



## wwPDB EM Validation Summary Report ⓘ

Apr 1, 2025 – 10:33 pm BST

PDB ID : 6ZKK / pdb\_00006zkk  
EMDB ID : EMD-11252  
Title : Complex I inhibited by rotenone, closed  
Authors : Kampjut, D.; Sazanov, L.A.  
Deposited on : 2020-06-30  
Resolution : 3.70 Å (reported)  
Based on initial model : 5LNK

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

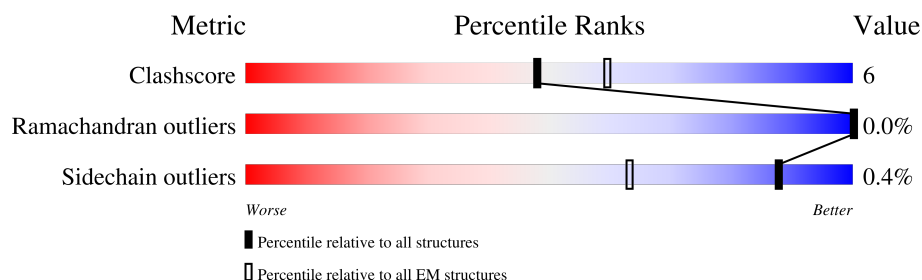
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.70 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	1	464	76% 17% 7%
2	2	246	77% 10% 13%
3	3	727	78% 16% 5%
4	4	463	76% 16% 7%
5	5	266	62% 17% 22%
6	6	223	57% 13% 30%
7	9	217	69% 12% 19%
8	A	115	84% 16%
9	H	318	81% 18%

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Mol	Chain	Length	Quality of chain
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	V	141	
16	W	189	
17	X	157	
17	j	157	
18	Y	172	
19	Z	175	
20	a	109	
21	b	124	
22	c	170	
23	d	380	
24	e	99	
25	f	116	
26	g	140	
27	h	114	
28	i	145	
29	k	355	
30	l	106	
31	m	84	
32	n	98	
33	o	122	

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Mol	Chain	Length	Quality of chain
34	p	130	 98%
35	q	144	 96%
36	r	128	 77% 23%
37	s	137	 88% 11%
38	t	179	 98%
39	u	108	 60% 40%
40	v	186	 83% 17%
41	w	154	 66% 34%
42	x	76	 64% 36%
43	y	58	 86% 14%
44	z	70	 100%

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	1	501	-	-	X	-
53	CDL	L	1004	X	-	-	-
53	CDL	L	1005	X	-	-	-
53	CDL	M	504	X	-	-	-
53	CDL	x	101	X	-	-	-

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 67950 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	1	430	Total	C	N	O	S	0	0
			3312	2086	593	613	20		

- Molecule 2 is a protein called Mitochondrial complex I, 24 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	213	Total	C	N	O	S	0	0
			1655	1058	278	309	10		

- Molecule 3 is a protein called NADH:ubiquinone oxidoreductase core subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	688	Total	C	N	O	S	0	0
			5275	3301	922	1011	41		

- Molecule 4 is a protein called Mitochondrial complex I, 49 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	430	Total	C	N	O	S	0	0
			3457	2207	594	631	25		

- Molecule 5 is a protein called NADH:ubiquinone oxidoreductase core subunit S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	208	Total	C	N	O	S	0	0
			1726	1112	296	315	3		

- Molecule 6 is a protein called Mitochondrial complex I, PSST subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	156	Total	C	N	O	S	0	0
			1247	795	225	213	14		

- Molecule 7 is a protein called Mitochondrial complex I, TYKY subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	9	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	115	Total	C	N	O	S	0	0
			922	621	133	161	7		

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	318	Total	C	N	O	S	0	0
			2528	1704	384	421	19		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	175	Total	C	N	O	S	0	0
			1344	904	192	235	13		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	98	Total	C	N	O	S	0	0
			749	490	112	132	15		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	606	Total	C	N	O	S	0	0
			4807	3188	746	829	44		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	459	Total	C	N	O	S	0	0
			3647	2429	571	607	40		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	347	Total	C	N	O	S	0	0
			2723	1808	416	459	40		

- Molecule 15 is a protein called Mitochondrial complex I, B14.7 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	V	140	Total	C	N	O	S	0	0
			1028	656	175	191	6		

- Molecule 16 is a protein called NADH:ubiquinone oxidoreductase subunit B5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	139	Total	C	N	O	S	0	0
			1155	761	194	198	2		

- Molecule 17 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	87	Total	C	N	O	S	0	0
			701	451	103	142	5		
17	j	82	Total	C	N	O	S	0	0
			660	425	98	132	5		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	171	Total	C	N	O	S	0	0
			1403	889	253	251	10		

- Molecule 19 is a protein called Mitochondrial complex I, PDSW subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	171	Total	C	N	O	S	0	0
			1441	905	266	262	8		

- Molecule 20 is a protein called Mitochondrial complex I, 10 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	a	44	Total	C	N	O	S	0	0
			371	233	66	71	1		

- Molecule 21 is a protein called Mitochondrial complex I, 13 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	b	95	Total	C	N	O	S	0	0
			737	451	139	144	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	c	126	Total	C	N	O	S	0	0
			1024	646	182	193	3		

- Molecule 23 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	340	Total	C	N	O	S	0	0
			2748	1775	489	478	6		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	e	86	Total	C	N	O	S	0	0
			691	434	129	126	2		

- Molecule 25 is a protein called Mitochondrial complex I, B13 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	f	113	Total	C	N	O	S	0	0
			917	595	153	167	2		

- Molecule 26 is a protein called NADH:ubiquinone oxidoreductase subunit A6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	g	114	Total	C	N	O	S	0	0
			969	619	180	166	4		

- Molecule 27 is a protein called Mitochondrial complex I, B14.5a subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	h	96	Total	C	N	O	S	0	0
			769	480	146	140	3		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	i	145	Total	C	N	O	S	0	0
			1209	778	216	210	5		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	k	320	Total	C	N	O	P	S	0	0
			2596	1659	432	494	1	10		

- Molecule 30 is a protein called NADH:ubiquinone oxidoreductase subunit S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	l	105	Total	C	N	O	S	0	0
			874	551	164	153	6		

- Molecule 31 is a protein called NADH:ubiquinone oxidoreductase subunit A3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	m	80	Total	C	N	O	S	0	0
			626	411	103	110	2		

- Molecule 32 is a protein called NADH:ubiquinone oxidoreductase subunit B3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	n	79	Total	C	N	O	S	0	0
			634	415	106	111	2		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	o	120	Total	C	N	O	S	0	0
			1004	652	175	172	5		

- Molecule 34 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	p	128	Total	C	N	O	S	0	0
			1059	675	189	194	1		

- Molecule 35 is a protein called Mitochondrial complex I, B16.6 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	q	139	Total	C	N	O	S	0	0
			1142	733	200	200	9		

- Molecule 36 is a protein called Mitochondrial complex I, B17 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	r	99	Total	C	N	O	S	0	0
			846	554	149	142	1		

- Molecule 37 is a protein called NADH:ubiquinone oxidoreductase subunit B7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	s	122	Total	C	N	O	S	0	0
			1047	653	199	186	9		

- Molecule 38 is a protein called NADH:ubiquinone oxidoreductase subunit B9.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	t	177	Total	C	N	O	S	0	0
			1520	973	279	262	6		

- Molecule 39 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	u	65	Total	C	N	O	S	0	0
			563	372	93	97	1		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	v	155	Total	C	N	O	S	0	0
			1307	846	213	239	9		

- Molecule 41 is a protein called Mitochondrial complex I, ESSS subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	w	101	Total	C	N	O	S	0	0
			846	542	140	160	4		

- Molecule 42 is a protein called Mitochondrial complex I, KFYI subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	x	49	Total	C	N	O	0	0
			412	271	70	71		

