



wwPDB EM Validation Summary Report ⓘ

Mar 19, 2026 – 07:53 PM UTC

PDB ID : 7W0R / pdb_00007w0r
EMDB ID : EMD-32248
Title : Active state CI from Q10-NADH dataset, Subclass 1
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-18
Resolution : 2.80 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

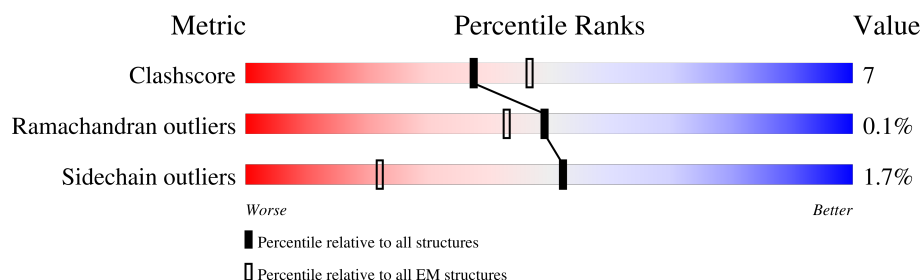
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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.



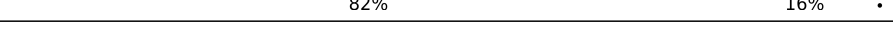
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	433	82% 18%
2	B	176	87% 13%
3	C	156	75% 24% .
4	E	115	88% 12%
5	F	86	72% 22% 6%
6	G	88	80% 20%
6	X	88	75% 24% .
7	H	112	78% 22%
8	I	112	74% 11% . 13%

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Mol	Chain	Length	Quality of chain
9	J	342	 85% 15%
10	K	43	 67% 33%
11	L	125	 82% 17% .
12	M	690	 83% 17%
13	N	144	 83% 17% .
14	O	217	 83% 16%
15	P	208	 85% 15%
16	Q	430	 83% 16% .
17	S	70	 81% 16% .
18	T	96	 89% 11%
19	U	83	 88% 12%
20	V	140	 82% 18%
21	W	142	 76% 24%
22	Y	67	 82% 16% .
23	Z	80	 88% 11% .
24	a	138	 85% 14% .
25	b	126	 61% 17% 22%
26	c	156	 86% 13% .
27	d	175	 80% 19% .
28	e	104	 79% 21%
29	f	49	 86% 14%
30	g	121	 89% 11%
31	h	105	 84% 16%
32	i	347	 81% 19%
33	j	115	 75% 24% .

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Mol	Chain	Length	Quality of chain
34	k	98	 72% 28%
35	l	606	 75% 25%
36	m	175	 81% 18% .
37	n	56	 82% 14% .
38	o	128	 86% 14%
39	p	178	 83% 17%
40	r	459	 80% 20%
41	s	318	 78% 21% .
42	u	171	 79% 19% .
43	v	124	 75% 24% .
44	w	320	 84% 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	SF4	A	501	-	-	X	-
45	SF4	C	301	-	-	X	-

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 68233 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	433	Total	C	N	O	S	0	0
			3330	2103	593	614	20		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	176	Total	C	N	O	S	0	0
			1412	887	243	269	13		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	156	Total	C	N	O	S	0	0
			1248	794	227	213	14		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	115	Total	C	N	O	S	0	0
			967	617	179	166	5		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	86	Total	C	N	O	S	0	0
			687	432	129	124	2		

- Molecule 6 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total	C	N	O	S	0	0
			690	446	102	137	5		
6	X	88	Total	C	N	O	S	0	0
			704	454	104	141	5		

- Molecule 7 is a protein called Complex I subunit B13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	112	Total	C	N	O	S	0	0
			910	588	154	165	3		

- Molecule 8 is a protein called Complex I-B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	97	Total	C	N	O	S	0	0
			780	491	147	139	3		

- Molecule 9 is a protein called NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	342	Total	C	N	O	S	0	0
			2751	1783	481	478	9		

- Molecule 10 is a protein called Complex I-9kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	43	Total	C	N	O	S	0	0
			366	228	68	69	1		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	125	Total	C	N	O	S	0	0
			1016	642	181	190	3		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	690	Total	C	N	O	S	0	0
			5296	3320	923	1014	39		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	144	Total	C	N	O	S	0	0
			1204	770	218	212	4		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	217	Total	C	N	O	S	0	0
			1671	1065	281	315	10		

- Molecule 15 is a protein called Complex I-30kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	208	Total	C	N	O	S	0	0
			1738	1124	298	314	2		

- Molecule 16 is a protein called Complex I-49kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	430	Total	C	N	O	S	0	0
			3459	2212	594	629	24		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	70	Total	C	N	O	S	0	0
			566	364	103	94	5		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	96	Total	C	N	O	S	0	0
			741	452	140	146	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	83	Total	C	N	O	S	0	0
			643	417	110	115	1		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	140	Total	C	N	O	S	0	0
			1021	651	174	190	6		

- Molecule 21 is a protein called Complex I-B16.6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	142	Total	C	N	O	S	0	0
			1167	752	200	206	9		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	67	Total	C	N	O	S	0	0
			584	385	95	103	1		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	80	Total	C	N	O	S	0	0
			641	418	108	114	1		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

- Molecule 25 is a protein called Complex I-B17.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	98	Total	C	N	O	S	0	0
			819	537	144	137	1		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	156	Total	C	N	O	S	0	0
			1315	853	213	241	8		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	175	Total	C	N	O	S	0	0
			1461	916	265	272	8		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	104	Total	C	N	O	S	0	0
			867	553	142	168	4		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	49	Total	C	N	O	0	0
			378	246	65	67		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	121	Total	C	N	O	S	0	0
			1000	650	173	171	6		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	105	Total	C	N	O	S	0	0
			867	550	161	150	6		

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	347	Total	C	N	O	S	0	0
			2710	1782	420	462	46		

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	115	Total	C	N	O	S	0	0
			914	615	134	158	7		

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	k	98	Total	C	N	O	S	0	0
			748	493	113	128	14		

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	606	Total	C	N	O	S	0	0
			4800	3182	744	823	51		

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	175	Total	C	N	O	S	0	0
			1295	864	188	230	13		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	56	Total	C	N	O	S	0	0
			479	311	88	79	1		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	o	128	Total	C	N	O	0	0
			1062	691	182	189		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	178	Total	C	N	O	S	0	0
			1530	980	279	263	8		

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	r	459	Total	C	N	O	S	0	0
			3631	2412	572	609	38		

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	318	Total	C	N	O	S	0	0
			2508	1678	385	424	21		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	u	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	124	Total	C	N	O	S	0	0
			1059	658	202	189	10		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2582	1643	438	491	10		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



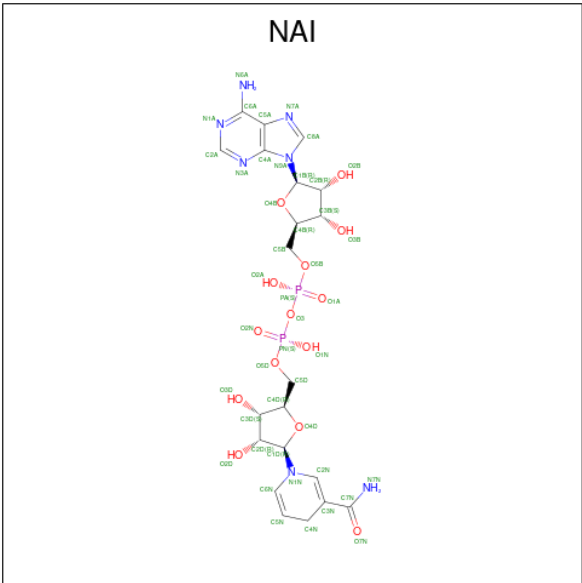
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



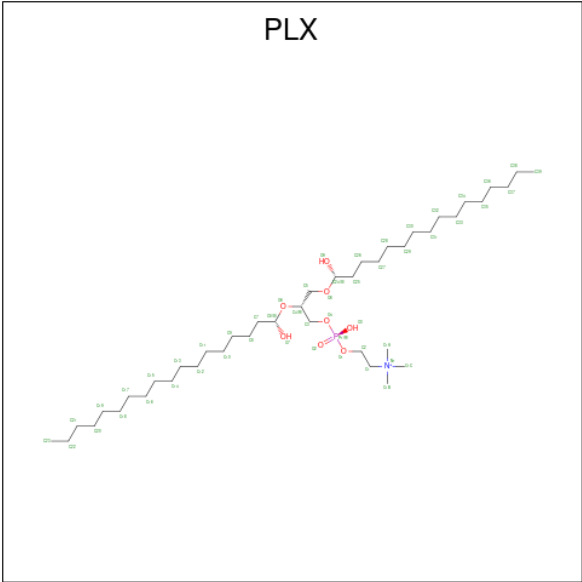
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 48 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



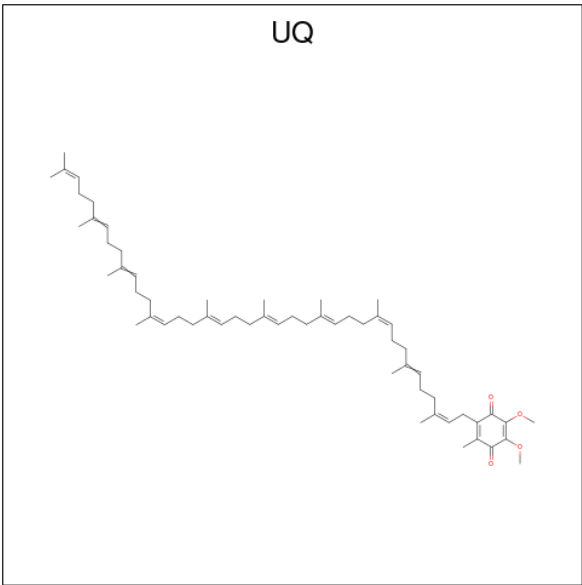
Mol	Chain	Residues	Atoms					AltConf
48	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	V	1	Total	C	N	O	P	0
			40	30	1	8	1	
48	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	i	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	j	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	j	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	l	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
48	r	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 49 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



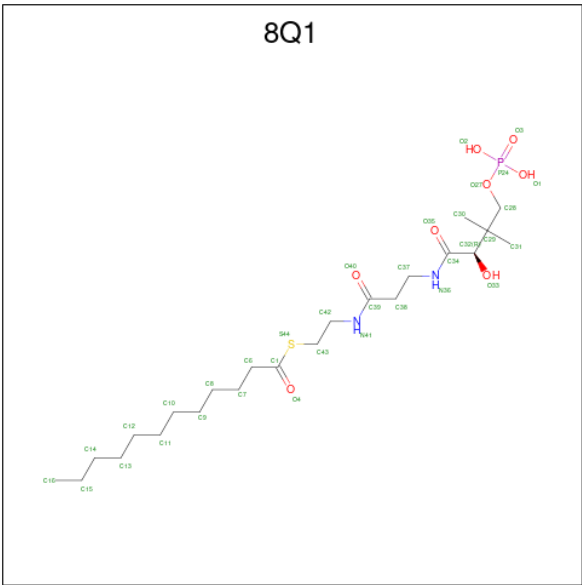
Mol	Chain	Residues	Atoms					AltConf
49	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	J	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 50 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: C₅₉H₉₀O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
50	C	1	Total	C	O	0
			38	34	4	
50	J	1	Total	C	O	0
			33	29	4	

- Molecule 51 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS) (labeled as "Ligand of Interest" by depositor).



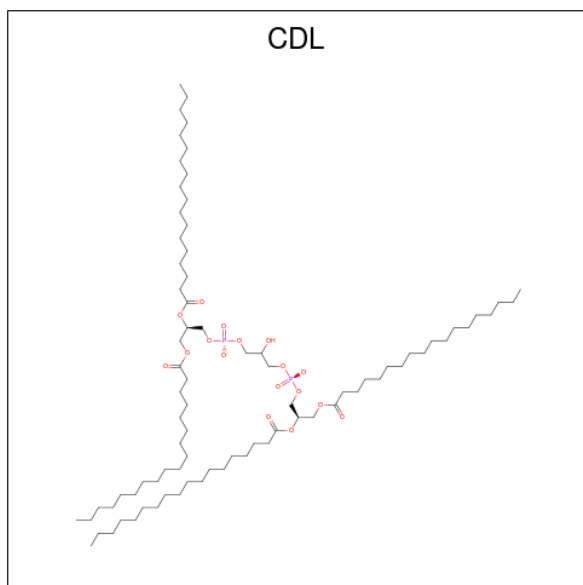
Mol	Chain	Residues	Atoms						AltConf
51	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

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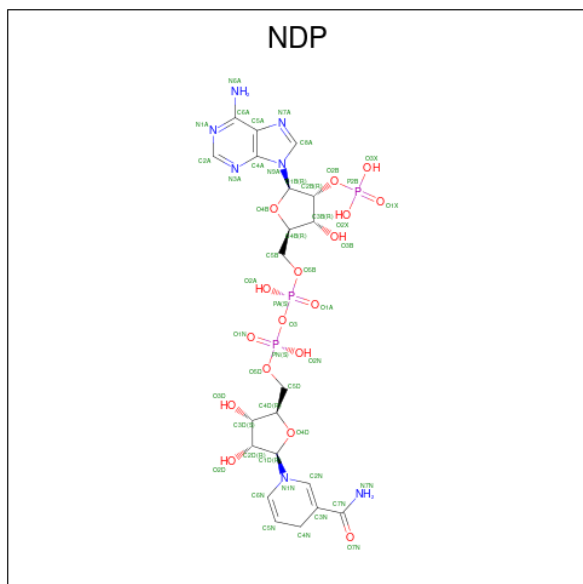
Mol	Chain	Residues	Atoms						AltConf
51	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 52 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



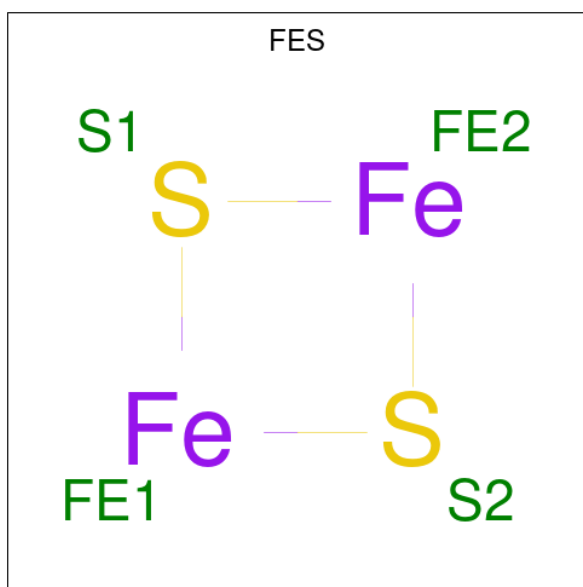
Mol	Chain	Residues	Atoms				AltConf
52	I	1	Total	C	O	P	0
			51	32	17	2	
52	V	1	Total	C	O	P	0
			94	75	17	2	
52	a	1	Total	C	O	P	0
			100	81	17	2	
52	k	1	Total	C	O	P	0
			100	81	17	2	
52	l	1	Total	C	O	P	0
			99	80	17	2	
52	l	1	Total	C	O	P	0
			100	81	17	2	
52	o	1	Total	C	O	P	0
			100	81	17	2	
52	r	1	Total	C	O	P	0
			100	81	17	2	
52	s	1	Total	C	O	P	0
			89	70	17	2	
52	u	1	Total	C	O	P	0
			55	36	17	2	

- Molecule 53 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
53	J	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 54 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
54	M	1	Total	Fe	S	0
			4	2	2	
54	O	1	Total	Fe	S	0
			4	2	2	

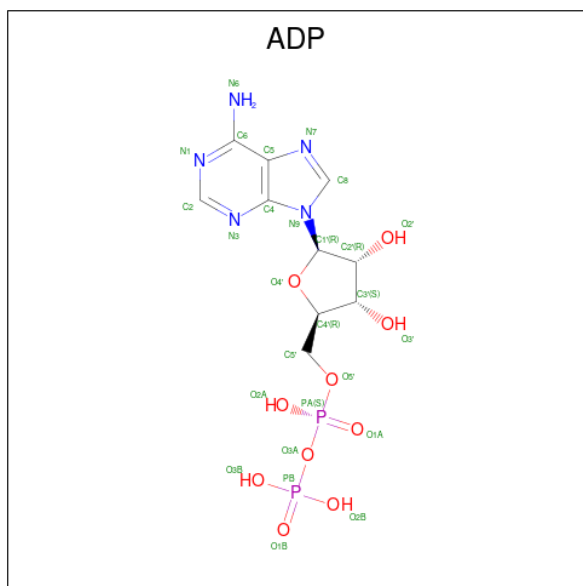
- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
55	M	1	Total	Mg	0
			1	1	

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
56	T	1	Total	Zn	0
			1	1	

- Molecule 57 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

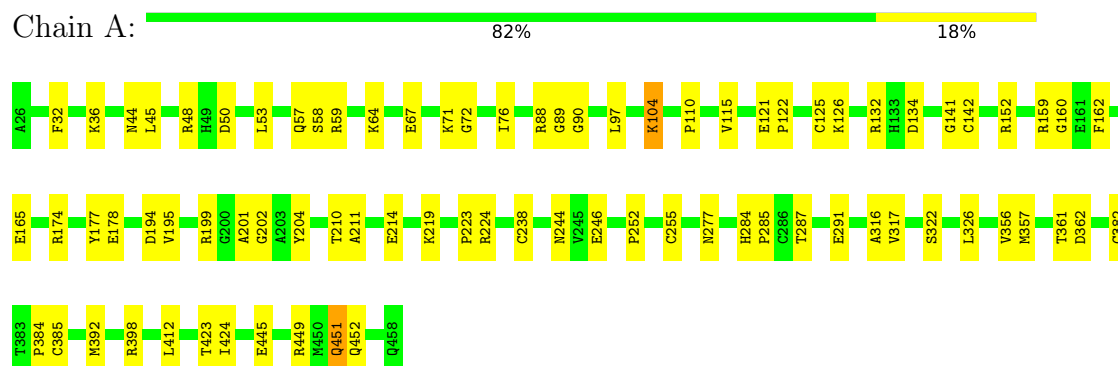


Mol	Chain	Residues	Atoms					AltConf
57	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

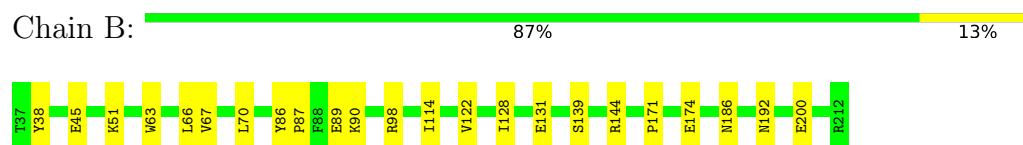
3 Residue-property plots [i](#)

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.

