



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 2, 2026 – 03:23 AM UTC

PDB ID : 1PJL / pdb_00001pjl
Title : Crystal structure of human m-NAD-ME in ternary complex with NAD and Lu3+
Authors : Yang, Z.; Batra, R.; Floyd, D.L.; Hung, H.-C.; Chang, G.-G.; Tong, L.
Deposited on : 2003-06-03
Resolution : 2.90 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

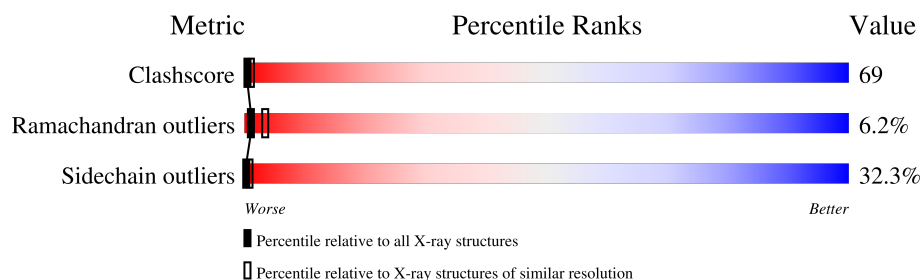
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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	584	19% 47% 26% • 6%
1	B	584	17% 47% 27% • 6%
1	C	584	20% 46% 26% • 6%
1	D	584	17% 48% 26% • 6%
1	E	584	20% 50% 22% • 6%
1	F	584	21% 49% 23% • 6%
1	G	584	15% 48% 27% • 6%
1	H	584	19% 48% 26% • 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 35527 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 NAD-dependent malic enzyme, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	Se	0	0	0
			4344	2781	738	802	9	14			
1	B	551	Total	C	N	O	S	Se	0	0	0
			4344	2781	738	802	9	14			
1	C	551	Total	C	N	O	S	Se	0	0	0
			4344	2781	738	802	9	14			
1	D	551	Total	C	N	O	S	Se	0	0	0
			4344	2781	738	802	9	14			
1	E	551	Total	C	N	O	S	Se	0	0	0
			4344	2781	738	802	9	14			
1	F	551	Total	C	N	O	S	Se	0	0	0
			4344	2781	738	802	9	14			
1	G	551	Total	C	N	O	S	Se	0	0	0
			4344	2781	738	802	9	14			
1	H	551	Total	C	N	O	S	Se	0	0	0
			4344	2781	738	802	9	14			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P23368
A	29	MSE	MET	modified residue	UNP P23368
A	38	MSE	MET	modified residue	UNP P23368
A	47	MSE	MET	modified residue	UNP P23368
A	75	MSE	MET	modified residue	UNP P23368
A	86	MSE	MET	modified residue	UNP P23368
A	108	MSE	MET	modified residue	UNP P23368
A	177	MSE	MET	modified residue	UNP P23368
A	219	MSE	MET	modified residue	UNP P23368
A	239	MSE	MET	modified residue	UNP P23368
A	325	MSE	MET	modified residue	UNP P23368
A	327	MSE	MET	modified residue	UNP P23368
A	343	MSE	MET	modified residue	UNP P23368

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Chain	Residue	Modelled	Actual	Comment	Reference
A	407	MSE	MET	modified residue	UNP P23368
A	539	MSE	MET	modified residue	UNP P23368
B	1001	MSE	MET	modified residue	UNP P23368
B	1029	MSE	MET	modified residue	UNP P23368
B	1038	MSE	MET	modified residue	UNP P23368
B	1047	MSE	MET	modified residue	UNP P23368
B	1075	MSE	MET	modified residue	UNP P23368
B	1086	MSE	MET	modified residue	UNP P23368
B	1108	MSE	MET	modified residue	UNP P23368
B	1177	MSE	MET	modified residue	UNP P23368
B	1219	MSE	MET	modified residue	UNP P23368
B	1239	MSE	MET	modified residue	UNP P23368
B	1325	MSE	MET	modified residue	UNP P23368
B	1327	MSE	MET	modified residue	UNP P23368
B	1343	MSE	MET	modified residue	UNP P23368
B	1407	MSE	MET	modified residue	UNP P23368
B	1539	MSE	MET	modified residue	UNP P23368
C	2001	MSE	MET	modified residue	UNP P23368
C	2029	MSE	MET	modified residue	UNP P23368
C	2038	MSE	MET	modified residue	UNP P23368
C	2047	MSE	MET	modified residue	UNP P23368
C	2075	MSE	MET	modified residue	UNP P23368
C	2086	MSE	MET	modified residue	UNP P23368
C	2108	MSE	MET	modified residue	UNP P23368
C	2177	MSE	MET	modified residue	UNP P23368
C	2219	MSE	MET	modified residue	UNP P23368
C	2239	MSE	MET	modified residue	UNP P23368
C	2325	MSE	MET	modified residue	UNP P23368
C	2327	MSE	MET	modified residue	UNP P23368
C	2343	MSE	MET	modified residue	UNP P23368
C	2407	MSE	MET	modified residue	UNP P23368
C	2539	MSE	MET	modified residue	UNP P23368
D	3001	MSE	MET	modified residue	UNP P23368
D	3029	MSE	MET	modified residue	UNP P23368
D	3038	MSE	MET	modified residue	UNP P23368
D	3047	MSE	MET	modified residue	UNP P23368
D	3075	MSE	MET	modified residue	UNP P23368
D	3086	MSE	MET	modified residue	UNP P23368
D	3108	MSE	MET	modified residue	UNP P23368
D	3177	MSE	MET	modified residue	UNP P23368
D	3219	MSE	MET	modified residue	UNP P23368
D	3239	MSE	MET	modified residue	UNP P23368

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Chain	Residue	Modelled	Actual	Comment	Reference
D	3325	MSE	MET	modified residue	UNP P23368
D	3327	MSE	MET	modified residue	UNP P23368
D	3343	MSE	MET	modified residue	UNP P23368
D	3407	MSE	MET	modified residue	UNP P23368
D	3539	MSE	MET	modified residue	UNP P23368
E	4001	MSE	MET	modified residue	UNP P23368
E	4029	MSE	MET	modified residue	UNP P23368
E	4038	MSE	MET	modified residue	UNP P23368
E	4047	MSE	MET	modified residue	UNP P23368
E	4075	MSE	MET	modified residue	UNP P23368
E	4086	MSE	MET	modified residue	UNP P23368
E	4108	MSE	MET	modified residue	UNP P23368
E	4177	MSE	MET	modified residue	UNP P23368
E	4219	MSE	MET	modified residue	UNP P23368
E	4239	MSE	MET	modified residue	UNP P23368
E	4325	MSE	MET	modified residue	UNP P23368
E	4327	MSE	MET	modified residue	UNP P23368
E	4343	MSE	MET	modified residue	UNP P23368
E	4407	MSE	MET	modified residue	UNP P23368
E	4539	MSE	MET	modified residue	UNP P23368
F	5001	MSE	MET	modified residue	UNP P23368
F	5029	MSE	MET	modified residue	UNP P23368
F	5038	MSE	MET	modified residue	UNP P23368
F	5047	MSE	MET	modified residue	UNP P23368
F	5075	MSE	MET	modified residue	UNP P23368
F	5086	MSE	MET	modified residue	UNP P23368
F	5108	MSE	MET	modified residue	UNP P23368
F	5177	MSE	MET	modified residue	UNP P23368
F	5219	MSE	MET	modified residue	UNP P23368
F	5239	MSE	MET	modified residue	UNP P23368
F	5325	MSE	MET	modified residue	UNP P23368
F	5327	MSE	MET	modified residue	UNP P23368
F	5343	MSE	MET	modified residue	UNP P23368
F	5407	MSE	MET	modified residue	UNP P23368
F	5539	MSE	MET	modified residue	UNP P23368
G	6001	MSE	MET	modified residue	UNP P23368
G	6029	MSE	MET	modified residue	UNP P23368
G	6038	MSE	MET	modified residue	UNP P23368
G	6047	MSE	MET	modified residue	UNP P23368
G	6075	MSE	MET	modified residue	UNP P23368
G	6086	MSE	MET	modified residue	UNP P23368
G	6108	MSE	MET	modified residue	UNP P23368

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Chain	Residue	Modelled	Actual	Comment	Reference
G	6177	MSE	MET	modified residue	UNP P23368
G	6219	MSE	MET	modified residue	UNP P23368
G	6239	MSE	MET	modified residue	UNP P23368
G	6325	MSE	MET	modified residue	UNP P23368
G	6327	MSE	MET	modified residue	UNP P23368
G	6343	MSE	MET	modified residue	UNP P23368
G	6407	MSE	MET	modified residue	UNP P23368
G	6539	MSE	MET	modified residue	UNP P23368
H	7001	MSE	MET	modified residue	UNP P23368
H	7029	MSE	MET	modified residue	UNP P23368
H	7038	MSE	MET	modified residue	UNP P23368
H	7047	MSE	MET	modified residue	UNP P23368
H	7075	MSE	MET	modified residue	UNP P23368
H	7086	MSE	MET	modified residue	UNP P23368
H	7108	MSE	MET	modified residue	UNP P23368
H	7177	MSE	MET	modified residue	UNP P23368
H	7219	MSE	MET	modified residue	UNP P23368
H	7239	MSE	MET	modified residue	UNP P23368
H	7325	MSE	MET	modified residue	UNP P23368
H	7327	MSE	MET	modified residue	UNP P23368
H	7343	MSE	MET	modified residue	UNP P23368
H	7407	MSE	MET	modified residue	UNP P23368
H	7539	MSE	MET	modified residue	UNP P23368

- Molecule 2 is LUTETIUM (III) ION (CCD ID: LU) (formula: Lu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Lu 1 1	0	0
2	B	1	Total Lu 1 1	0	0
2	C	1	Total Lu 1 1	0	0
2	D	1	Total Lu 1 1	0	0
2	E	1	Total Lu 1 1	0	0
2	F	1	Total Lu 1 1	0	0
2	G	1	Total Lu 1 1	0	0
2	H	1	Total Lu 1 1	0	0

- # NAD

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	G	1	Total	C	N	O	P	18	0
			44	21	7	14	2		
3	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	H	1	Total	C	N	O	P	18	0
			44	21	7	14	2		

- Molecule 4 is water.

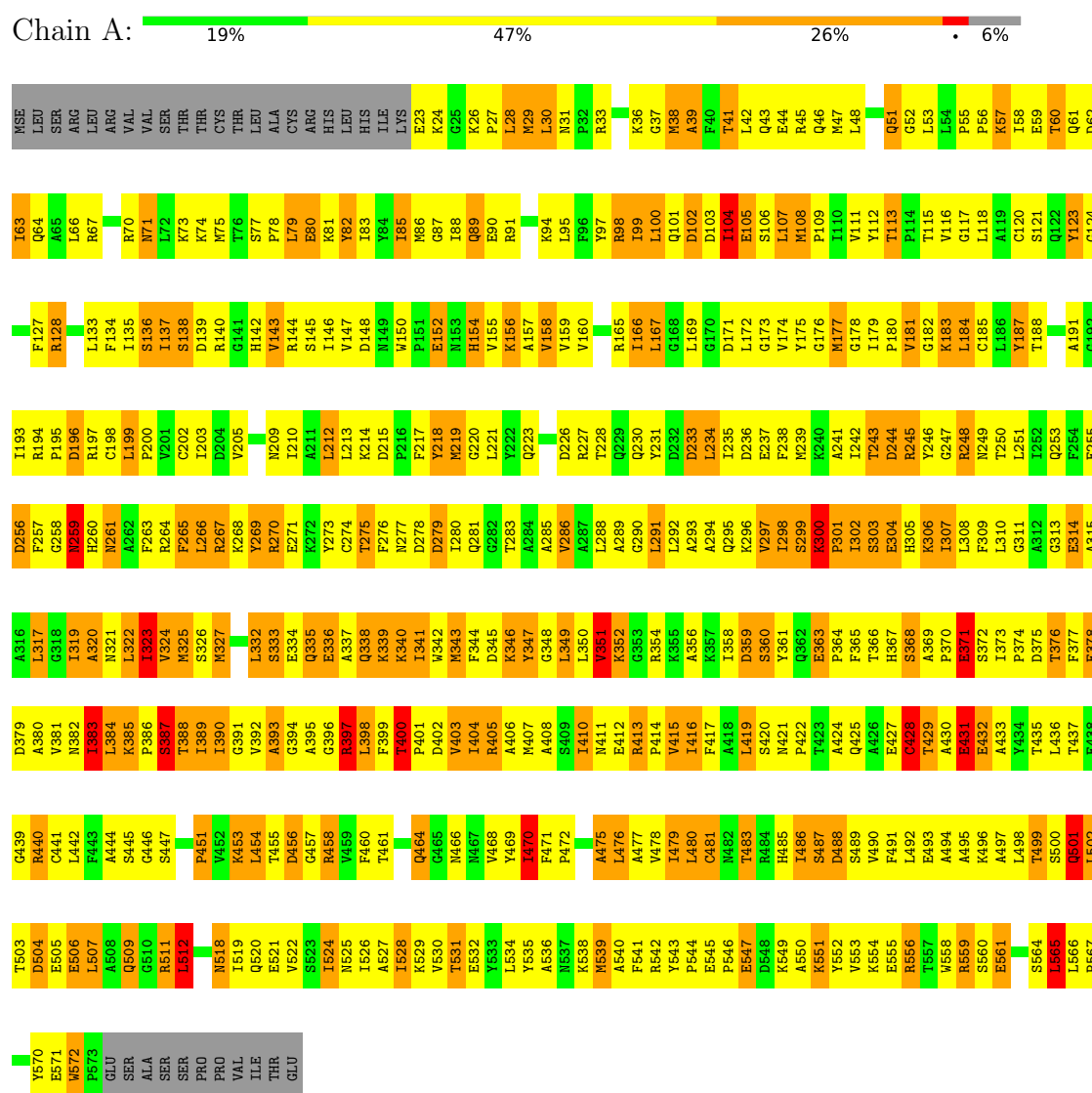
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		
4	B	6	Total	O	0	0
			6	6		
4	C	11	Total	O	0	0
			11	11		
4	D	6	Total	O	0	0
			6	6		
4	E	6	Total	O	0	0
			6	6		
4	F	10	Total	O	0	0
			10	10		
4	G	5	Total	O	0	0
			5	5		
4	H	10	Total	O	0	0
			10	10		