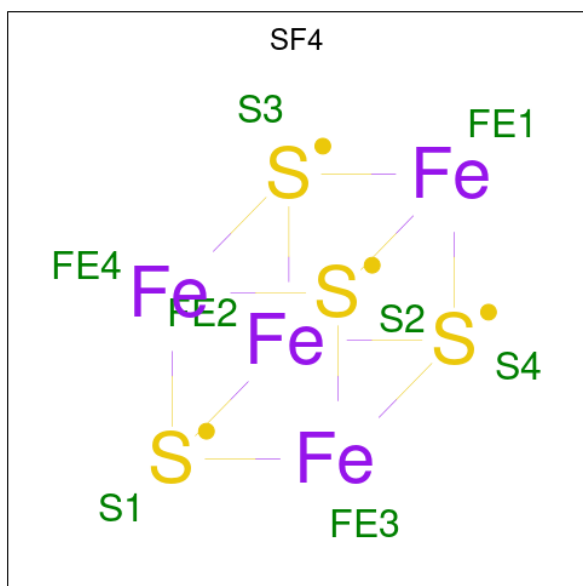
- Molecule 43 is a protein called Mitochondrial complex I, MNLL subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	y	50	Total	C	N	O	0	0
			436	287	77	72		

- Molecule 44 is a protein called Mitochondrial complex I, MWFE subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	z	70	Total	C	N	O	S	0	0
			576	369	106	96	5		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



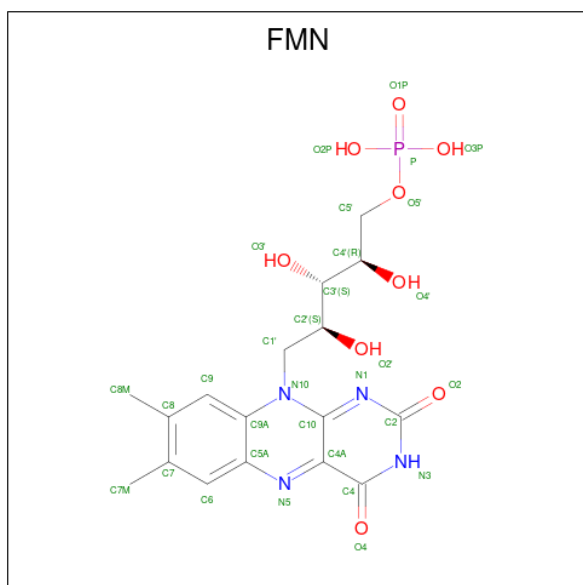
Mol	Chain	Residues	Atoms			AltConf
45	1	1	Total	Fe	S	0
			8	4	4	
45	3	1	Total	Fe	S	0
			8	4	4	
45	3	1	Total	Fe	S	0
			8	4	4	
45	6	1	Total	Fe	S	0
			8	4	4	

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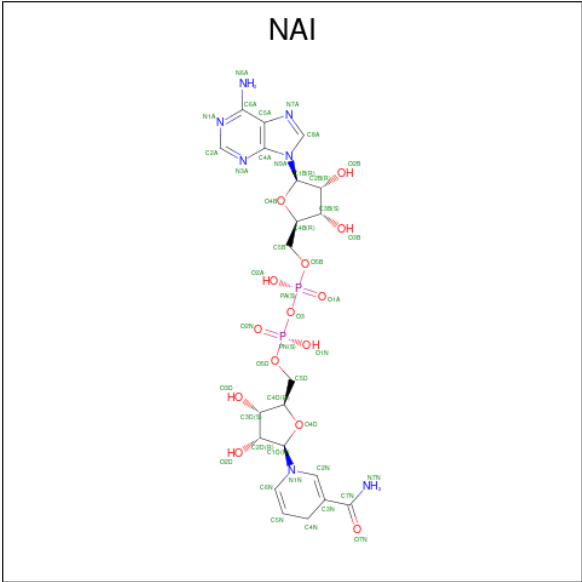
Mol	Chain	Residues	Atoms			AltConf
45	9	1	Total	Fe	S	0
			8	4	4	
45	9	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ).



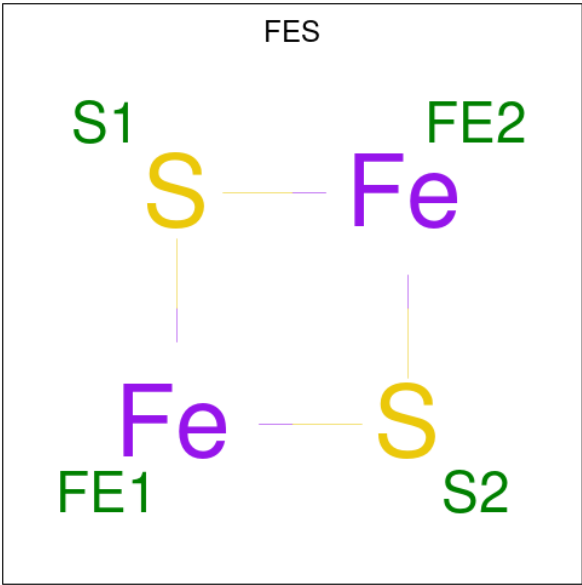
Mol	Chain	Residues	Atoms					AltConf
46	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula:  $C_{21}H_{29}N_7O_{14}P_2$ ).



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

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).

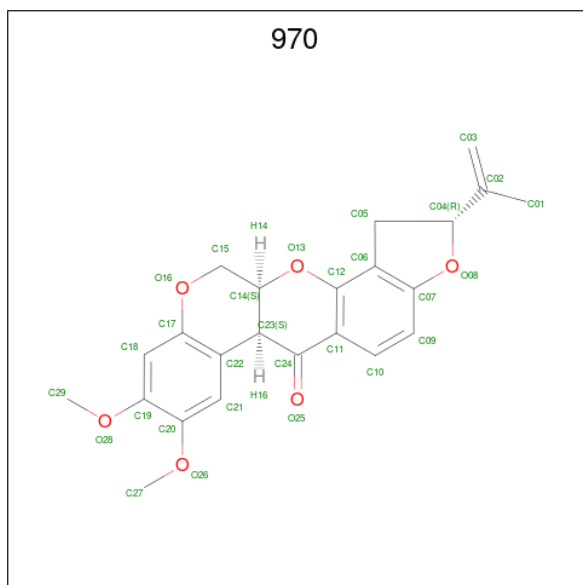


Mol	Chain	Residues	Atoms			AltConf
48	2	1	Total	Fe	S	0
			4	2	2	
48	3	1	Total	Fe	S	0
			4	2	2	

- Molecule 49 is POTASSIUM ION (CCD ID: K) (formula: K).