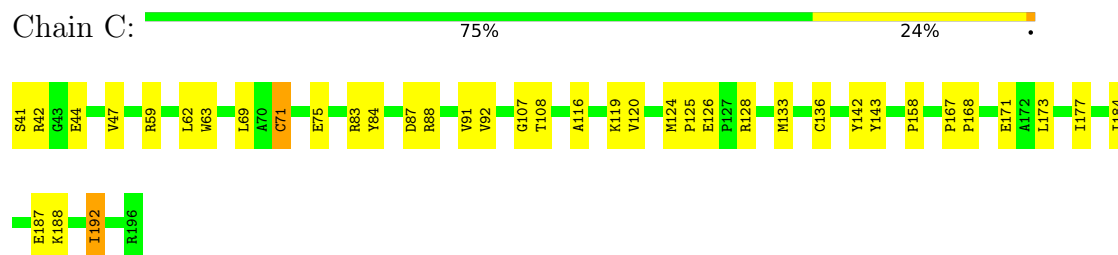
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



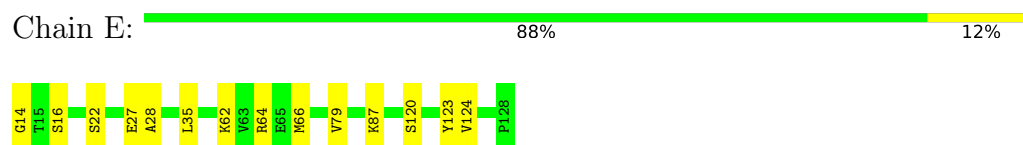
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

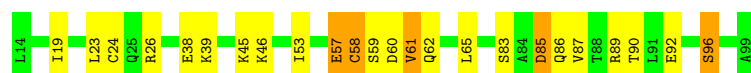


- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain F:  72% 22% 6%



- Molecule 6: Acyl carrier protein

Chain G:  80% 20%



- Molecule 6: Acyl carrier protein

Chain X:  75% 24% .



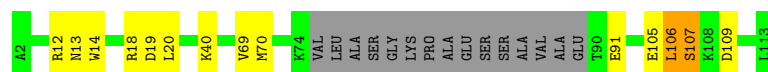
- Molecule 7: Complex I subunit B13

Chain H:  78% 22%



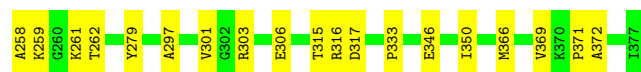
- Molecule 8: Complex I-B14.5a

Chain I:  74% 11% . 13%



- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial

Chain J:  85% 15%



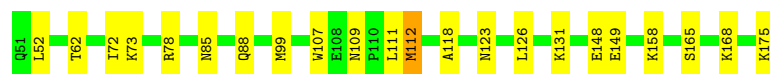
- Molecule 10: Complex I-9kD

Chain K:  67% 33%



- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain L:  82% 17%



- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain M:  83% 17%



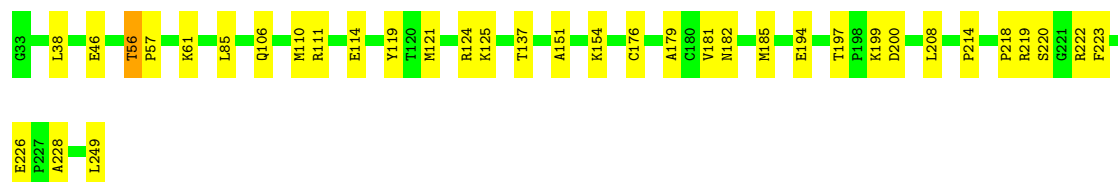
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain N:  83% 17%



- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain O:  83% 16%



- Molecule 15: Complex I-30kD

Chain P:  85% 15%



- Molecule 16: Complex I-49kD

R418	T198	A34
S439	F199	W37
V447	F200	Q38
T451	R207	P39
G452	E208	W43
T453	E212	F47
F458	F213	A50
D462	Y214	V51
R463	E215	M52
	R216	
	V217	D74
	R221	T75
	M222	L76
	H223	F84
	A224	Q87
	P229	L95
	L241	R96
	D242	L97
	D243	V106
	E260	G114
	R271	R118
	E281	P134
	L302	D137
	R303	M144
	D309	Q149
	E335	A150
	Q339	V155
	L348	E156
	A351	K157
	M375	R171
	E376	T178
	L379	L181
	K383	N182
	L384	M185
	Y385	T188
	L400	T189
	E401	L192
	K404	M197
	G405	
	E406	

-
- | Category | Value (approximate) |
|----------|---------------------|
| M1 | 1.0 |
| E4 | 0.8 |
| P7 | 0.8 |
| M12 | 0.8 |
| P19 | 0.8 |
| H27 | 0.8 |
| N31 | 0.8 |
| K36 | 0.8 |
| Y43 | 0.8 |
| I54 | 1.2 |
| L66 | 1.2 |
| I69 | 0.8 |
| D70 | 0.8 |

-
- | Category | Count |
|----------|-------|
| G28 | 1 |
| D47 | 1 |
| R51 | 1 |
| R52 | 1 |
| V53 | 1 |
| R54 | 1 |
| N63 | 1 |
| E64 | 1 |
| D69 | 1 |
| E73 | 1 |
| V79 | 1 |
| I84 | 1 |
| P121 | 1 |
| H122 | 1 |
| H123 | 1 |

-

- | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|
| A2 | K3 | T4 | T16 | E17 | R20 | T26 | G29 | A38 | V53 | T56 | S63 | G67 | A68 | D86 | P87 | C95 | L101 | T105 | R106 | I110 | C115 | L120 | A123 | L124 | M127 | V141 |
|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|

- [illegible]

- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain Y:  82% 16%



- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain Z:  88% 11%



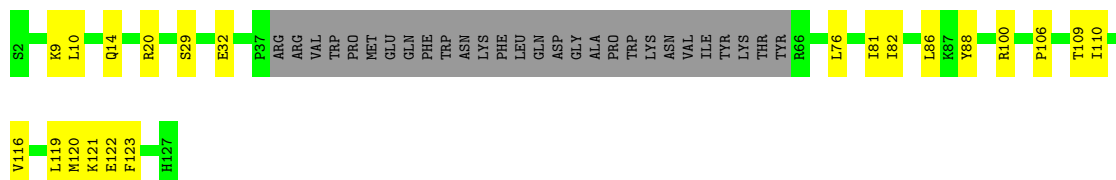
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain a:  85% 14%



- Molecule 25: Complex I-B17

Chain b:  61% 17% 22%



- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c:  86% 13%



- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

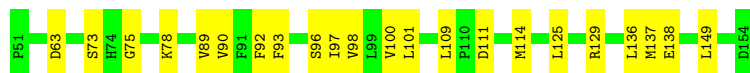
Chain d:  80% 19%





- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e: 79% 21%



- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain f: 86% 14%



- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g: 89% 11%



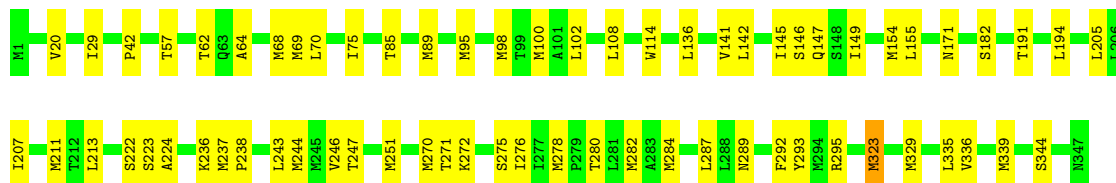
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain h: 84% 16%



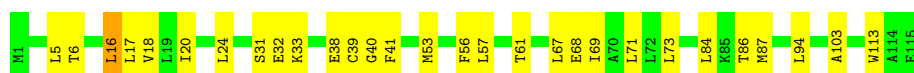
- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

Chain i: 81% 19%



- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

Chain j: 75% 24%



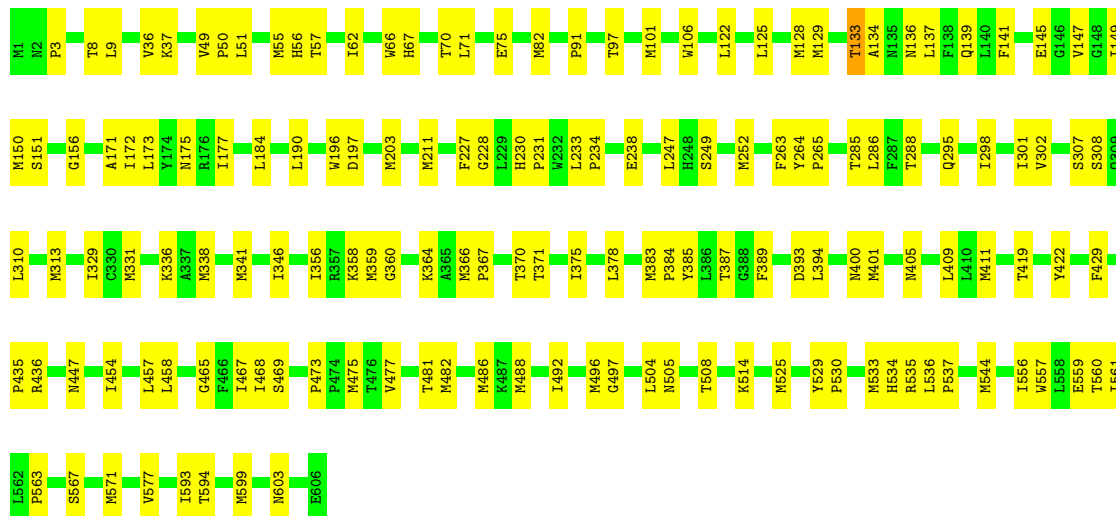
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

Chain k:  72% 28%



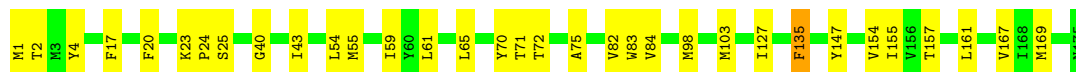
- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

Chain l:  75% 25%



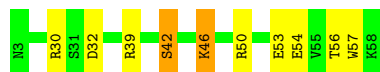
- Molecule 36: NADH-ubiquinone oxidoreductase chain 6

Chain m:  81% 18% .



- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain n:  82% 14% .



- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain o:  86% 14%



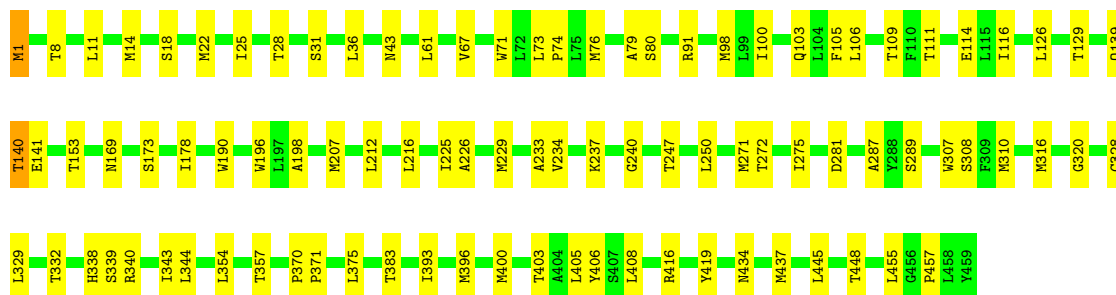
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain p:  83% 17%



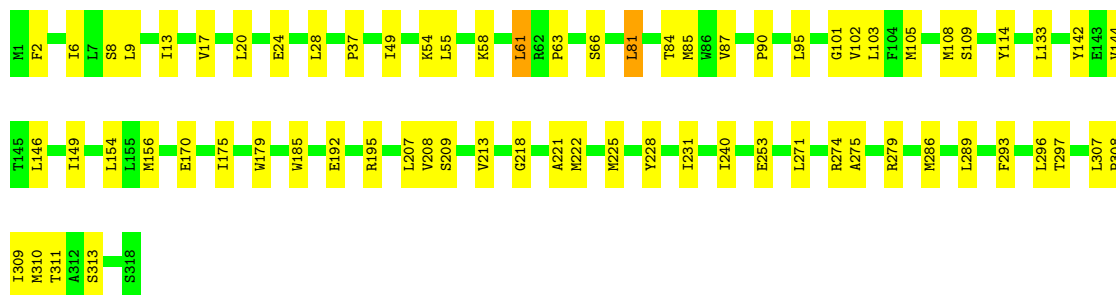
- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain r:  80% 20%



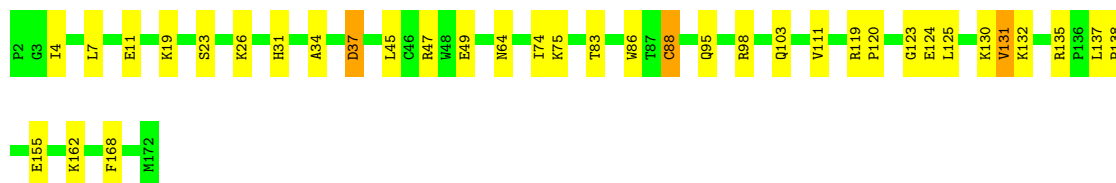
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain s:  78% 21% .



- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u:  79% 19% .

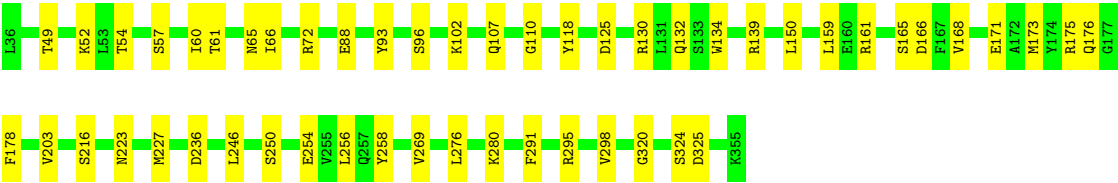
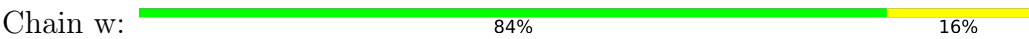


- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v:  75% 24% .



● Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	124399	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, NDP, MG, ZN, FES, 2MR, ADP, 8Q1, PLX, UQ, SF4, NAI, FMN, PEE

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	0.17	0/3406	0.32	0/4603
2	B	0.22	0/1443	0.34	0/1952
3	C	0.22	0/1279	0.32	0/1730
4	E	0.17	0/991	0.30	0/1335
5	F	0.20	0/698	0.49	3/940 (0.3%)
6	G	0.19	0/702	0.45	0/952
6	X	0.16	0/716	0.34	0/968
7	H	0.19	0/929	0.35	0/1258
8	I	0.20	0/798	0.54	2/1079 (0.2%)
9	J	0.18	0/2828	0.31	0/3834
10	K	0.14	0/377	0.24	0/509
11	L	0.20	0/1039	0.31	0/1403
12	M	0.19	0/5384	0.35	0/7295
13	N	0.20	0/1245	0.40	0/1694
14	O	0.16	0/1711	0.33	0/2328
15	P	0.21	0/1789	0.33	0/2436
16	Q	0.22	0/3538	0.36	0/4796
17	S	0.21	0/581	0.41	0/781
18	T	0.17	0/755	0.30	0/1018
19	U	0.15	0/664	0.31	0/912
20	V	0.24	0/1042	0.41	0/1411
21	W	0.19	0/1198	0.32	0/1617
22	Y	0.15	0/610	0.29	0/836
23	Z	0.14	0/660	0.29	0/892
24	a	0.19	0/1184	0.31	0/1603
25	b	0.17	0/844	0.33	0/1149
26	c	0.18	0/1371	0.36	0/1875
27	d	0.20	0/1494	0.51	6/2015 (0.3%)
28	e	0.17	0/891	0.33	0/1210
29	f	0.18	0/386	0.35	0/523
30	g	0.17	0/1031	0.31	0/1394
31	h	0.17	0/889	0.32	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.21	0/2773	0.38	0/3768
33	j	0.23	0/938	0.41	0/1281
34	k	0.22	0/759	0.37	0/1029
35	l	0.18	0/4929	0.35	0/6704
36	m	0.20	0/1328	0.36	0/1804
37	n	0.14	0/491	0.28	0/663
38	o	0.16	0/1092	0.30	0/1481
39	p	0.17	0/1586	0.31	0/2150
40	r	0.21	0/3723	0.36	0/5078
41	s	0.22	0/2581	0.39	0/3529
42	u	0.17	0/1436	0.36	0/1938
43	v	0.15	0/1083	0.31	0/1448
44	w	0.16	0/2642	0.31	0/3580
All	All	0.19	0/67834	0.35	11/91991 (0.0%)

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
8	I	106	LEU	N-CA-C	7.86	121.41	109.62
8	I	107	SER	N-CA-C	7.71	120.66	111.02
27	d	13	PRO	CA-C-N	7.69	127.40	119.56
27	d	13	PRO	C-N-CA	7.69	127.40	119.56
27	d	12	GLU	CA-C-N	6.57	127.14	120.38

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	3330	0	3292	57	0
2	B	1412	0	1363	19	0
3	C	1248	0	1254	29	0
4	E	967	0	971	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	687	0	700	16	0
6	G	690	0	669	13	0
6	X	704	0	695	14	0
7	H	910	0	950	15	0
8	I	780	0	808	14	0
9	J	2751	0	2773	31	0
10	K	366	0	338	12	0
11	L	1016	0	1016	17	0
12	M	5296	0	5326	72	0
13	N	1204	0	1162	18	0
14	O	1671	0	1673	29	0
15	P	1738	0	1693	21	0
16	Q	3459	0	3396	49	0
17	S	566	0	561	13	0
18	T	741	0	702	7	0
19	U	643	0	642	7	0
20	V	1021	0	1027	16	0
21	W	1167	0	1155	32	0
22	Y	584	0	529	11	0
23	Z	641	0	620	9	0
24	a	1151	0	1164	17	0
25	b	819	0	835	18	0
26	c	1315	0	1208	19	0
27	d	1461	0	1429	26	0
28	e	867	0	817	20	0
29	f	378	0	356	3	0
30	g	1000	0	994	10	0
31	h	867	0	873	15	0
32	i	2710	0	2874	52	0
33	j	914	0	951	26	0
34	k	748	0	799	24	0
35	l	4800	0	4939	111	0
36	m	1295	0	1263	31	0
37	n	479	0	486	8	0
38	o	1062	0	1072	12	0
39	p	1530	0	1466	22	0
40	r	3631	0	3839	68	0
41	s	2508	0	2607	54	0
42	u	1398	0	1374	29	0
43	v	1059	0	1029	25	0
44	w	2582	0	2531	29	0
45	A	8	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	B	16	0	0	0	0
45	C	8	0	0	2	0
45	M	16	0	0	0	0
46	A	31	0	19	3	0
47	A	44	0	27	6	0
48	B	51	0	82	4	0
48	C	47	0	71	2	0
48	V	40	0	54	3	0
48	W	41	0	59	1	0
48	i	47	0	71	4	0
48	j	92	0	141	5	0
48	l	97	0	151	11	0
48	r	51	0	82	4	0
49	C	52	0	88	4	0
49	J	52	0	88	5	0
49	a	52	0	88	1	0
49	g	52	0	88	4	0
49	j	52	0	88	2	0
49	r	104	0	176	10	0
50	C	38	0	47	5	0
50	J	33	0	39	6	0
51	G	35	0	0	0	0
51	X	35	0	0	2	0
52	I	51	0	46	1	0
52	V	94	0	138	5	0
52	a	100	0	156	8	0
52	k	100	0	156	11	0
52	l	199	0	307	15	0
52	o	100	0	156	5	0
52	r	100	0	156	10	0
52	s	89	0	125	5	0
52	u	55	0	54	3	0
53	J	48	0	24	1	0
54	M	4	0	0	0	0
54	O	4	0	0	0	0
55	M	1	0	0	0	0
56	T	1	0	0	0	0
57	w	27	0	11	2	0
All	All	68233	0	69009	1024	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 7.