3 Residue-property plots

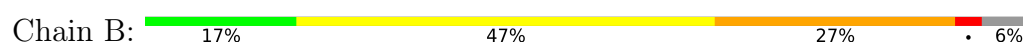
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

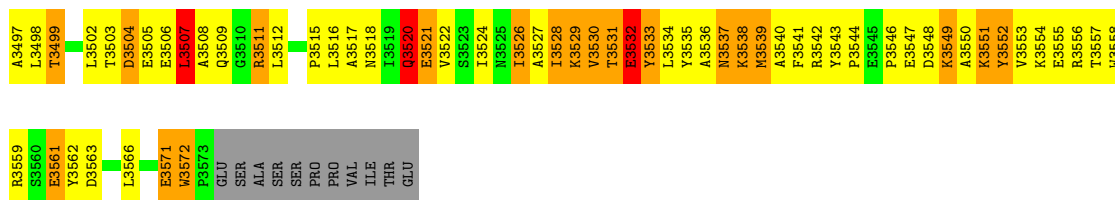


- Molecule 1: NAD-dependent malic enzyme, mitochondrial



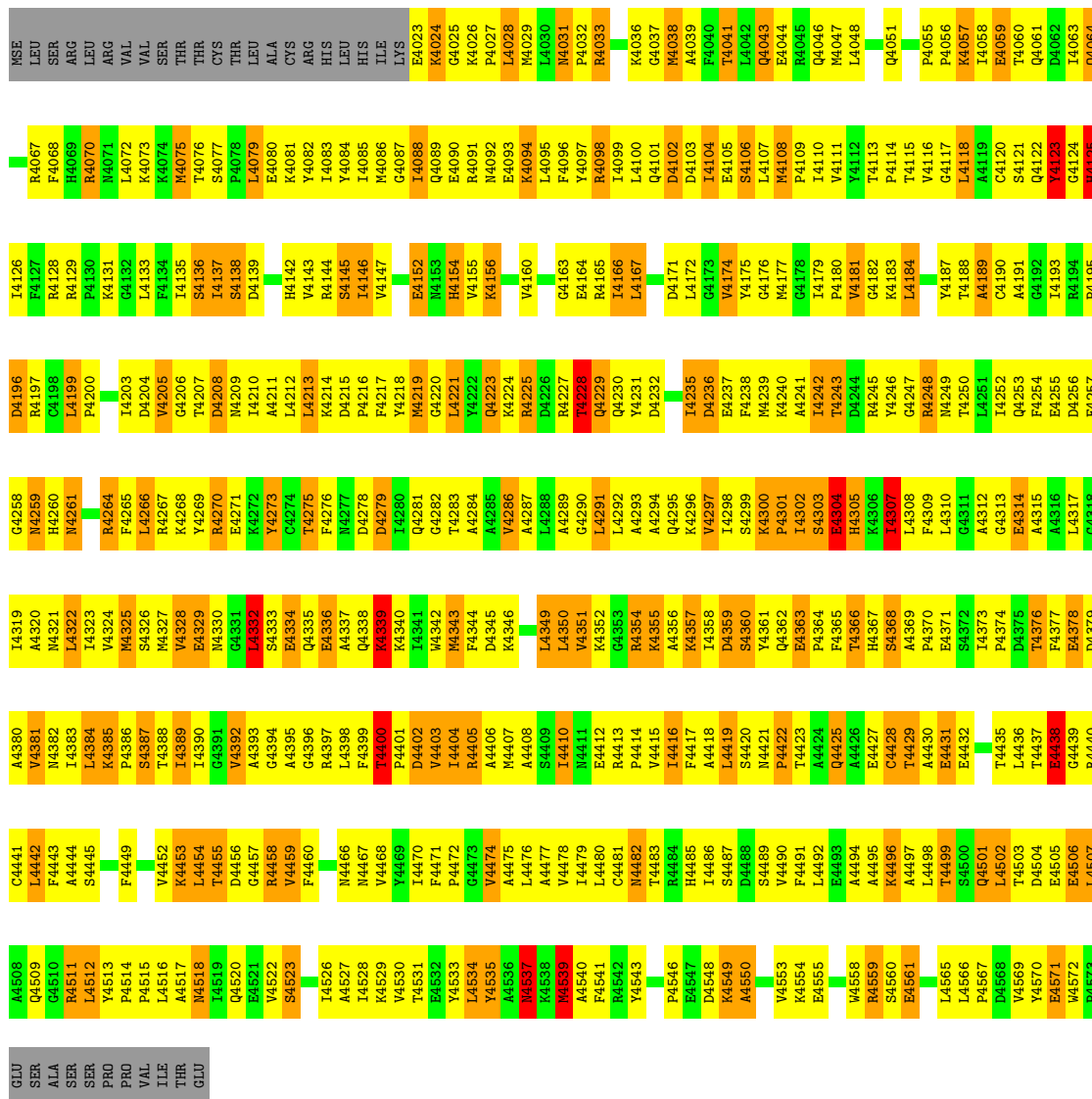
- Molecule 1: NAD-dependent malic enzyme, mitochondrial

[illegible]



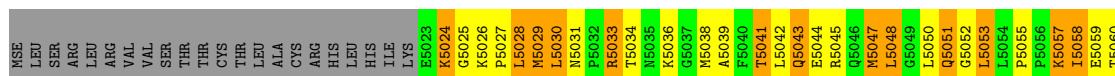
• Molecule 1: NAD-dependent malic enzyme, mitochondrial