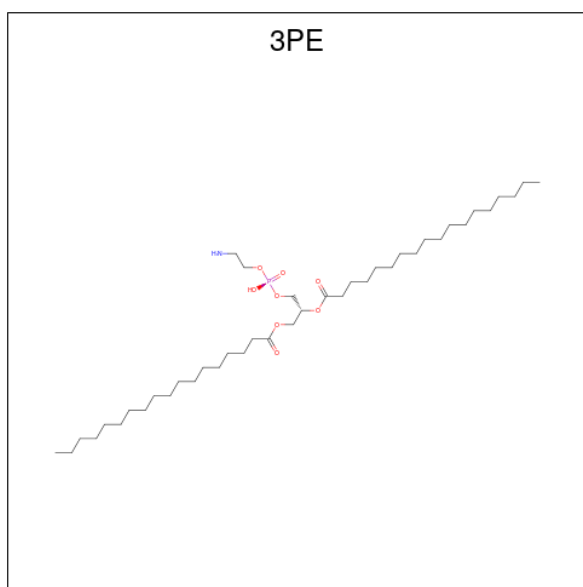
Mol	Chain	Residues	Atoms		AltConf
49	3	1	Total	K	0
			1	1	

- Molecule 50 is (2R,6aS,12aS)-8,9-dimethoxy-2-(prop-1-en-2-yl)-1,2,12,12a-tetrahydrofuro[2',3':7,8][1]benzopyrano[2,3-c][1]benzopyran-6(6aH)-one (CCD ID: 970) (formula: C<sub>23</sub>H<sub>22</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
50	4	1	Total	C	O	0
			29	23	6	

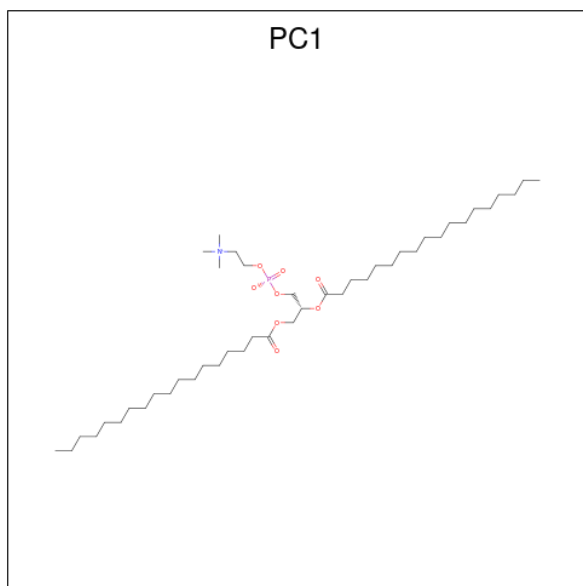
- Molecule 51 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C<sub>41</sub>H<sub>82</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
51	4	1	Total	C	N	O	P	0
			40	30	1	8	1	
51	6	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	J	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	J	1	Total	C	N	O	P	0
			40	30	1	8	1	
51	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	L	1	Total	C	N	O	P	0
			31	21	1	8	1	
51	M	1	Total	C	N	O	P	0
			44	34	1	8	1	
51	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	V	1	Total	C	O	P		0
			27	18	8	1		
51	V	1	Total	C	N	O	P	0
			37	27	1	8	1	
51	i	1	Total	C	N	O	P	0
			51	41	1	8	1	
51	o	1	Total	C	N	O	P	0
			31	21	1	8	1	

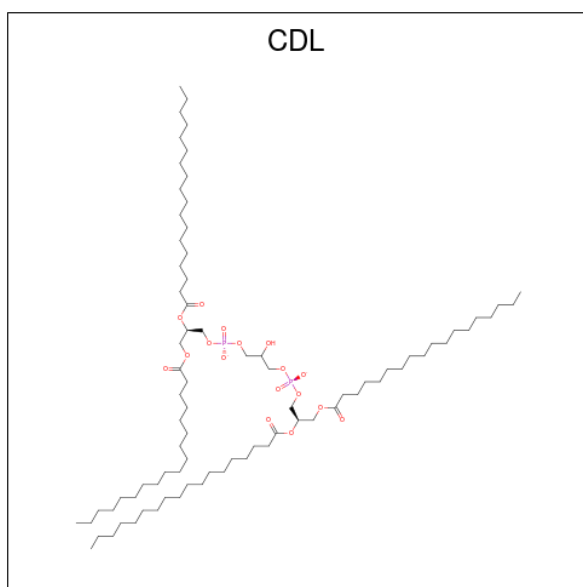
- Molecule 52 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1)

(formula:  $C_{44}H_{88}NO_8P$ ).



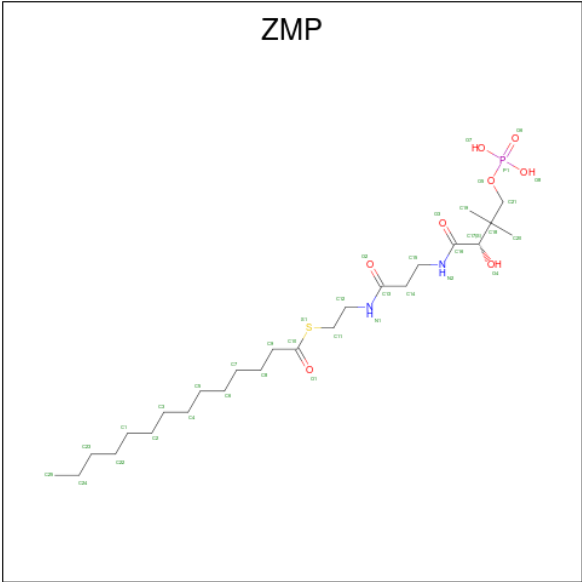
Mol	Chain	Residues	Atoms					AltConf
52	6	1	Total	C	N	O	P	0
			46	36	1	8	1	
52	9	1	Total	C	N	O	P	0
			54	44	1	8	1	
52	L	1	Total	C	N	O	P	0
			54	44	1	8	1	
52	M	1	Total	C	N	O	P	0
			54	44	1	8	1	
52	M	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 53 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



Mol	Chain	Residues	Atoms				AltConf
53	L	1	Total	C	O	P	0
			85	66	17	2	
53	L	1	Total	C	O	P	0
			100	81	17	2	
53	M	1	Total	C	O	P	0
			100	81	17	2	
53	N	1	Total	C	O	P	0
			90	71	17	2	
53	V	1	Total	C	O	P	0
			94	75	17	2	
53	W	1	Total	C	O	P	0
			100	81	17	2	
53	h	1	Total	C	O	P	0
			58	39	17	2	
53	x	1	Total	C	O	P	0
			75	56	17	2	

- Molecule 54 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C<sub>25</sub>H<sub>49</sub>N<sub>2</sub>O<sub>8</sub>PS).

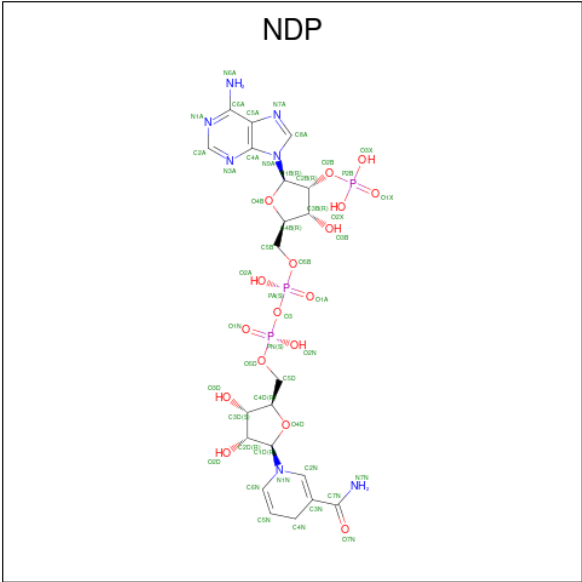


Mol	Chain	Residues	Atoms					AltConf
54	X	1	Total	C	N	O	P	S
			31	20	2	7	1	1
54	g	1	Total	C	N	O	P	S
			34	23	2	7	1	1

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

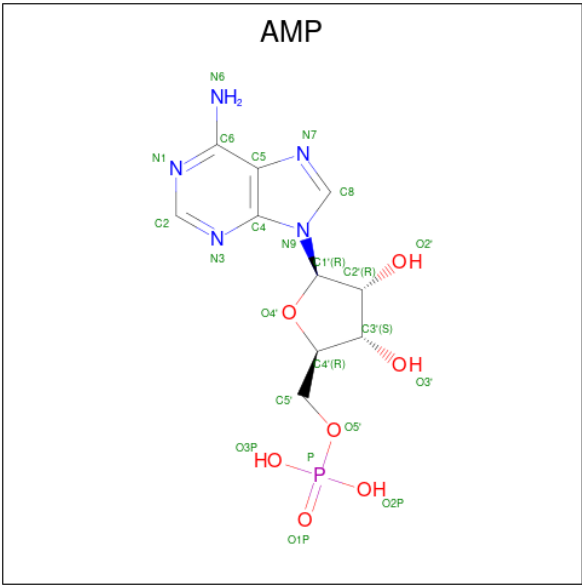
Mol	Chain	Residues	Atoms		AltConf
55	b	1	Total	Zn	0
			1	1	