The worst 5 of 1024 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)
20:V:95:CYS:SG	20:V:115:CYS:SG	1.39	1.39
47:A:503:NAI:C1B	47:A:503:NAI:O4B	1.63	1.22
53:J:401:NDP:O4D	53:J:401:NDP:C4D	1.68	1.12
20:V:110:ILE:HD13	48:V:202:PEE:H49	1.51	0.90
32:i:68:MET:HE1	34:k:37:MET:HE2	1.58	0.84

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 PDB entries followed by that with respect to all EM entries.

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	431/433 (100%)	420 (97%)	11 (3%)	0	100	100
2	B	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
3	C	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
4	E	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
5	F	84/86 (98%)	78 (93%)	6 (7%)	0	100	100
6	G	86/88 (98%)	81 (94%)	4 (5%)	1 (1%)	10	34
6	X	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
7	H	110/112 (98%)	104 (94%)	6 (6%)	0	100	100
8	I	93/112 (83%)	83 (89%)	10 (11%)	0	100	100
9	J	340/342 (99%)	325 (96%)	14 (4%)	1 (0%)	36	66
10	K	41/43 (95%)	39 (95%)	2 (5%)	0	100	100
11	L	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
12	M	688/690 (100%)	666 (97%)	22 (3%)	0	100	100
13	N	142/144 (99%)	139 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	O	215/217 (99%)	205 (95%)	10 (5%)	0	100	100
15	P	206/208 (99%)	199 (97%)	7 (3%)	0	100	100
16	Q	427/430 (99%)	412 (96%)	15 (4%)	0	100	100
17	S	68/70 (97%)	62 (91%)	6 (9%)	0	100	100
18	T	94/96 (98%)	91 (97%)	3 (3%)	0	100	100
19	U	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
20	V	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
21	W	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
22	Y	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
23	Z	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
24	a	136/138 (99%)	133 (98%)	3 (2%)	0	100	100
25	b	94/126 (75%)	88 (94%)	6 (6%)	0	100	100
26	c	154/156 (99%)	143 (93%)	11 (7%)	0	100	100
27	d	173/175 (99%)	172 (99%)	1 (1%)	0	100	100
28	e	102/104 (98%)	94 (92%)	8 (8%)	0	100	100
29	f	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
30	g	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
31	h	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
32	i	345/347 (99%)	329 (95%)	16 (5%)	0	100	100
33	j	113/115 (98%)	109 (96%)	3 (3%)	1 (1%)	14	41
34	k	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
35	l	604/606 (100%)	578 (96%)	26 (4%)	0	100	100
36	m	173/175 (99%)	161 (93%)	11 (6%)	1 (1%)	21	51
37	n	54/56 (96%)	54 (100%)	0	0	100	100
38	o	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
39	p	176/178 (99%)	169 (96%)	6 (3%)	1 (1%)	21	51
40	r	457/459 (100%)	450 (98%)	7 (2%)	0	100	100
41	s	316/318 (99%)	304 (96%)	11 (4%)	1 (0%)	36	66
42	u	169/171 (99%)	165 (98%)	4 (2%)	0	100	100
43	v	122/124 (98%)	117 (96%)	5 (4%)	0	100	100
44	w	318/320 (99%)	306 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	8174/8312 (98%)	7861 (96%)	307 (4%)	6 (0%)	49 77

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	G	133	ILE
9	J	38	HIS
41	s	208	VAL
36	m	25	SER
39	p	174	PRO

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 PDB entries followed by that with respect to all EM entries.

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	346/346 (100%)	342 (99%)	4 (1%)	63 87
2	B	151/151 (100%)	149 (99%)	2 (1%)	61 86
3	C	132/132 (100%)	129 (98%)	3 (2%)	44 78
4	E	106/107 (99%)	106 (100%)	0	100 100
5	F	75/76 (99%)	70 (93%)	5 (7%)	15 42
6	G	75/81 (93%)	75 (100%)	0	100 100
6	X	79/81 (98%)	77 (98%)	2 (2%)	42 76
7	H	99/99 (100%)	98 (99%)	1 (1%)	68 88
8	I	87/97 (90%)	87 (100%)	0	100 100
9	J	296/296 (100%)	295 (100%)	1 (0%)	86 95
10	K	42/42 (100%)	40 (95%)	2 (5%)	23 56
11	L	113/113 (100%)	111 (98%)	2 (2%)	51 82
12	M	580/580 (100%)	572 (99%)	8 (1%)	59 85
13	N	130/130 (100%)	129 (99%)	1 (1%)	73 90
14	O	183/183 (100%)	179 (98%)	4 (2%)	45 78
15	P	190/190 (100%)	186 (98%)	4 (2%)	47 79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	Q	370/370 (100%)	364 (98%)	6 (2%)	55	83
17	S	57/58 (98%)	55 (96%)	2 (4%)	32	67
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	69/69 (100%)	69 (100%)	0	100	100
20	V	101/101 (100%)	98 (97%)	3 (3%)	36	72
21	W	122/123 (99%)	118 (97%)	4 (3%)	33	69
22	Y	62/62 (100%)	60 (97%)	2 (3%)	34	70
23	Z	62/62 (100%)	60 (97%)	2 (3%)	34	70
24	a	121/121 (100%)	118 (98%)	3 (2%)	42	76
25	b	90/119 (76%)	88 (98%)	2 (2%)	45	78
26	c	141/141 (100%)	139 (99%)	2 (1%)	59	85
27	d	155/155 (100%)	152 (98%)	3 (2%)	50	81
28	e	96/96 (100%)	96 (100%)	0	100	100
29	f	36/45 (80%)	35 (97%)	1 (3%)	38	73
30	g	108/108 (100%)	107 (99%)	1 (1%)	70	89
31	h	93/93 (100%)	90 (97%)	3 (3%)	34	70
32	i	311/311 (100%)	306 (98%)	5 (2%)	55	83
33	j	100/100 (100%)	95 (95%)	5 (5%)	22	54
34	k	85/85 (100%)	85 (100%)	0	100	100
35	l	537/540 (99%)	532 (99%)	5 (1%)	70	89
36	m	130/141 (92%)	129 (99%)	1 (1%)	73	90
37	n	53/53 (100%)	50 (94%)	3 (6%)	18	49
38	o	113/113 (100%)	112 (99%)	1 (1%)	70	89
39	p	158/159 (99%)	156 (99%)	2 (1%)	61	86
40	r	410/410 (100%)	402 (98%)	8 (2%)	48	80
41	s	275/275 (100%)	268 (98%)	7 (2%)	42	76
42	u	153/153 (100%)	147 (96%)	6 (4%)	28	64
43	v	111/111 (100%)	110 (99%)	1 (1%)	70	89
44	w	281/283 (99%)	277 (99%)	4 (1%)	59	85
All	All	7163/7240 (99%)	7042 (98%)	121 (2%)	52	83

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	Z	34	GLU
42	u	23	SER
31	h	80	LYS
41	s	296	LEU
44	w	107	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
39	p	51	HIS
39	p	141	GLN
42	u	65	GLN
16	Q	162	GLN
16	Q	92	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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
16	2MR	Q	118	16	10,12,13	2.02	2 (20%)	5,13,15	6.32	3 (60%)

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
16	2MR	Q	118	16	-	3/10/13/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.57	1.46	1.34
16	Q	118	2MR	CQ2-NH2	-2.13	1.41	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	118	2MR	NE-CZ-NH2	12.93	131.33	119.48
16	Q	118	2MR	CD-NE-CZ	4.66	132.12	123.36
16	Q	118	2MR	CQ2-NH2-CZ	3.06	130.21	123.65

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	Q	118	2MR	NE-CD-CG-CB
16	Q	118	2MR	CA-CB-CG-CD
16	Q	118	2MR	CG-CD-NE-CZ

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Q	118	2MR	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 2 are monoatomic - leaving 43 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
57	ADP	w	401	-	28,29,29	3.16	9 (32%)	43,45,45	1.92	10 (23%)
48	PEE	W	201	-	40,40,50	1.17	5 (12%)	43,45,55	0.94	2 (4%)
52	CDL	k	101	-	99,99,99	1.11	8 (8%)	105,111,111	0.87	4 (3%)
45	SF4	C	301	3	0,12,12	-	-	-	-	-
49	PLX	J	403	-	51,51,51	1.19	3 (5%)	53,59,59	0.62	1 (1%)
49	PLX	r	503	-	51,51,51	1.20	4 (7%)	53,59,59	0.62	1 (1%)
52	CDL	u	201	-	54,54,99	1.39	9 (16%)	60,66,111	1.09	4 (6%)
52	CDL	l	702	-	99,99,99	1.11	9 (9%)	105,111,111	0.88	4 (3%)
52	CDL	a	201	-	99,99,99	1.11	8 (8%)	105,111,111	0.86	4 (3%)
52	CDL	o	201	-	99,99,99	1.11	8 (8%)	105,111,111	0.88	4 (3%)
45	SF4	B	302	2	0,12,12	-	-	-	-	-
54	FES	M	803	12	0,4,4	-	-	-	-	-
48	PEE	B	303	-	50,50,50	1.18	6 (12%)	53,55,55	1.06	2 (3%)
48	PEE	r	501	-	50,50,50	1.17	6 (12%)	53,55,55	1.03	2 (3%)
52	CDL	l	701	-	98,98,99	1.11	8 (8%)	104,110,111	0.92	4 (3%)
50	UQ	C	304	-	38,38,63	3.60	12 (31%)	48,49,79	2.87	18 (37%)
52	CDL	V	201	-	93,93,99	1.13	9 (9%)	99,105,111	0.90	5 (5%)
45	SF4	M	801	12	0,12,12	-	-	-	-	-
48	PEE	i	401	-	46,46,50	1.21	6 (13%)	49,51,55	1.03	2 (4%)
54	FES	O	301	14	0,4,4	-	-	-	-	-
48	PEE	j	202	-	40,40,50	1.16	5 (12%)	43,45,55	1.13	3 (6%)
48	PEE	C	302	-	46,46,50	1.22	6 (13%)	49,51,55	1.01	2 (4%)
48	PEE	V	202	-	39,39,50	1.33	6 (15%)	42,44,55	1.11	3 (7%)
45	SF4	M	802	12	0,12,12	-	-	-	-	-
53	NDP	J	401	-	51,52,52	4.28	24 (47%)	71,80,80	2.21	13 (18%)
45	SF4	B	301	2	0,12,12	-	-	-	-	-
48	PEE	l	703	-	50,50,50	1.18	6 (12%)	53,55,55	0.95	2 (3%)
51	8Q1	X	201	6	32,34,34	1.62	6 (18%)	39,43,43	1.63	7 (17%)
48	PEE	l	704	-	45,45,50	1.23	6 (13%)	48,50,55	1.01	2 (4%)
52	CDL	I	201	-	50,50,99	1.41	8 (16%)	56,62,111	1.13	4 (7%)
49	PLX	g	201	-	51,51,51	1.19	3 (5%)	53,59,59	0.68	1 (1%)
52	CDL	s	401	-	88,88,99	1.15	7 (7%)	94,100,111	0.96	4 (4%)
51	8Q1	G	201	6	32,34,34	1.60	5 (15%)	39,43,43	1.75	6 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	PLX	r	502	-	51,51,51	1.20	5 (9%)	53,59,59	0.64	1 (1%)
49	PLX	a	202	-	51,51,51	1.22	5 (9%)	53,59,59	0.58	1 (1%)
50	UQ	J	402	-	33,33,63	3.55	11 (33%)	42,43,79	2.62	14 (33%)
52	CDL	r	504	-	99,99,99	1.09	8 (8%)	105,111,111	0.91	4 (3%)
47	NAI	A	503	-	47,48,48	4.00	22 (46%)	64,73,73	1.71	12 (18%)
49	PLX	C	303	-	51,51,51	1.20	5 (9%)	53,59,59	0.66	1 (1%)
45	SF4	A	501	1	0,12,12	-	-	-	-	-
49	PLX	j	203	-	51,51,51	1.20	4 (7%)	53,59,59	0.65	1 (1%)
46	FMN	A	502	-	33,33,33	1.09	2 (6%)	48,50,50	1.30	8 (16%)
48	PEE	j	201	-	50,50,50	1.17	6 (12%)	53,55,55	0.96	2 (3%)

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
57	ADP	w	401	-	-	5/16/32/32	0/3/3/3
48	PEE	W	201	-	-	19/44/44/54	-
52	CDL	k	101	-	-	61/110/110/110	-
45	SF4	C	301	3	-	-	0/6/5/5
49	PLX	J	403	-	-	34/55/55/55	-
49	PLX	r	503	-	-	30/55/55/55	-
52	CDL	u	201	-	-	35/65/65/110	-
52	CDL	l	702	-	-	56/110/110/110	-
52	CDL	a	201	-	-	49/110/110/110	-
52	CDL	o	201	-	-	65/110/110/110	-
45	SF4	B	302	2	-	-	0/6/5/5
54	FES	M	803	12	-	-	0/1/1/1
48	PEE	B	303	-	-	26/54/54/54	-
48	PEE	r	501	-	-	31/54/54/54	-
52	CDL	l	701	-	-	61/109/109/110	-
50	UQ	C	304	-	-	14/33/57/87	0/1/1/1
52	CDL	V	201	-	-	58/104/104/110	-
45	SF4	M	801	12	-	-	0/6/5/5
48	PEE	i	401	-	-	20/50/50/54	-
54	FES	O	301	14	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PEE	j	202	-	-	20/44/44/54	-
48	PEE	C	302	-	-	26/50/50/54	-
48	PEE	V	202	-	-	26/43/43/54	-
53	NDP	J	401	-	-	11/34/77/77	0/5/5/5
45	SF4	M	802	12	-	-	0/6/5/5
51	8Q1	X	201	6	-	14/41/41/41	-
48	PEE	l	703	-	-	30/54/54/54	-
45	SF4	B	301	2	-	-	0/6/5/5
48	PEE	l	704	-	-	27/49/49/54	-
52	CDL	I	201	-	-	30/61/61/110	-
49	PLX	g	201	-	-	31/55/55/55	-
52	CDL	s	401	-	-	47/99/99/110	-
51	8Q1	G	201	6	-	13/41/41/41	-
49	PLX	r	502	-	-	32/55/55/55	-
49	PLX	a	202	-	-	30/55/55/55	-
50	UQ	J	402	-	-	10/27/51/87	0/1/1/1
52	CDL	r	504	-	-	64/110/110/110	-
47	NAI	A	503	-	-	8/29/72/72	0/5/5/5
49	PLX	C	303	-	-	30/55/55/55	-
45	SF4	A	501	1	-	-	0/6/5/5
49	PLX	j	203	-	-	27/55/55/55	-
46	FMN	A	502	-	-	3/18/18/18	0/3/3/3
48	PEE	j	201	-	-	26/54/54/54	-

The worst 5 of 260 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	J	401	NDP	C3B-C2B	-13.23	1.24	1.53
53	J	401	NDP	O4D-C4D	10.74	1.68	1.45
47	A	503	NAI	C3D-C4D	-10.36	1.26	1.53
53	J	401	NDP	C3D-C4D	-10.05	1.27	1.53
50	J	402	UQ	C18-C19	10.00	1.56	1.33

The worst 5 of 158 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	C	304	UQ	C7-C8-C9	-8.10	112.88	126.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	J	401	NDP	C3N-C2N-N1N	-7.64	111.98	123.20
50	J	402	UQ	C7-C8-C9	-7.64	113.67	126.83
53	J	401	NDP	C1D-N1N-C2N	-7.05	109.53	121.14
51	G	201	8Q1	C6-C1-S44	6.98	121.72	113.40

There are no chirality outliers.

5 of 1069 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
48	B	303	PEE	C11-C10-O2-C2
48	B	303	PEE	O4-C10-O2-C2
48	C	302	PEE	C11-C10-O2-C2

There are no ring outliers.