Chain E: 20% 50% 22% 6%



• Molecule 1: NAD-dependent malic enzyme, mitochondrial

Chain F: 21% 49% 23% 6%

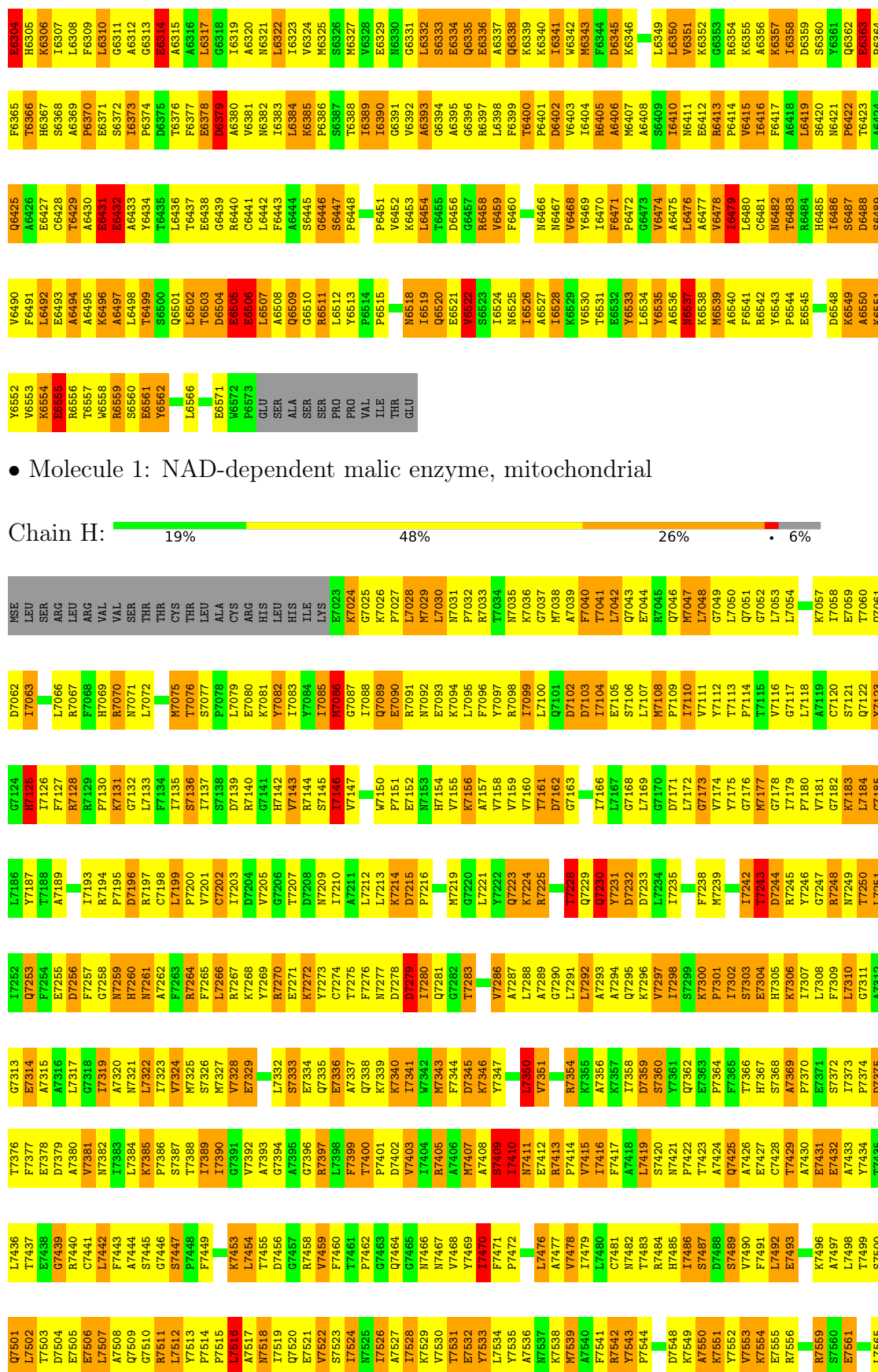


Q5061	Q5122	Q5194	Q5257	Q5318	Q5440	L5502	P5567
D5062	Y5123	P5195	G5258	I5319	C5441	T5503	D5568
I5063	G5124	D5196	N5259	N5321	L5442	E5504	Y5569
A5064	H5125	N5197	H5260	N5322	F5443	E5505	Y5570
A5065	H5126	C5198	N5261	I5323	A5444	E5506	N5571
	F5127	L5199		L5324	S5445	L5507	N5572
	R5128	P5200		V5324	G5446	A5508	P5573
F5068		F5201	R5264	V5325	S5447	Q5509	GLU
H5069		G5202	F5265	S5326	P5448	Q5510	SER
R5070	L5133	C5202	F5266	N5327	F5449	G5511	ALA
N5071	F5134	L5203	N5267	V5328	F5450	L5512	SER
L5072	I5135	D5204	K5268	V5329	G5451	S5513	CYS
K5073	S5136	V5205	V5269	N5330	P5452	P5514	THR
K5074	I5137	R5270	R5270	N5331	K5453	P5515	LEU
K5075	S5138	T5207	E5271	G5332	L5454	L5516	ALA
T5076	D5139	D5208	K5272	L5332	T5455	A5517	CYS
S5077	R5140	N5209	F5273	S5333	T5456	A5518	THR
P5078	H5141	D5209	T5274	G5334	G5456	N5519	THR
L5079	H5142	E5211	T5275	Q5335	G5457	L5520	HIS
F5080	V5143	L5212	F5276	E5336	R5458	Q5520	LEU
K5081	R5144	L5213	N5277	F5337	V5459	E5521	HIS
Y5082	S5145	K5214	D5278	Q5338	F5460	S5522	ILE
L5083	I5146		E5279	K5339	T5461	S5523	LYS
Y5084	V5147	F5217	K5281	K5340	P5462	I5524	
T5085	D5148	Y5218	Q5281	V5403	G5463	N5525	
H5086	N5149	E5219	G5282	I5341	G5464	I5526	
G5087		G5220	T5283	N5342	G5465	A5527	
	E5152	L5221	A5284	N5343	N5466	L5528	
N5088	N5153	F5222	A5285	P5344	N5467	K5529	
K5089	H5154	L5291	V5286	K5346	V5468	V5530	
R5091	A5157	K5224	E5287	A5408	S5409	T5531	
N5092	V5158	R5225	L5288	I5410	F5411	E5532	
E5093	V5159	R5226	A5289	L5349	F5471	Y5533	
L5094	V5160	R5227	E5290	L5350	P5472	L5534	
F5095	T5161	Y5228	K5291	V5351	E5412	E5535	
Y5097	D5162	Q5230	L5292	G5352	P5413	G5473	
		Y5231	A5293	K5353	V5474	V5475	
	I5166		A5294	K5354	L5415	L5476	
	L5167		Q5295	A5355	F5417	A5477	
L5100	L5168	L5234	K5296	K5356	A5418	V5478	
D5102	L5169	L5235	Y5297	K5357	L5419	L5479	
D5103			L5298	D5359	S5420	L5480	
F5104	L5172	F5238	S5299	S5360	N5421	C5481	
E5105	G5173	N5239	P5300	Q5361	T5422	R5484	
S5106	V5174	A5240	P5301	E5362	A5423	H5485	
L5107	G5175	L5242	L5302	E5363	A5424	A5486	
M5108	G5176	T5243	S5303	P5364	Q5425	K5550	
P5109	M5177	D5244	E5304	F5365	A5426	K5551	
L5110	G5178	R5245	H5305	T5366	E5427	V5552	
Y5111	L5179	R5246	K5306	H5367	C5428	K5554	
Y5112	P5180	G5247	L5307	S5368	T5429	F5491	
Y5113	V5181	R5248	L5308	A5369	A5430	L5492	
P5114	L5184	N5249	P5309	E5371	E5431	E5493	
L5115	G5185	L5250	G5311	S5372	E5432	A5494	
G5116	L5186	L5251	A5312	Y5373	Y5434	S5560	
L5117	Y5187	L5252	G5313	P5374	F5435	E5561	
A5119	T5188	Q5253	E5314	D5375	L5436	D5562	
C5120		F5254	A5315	F5376	T5437	S5563	
S5121		E5255	A5316	F5377	T5499	S5564	
		D5256	L5317	E5378	Q5501	L5566	

● Molecule 1: NAD-dependent malic enzyme, mitochondrial

Chain G: 15% 48% 27% 6%

K5E	D6062	Y6123	K6183	D6244
LEU	I6063	G6124	L6184	R6245
SER	Q6064	H6125	C6185	Y6246
ARG	A6065	R6126	L6186	G6247
LEU	L6066	F6127	Y6187	R6248
ARG	R6067	R6128	T6188	N6249
VAL	F6068	R6129	A6189	T6250
VAL	H6069	P6130	G6190	L6251
SER	R6070	G6131	A6191	T6252
THR	N6071	G6132	G6192	Q6253
THR	L6072	L6133	L6193	F6254
CYS	K6073	F6134	R6194	E6255
THR	K6074	L6135	P6195	D6256
LEU	M6075	S6136	D6196	F6257
ALA	T6076	L6137	R6197	G6258
CYS	S6077	S6138	C6198	G6259
ARG	P6078	D6139	L6199	H6260
HIS	R6079	R6140	P6200	N6261
LEU	E6080	G6141	V6201	A6262
HIS	K6081	H6142	G6202	F6263
ILE	Y6082	R6144	L6203	L6264
LYS	I6083	S6145	D6204	F6265
		G6086	G6205	L6266
		G6087	K6086	R6267
		T6146	G6087	H6268
		D6148	D6206	R6269
		N6149	P6027	R6270
		L6150	L6207	E5271
		P6151	N6029	K6272
		E6152	L6030	Y6273
		N6153	E6093	C6274
		H6154	K6094	T6275
		V6155	L6095	F6276
		A6156	F6096	N6277
		G6157	R6097	G6278
		V6158	R6098	M6279
		V6159	L6099	G6280
		L6100	L6101	L6281
		Q6101	D6102	G6282
		D6103	L6104	T6283
		E6104	R6105	A6284
		S6106	L6107	A6285
		L6107	R6108	V6286
		G6108	P6109	R6287
		L6109	L6110	L6288
		V6111	L6112	G6289
		Y6112	T6113	L6290
		T6113	P6114	G6291
		T6115	G6115	Y6292
		V6116	P6055	L6293
		G6117	P6056	A6293
		H6118	G6177	G6294
		A6119	T6179	K6300
		P6120	P6180	P6301
		S6121	V6181	L6302
		Q6122	G6182	S6303



• Molecule 1: NAD-dependent malic enzyme, mitochondrial

L7566	Y7570	GLU
P7567	E7571	SER
	W7572	ALA
	P7573	SER
		SER
		PRO
		PRO
		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	P 1	Depositor
Cell constants a, b, c, α , β , γ	113.30Å 119.00Å 125.90Å 116.50° 94.80° 102.80°	Depositor
Resolution (Å)	20.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.90)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.204 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	35527	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LU, 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	0.56	0/4424	1.06	33/5969 (0.6%)
1	B	0.56	0/4424	1.04	30/5969 (0.5%)
1	C	0.56	0/4424	1.05	27/5969 (0.5%)
1	D	0.57	0/4424	1.06	33/5969 (0.6%)
1	E	0.59	0/4424	1.05	25/5969 (0.4%)
1	F	0.58	0/4424	1.06	33/5969 (0.6%)
1	G	0.56	0/4424	1.12	38/5969 (0.6%)
1	H	0.56	0/4424	1.06	33/5969 (0.6%)
All	All	0.57	0/35392	1.06	252/47752 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

The worst 5 of 252 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	6446	GLY	N-CA-C	-9.97	100.94	112.50
1	F	5125	HIS	N-CA-C	-9.65	101.27	113.43
1	G	6125	HIS	N-CA-C	-9.07	104.28	114.62
1	D	3438	GLU	N-CA-C	-8.82	101.82	112.58
1	D	3507	LEU	N-CA-C	-8.74	101.33	111.03

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	TYR	Sidechain

5.2 Too-close contacts

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	4344	0	4372	630	0
1	B	4344	0	4372	651	0
1	C	4344	0	4372	624	0
1	D	4344	0	4372	686	0
1	E	4344	0	4372	560	0
1	F	4344	0	4372	532	0
1	G	4344	0	4372	684	0
1	H	4344	0	4372	599	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	88	0	52	3	0
3	B	88	0	52	5	0
3	C	88	0	52	2	0
3	D	88	0	52	4	0
3	E	88	0	52	3	0
3	F	88	0	52	3	0
3	G	88	0	52	4	0
3	H	88	0	52	3	0
4	A	9	0	0	3	0
4	B	6	0	0	1	0
4	C	11	0	0	1	0
4	D	6	0	0	6	0
4	E	6	0	0	0	0
4	F	10	0	0	1	0
4	G	5	0	0	3	0
4	H	10	0	0	1	0
All	All	35527	0	35392	4886	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 69.

The worst 5 of 4886 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3061:GLN:HA	1:D:3064:GLN:HE21	1.04	1.18
1:D:3388:THR:HG23	1:D:3415:VAL:HB	1.27	1.15
1:H:7210:ILE:HG22	1:H:7214:LYS:HZ1	1.01	1.14
1:H:7388:THR:HG23	1:H:7415:VAL:HB	1.27	1.14
1:D:3253:GLN:HE22	1:D:3255:GLU:HG2	1.13	1.13

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	549/584 (94%)	415 (76%)	99 (18%)	35 (6%)	1	3
1	B	549/584 (94%)	406 (74%)	107 (20%)	36 (7%)	1	3
1	C	549/584 (94%)	407 (74%)	102 (19%)	40 (7%)	1	2
1	D	549/584 (94%)	394 (72%)	119 (22%)	36 (7%)	1	3
1	E	549/584 (94%)	429 (78%)	94 (17%)	26 (5%)	2	7
1	F	549/584 (94%)	437 (80%)	83 (15%)	29 (5%)	1	5
1	G	549/584 (94%)	398 (72%)	111 (20%)	40 (7%)	1	2
1	H	549/584 (94%)	398 (72%)	120 (22%)	31 (6%)	1	4
All	All	4392/4672 (94%)	3284 (75%)	835 (19%)	273 (6%)	1	3

5 of 273 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	ILE

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Mol	Chain	Res	Type
1	A	167	LEU
1	A	256	ASP
1	A	259	ASN
1	A	268	LYS

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	466/483 (96%)	313 (67%)	153 (33%)	0	1
1	B	466/483 (96%)	302 (65%)	164 (35%)	0	0
1	C	466/483 (96%)	323 (69%)	143 (31%)	0	1
1	D	466/483 (96%)	306 (66%)	160 (34%)	0	0
1	E	466/483 (96%)	324 (70%)	142 (30%)	0	1
1	F	466/483 (96%)	324 (70%)	142 (30%)	0	1
1	G	466/483 (96%)	309 (66%)	157 (34%)	0	0
1	H	466/483 (96%)	323 (69%)	143 (31%)	0	1
All	All	3728/3864 (96%)	2524 (68%)	1204 (32%)	0	1

5 of 1204 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	6118	LEU
1	H	7350	LEU
1	G	6227	ARG
1	G	6115	THR
1	G	6506	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 118 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	3525	ASN

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Mol	Chain	Res	Type
1	H	7411	ASN
1	E	4482	ASN
1	H	7338	GLN
1	G	6425	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	$\# Z > 2$
3	NAD	G	6601	-	46,48,48	2.11	13 (28%)	64,73,73	1.91	12 (18%)
3	NAD	D	3602	-	46,48,48	2.14	12 (26%)	64,73,73	1.82	11 (17%)
3	NAD	B	1601	-	46,48,48	1.97	13 (28%)	64,73,73	1.89	10 (15%)
3	NAD	H	7601	-	46,48,48	2.19	12 (26%)	64,73,73	1.91	11 (17%)
3	NAD	A	601	-	46,48,48	2.11	10 (21%)	64,73,73	1.91	12 (18%)
3	NAD	C	2602	-	46,48,48	2.17	10 (21%)	64,73,73	1.85	11 (17%)
3	NAD	F	5602	-	46,48,48	2.05	12 (26%)	64,73,73	1.89	11 (17%)
3	NAD	C	2601	-	46,48,48	2.18	13 (28%)	64,73,73	1.88	11 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAD	E	4602	-	46,48,48	2.04	10 (21%)	64,73,73	1.87	10 (15%)
3	NAD	D	3601	-	46,48,48	2.43	16 (34%)	64,73,73	1.93	12 (18%)
3	NAD	G	6602	-	46,48,48	2.06	12 (26%)	64,73,73	1.86	10 (15%)
3	NAD	H	7602	-	46,48,48	2.05	10 (21%)	64,73,73	1.89	13 (20%)
3	NAD	E	4601	-	46,48,48	2.11	13 (28%)	64,73,73	1.91	10 (15%)
3	NAD	F	5601	-	46,48,48	1.87	12 (26%)	64,73,73	1.87	11 (17%)
3	NAD	B	1602	-	46,48,48	2.12	10 (21%)	64,73,73	1.88	10 (15%)
3	NAD	A	602	-	46,48,48	2.11	13 (28%)	64,73,73	1.87	10 (15%)