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



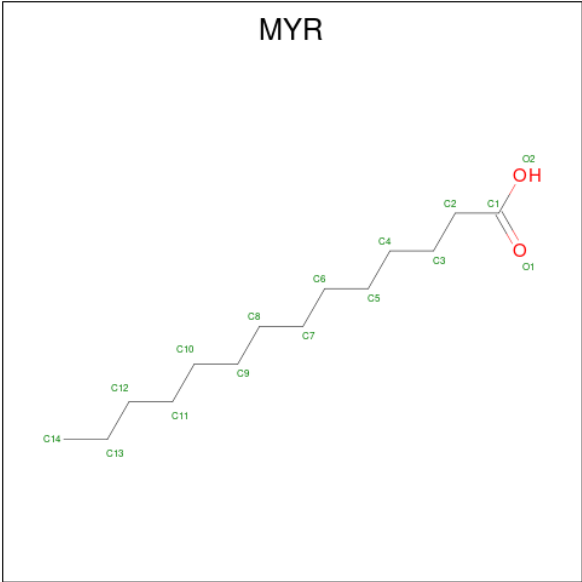
Mol	Chain	Residues	Atoms					AltConf
56	d	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 57 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula:  $C_{10}H_{14}N_5O_7P$ ).



Mol	Chain	Residues	Atoms					AltConf
57	k	1	Total	C	N	O	P	0
			23	10	5	7	1	

- Molecule 58 is MYRISTIC ACID (CCD ID: MYR) (formula:  $C_{14}H_{28}O_2$ ).

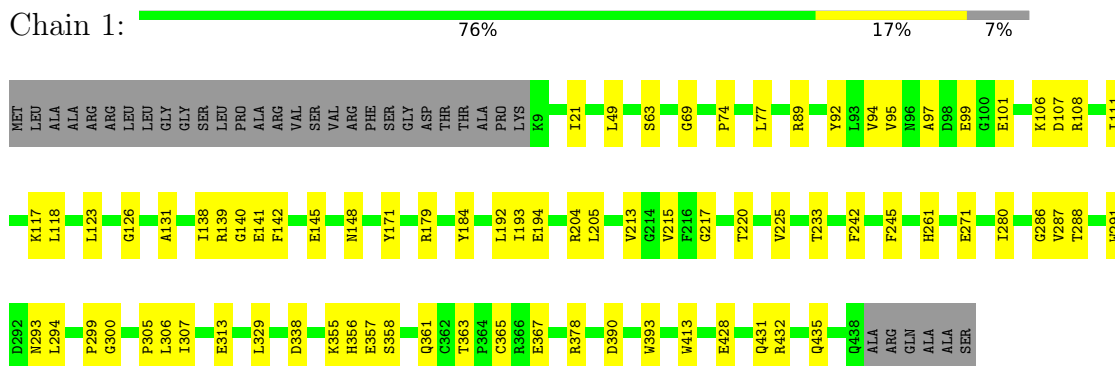


Mol	Chain	Residues	Atoms			AltConf
58	s	1	Total	C	O	0
			15	14	1	

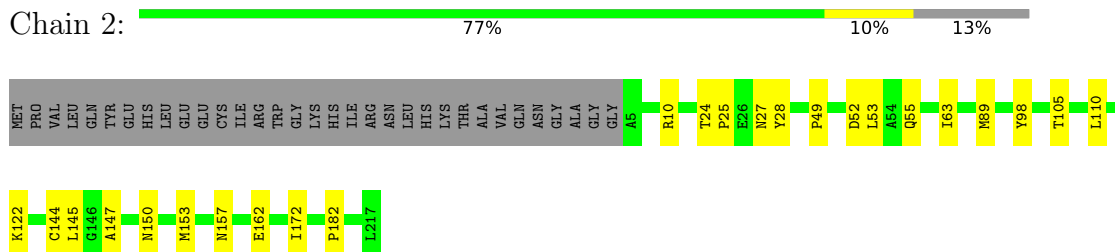
### 3 Residue-property plots

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.

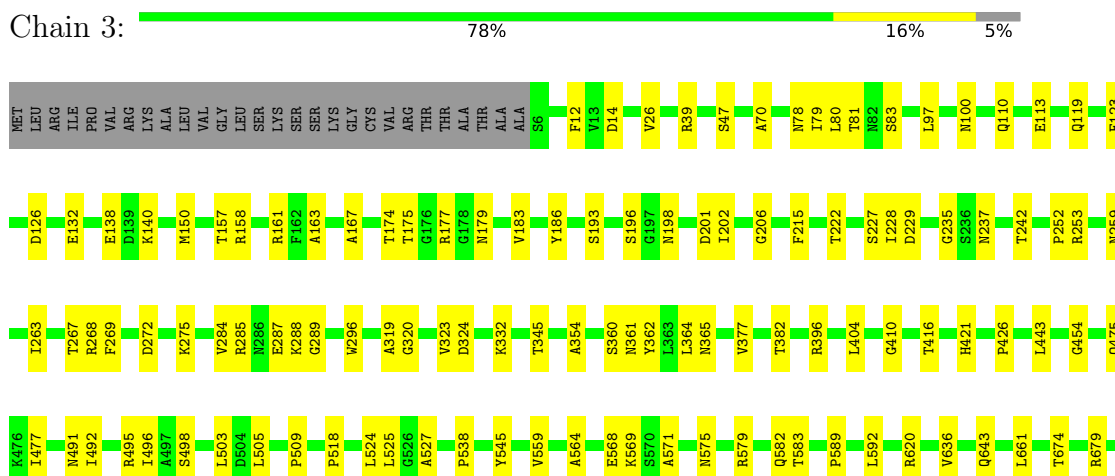
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

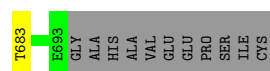


- Molecule 2: Mitochondrial complex I, 24 kDa subunit



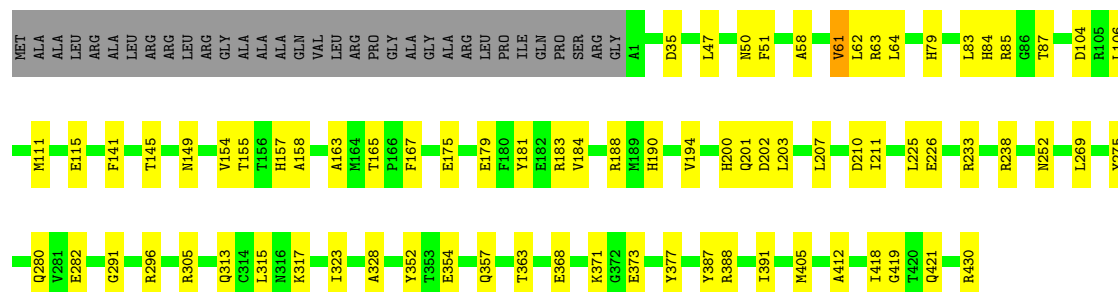
- Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1