36 monomers are involved in 144 short contacts:

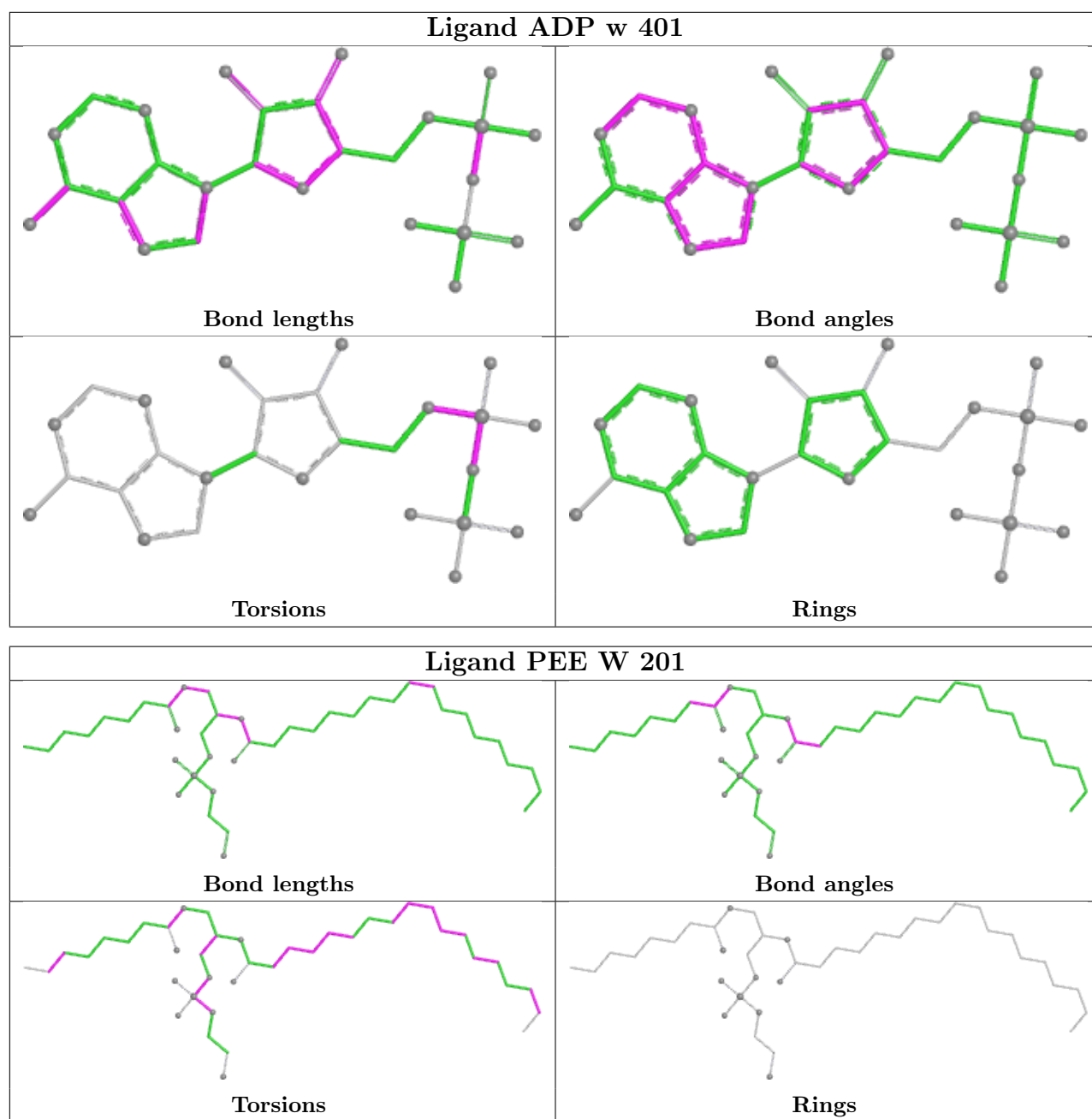
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	w	401	ADP	2	0
48	W	201	PEE	1	0
52	k	101	CDL	11	0
45	C	301	SF4	2	0
49	J	403	PLX	5	0
49	r	503	PLX	5	0
52	u	201	CDL	3	0
52	l	702	CDL	4	0
52	a	201	CDL	8	0
52	o	201	CDL	5	0
48	B	303	PEE	4	0
48	r	501	PEE	4	0
52	l	701	CDL	11	0
50	C	304	UQ	5	0
52	V	201	CDL	5	0
48	i	401	PEE	4	0
48	j	202	PEE	2	0
48	C	302	PEE	2	0
48	V	202	PEE	3	0
53	J	401	NDP	1	0
48	l	703	PEE	4	0
51	X	201	8Q1	2	0

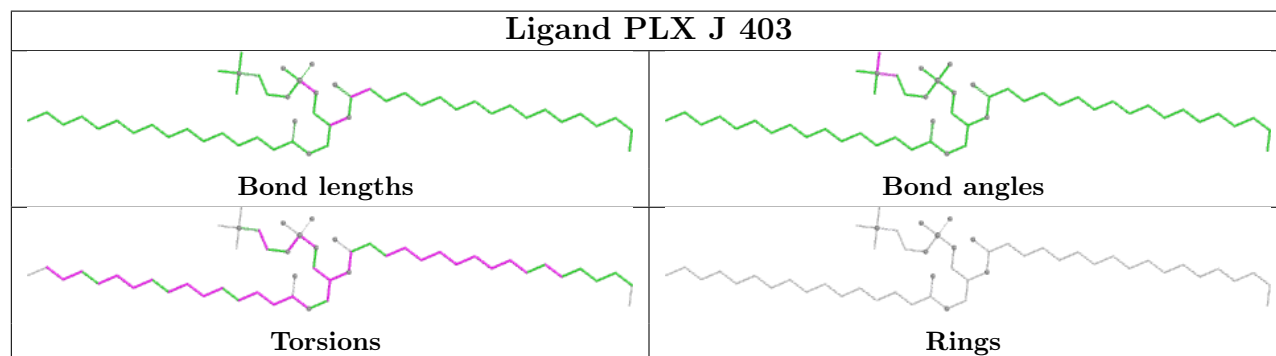
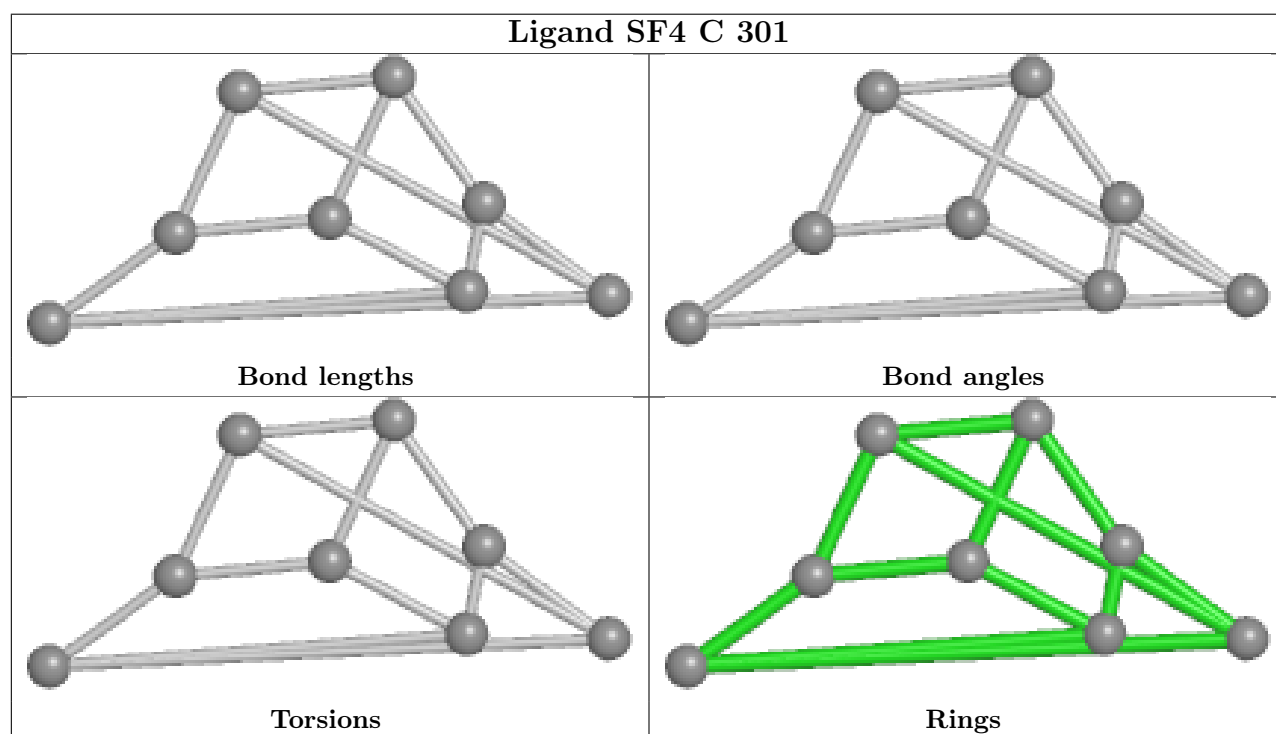
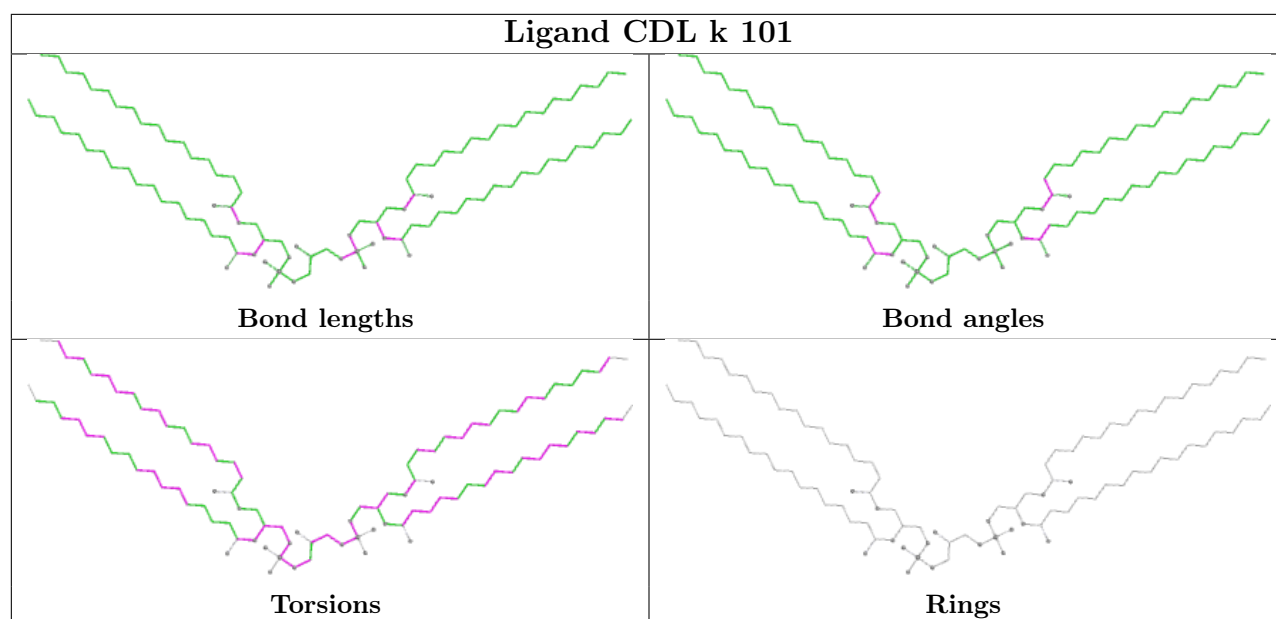
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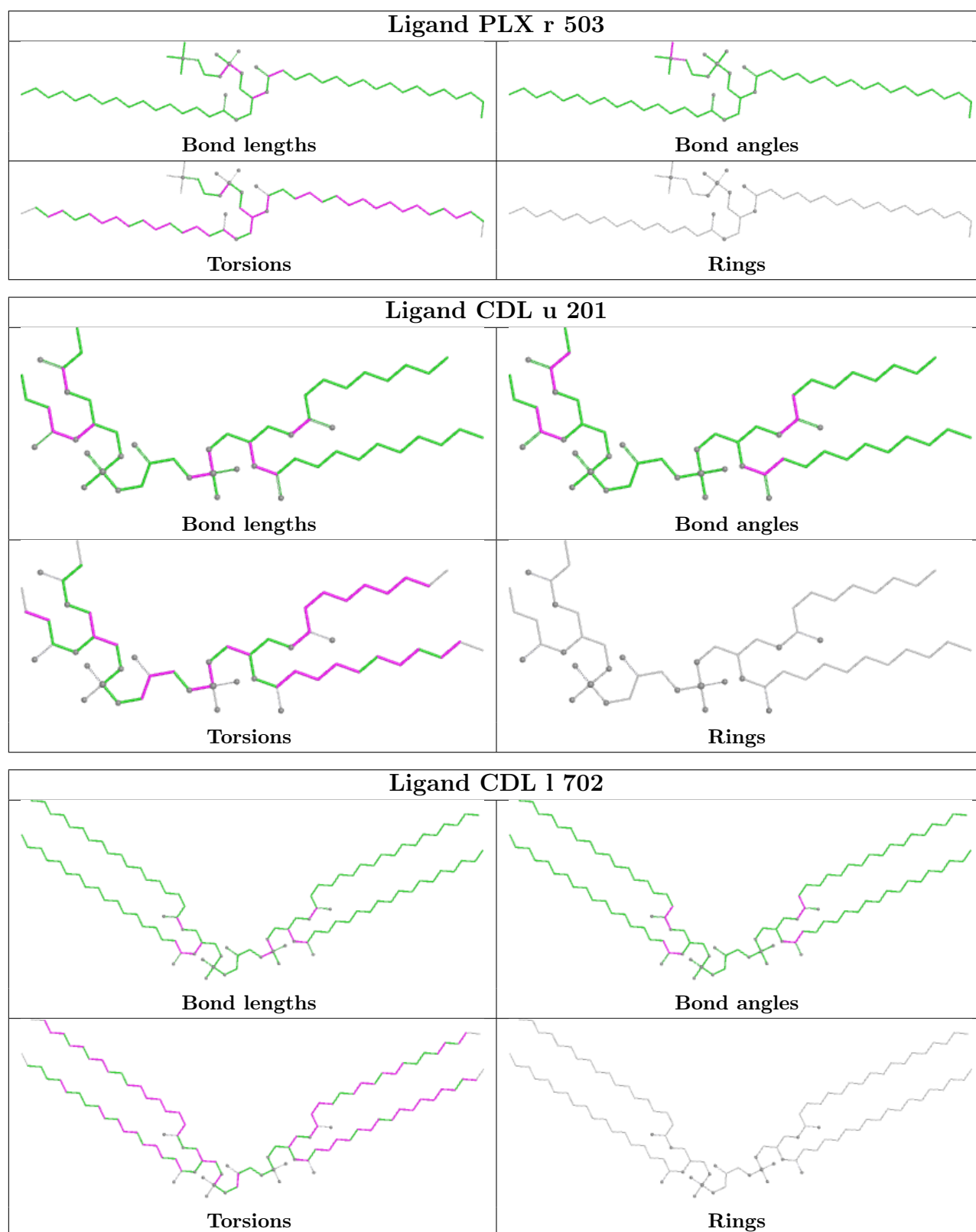
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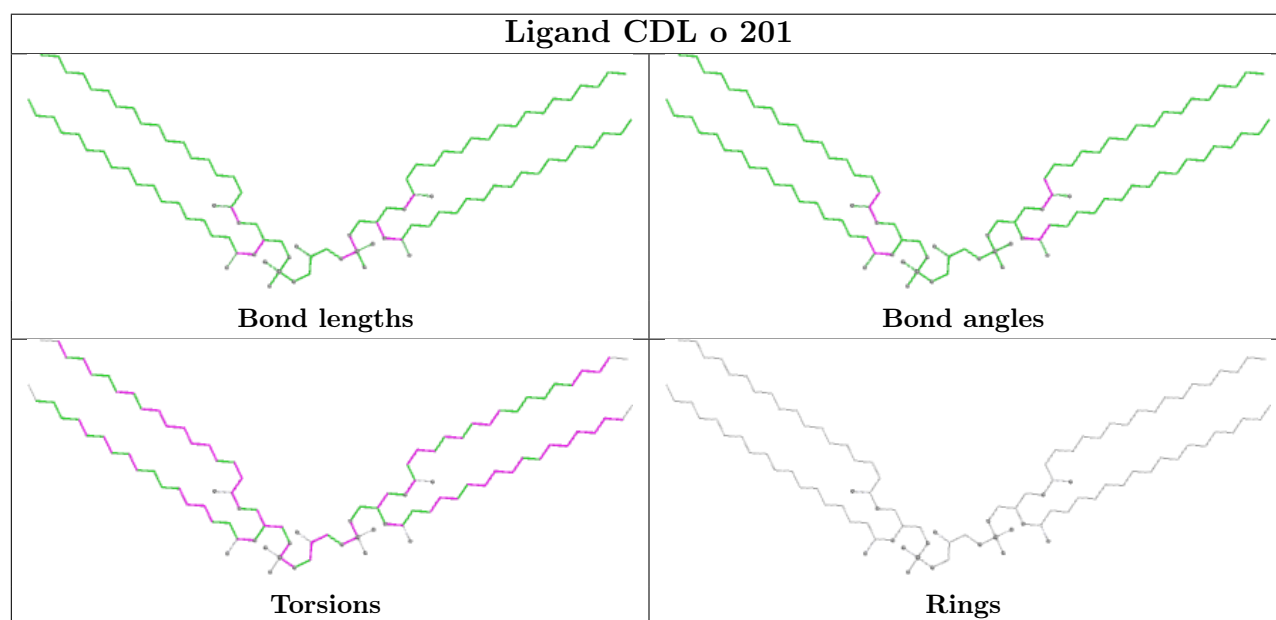
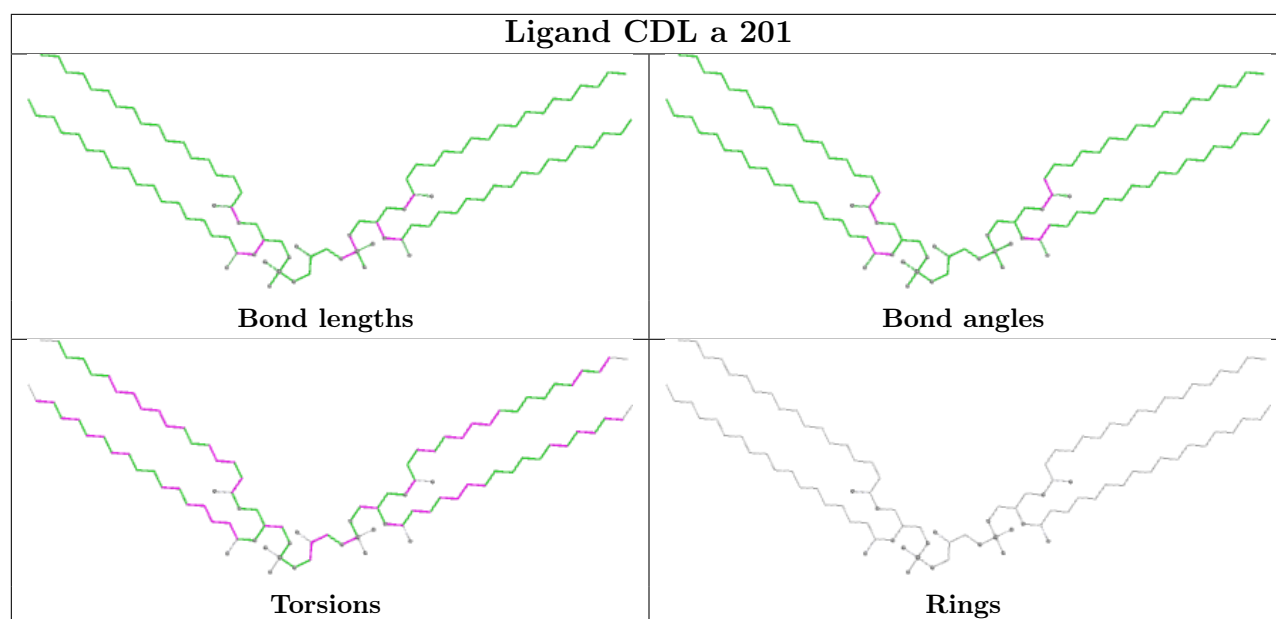
Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	l	704	PEE	7	0
52	I	201	CDL	1	0
49	g	201	PLX	4	0
52	s	401	CDL	5	0
49	r	502	PLX	5	0
49	a	202	PLX	1	0
50	J	402	UQ	6	0
52	r	504	CDL	10	0
47	A	503	NAI	6	0
49	C	303	PLX	4	0
45	A	501	SF4	2	0
49	j	203	PLX	2	0
46	A	502	FMN	3	0
48	j	201	PEE	3	0

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.