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
3	NAD	G	6601	-	-	0/30/62/62	0/5/5/5
3	NAD	D	3602	-	-	8/30/62/62	0/5/5/5
3	NAD	B	1601	-	-	10/30/62/62	0/5/5/5
3	NAD	H	7601	-	-	1/30/62/62	0/5/5/5
3	NAD	A	601	-	-	0/30/62/62	0/5/5/5
3	NAD	C	2602	-	-	4/30/62/62	0/5/5/5
3	NAD	F	5602	-	-	5/30/62/62	0/5/5/5
3	NAD	C	2601	-	-	5/30/62/62	0/5/5/5
3	NAD	E	4602	-	-	6/30/62/62	0/5/5/5
3	NAD	D	3601	-	-	3/30/62/62	0/5/5/5
3	NAD	G	6602	-	-	7/30/62/62	0/5/5/5
3	NAD	H	7602	-	-	6/30/62/62	0/5/5/5
3	NAD	E	4601	-	-	2/30/62/62	0/5/5/5
3	NAD	F	5601	-	-	1/30/62/62	0/5/5/5
3	NAD	B	1602	-	-	7/30/62/62	0/5/5/5
3	NAD	A	602	-	-	5/30/62/62	0/5/5/5

The worst 5 of 191 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1602	NAD	C2N-N1N	8.93	1.44	1.35
3	D	3601	NAD	C2N-N1N	8.43	1.44	1.35
3	C	2602	NAD	C2N-N1N	8.25	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	7601	NAD	C2N-N1N	8.02	1.43	1.35
3	D	3602	NAD	C2N-N1N	7.92	1.43	1.35

The worst 5 of 175 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3601	NAD	C5A-C4A-N3A	-6.28	118.08	126.72
3	B	1602	NAD	C5A-C4A-N3A	-6.18	118.21	126.72
3	H	7601	NAD	C5A-C4A-N3A	-6.13	118.28	126.72
3	H	7602	NAD	C5A-C4A-N3A	-6.08	118.35	126.72
3	F	5602	NAD	C5A-C4A-N3A	-6.08	118.35	126.72

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	NAD	C5B-O5B-PA-O1A
3	A	602	NAD	C5B-O5B-PA-O3
3	B	1601	NAD	C5B-O5B-PA-O1A
3	B	1601	NAD	C5B-O5B-PA-O2A
3	B	1601	NAD	C5B-O5B-PA-O3

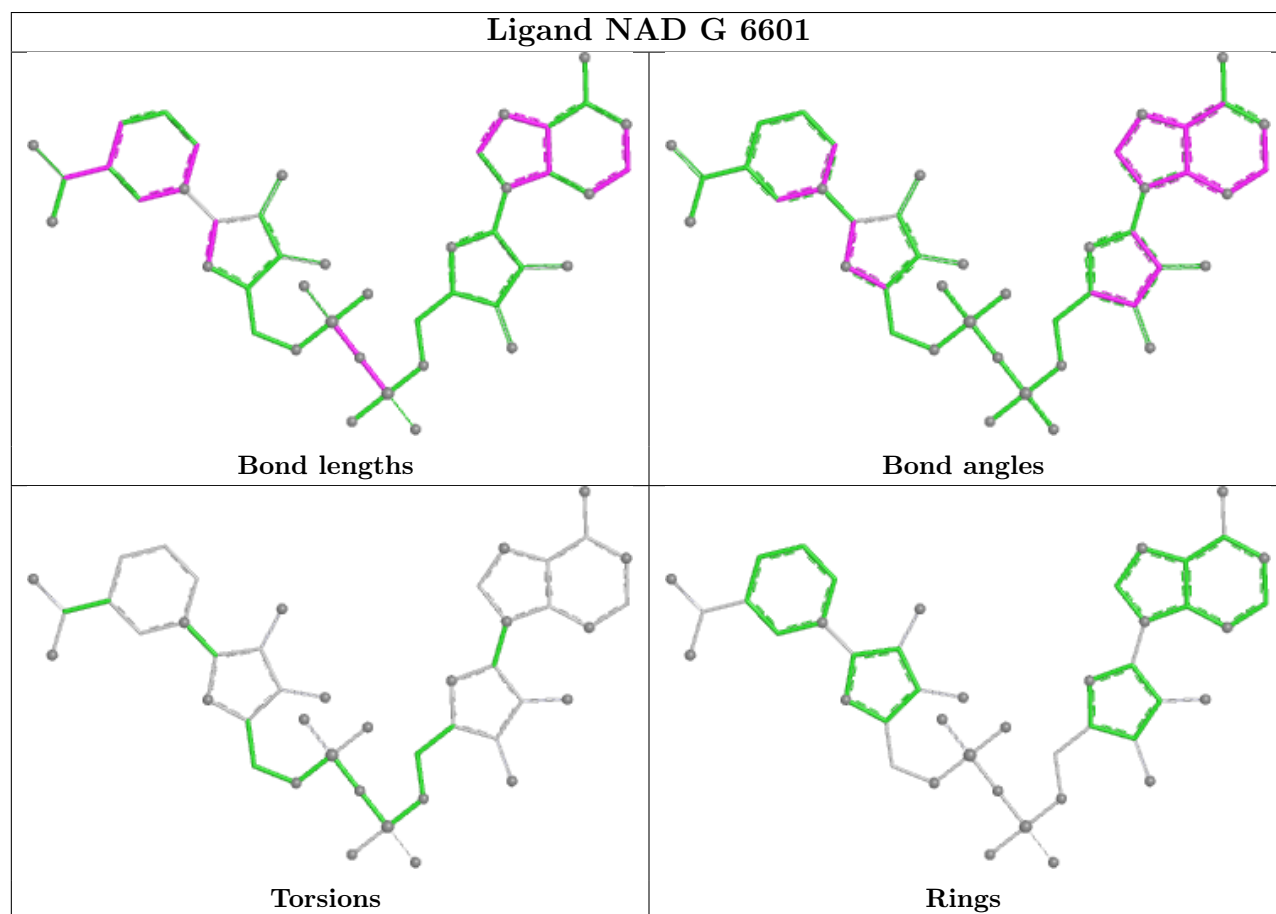
There are no ring outliers.

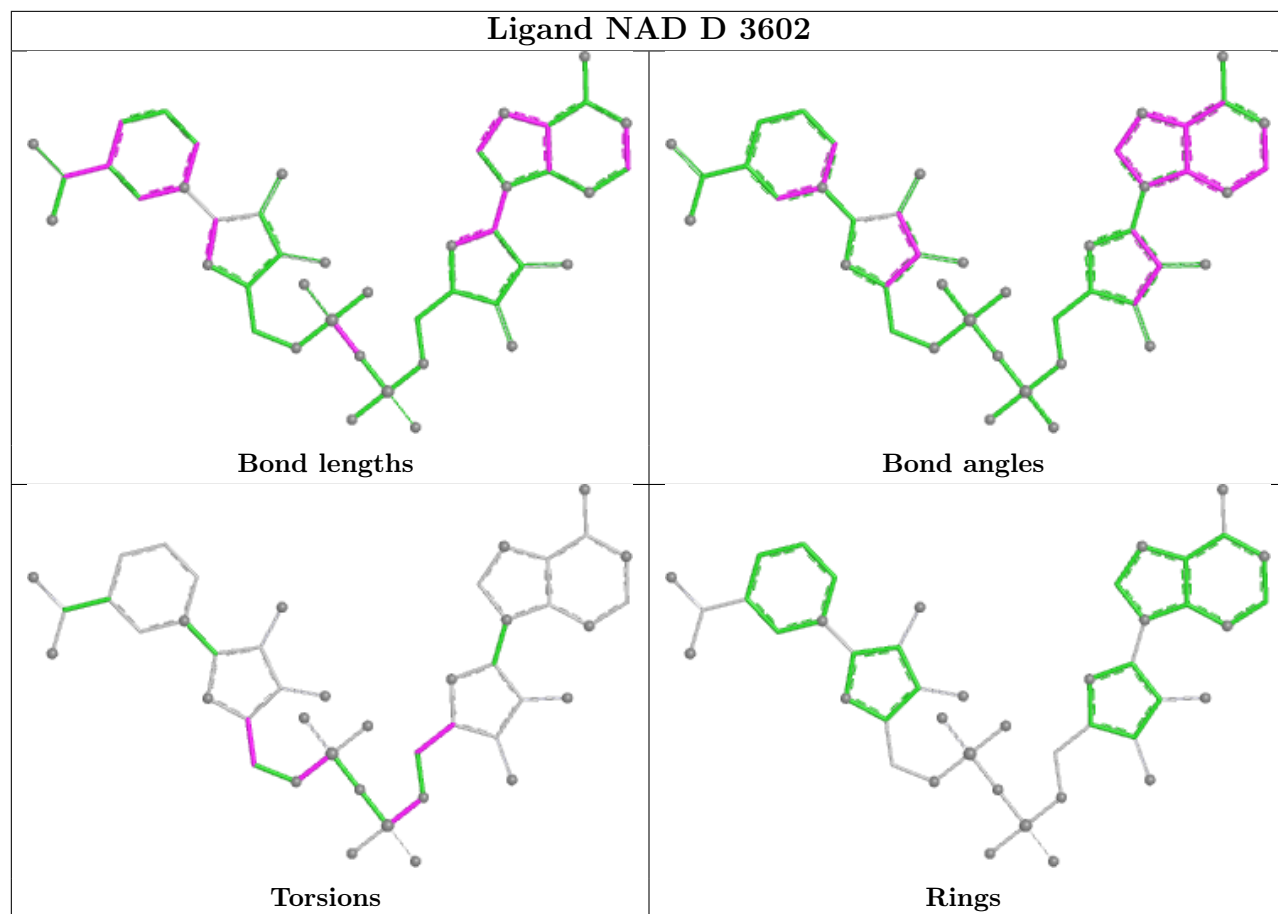
11 monomers are involved in 27 short contacts:

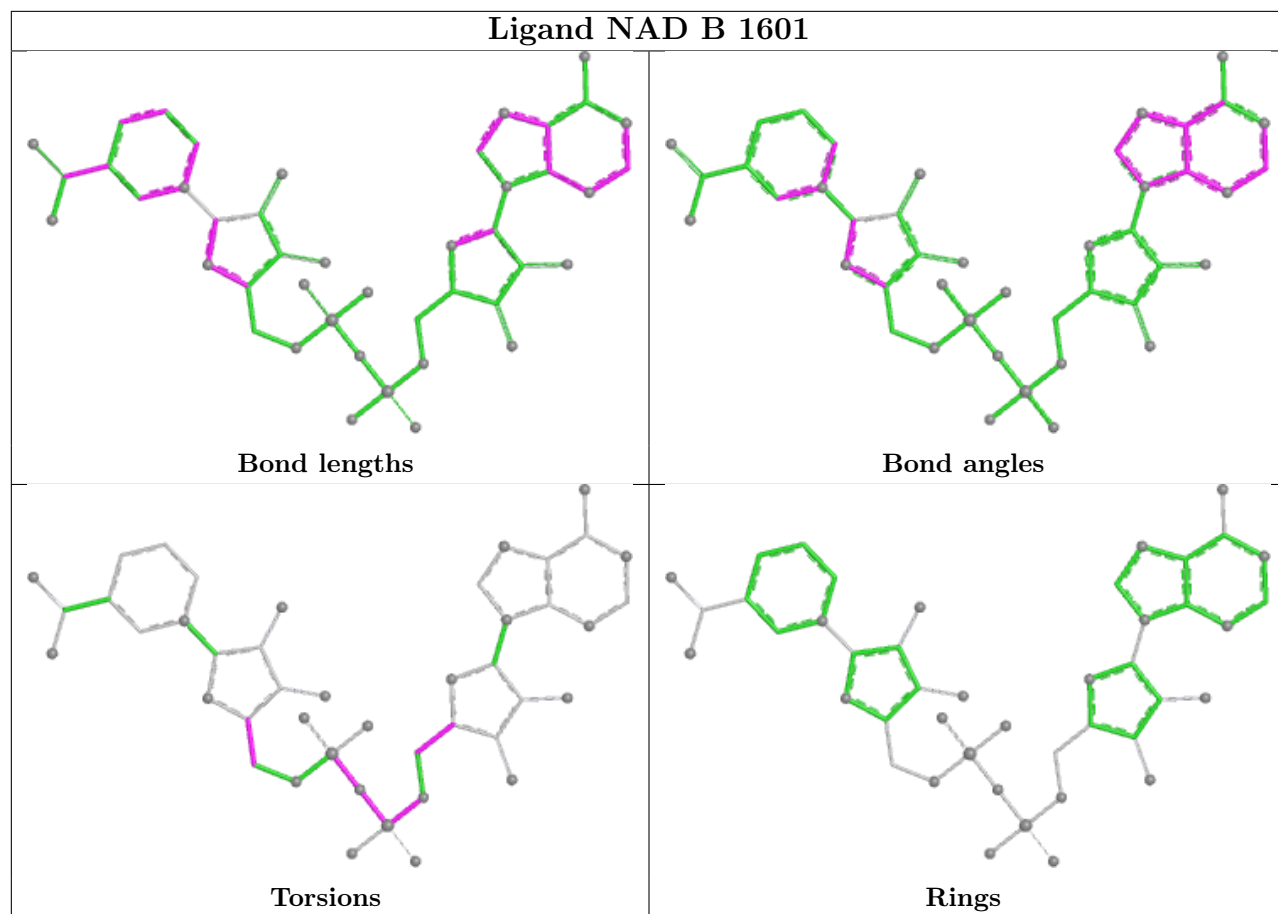
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	6601	NAD	4	0
3	D	3602	NAD	1	0
3	B	1601	NAD	4	0
3	H	7601	NAD	2	0
3	A	601	NAD	3	0
3	C	2601	NAD	2	0
3	D	3601	NAD	3	0
3	H	7602	NAD	1	0
3	E	4601	NAD	3	0
3	F	5601	NAD	3	0
3	B	1602	NAD	1	0