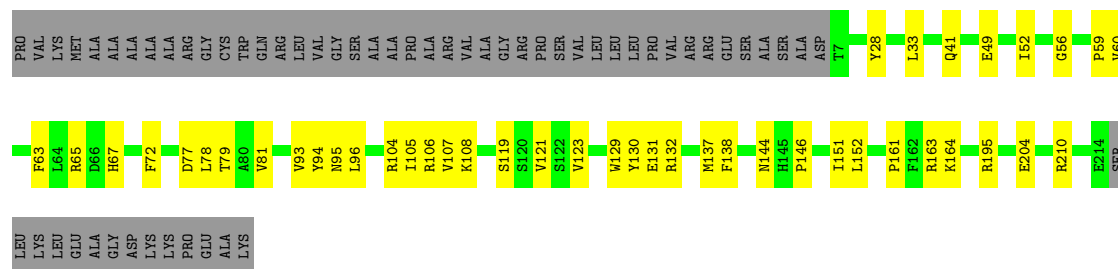
- Molecule 4: Mitochondrial complex I, 49 kDa subunit

Chain 4: 76% 16% 7%



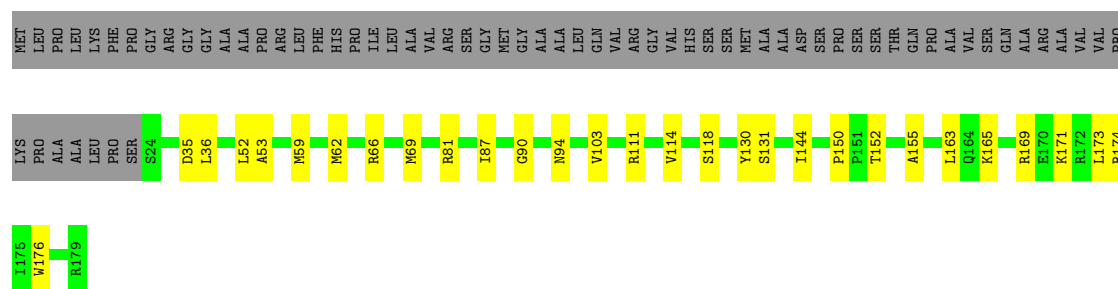
- Molecule 5: NADH:ubiquinone oxidoreductase core subunit S3

Chain 5: 62% 17% 22%



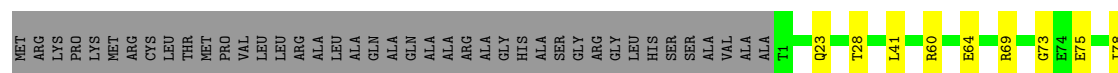
- Molecule 6: Mitochondrial complex I, PSST subunit

Chain 6: 57% 13% 30%



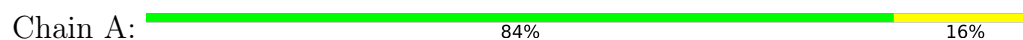
- Molecule 7: Mitochondrial complex I, TYKY subunit

Chain 9: 69% 12% 19%

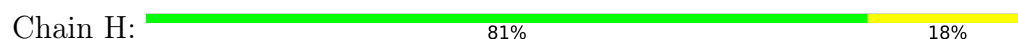




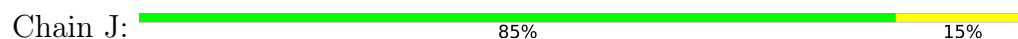
- Molecule 8: NADH-ubiquinone oxidoreductase chain 3



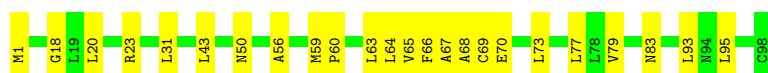
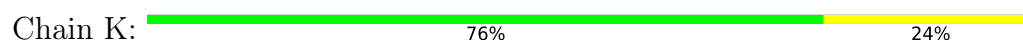
- Molecule 9: NADH-ubiquinone oxidoreductase chain 1



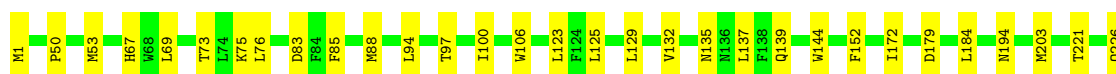
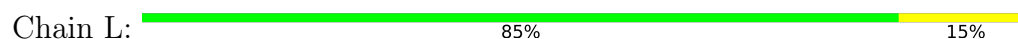
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6



- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



- Molecule 12: NADH-ubiquinone oxidoreductase chain 5



- Molecule 13: NADH-ubiquinone oxidoreductase chain 4



I412	N188	M1
H440	V196	L2
M441	L197	K3
L449	M204	L11
I453	P208	S18
I454	L209	I23
P457	L214	L50
L458	W215	N51
Y459	L216	F57
	I225	L61
	A232	P64
	L236	M70
	K237	L75
	M243	R91
	I246	K92
	L249	K93
	I301	L94
	A318	I100
	M325	Q103
	L329	I116
	A330	F117
	M331	F118
	R340	Y119
	L352	F122
	M355	I132
	W359	R135
	L369	G137
	P370	N138
	I373	Q139
	I376	A155
	L379	G156
	M383	S157
	I393	L158
	L408	P159
		L160
		L161
		I167
		N175
		L172

- |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| A180 | A181 | T17  | V20  | L27  | W30  | I41  | M49  | P50  | R51  | E54  | T57  | K58  | S67  | Q83  | H84  | T85  | N91  | A109 | P110 | F111 | H112 | V115 | I122 | L128 | M133 | A137 | L142 | L146 | I149 | I159 | S161 | I162 | W167 | L170 | P176 |
| G188 | W199 | V193 | L194 | L195 | M211 | T212 | T213 | S214 | F216 | M236 | P238 | L239 | M240 | T241 | L242 | L243 | V244 | L245 | L246 | S258 | M261 | L266 | M270 | S275 | L278 | A283 | L284 | T285 | Y291 | T330 | S333 | T340 | E347 |      |      |

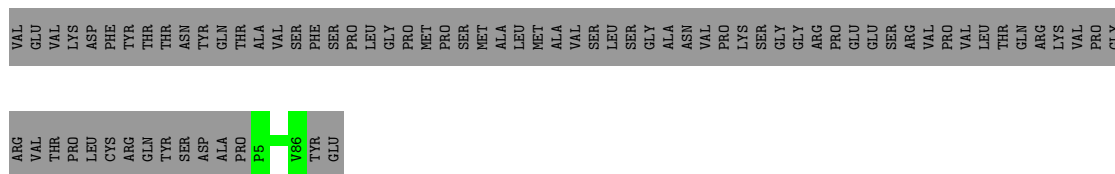
- |     |    |    |    |    |  |     |  |     |  |     |  |     |     |     |     |     |  |     |  |     |  |     |  |      |  |      |  |      |
|-----|----|----|----|----|--|-----|--|-----|--|-----|--|-----|-----|-----|-----|-----|--|-----|--|-----|--|-----|--|------|--|------|--|------|
| MET | A1 | K2 | T3 | L4 |  | I11 |  | K20 |  | G32 |  | S39 | V40 | A41 | L42 | K43 |  | R54 |  | T59 |  | I65 |  | L100 |  | G127 |  | V140 |
|-----|----|----|----|----|--|-----|--|-----|--|-----|--|-----|-----|-----|-----|-----|--|-----|--|-----|--|-----|--|------|--|------|--|------|

- [illegible]

- [illegible]

- WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

Chain j:  52% 48%




- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain Y:  93% 6%



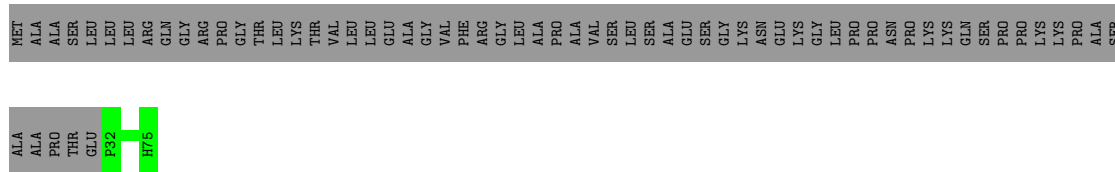
- Molecule 19: Mitochondrial complex I, PDSW subunit