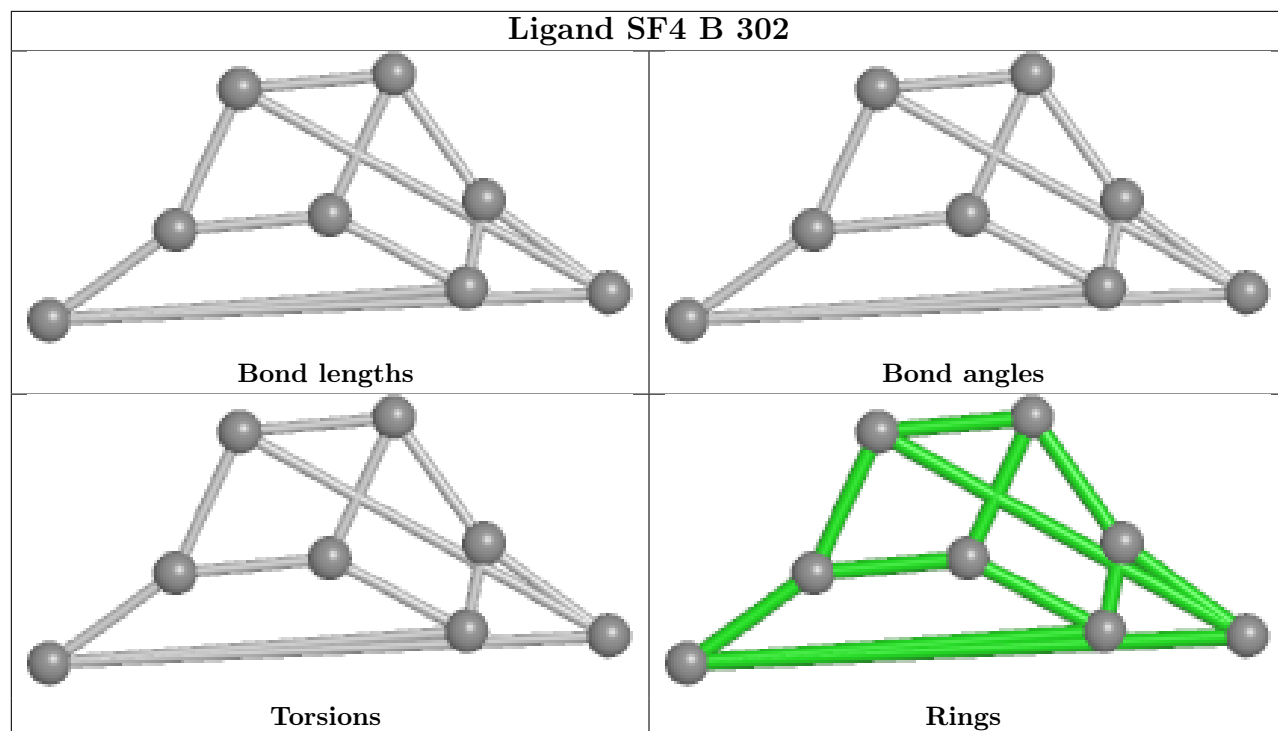




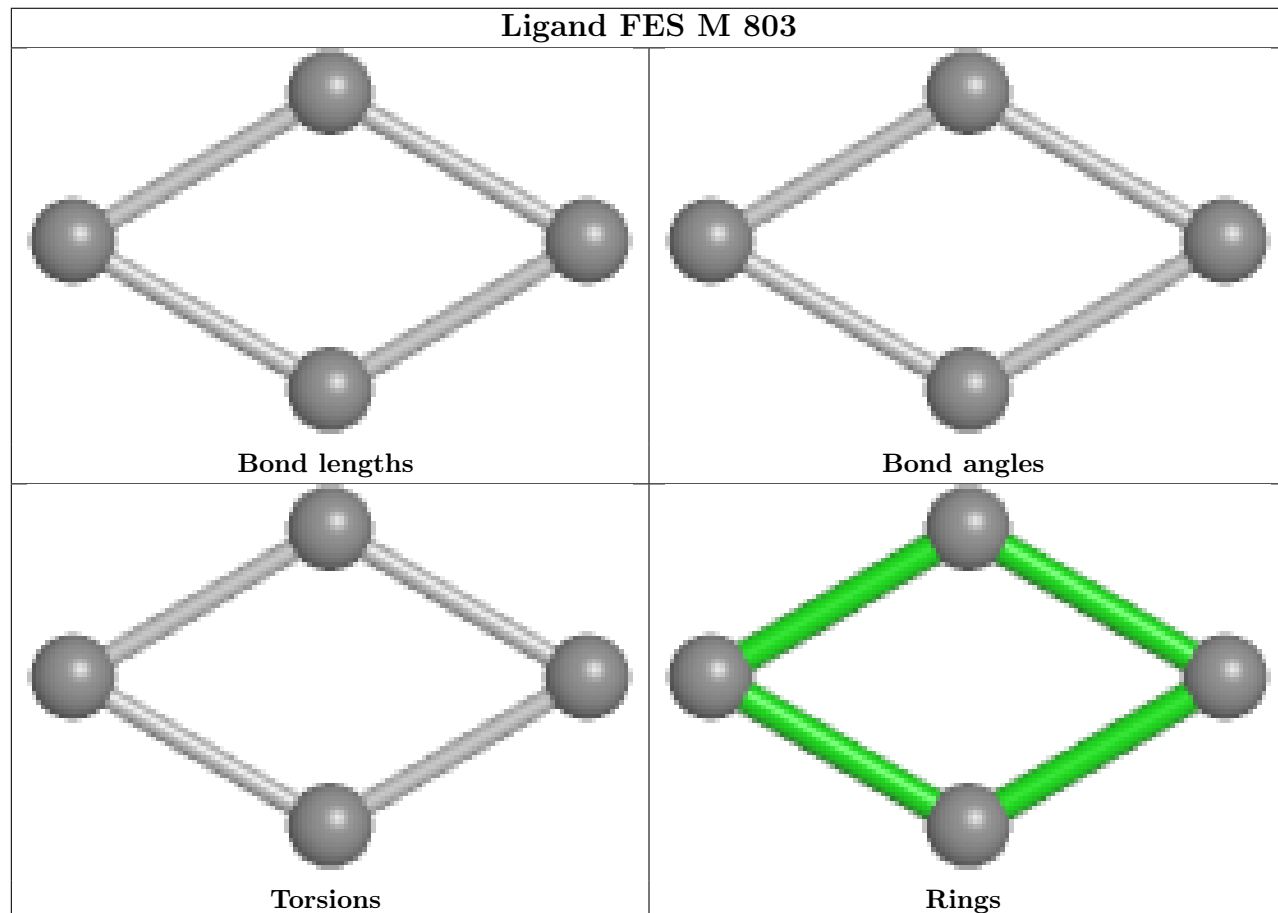


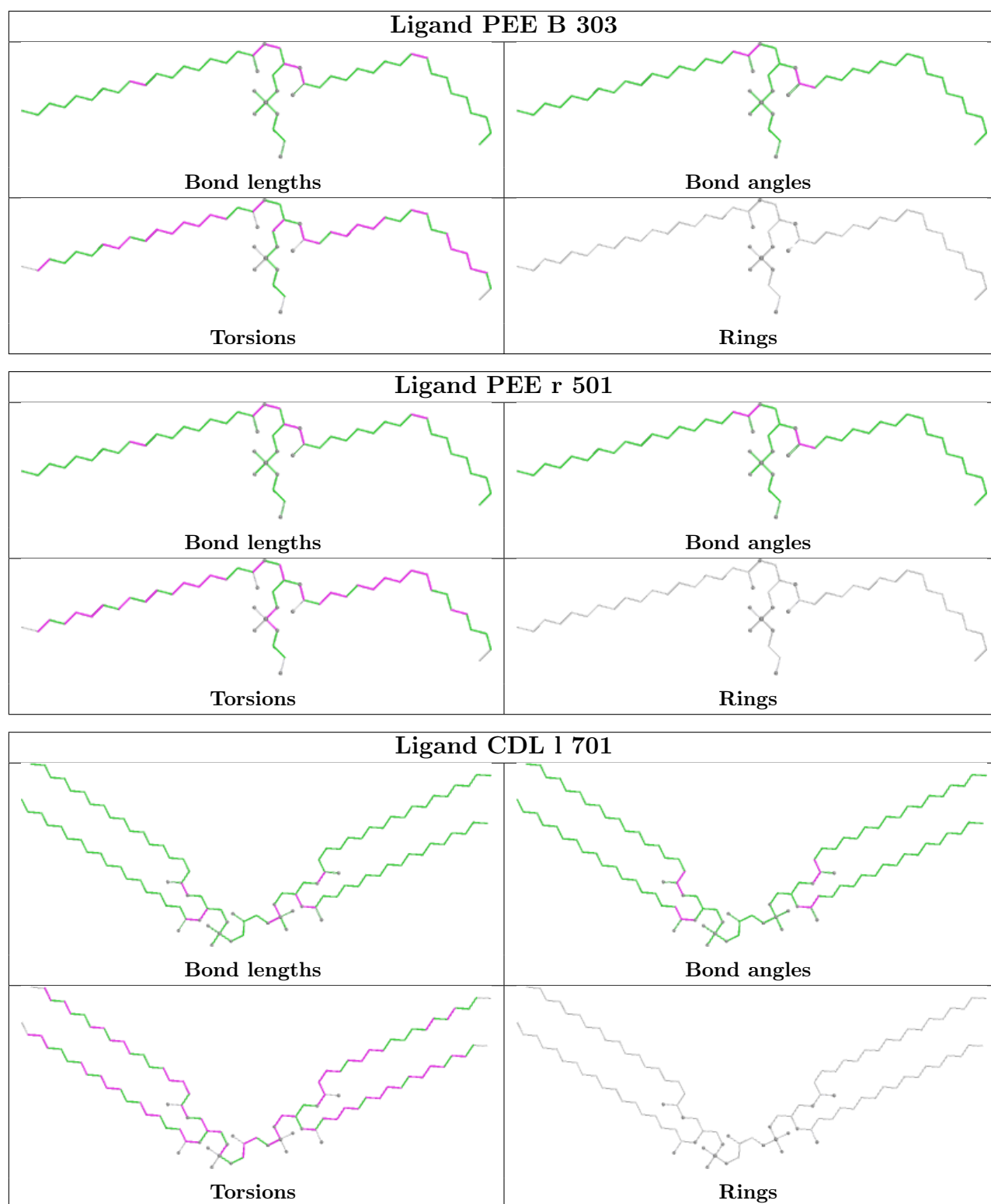


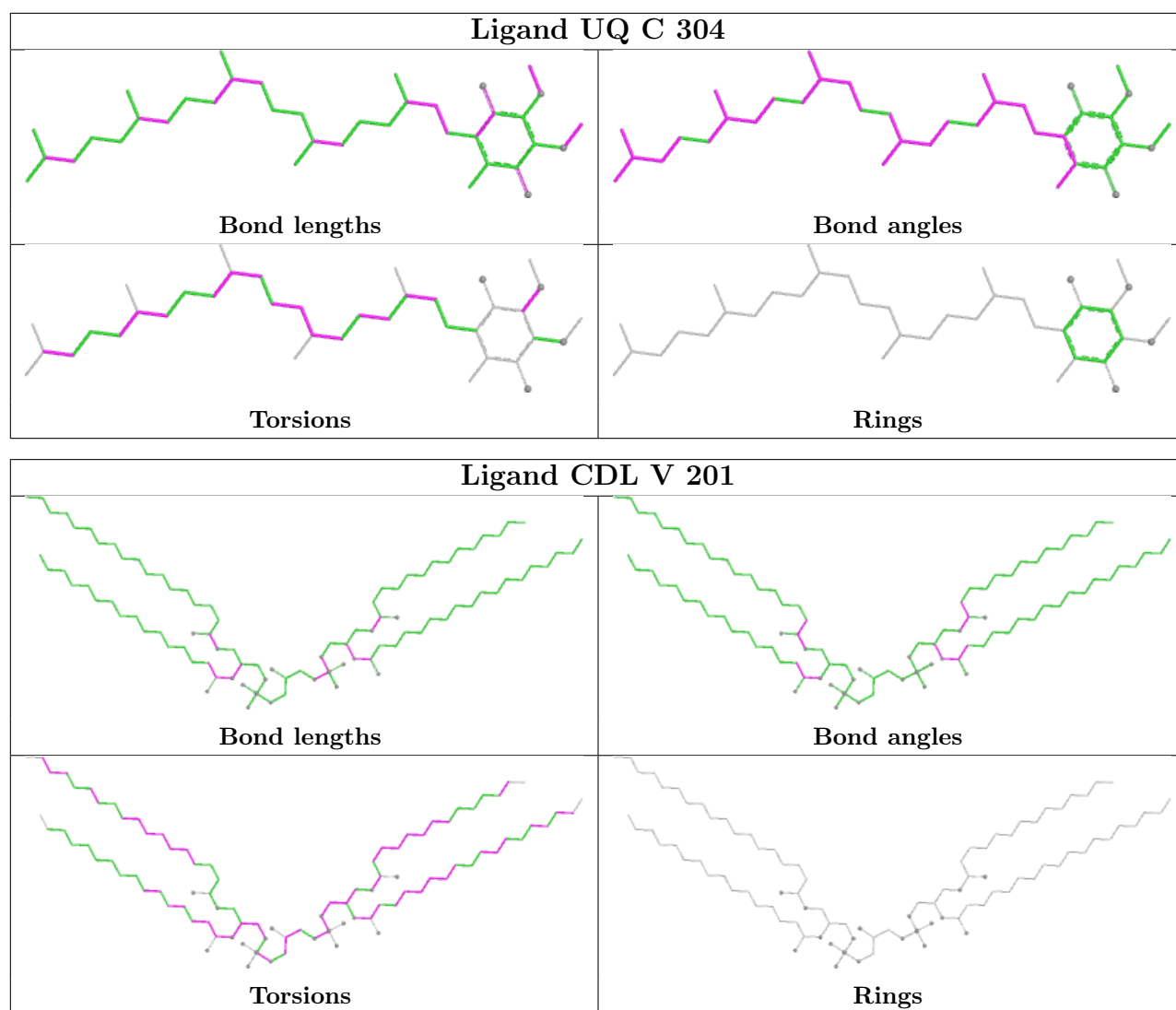
Ligand SF4 B 302

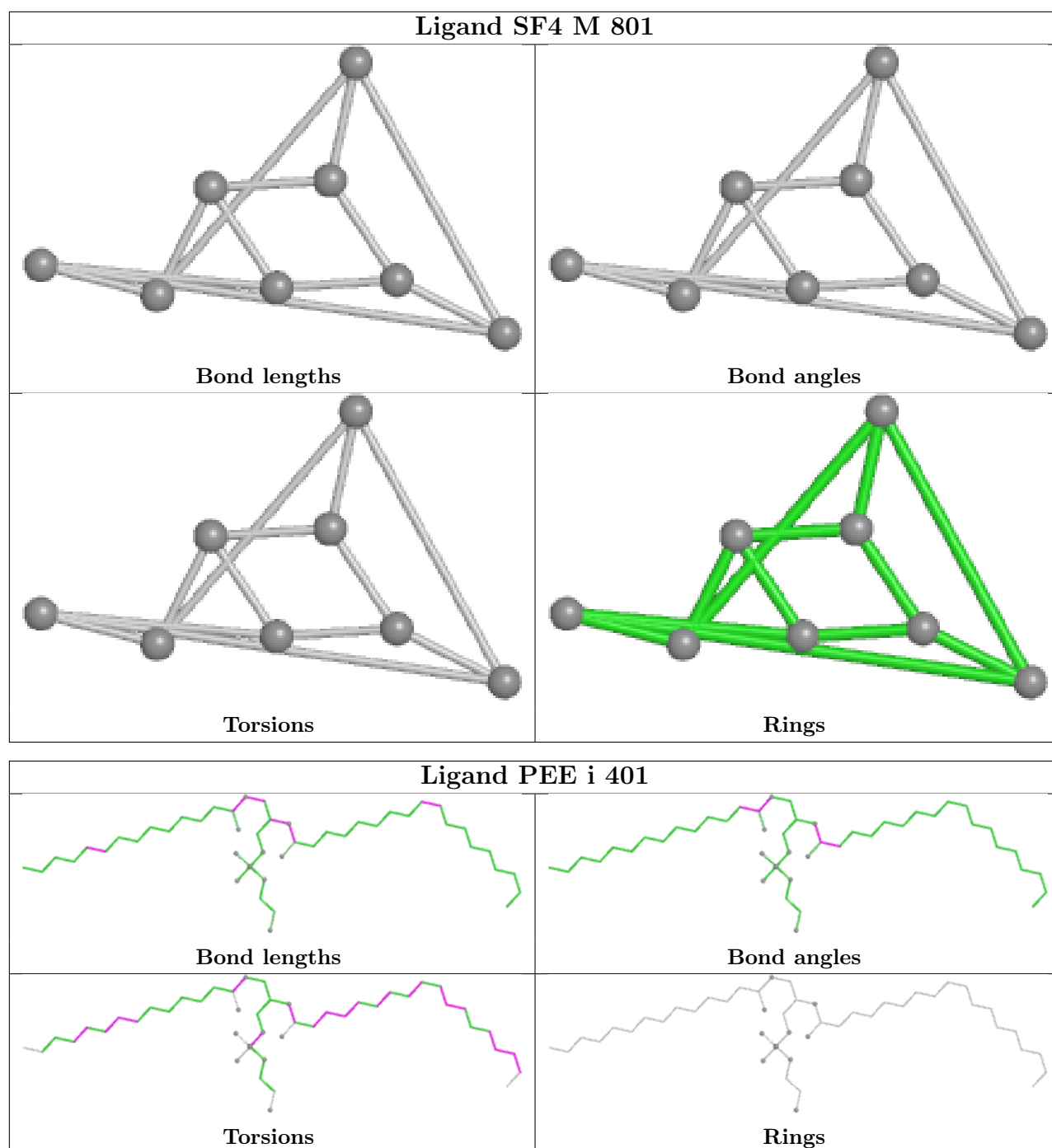


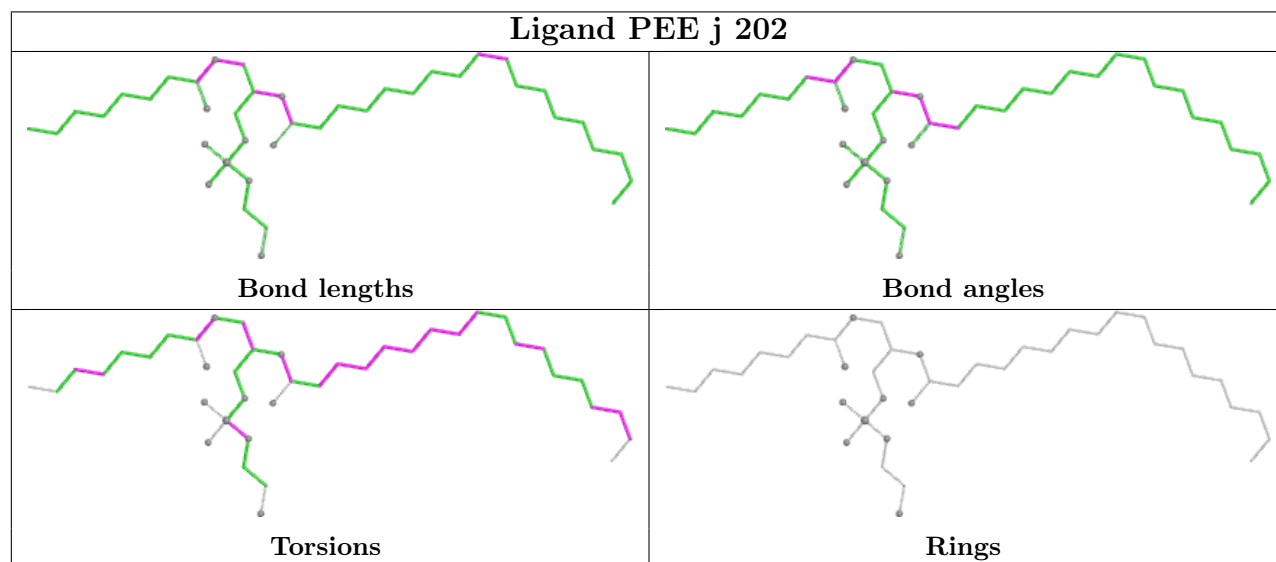
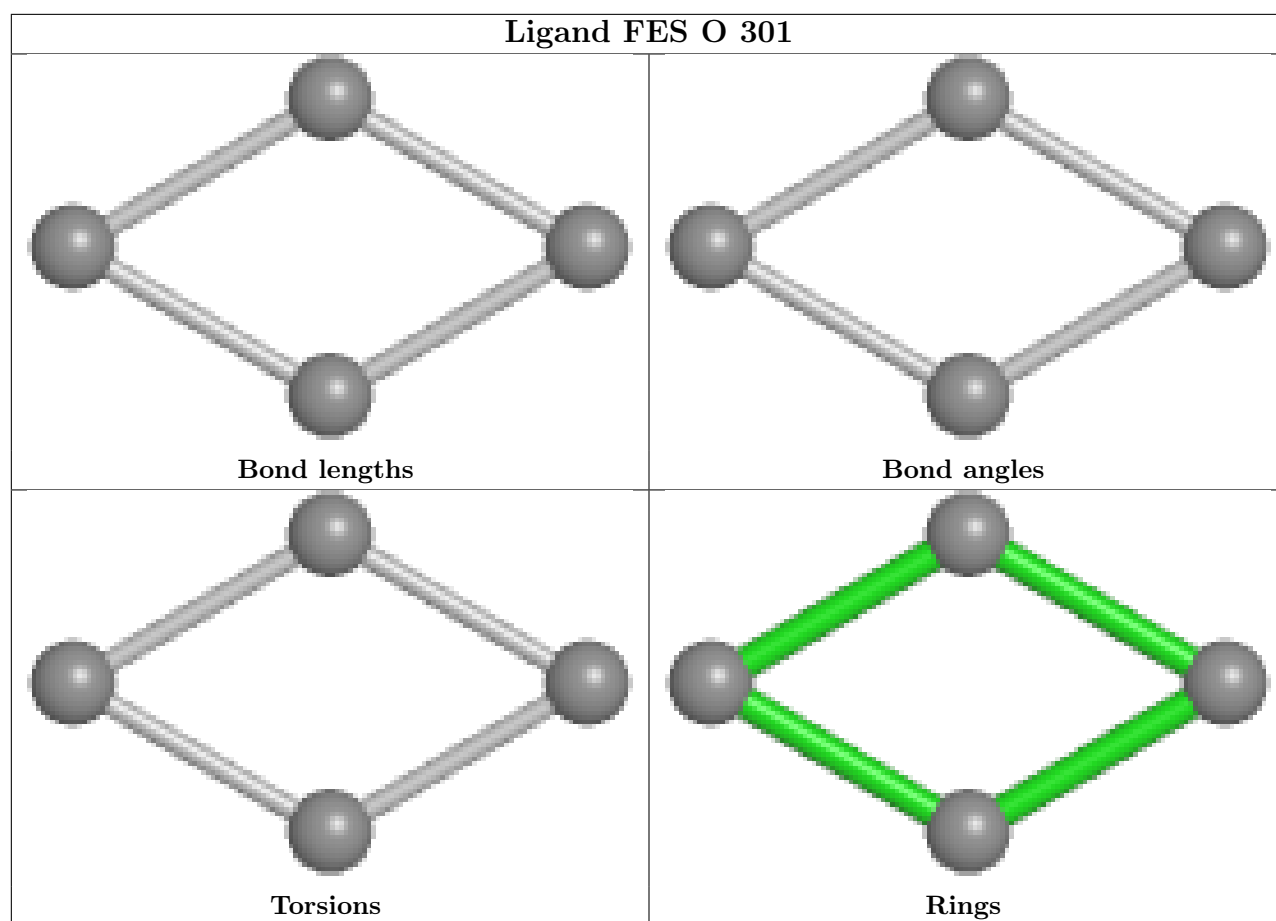
Ligand FES M 803

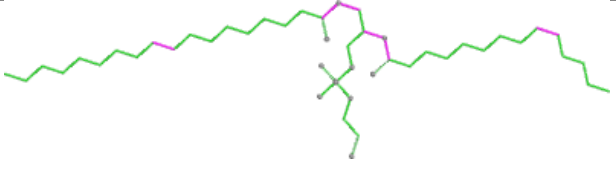
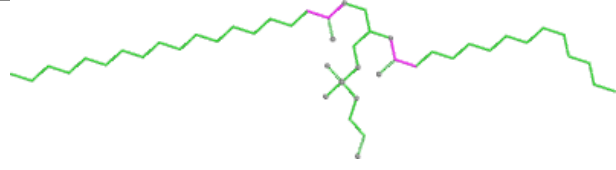