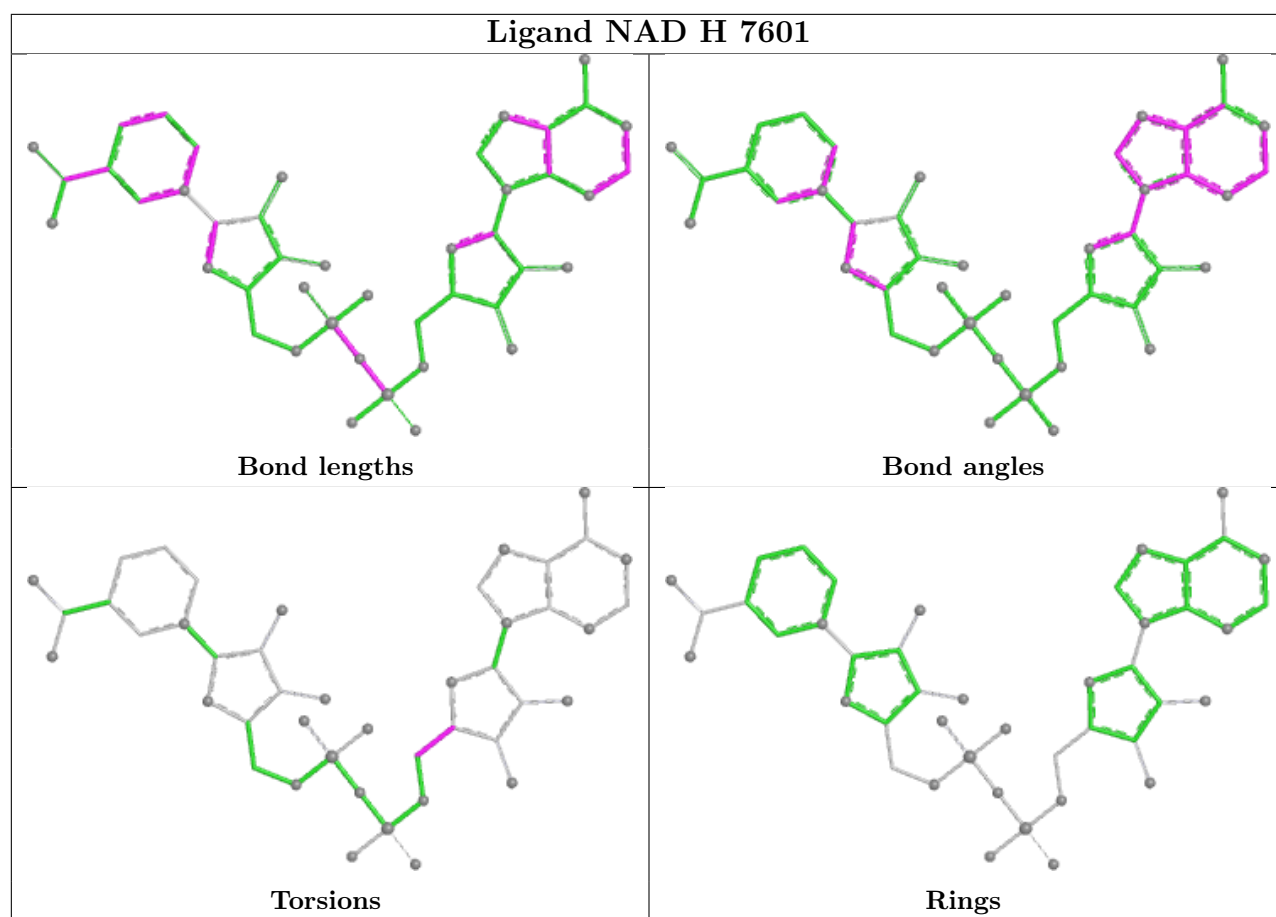
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

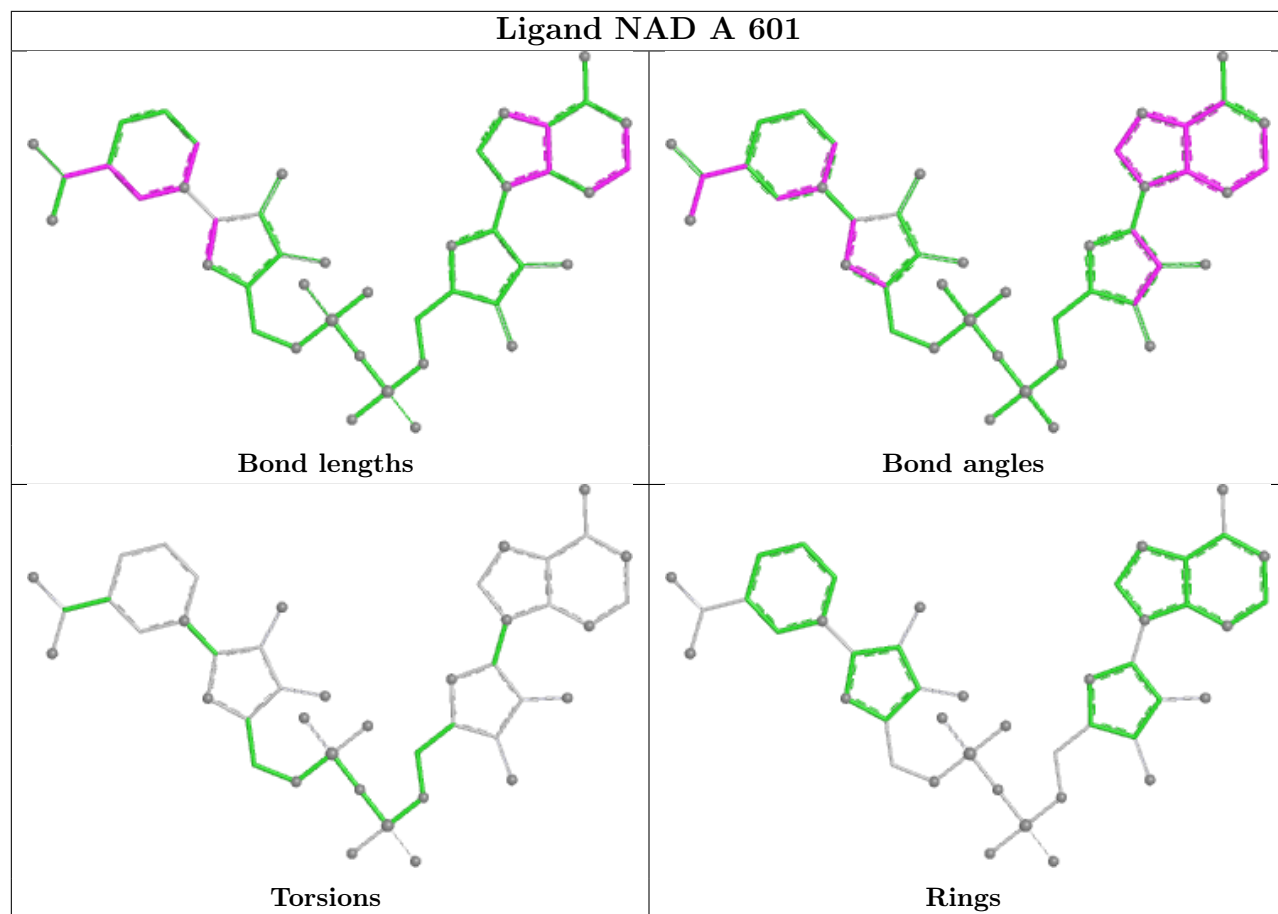
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

