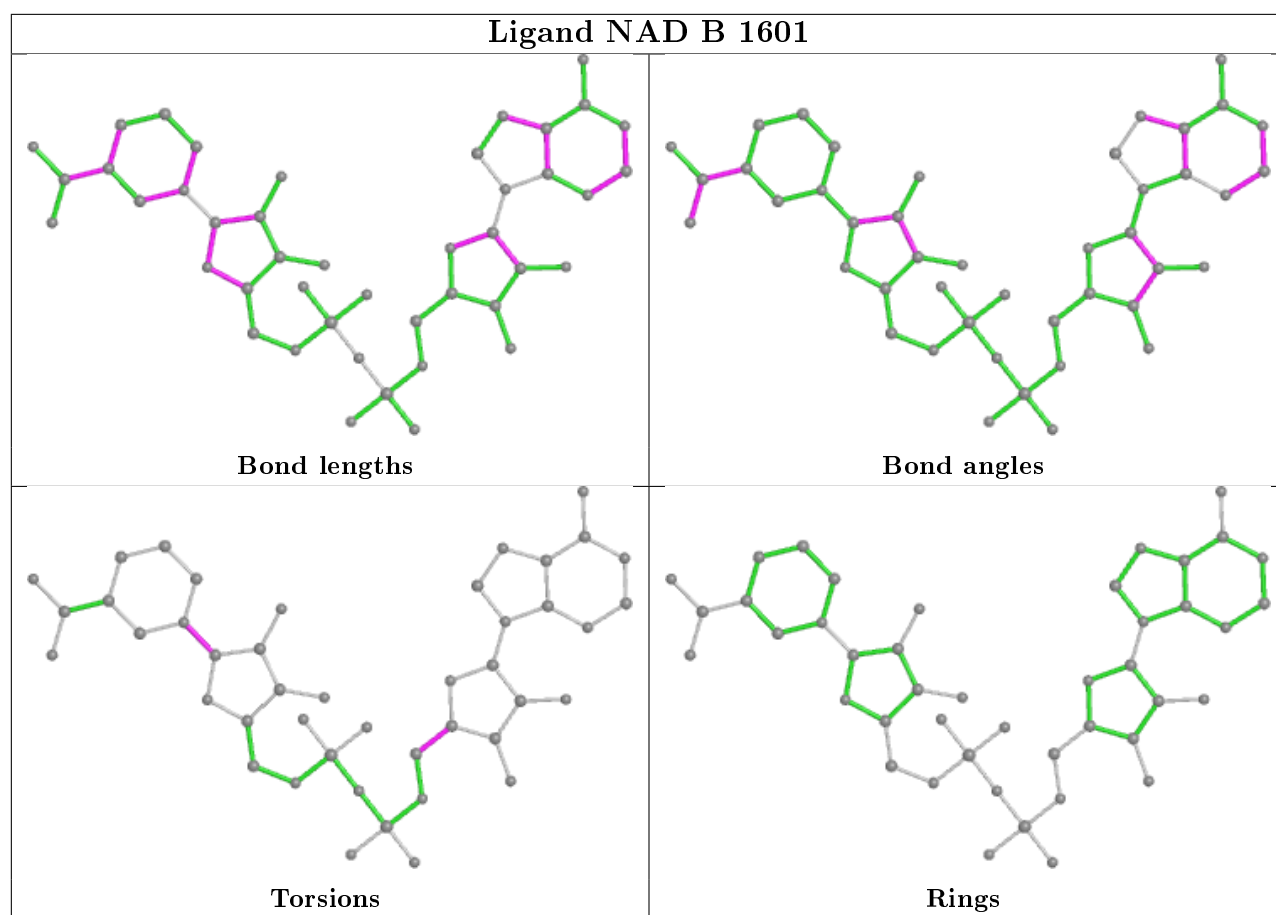












5.7 Other polymers [i](#)

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.