Chain Z:  89% 9%



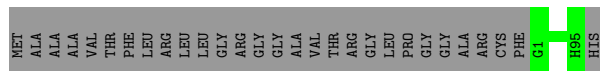
- Molecule 20: Mitochondrial complex I, 10 kDa subunit

Chain a:  40% 60%



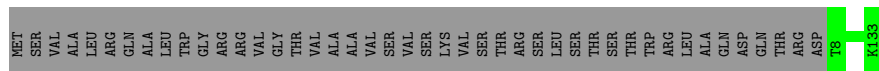
- Molecule 21: Mitochondrial complex I, 13 kDa subunit

Chain b:  77% 23%




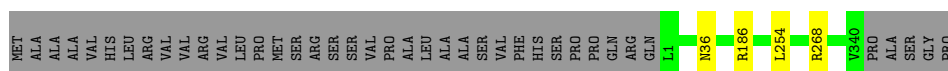
- Molecule 22: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain c:  74% 26%

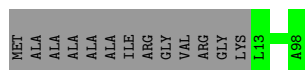
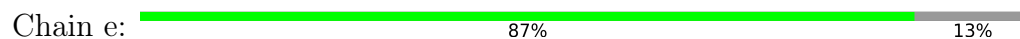


- Molecule 23: NADH:ubiquinone oxidoreductase subunit A9

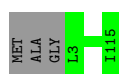
Chain d:  88% 11%



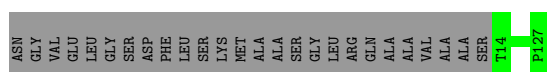
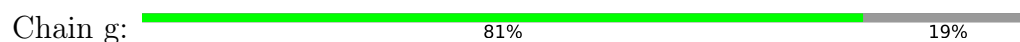
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



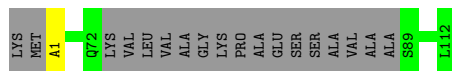
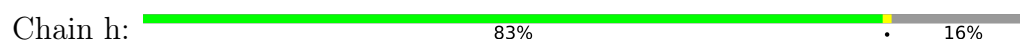
- Molecule 25: Mitochondrial complex I, B13 subunit



- Molecule 26: NADH:ubiquinone oxidoreductase subunit A6



- Molecule 27: Mitochondrial complex I, B14.5a subunit

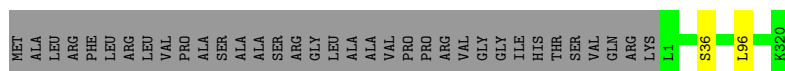
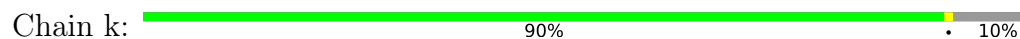


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



There are no outlier residues recorded for this chain.

- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



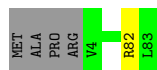
- Molecule 30: NADH:ubiquinone oxidoreductase subunit S5





- Molecule 31: NADH:ubiquinone oxidoreductase subunit A3

Chain m: 94% 5%



- Molecule 32: NADH:ubiquinone oxidoreductase subunit B3

Chain n: 81% 19%



- Molecule 33: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain o: 98% .



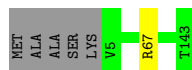
- Molecule 34: NADH:ubiquinone oxidoreductase subunit B4

Chain p: 98% .



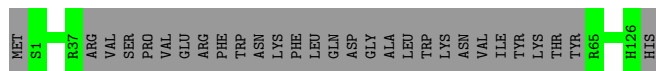
- Molecule 35: Mitochondrial complex I, B16.6 subunit

Chain q: 96% . .



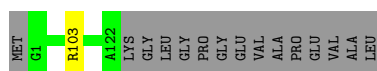
- Molecule 36: Mitochondrial complex I, B17 subunit

Chain r: 77% 23%



- Molecule 37: NADH:ubiquinone oxidoreductase subunit B7

Chain s: 88% . 11%



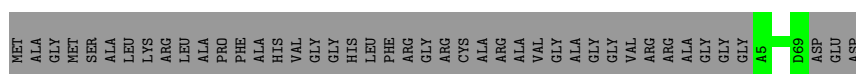
- Molecule 38: NADH:ubiquinone oxidoreductase subunit B9

Chain t: 98%



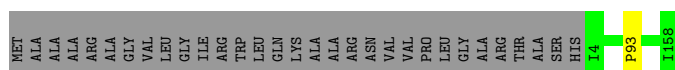
- Molecule 39: NADH:ubiquinone oxidoreductase subunit B2

Chain u: 60%



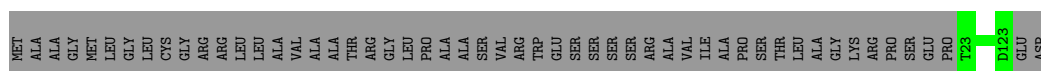
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain v: 83%



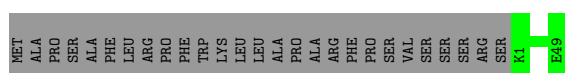
- Molecule 41: Mitochondrial complex I, ESSS subunit

Chain w: 66%



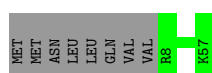
- Molecule 42: Mitochondrial complex I, KFYI subunit

Chain x: 64%



- Molecule 43: Mitochondrial complex I, MNLL subunit

Chain y: 86%



- Molecule 44: Mitochondrial complex I, MWFE subunit

Chain z: 100%

There are no outlier residues recorded for this chain.

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7162	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 ( $e^-/\text{\AA}^2$ )	100	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k 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: 3PE, NDP, K, FMN, PC1, 970, AYA, CDL, FES, SEP, 2MR, ZMP, AMP, NAI, ZN, MYR, SF4, FME

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	1	0.35	0/3386	0.56	0/4575
2	2	0.33	0/1695	0.54	0/2306
3	3	0.34	0/5362	0.55	0/7266
4	4	0.38	0/3535	0.56	0/4791
5	5	0.35	0/1776	0.55	2/2417 (0.1%)
6	6	0.41	0/1278	0.56	0/1728
7	9	0.39	0/1445	0.56	0/1956
8	A	0.33	0/947	0.63	2/1296 (0.2%)
9	H	0.35	0/2603	0.64	0/3561
10	J	0.36	0/1378	0.65	2/1868 (0.1%)
11	K	0.31	0/749	0.62	0/1014
12	L	0.32	0/4925	0.56	0/6700
13	M	0.33	0/3731	0.61	1/5085 (0.0%)
14	N	0.34	0/2787	0.59	1/3795 (0.0%)
15	V	0.27	0/1041	0.51	0/1412
16	W	0.30	0/1188	0.52	0/1607
17	X	0.27	0/713	0.51	0/963
17	j	0.29	0/670	0.51	0/902
18	Y	0.30	0/1440	0.53	0/1942
19	Z	0.30	0/1475	0.50	0/1989
20	a	0.28	0/383	0.48	0/518
21	b	0.32	0/749	0.47	0/1009
22	c	0.30	0/1047	0.51	0/1415
23	d	0.30	0/2824	0.55	1/3830 (0.0%)
24	e	0.28	0/702	0.51	0/945
25	f	0.29	0/937	0.51	0/1271
26	g	0.32	0/993	0.52	0/1336
27	h	0.31	0/779	0.55	0/1053
28	i	0.33	0/1250	0.51	0/1698
29	k	0.30	0/2646	0.50	1/3579 (0.0%)
30	l	0.30	0/896	0.52	0/1200