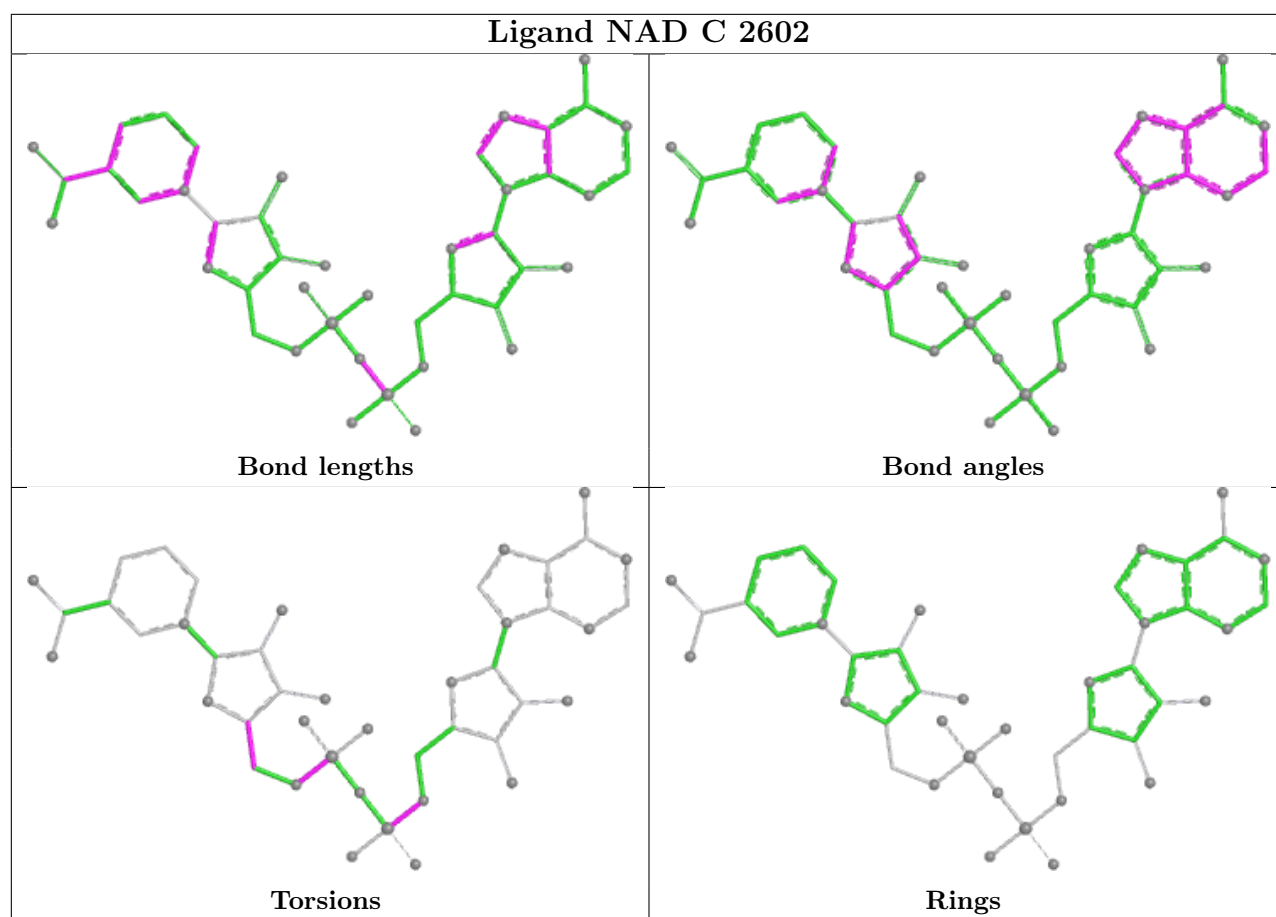


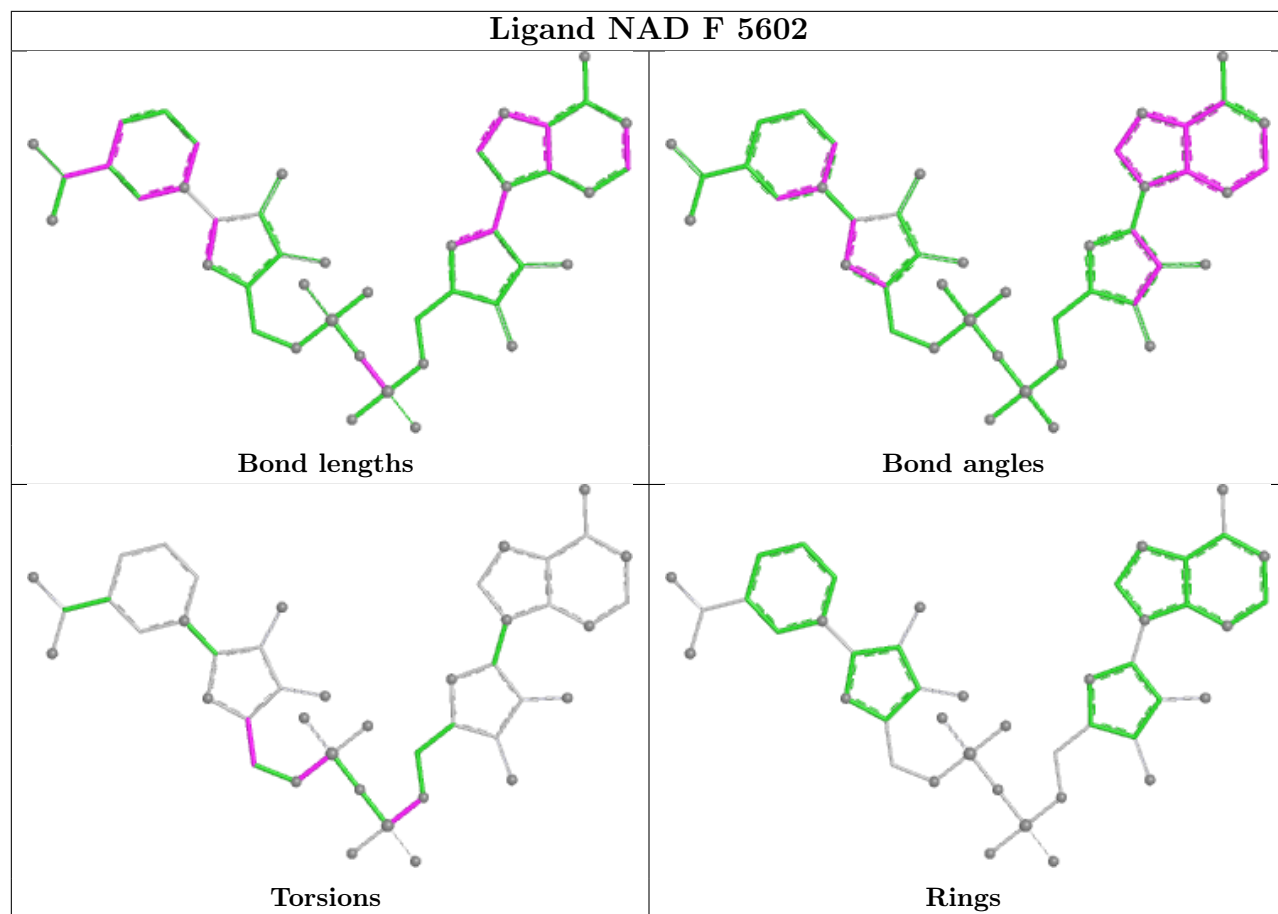


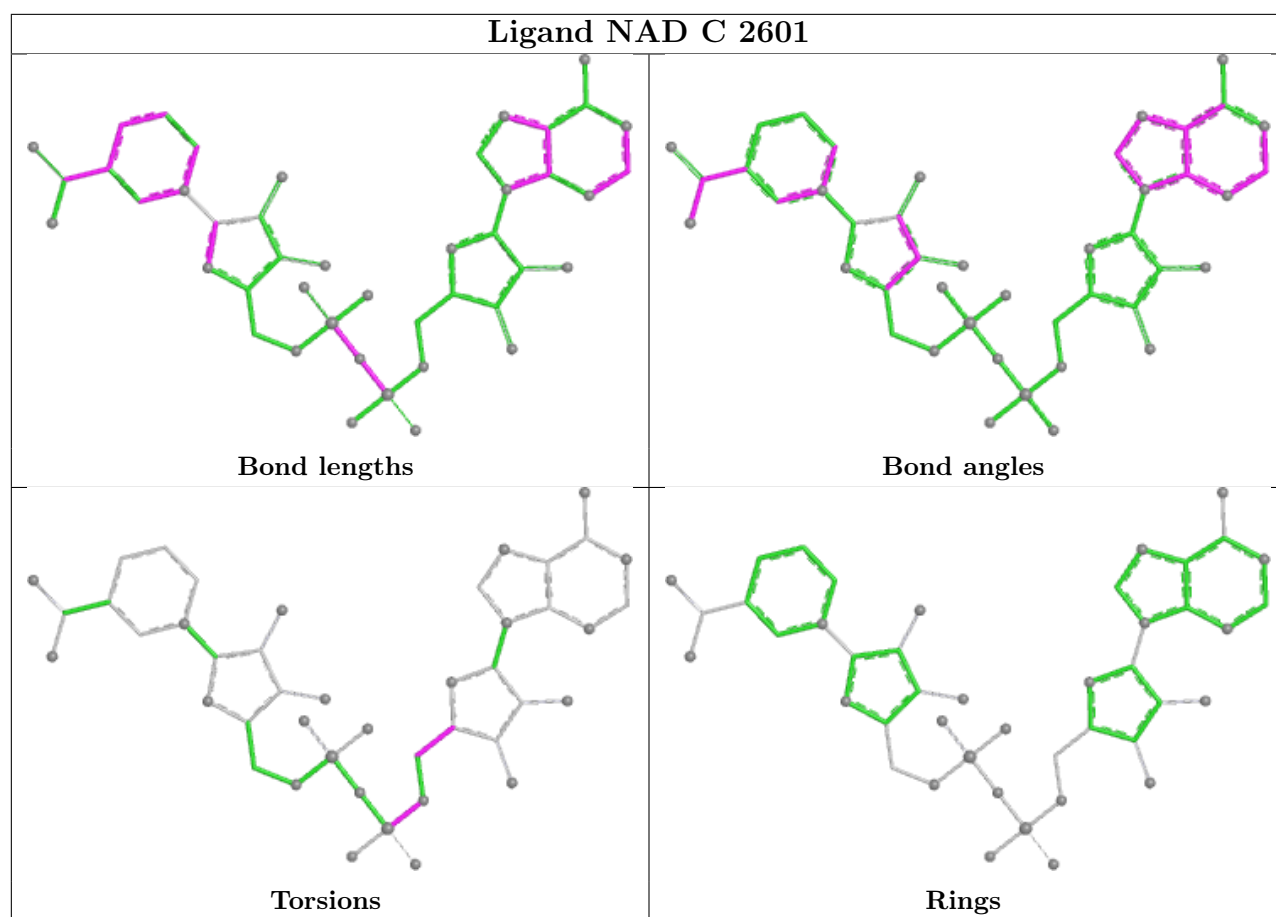


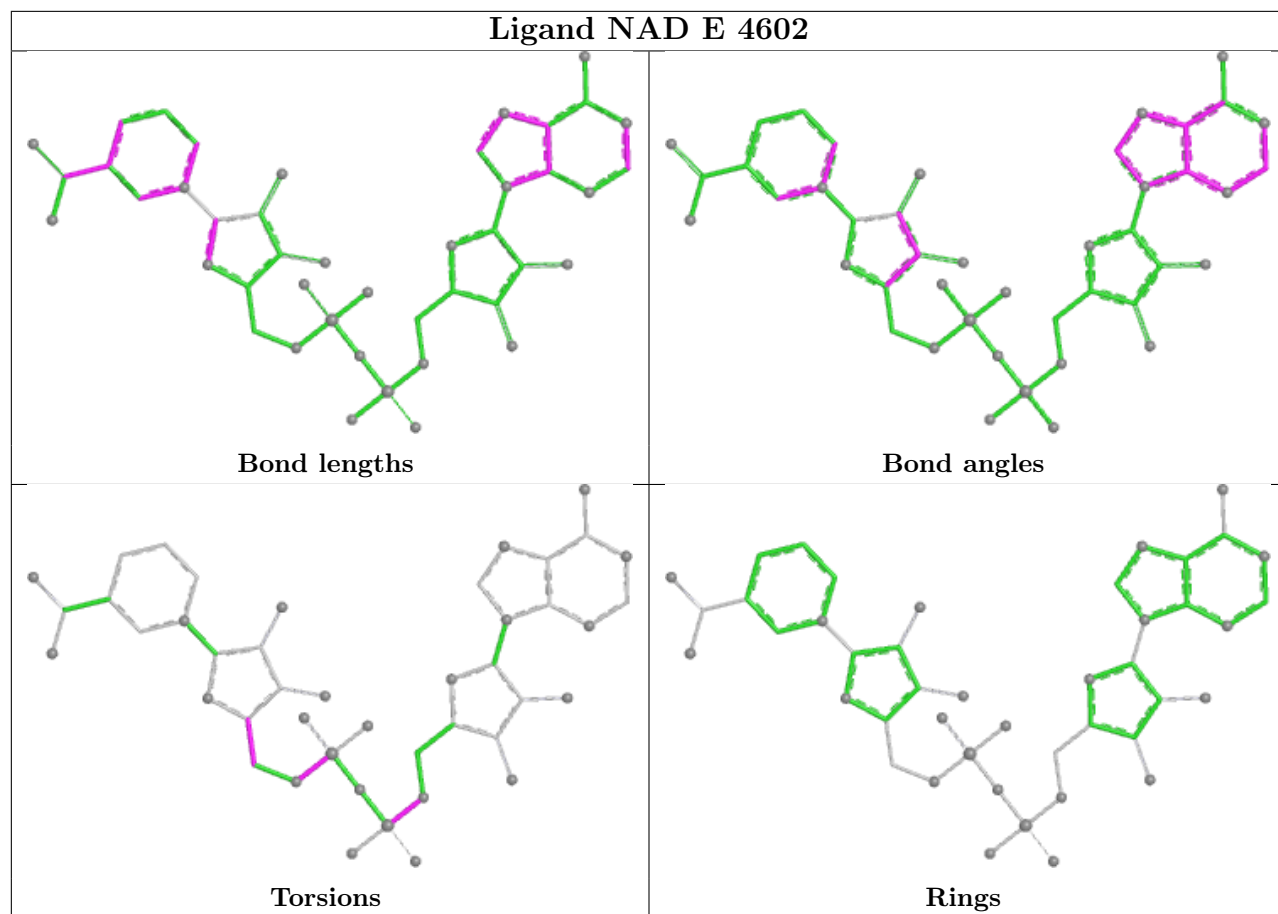