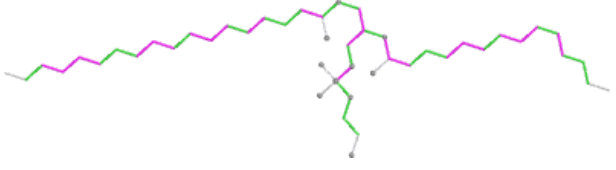
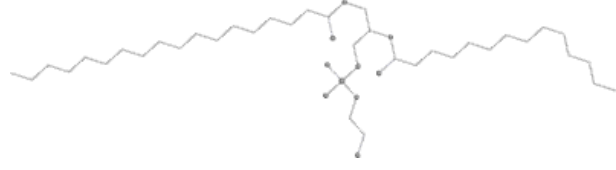


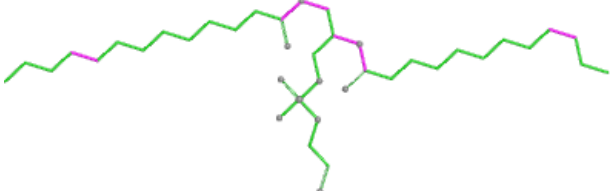
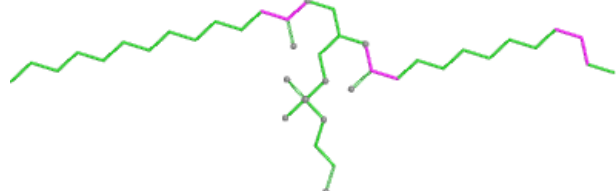
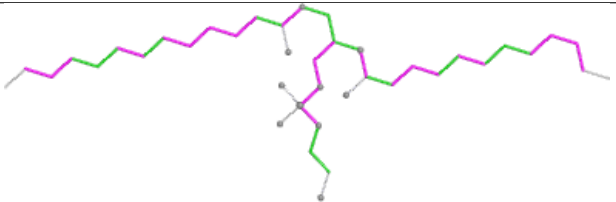
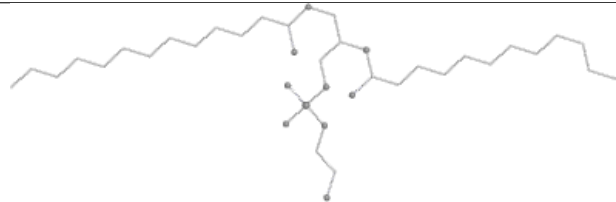


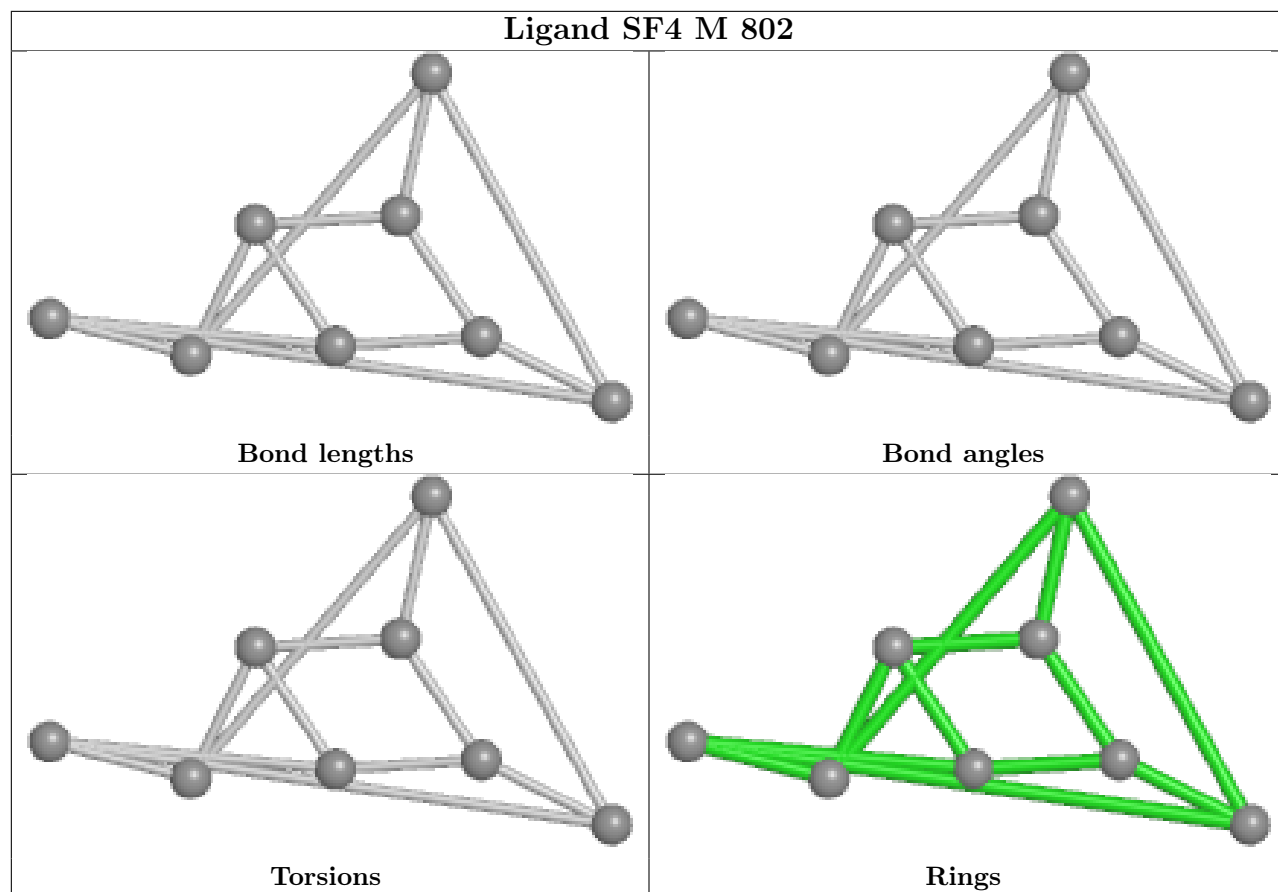


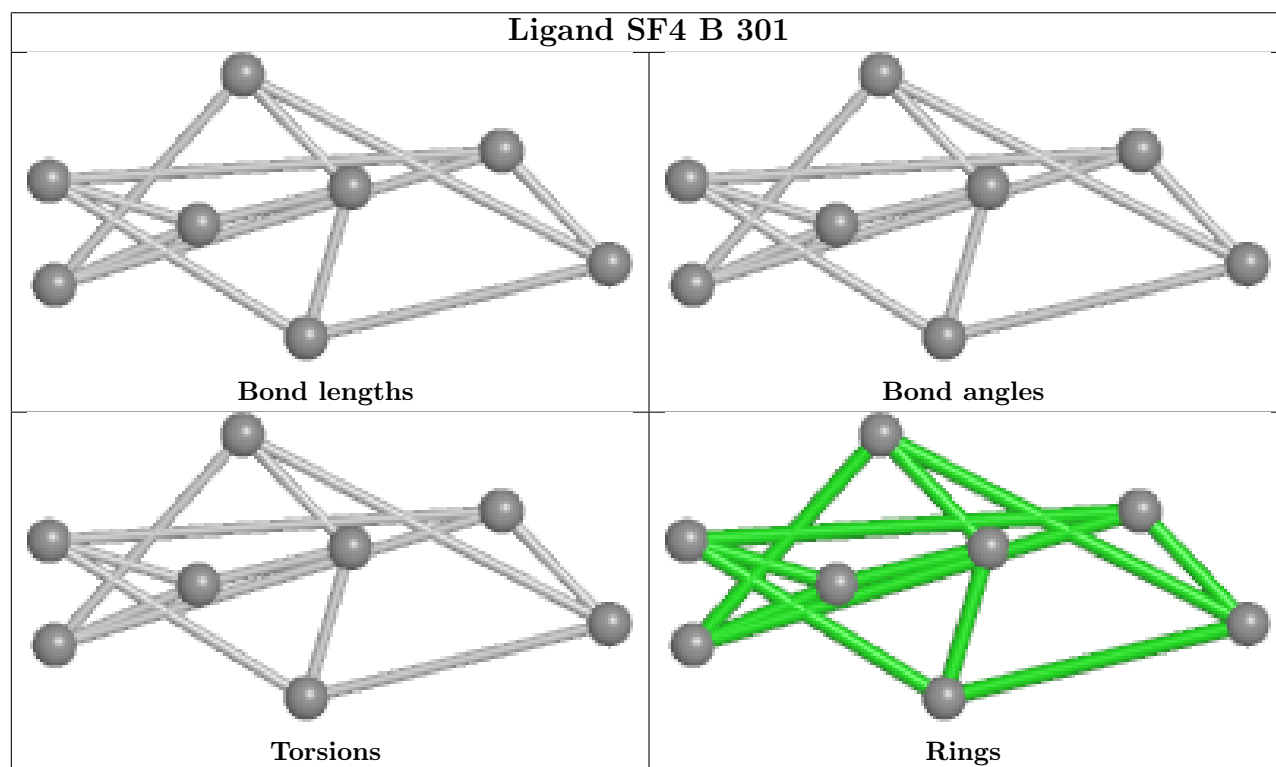
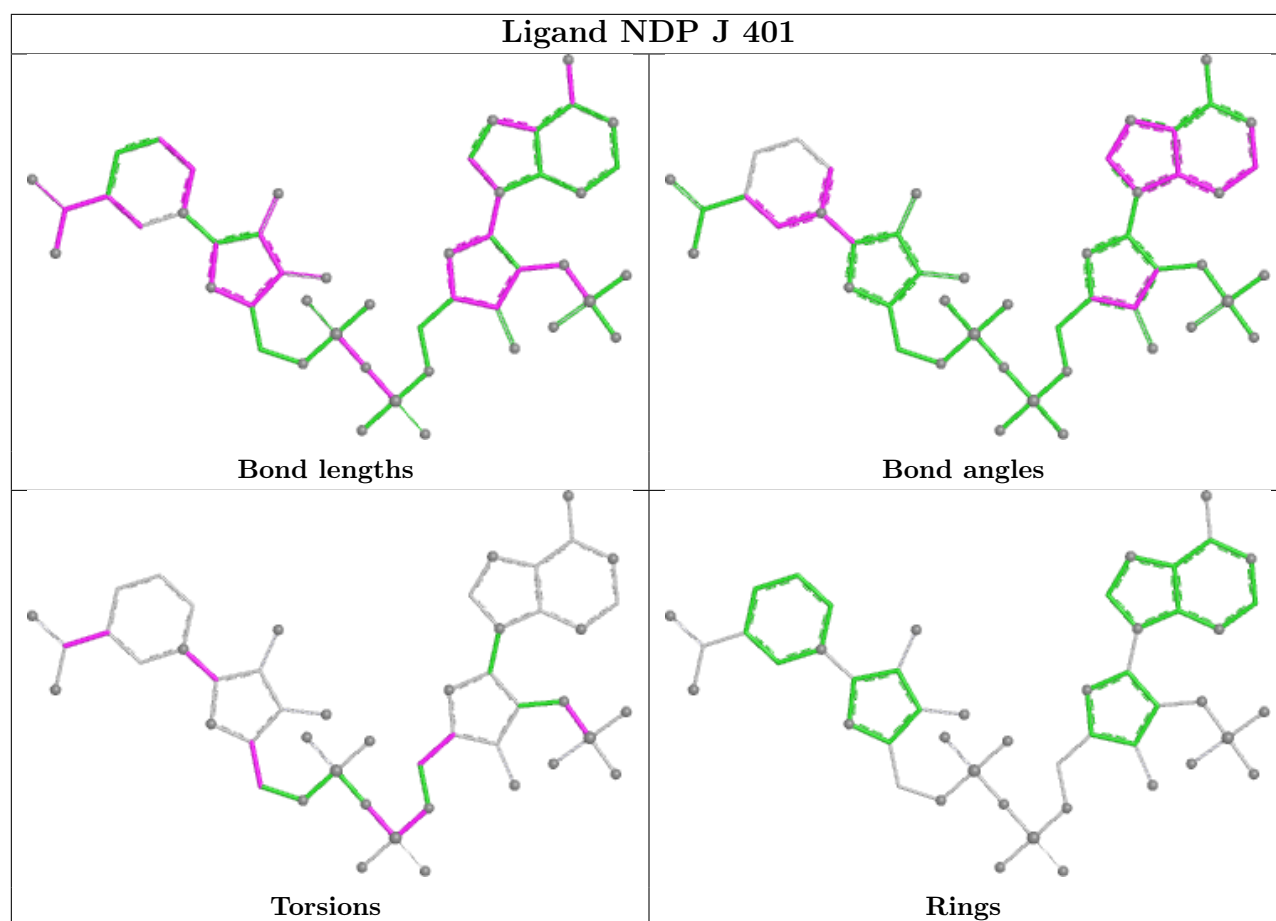