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
31	m	0.28	0/647	0.49	0/890
32	n	0.30	0/653	0.45	0/882
33	o	0.32	0/1035	0.49	0/1398
34	p	0.28	0/1085	0.49	0/1467
35	q	0.30	0/1171	0.50	0/1579
36	r	0.29	0/874	0.52	0/1188
37	s	0.27	0/1072	0.48	0/1436
38	t	0.30	0/1573	0.51	1/2130 (0.0%)
39	u	0.30	0/590	0.47	0/810
40	v	0.29	0/1361	0.52	1/1861 (0.1%)
41	w	0.30	0/872	0.51	0/1185
42	x	0.27	0/425	0.41	0/576
43	y	0.27	0/449	0.50	0/605
44	z	0.36	0/591	0.52	0/795
All	All	0.33	0/67728	0.55	12/91829 (0.0%)

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
2	2	0	1
3	3	0	1
4	4	0	1
10	J	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	254	LEU	CA-CB-CG	6.64	130.56	115.30
10	J	146	LEU	CA-CB-CG	6.30	129.79	115.30
5	5	52	ILE	C-N-CA	6.28	137.40	121.70
10	J	52	LEU	CA-CB-CG	5.94	128.96	115.30
8	A	3	LEU	CA-CB-CG	5.83	128.72	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	63	ILE	Peptide
3	3	259	ASN	Peptide
4	4	275	TYR	Peptide
10	J	115	ILE	Peptide

## 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	1	3312	0	3269	53	0
2	2	1655	0	1668	14	0
3	3	5275	0	5300	66	0
4	4	3457	0	3397	56	0
5	5	1726	0	1676	27	0
6	6	1247	0	1259	20	0
7	9	1414	0	1371	20	0
8	A	922	0	953	17	0
9	H	2528	0	2641	43	0
10	J	1344	0	1364	19	0
11	K	749	0	793	20	0
12	L	4807	0	4949	55	0
13	M	3647	0	3849	46	0
14	N	2723	0	2930	43	0
15	V	1028	0	1036	10	0
16	W	1155	0	1177	11	0
17	X	701	0	692	5	0
17	j	660	0	663	0	0
18	Y	1403	0	1392	7	0
19	Z	1441	0	1419	9	0
20	a	371	0	344	0	0
21	b	737	0	710	0	0
22	c	1024	0	1023	0	0
23	d	2748	0	2763	0	0
24	e	691	0	706	0	0
25	f	917	0	958	0	0
26	g	969	0	980	0	0
27	h	769	0	780	0	0
28	i	1209	0	1182	0	0
29	k	2596	0	2559	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	l	874	0	869	0	0
31	m	626	0	635	0	0
32	n	634	0	616	0	0
33	o	1004	0	995	0	0
34	p	1059	0	1062	0	0
35	q	1142	0	1137	0	0
36	r	846	0	864	0	0
37	s	1047	0	1013	0	0
38	t	1520	0	1477	0	0
39	u	563	0	509	0	0
40	v	1307	0	1207	0	0
41	w	846	0	792	0	0
42	x	412	0	411	0	0
43	y	436	0	437	0	0
44	z	576	0	570	0	0
45	1	8	0	0	3	0
45	3	16	0	0	1	0
45	6	8	0	0	1	0
45	9	16	0	0	0	0
46	1	31	0	19	0	0
47	1	44	0	27	2	0
48	2	4	0	0	1	0
48	3	4	0	0	0	0
49	3	1	0	0	0	0
50	4	29	0	0	0	0
51	4	40	0	54	1	0
51	6	51	0	82	3	0
51	A	51	0	82	0	0
51	J	91	0	136	2	0
51	L	82	0	118	1	0
51	M	44	0	65	1	0
51	N	51	0	82	0	0
51	V	64	0	75	1	0
51	i	51	0	82	0	0
51	o	31	0	36	0	0
52	6	46	0	69	1	0
52	9	54	0	88	4	0
52	L	54	0	88	5	0
52	M	108	0	176	8	0
53	L	185	0	276	12	0
53	M	100	0	156	3	0
53	N	90	0	133	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	V	94	0	141	4	0
53	W	100	0	156	7	0
53	h	58	0	60	0	0
53	x	75	0	97	0	0
54	X	31	0	34	1	0
54	g	34	0	40	0	0
55	b	1	0	0	0	0
56	d	48	0	26	0	0
57	k	23	0	12	0	0
58	s	15	0	27	0	0
All	All	67950	0	68834	489	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 6.

The worst 5 of 489 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)
14:N:242:ILE:HG23	53:N:402:CDL:H791	1.73	0.71
5:5:129:TRP:O	5:5:132:ARG:HB3	1.92	0.70
7:9:92:ILE:HG12	7:9:111:ILE:HG12	1.74	0.69
11:K:70:GLU:O	11:K:73:LEU:HB3	1.92	0.68
4:4:405:MET:SD	4:4:421:GLN:NE2	2.68	0.66

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	1	428/464 (92%)	408 (95%)	20 (5%)	0	100	100
2	2	211/246 (86%)	195 (92%)	16 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	3	686/727 (94%)	641 (93%)	45 (7%)	0	100	100
4	4	427/463 (92%)	398 (93%)	29 (7%)	0	100	100
5	5	206/266 (77%)	190 (92%)	16 (8%)	0	100	100
6	6	154/223 (69%)	148 (96%)	6 (4%)	0	100	100
7	9	174/217 (80%)	159 (91%)	15 (9%)	0	100	100
8	A	113/115 (98%)	103 (91%)	10 (9%)	0	100	100
9	H	316/318 (99%)	302 (96%)	14 (4%)	0	100	100
10	J	173/175 (99%)	164 (95%)	8 (5%)	1 (1%)	22	54
11	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
12	L	604/606 (100%)	564 (93%)	40 (7%)	0	100	100
13	M	457/459 (100%)	440 (96%)	17 (4%)	0	100	100
14	N	345/347 (99%)	333 (96%)	12 (4%)	0	100	100
15	V	138/141 (98%)	134 (97%)	4 (3%)	0	100	100
16	W	137/189 (72%)	132 (96%)	5 (4%)	0	100	100
17	X	85/157 (54%)	80 (94%)	5 (6%)	0	100	100
17	j	80/157 (51%)	73 (91%)	7 (9%)	0	100	100
18	Y	169/172 (98%)	159 (94%)	10 (6%)	0	100	100
19	Z	169/175 (97%)	166 (98%)	3 (2%)	0	100	100
20	a	42/109 (38%)	40 (95%)	2 (5%)	0	100	100
21	b	93/124 (75%)	91 (98%)	2 (2%)	0	100	100
22	c	124/170 (73%)	122 (98%)	2 (2%)	0	100	100
23	d	338/380 (89%)	318 (94%)	20 (6%)	0	100	100
24	e	84/99 (85%)	81 (96%)	3 (4%)	0	100	100
25	f	111/116 (96%)	107 (96%)	4 (4%)	0	100	100
26	g	112/140 (80%)	109 (97%)	3 (3%)	0	100	100
27	h	92/114 (81%)	89 (97%)	3 (3%)	0	100	100
28	i	143/145 (99%)	139 (97%)	4 (3%)	0	100	100
29	k	317/355 (89%)	299 (94%)	18 (6%)	0	100	100
30	l	103/106 (97%)	94 (91%)	9 (9%)	0	100	100
31	m	78/84 (93%)	72 (92%)	6 (8%)	0	100	100
32	n	77/98 (79%)	73 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	o	118/122 (97%)	115 (98%)	3 (2%)	0	100	100
34	p	126/130 (97%)	119 (94%)	7 (6%)	0	100	100
35	q	137/144 (95%)	134 (98%)	3 (2%)	0	100	100
36	r	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
37	s	120/137 (88%)	118 (98%)	2 (2%)	0	100	100
38	t	175/179 (98%)	165 (94%)	10 (6%)	0	100	100
39	u	63/108 (58%)	61 (97%)	2 (3%)	0	100	100
40	v	153/186 (82%)	143 (94%)	10 (6%)	0	100	100
41	w	99/154 (64%)	93 (94%)	6 (6%)	0	100	100
42	x	47/76 (62%)	45 (96%)	2 (4%)	0	100	100
43	y	48/58 (83%)	48 (100%)	0	0	100	100
44	z	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
All	All	8131/9247 (88%)	7712 (95%)	418 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	116	VAL