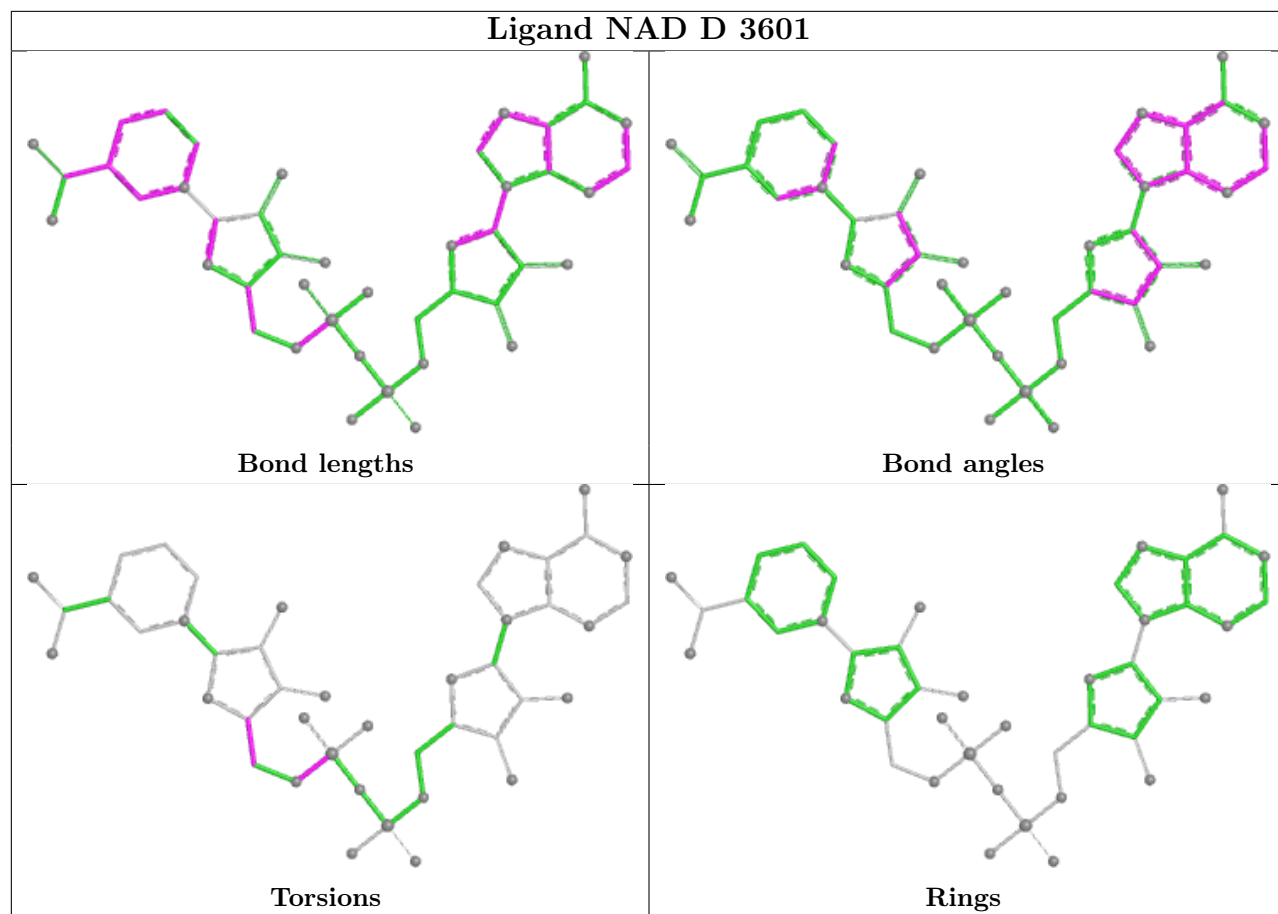


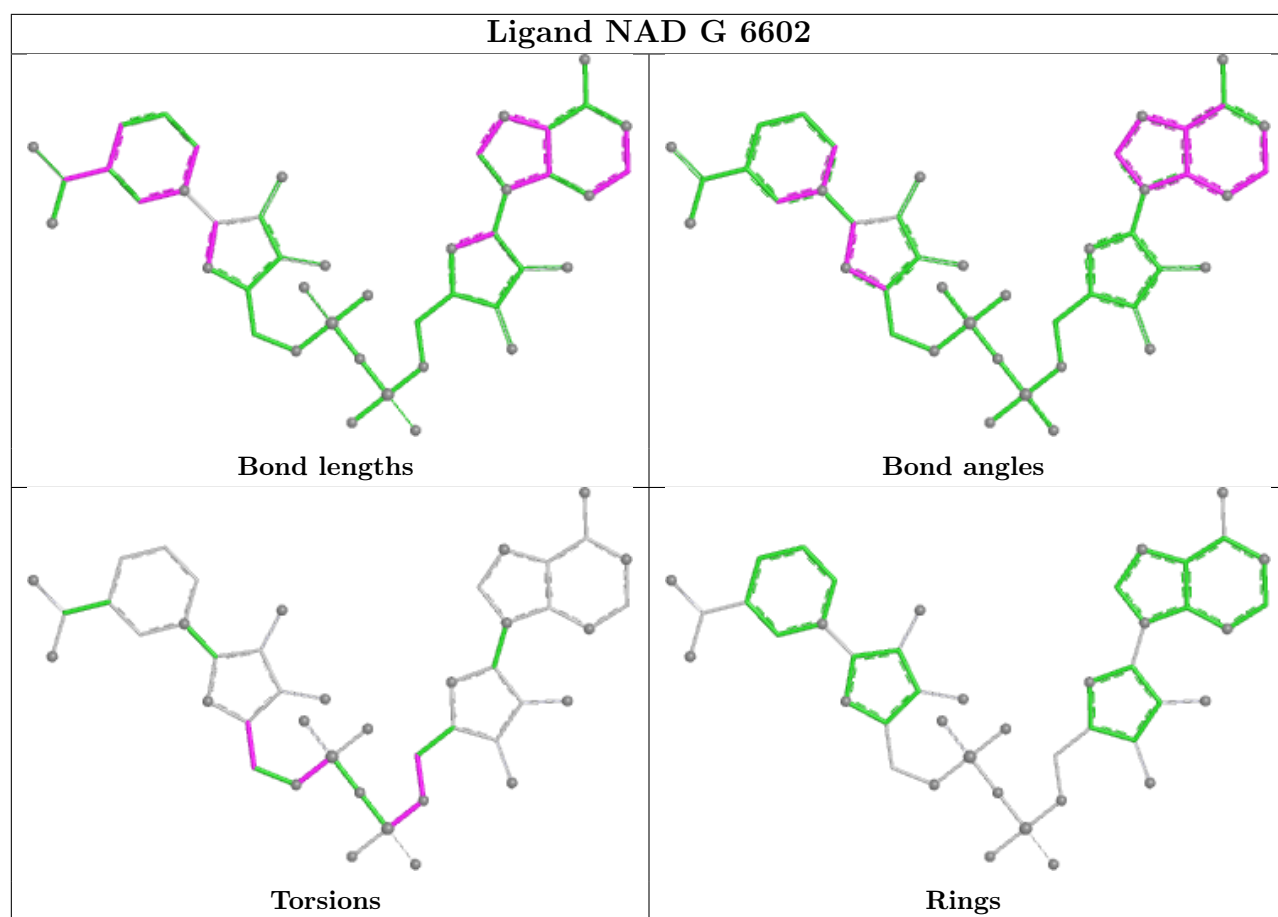


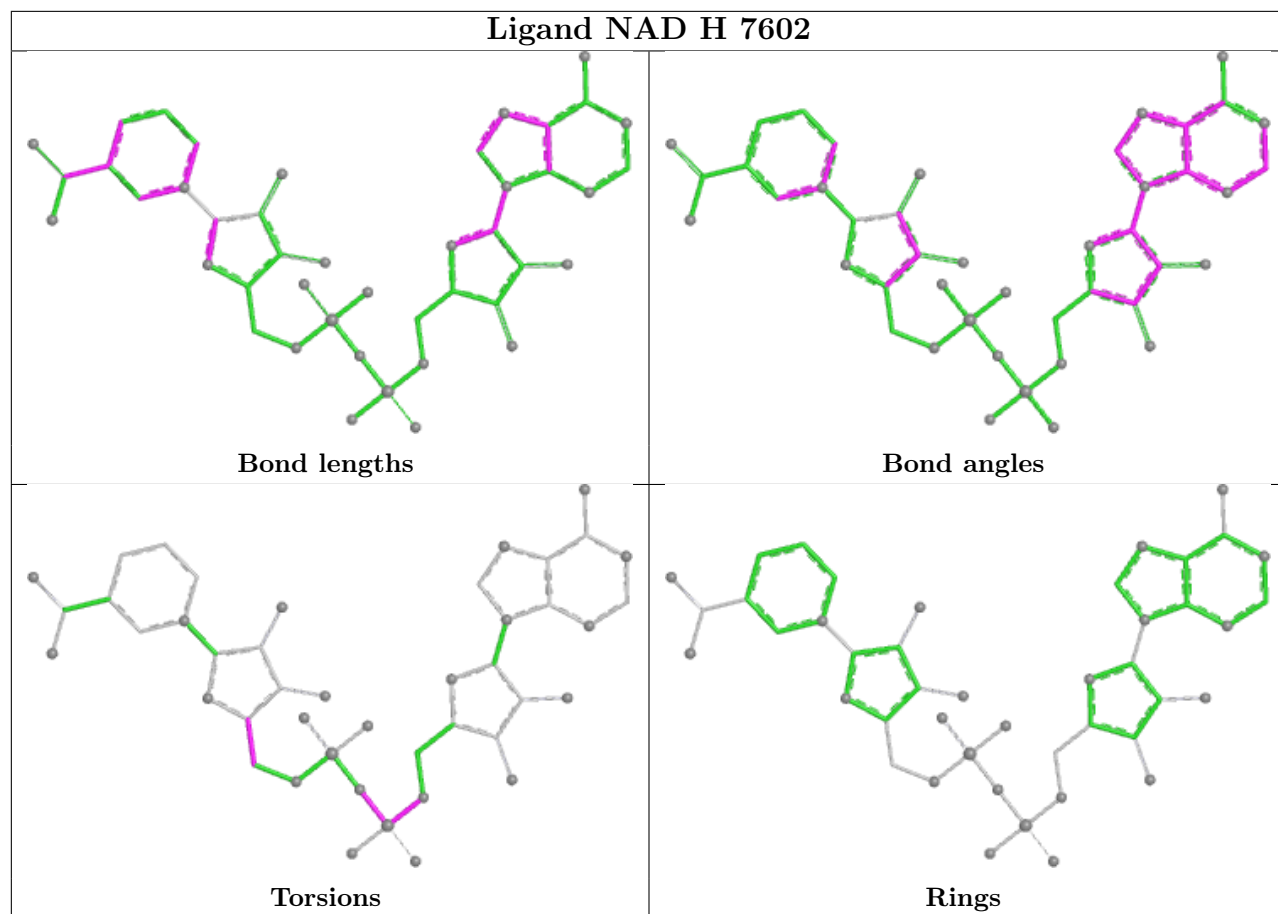


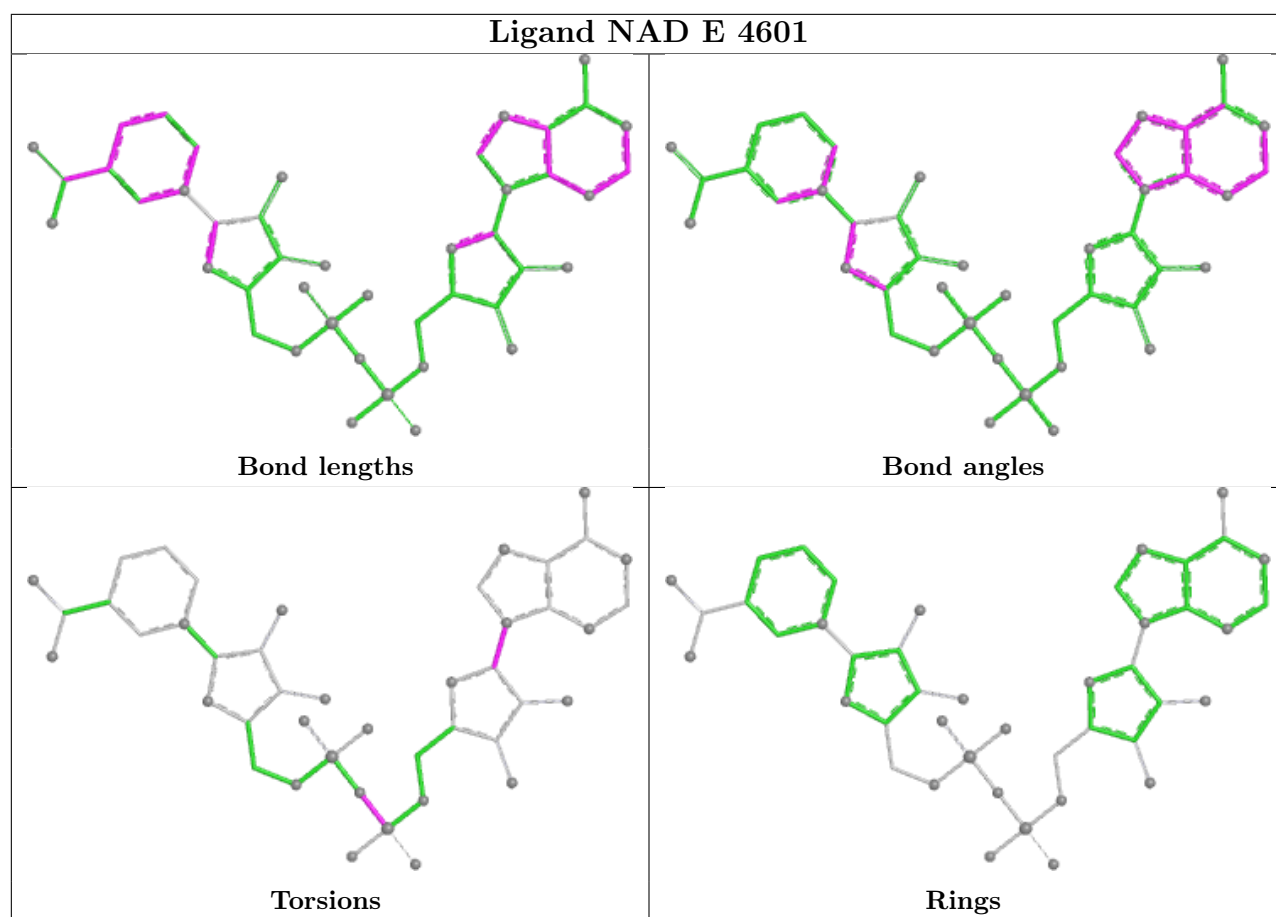