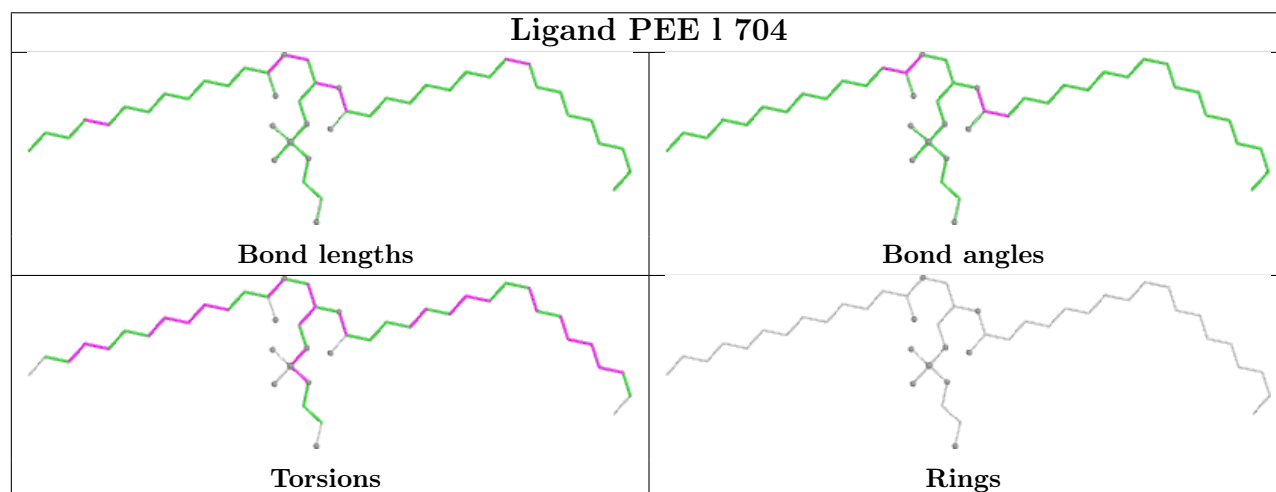
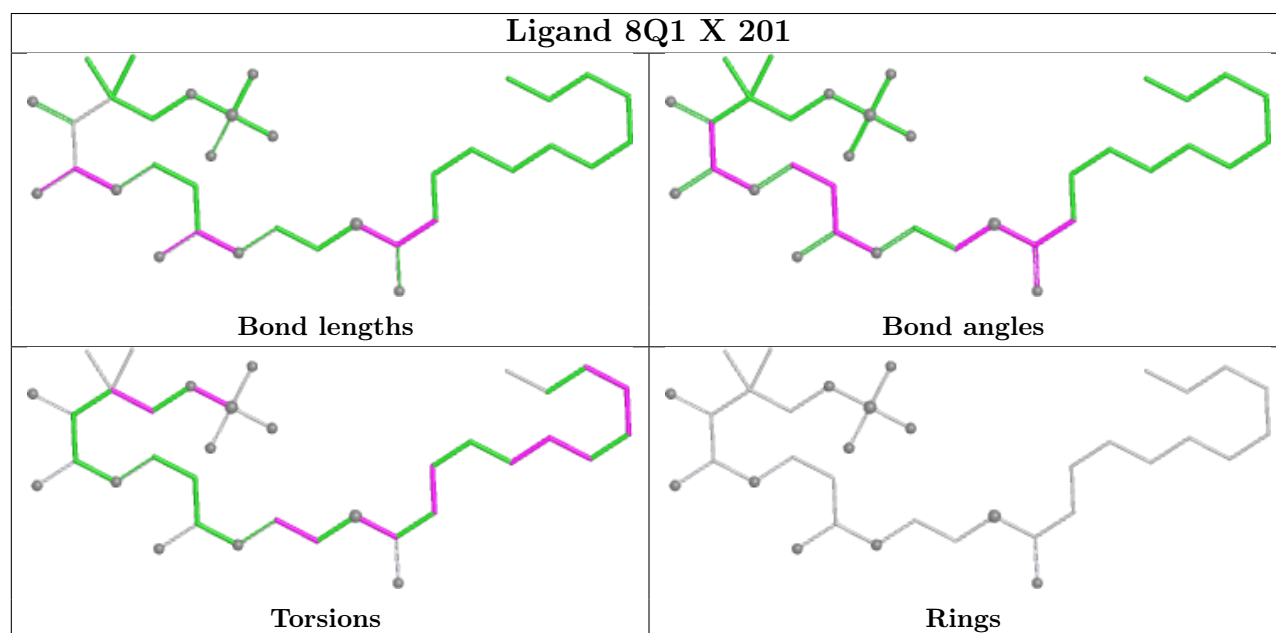
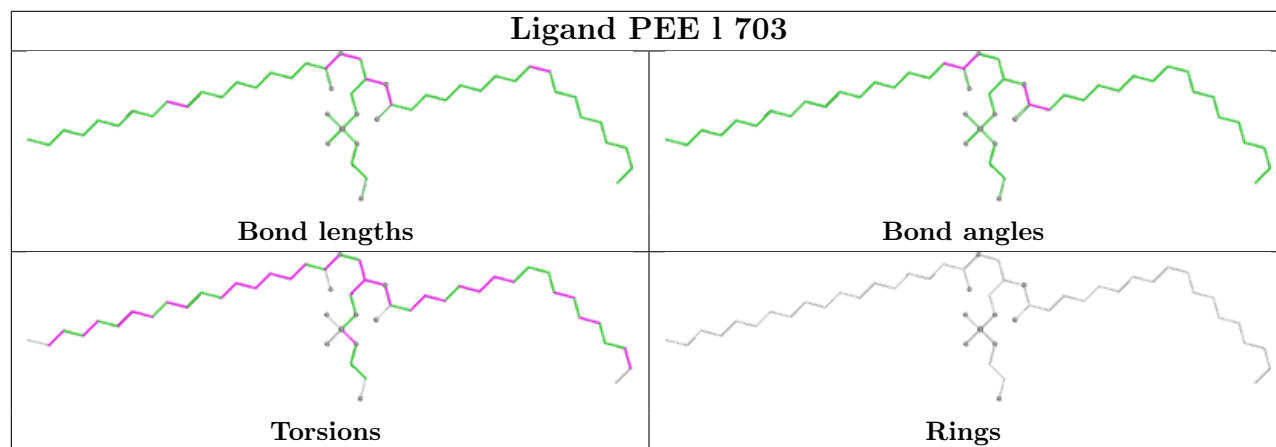


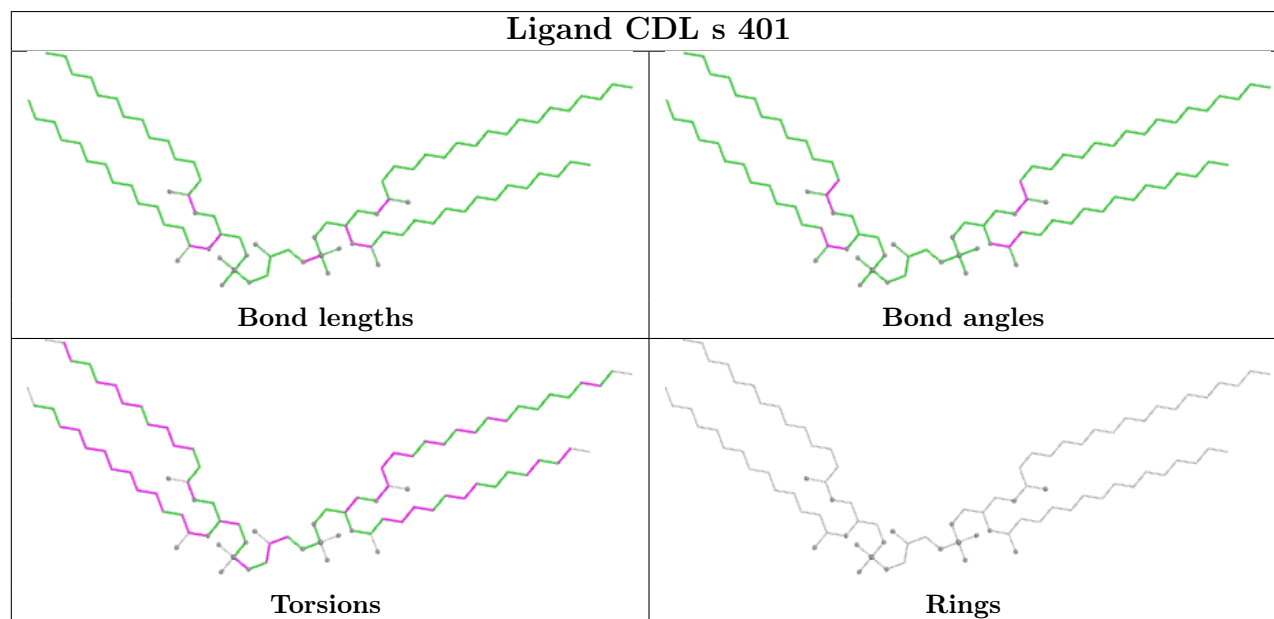
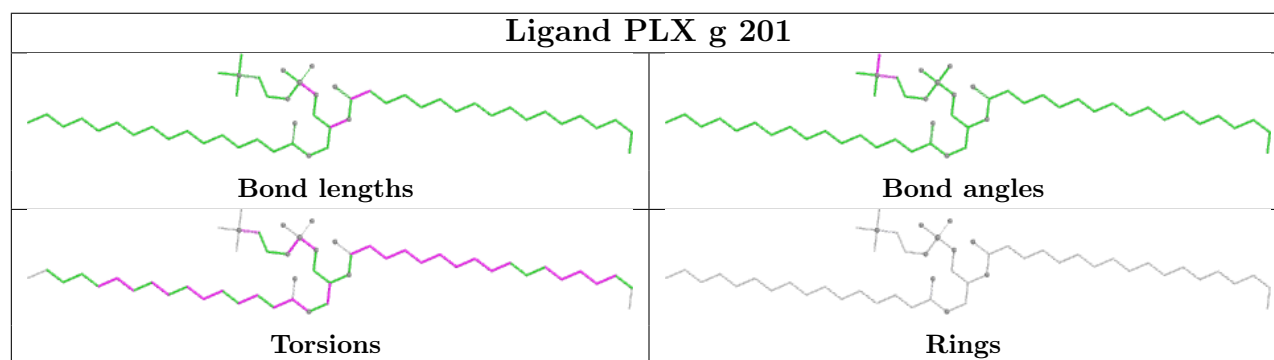
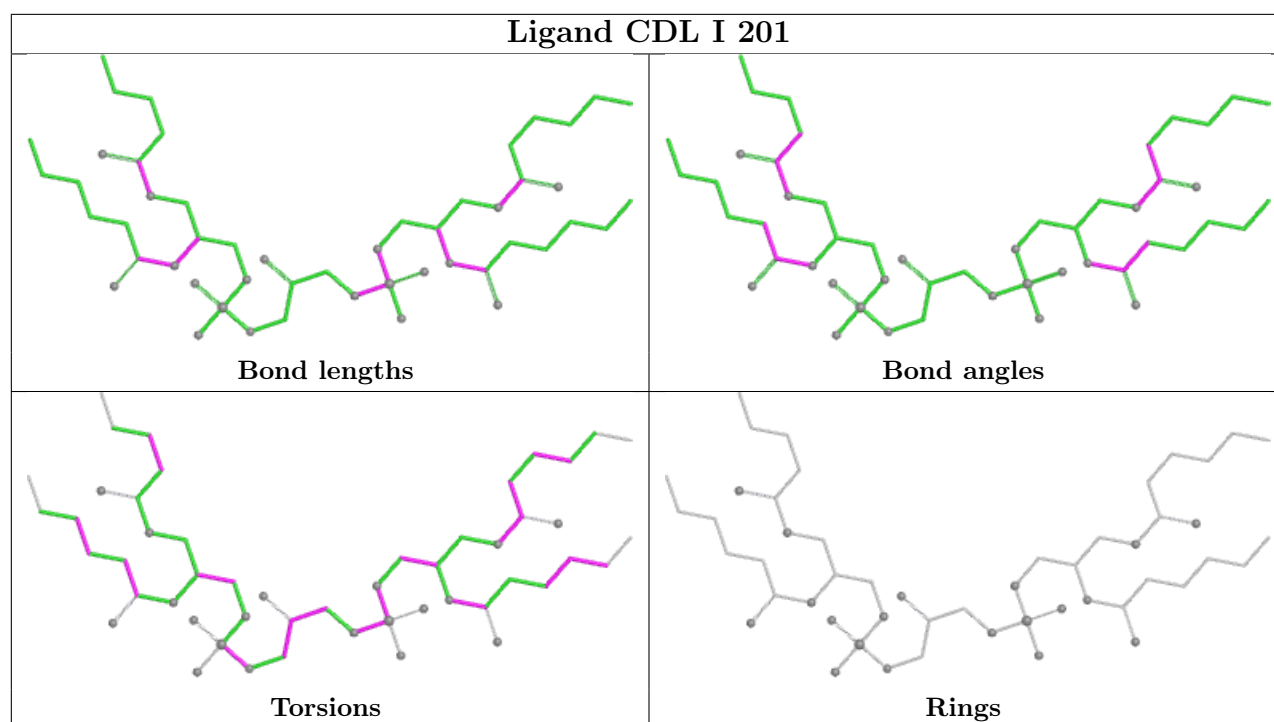
Ligand PEE C 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

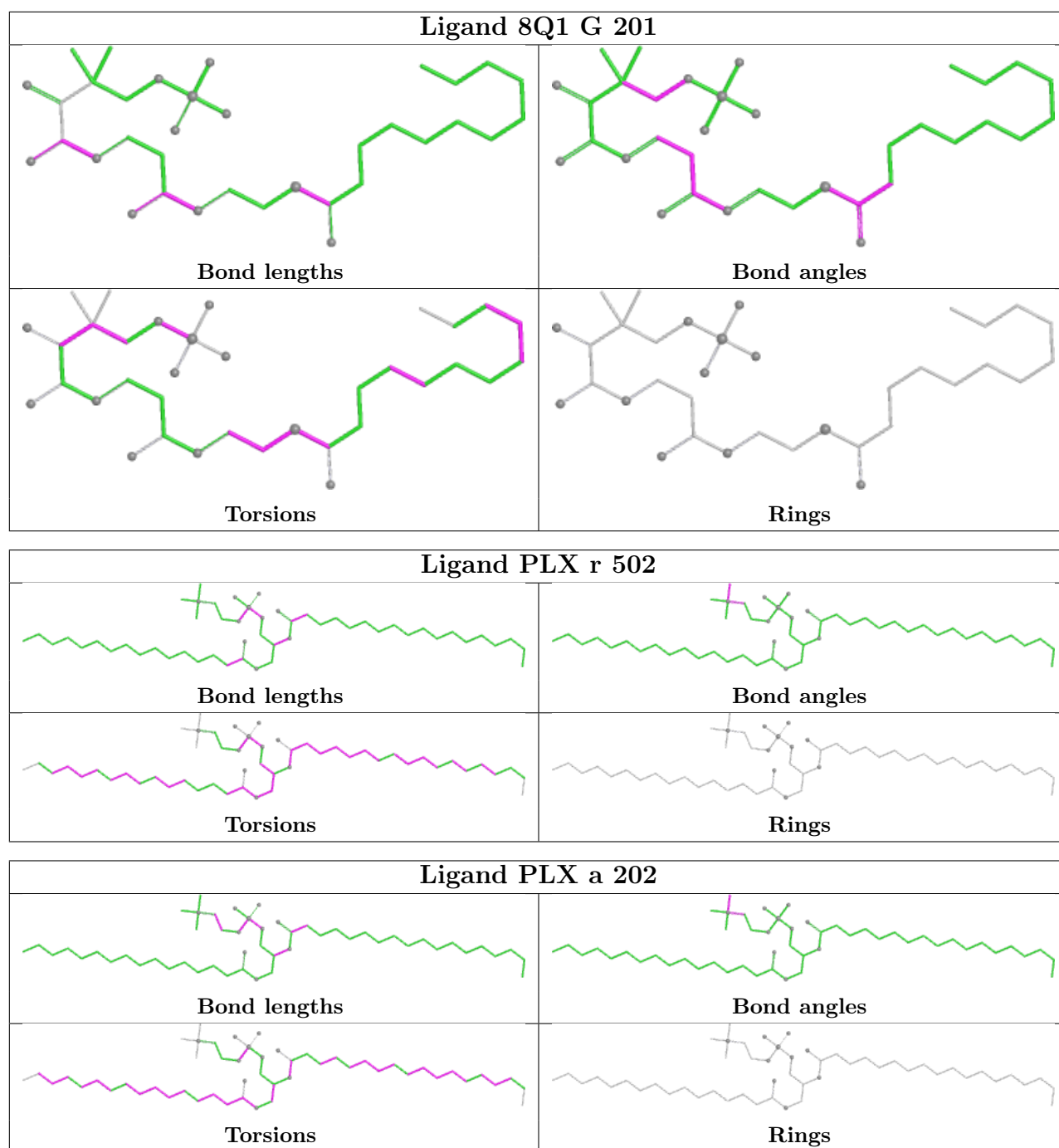
Ligand PEE V 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