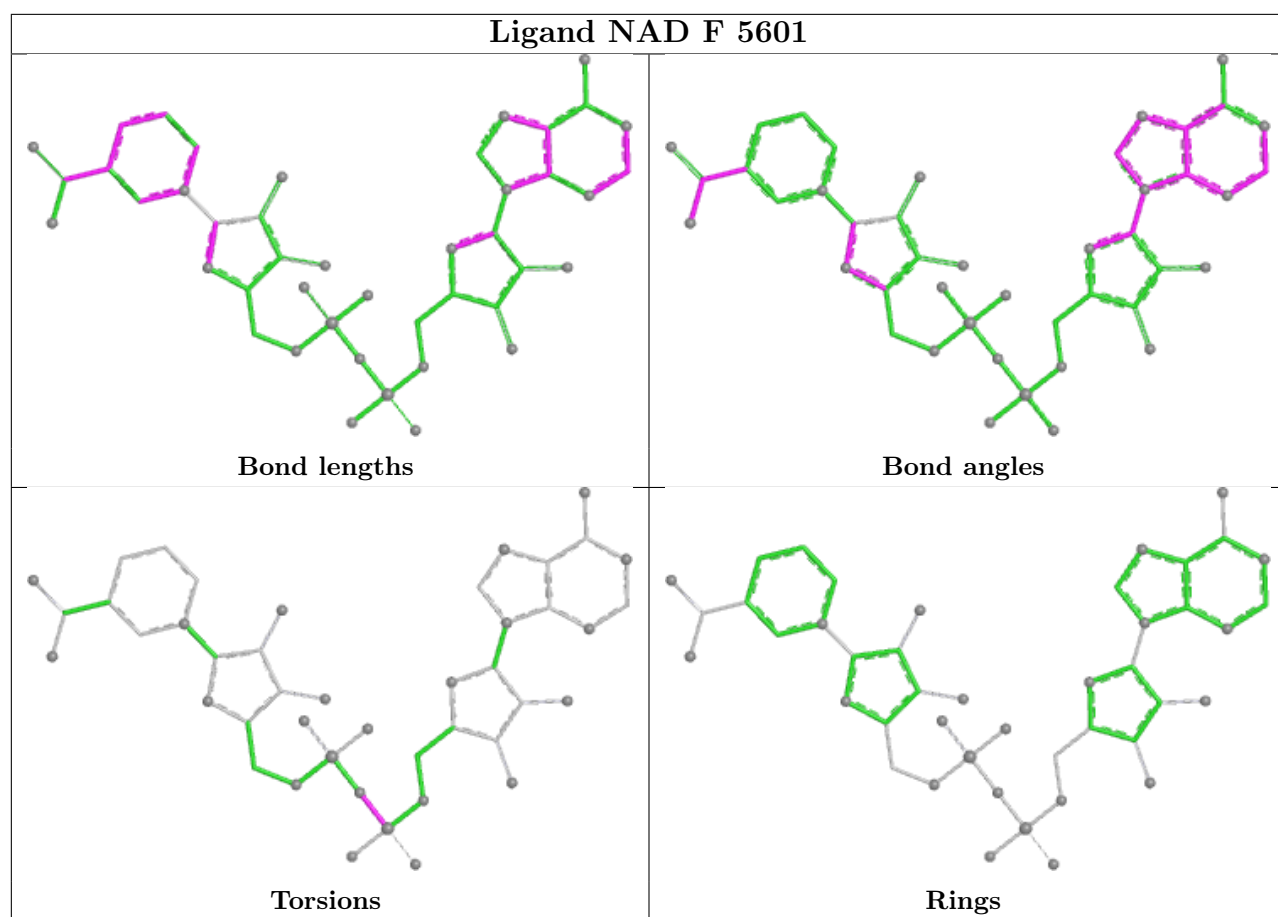


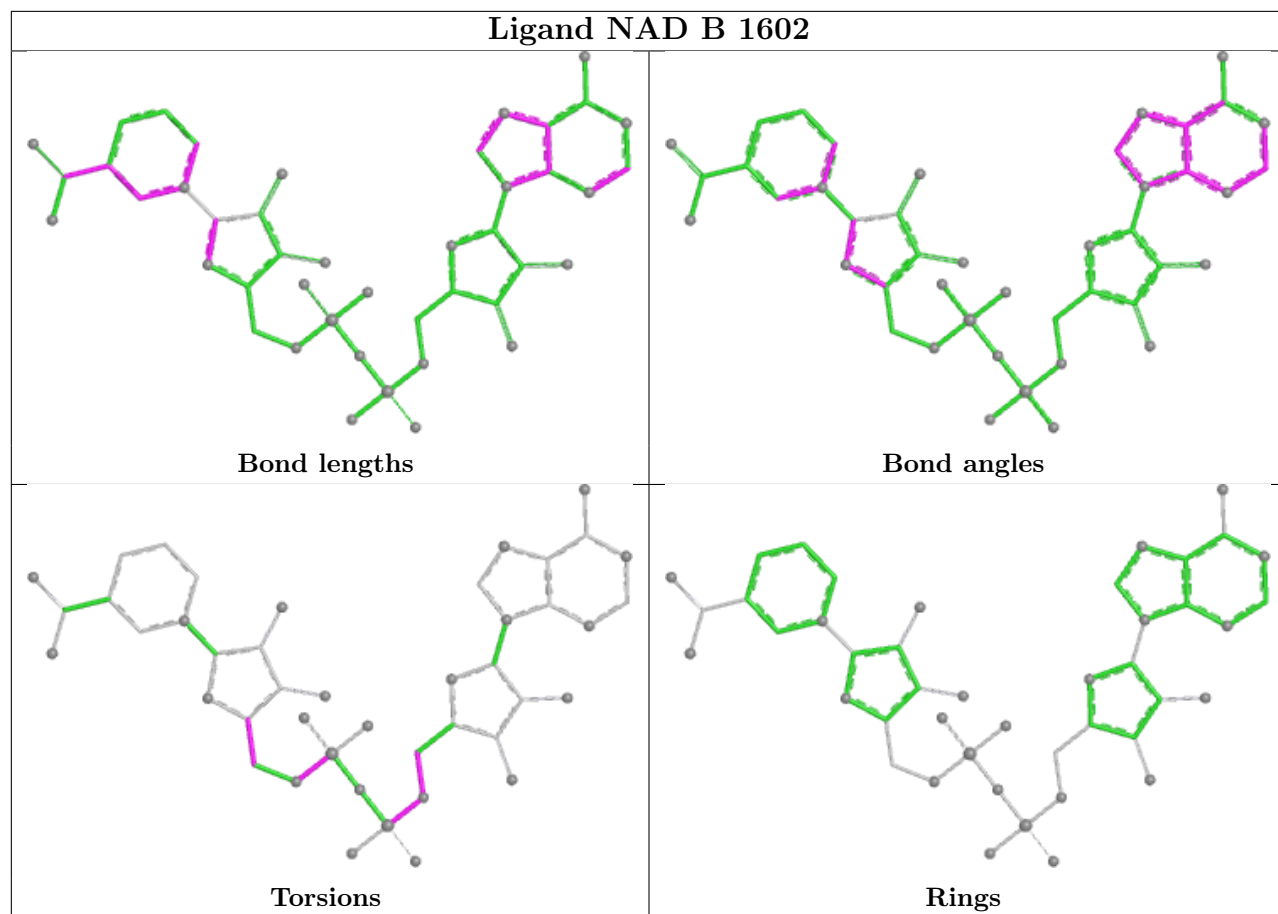


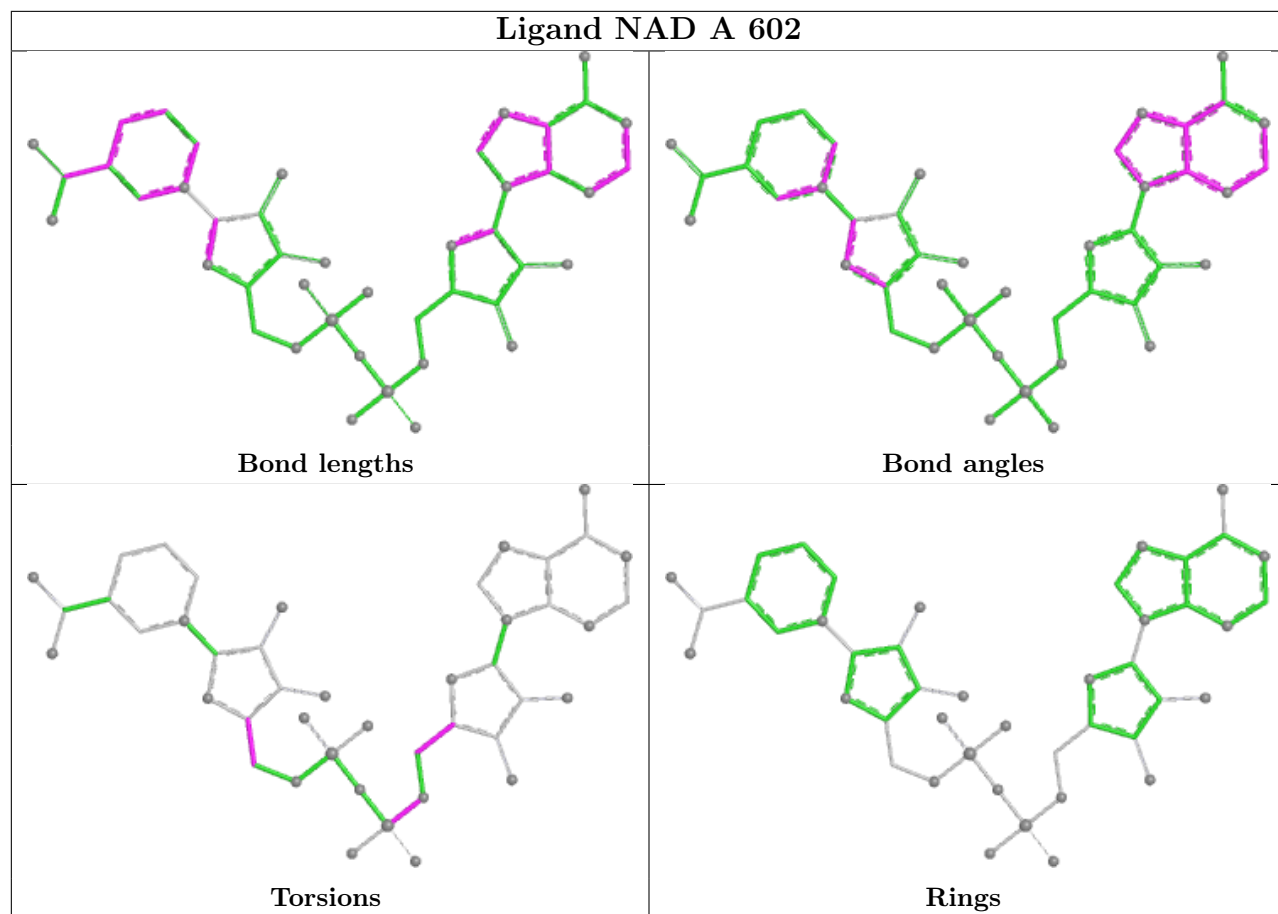












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.