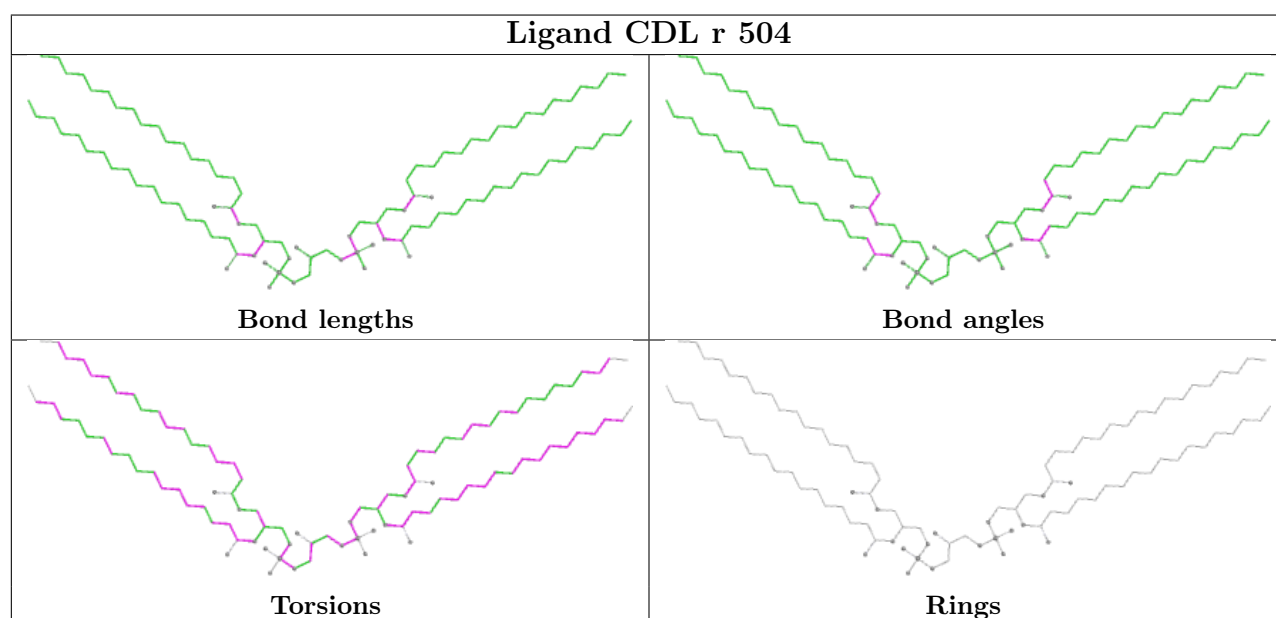
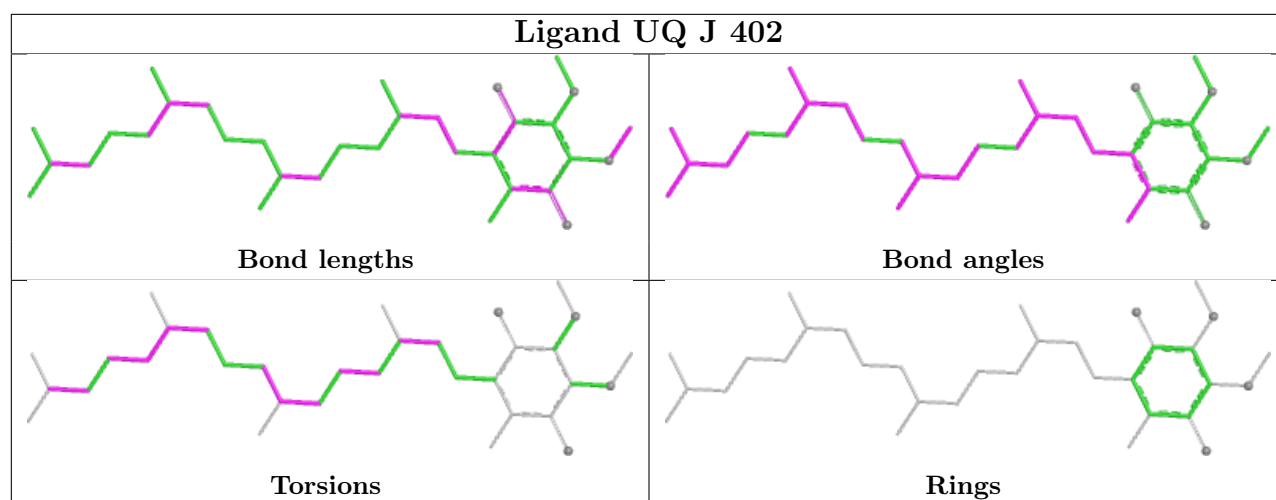


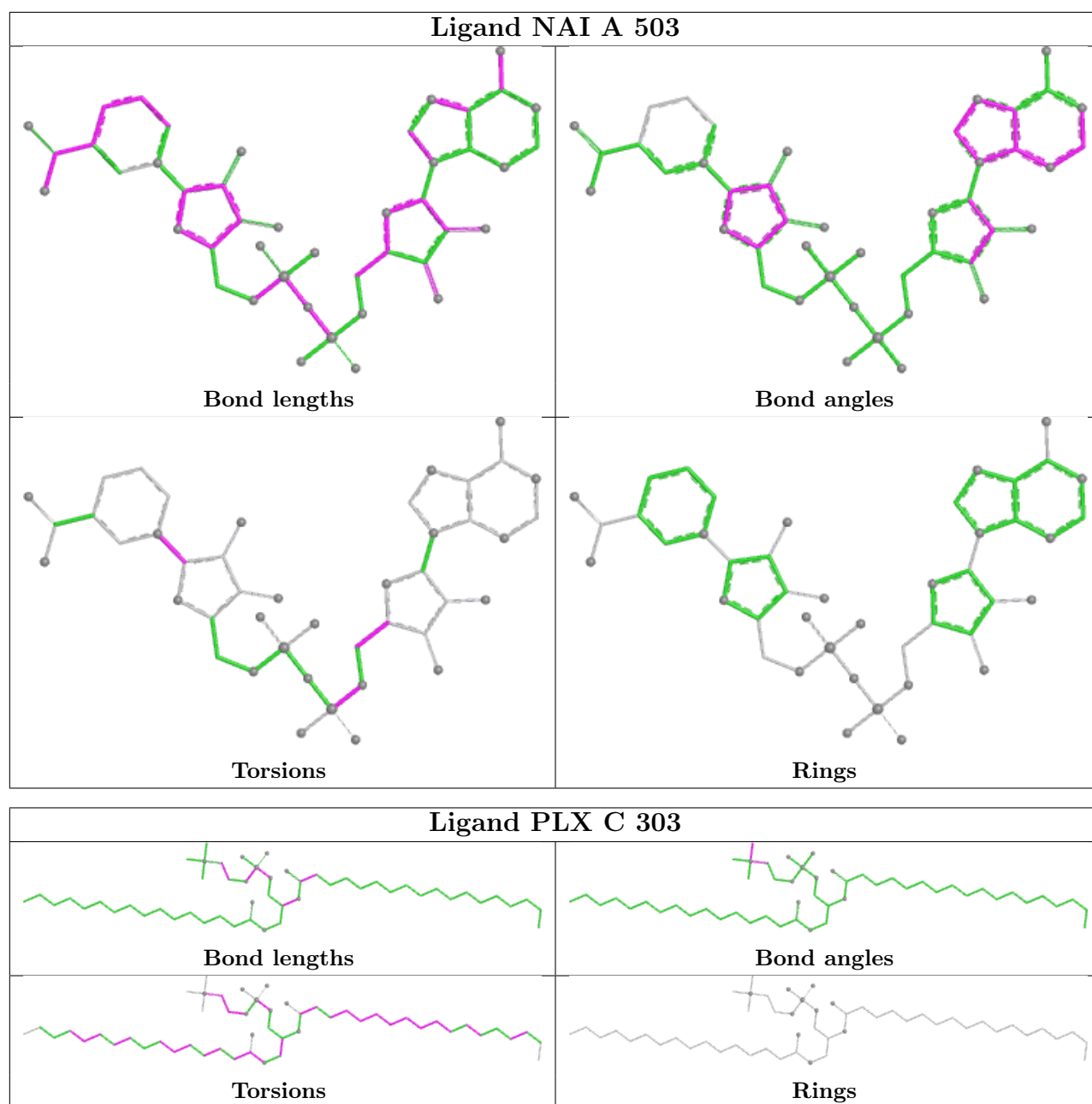


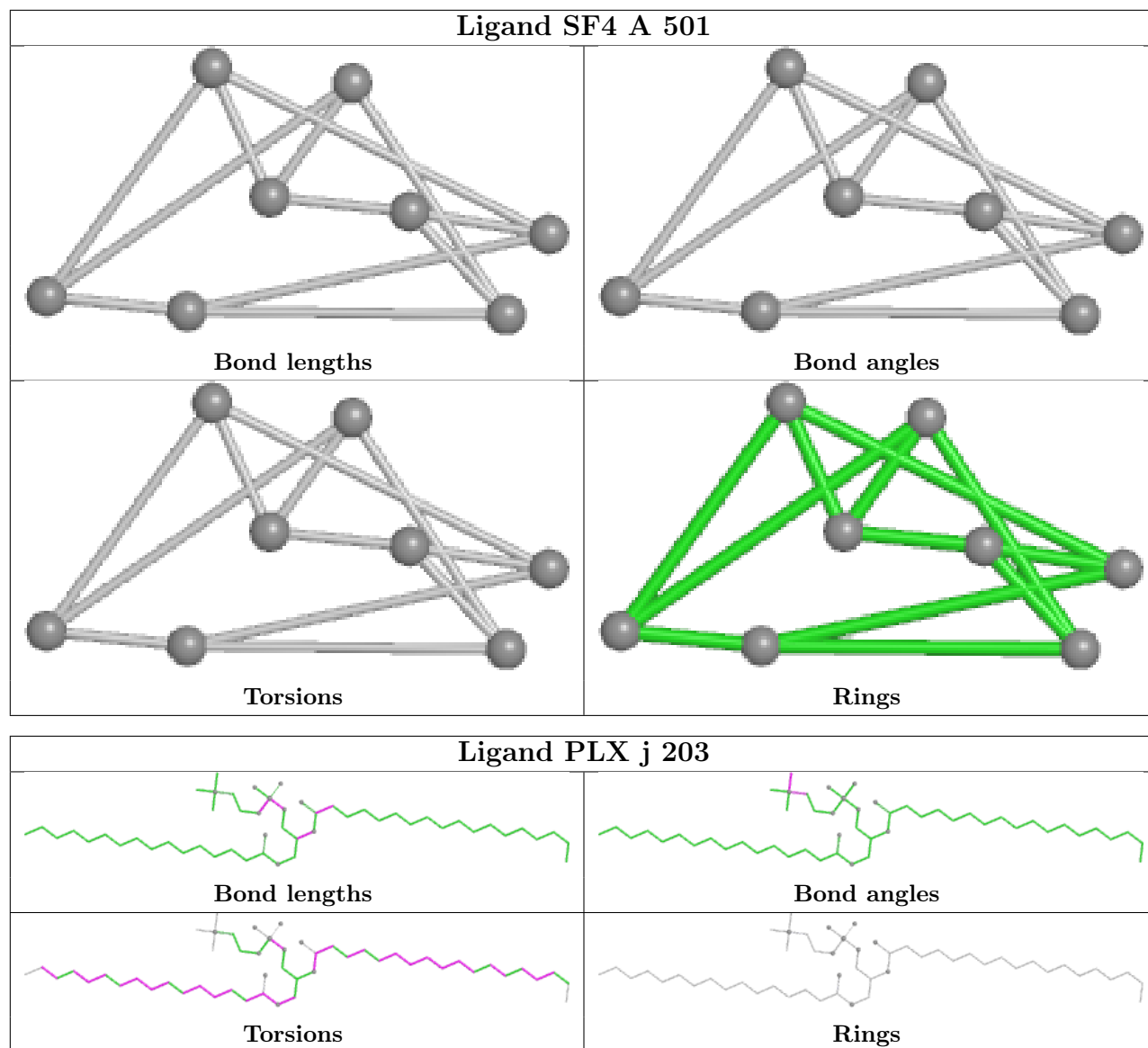


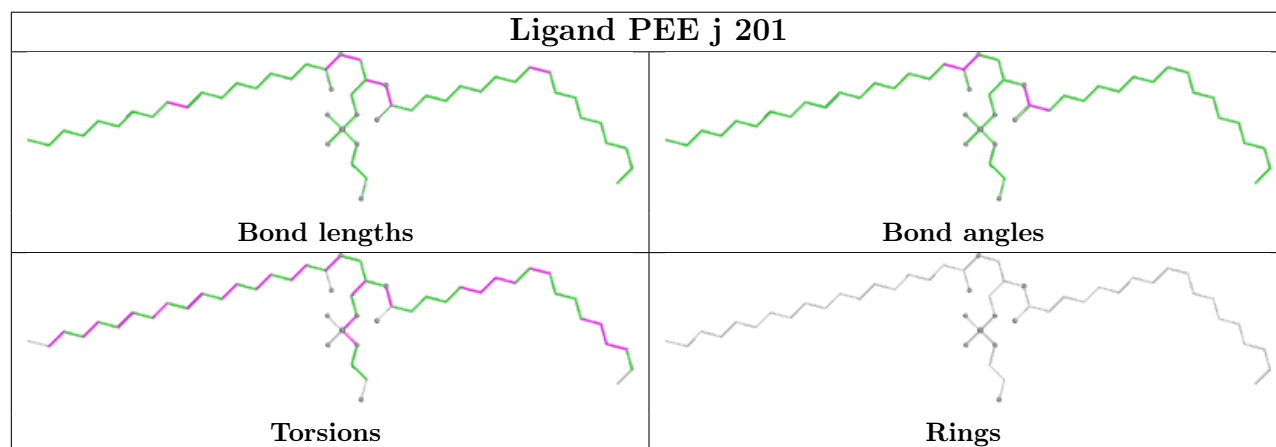
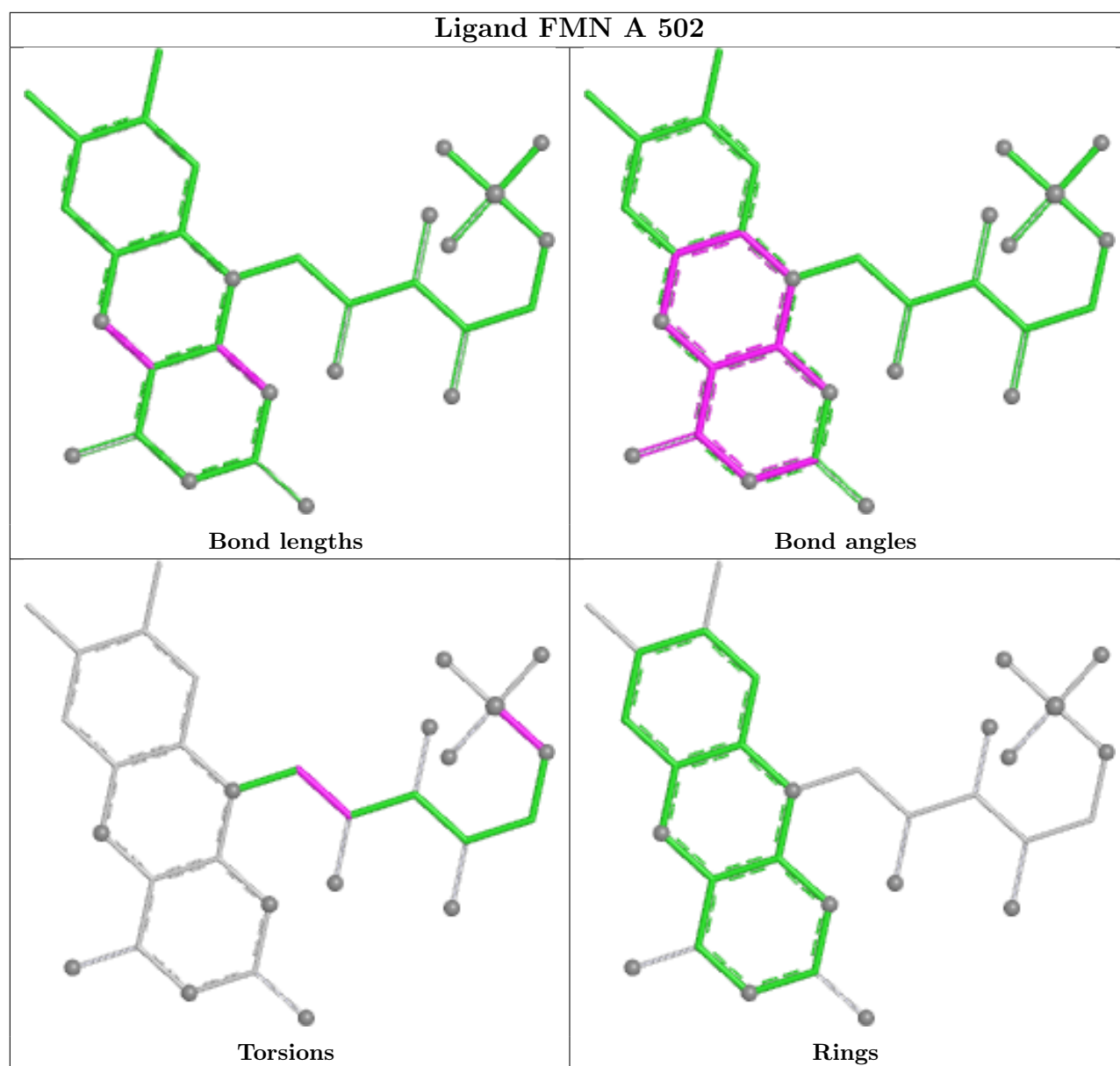












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32248. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.