### 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	1	344/368 (94%)	343 (100%)	1 (0%)	91	94
2	2	183/210 (87%)	182 (100%)	1 (0%)	86	92
3	3	578/608 (95%)	576 (100%)	2 (0%)	91	94
4	4	370/391 (95%)	367 (99%)	3 (1%)	79	85
5	5	189/230 (82%)	189 (100%)	0	100	100
6	6	132/181 (73%)	130 (98%)	2 (2%)	60	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	9	151/179 (84%)	151 (100%)	0	100	100
8	A	103/103 (100%)	103 (100%)	0	100	100
9	H	278/278 (100%)	276 (99%)	2 (1%)	81	88
10	J	144/144 (100%)	143 (99%)	1 (1%)	81	88
11	K	86/86 (100%)	85 (99%)	1 (1%)	67	79
12	L	538/538 (100%)	535 (99%)	3 (1%)	84	90
13	M	411/411 (100%)	410 (100%)	1 (0%)	92	96
14	N	315/315 (100%)	314 (100%)	1 (0%)	91	94
15	V	101/102 (99%)	101 (100%)	0	100	100
16	W	122/160 (76%)	122 (100%)	0	100	100
17	X	80/141 (57%)	80 (100%)	0	100	100
17	j	76/141 (54%)	76 (100%)	0	100	100
18	Y	154/155 (99%)	153 (99%)	1 (1%)	84	90
19	Z	155/157 (99%)	155 (100%)	0	100	100
20	a	43/93 (46%)	43 (100%)	0	100	100
21	b	79/97 (81%)	79 (100%)	0	100	100
22	c	113/150 (75%)	113 (100%)	0	100	100
23	d	294/326 (90%)	291 (99%)	3 (1%)	73	82
24	e	76/82 (93%)	76 (100%)	0	100	100
25	f	101/102 (99%)	101 (100%)	0	100	100
26	g	107/124 (86%)	107 (100%)	0	100	100
27	h	84/96 (88%)	84 (100%)	0	100	100
28	i	131/131 (100%)	131 (100%)	0	100	100
29	k	283/309 (92%)	283 (100%)	0	100	100
30	l	94/95 (99%)	94 (100%)	0	100	100
31	m	69/72 (96%)	68 (99%)	1 (1%)	62	76
32	n	61/76 (80%)	61 (100%)	0	100	100
33	o	107/109 (98%)	107 (100%)	0	100	100
34	p	114/116 (98%)	114 (100%)	0	100	100
35	q	119/122 (98%)	118 (99%)	1 (1%)	79	85
36	r	95/122 (78%)	95 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	s	110/120 (92%)	109 (99%)	1 (1%)	75	84
38	t	159/161 (99%)	158 (99%)	1 (1%)	84	90
39	u	59/84 (70%)	59 (100%)	0	100	100
40	v	140/160 (88%)	140 (100%)	0	100	100
41	w	92/130 (71%)	92 (100%)	0	100	100
42	x	44/67 (66%)	44 (100%)	0	100	100
43	y	46/54 (85%)	46 (100%)	0	100	100
44	z	59/59 (100%)	59 (100%)	0	100	100
All	All	7189/7955 (90%)	7163 (100%)	26 (0%)	88	93

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	270	ASN
14	N	235	ASN
37	s	103	ARG
13	M	138	ASN
18	Y	63	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
23	d	87	HIS
29	k	153	ASN
23	d	288	HIS
28	i	5	GLN
33	o	46	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues are 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	$\# Z  > 2$
12	FME	L	1	12	8,9,10	0.95	0	7,9,11	1.12	1 (14%)
15	AYA	V	1	15	6,7,8	1.16	0	5,8,10	2.00	2 (40%)
29	SEP	k	36	29	8,9,10	1.52	1 (12%)	8,12,14	1.78	2 (25%)
13	FME	M	1	13	8,9,10	1.01	1 (12%)	7,9,11	0.86	0
4	2MR	4	85	4	10,12,13	2.34	3 (30%)	5,13,15	1.69	1 (20%)
11	FME	K	1	11	8,9,10	0.99	1 (12%)	7,9,11	0.81	0
27	AYA	h	1	27	6,7,8	1.14	1 (16%)	5,8,10	1.69	1 (20%)

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
12	FME	L	1	12	-	3/7/9/11	-
15	AYA	V	1	15	-	2/4/6/8	-
29	SEP	k	36	29	-	3/5/8/10	-
13	FME	M	1	13	-	5/7/9/11	-
4	2MR	4	85	4	-	0/10/13/15	-
11	FME	K	1	11	-	4/7/9/11	-
27	AYA	h	1	27	-	0/4/6/8	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	85	2MR	CZ-NE	4.80	1.44	1.34
4	4	85	2MR	CZ-NH2	4.73	1.43	1.33
29	k	36	SEP	P-O1P	3.34	1.61	1.50
13	M	1	FME	CA-N	-2.16	1.43	1.46
4	4	85	2MR	CQ1-NH1	-2.10	1.42	1.46

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	h	1	AYA	CB-CA-N	3.55	113.56	109.61
29	k	36	SEP	P-OG-CB	-3.34	109.09	118.30
29	k	36	SEP	OG-CB-CA	3.31	111.36	108.14
15	V	1	AYA	CB-CA-N	3.30	113.28	109.61
4	4	85	2MR	NE-CZ-NH2	-2.93	116.80	119.48

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	K	1	FME	CA-CB-CG-SD
12	L	1	FME	O-C-CA-CB
12	L	1	FME	CA-CB-CG-SD
13	M	1	FME	C-CA-CB-CG
13	M	1	FME	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	V	1	AYA	3	0
13	M	1	FME	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 44 ligands modelled in this entry, 2 are monoatomic - leaving 42 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	$\# Z  > 2$
50	970	4	501	-	33,33,33	0.42	0	48,50,50	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
52	PC1	L	1003	-	53,53,53	0.32	0	59,61,61	0.62	2 (3%)
53	CDL	L	1004	-	84,84,99	0.28	0	90,96,111	0.22	0
52	PC1	M	503	-	53,53,53	0.30	0	59,61,61	0.36	0
45	SF4	6	201	6	0,12,12	-	-	-		
45	SF4	9	403	7	0,12,12	-	-	-		
51	3PE	N	401	-	50,50,50	0.34	0	53,55,55	0.55	1 (1%)
51	3PE	L	1001	-	50,50,50	0.30	0	53,55,55	0.33	0
51	3PE	J	201	-	50,50,50	0.32	0	53,55,55	0.37	0
51	3PE	V	201	-	26,26,50	0.48	0	30,31,55	0.48	1 (3%)
51	3PE	A	201	-	50,50,50	0.32	0	53,55,55	0.33	0
51	3PE	M	501	-	43,43,50	0.34	0	46,48,55	0.40	0
47	NAI	1	503	-	42,48,48	0.60	0	47,73,73	1.99	4 (8%)
53	CDL	L	1005	-	99,99,99	0.25	0	105,111,111	0.30	0
51	3PE	J	202	-	39,39,50	0.35	0	42,44,55	0.48	0
48	FES	3	803	3	0,4,4	-	-	-		
52	PC1	6	202	-	45,45,53	0.32	0	51,53,61	0.37	0
53	CDL	W	201	-	99,99,99	0.26	0	105,111,111	0.30	0
45	SF4	9	402	7	0,12,12	-	-	-		
52	PC1	9	401	-	53,53,53	0.31	0	59,61,61	0.51	1 (1%)
53	CDL	x	101	-	74,74,99	0.30	0	80,86,111	0.43	1 (1%)
53	CDL	h	201	-	57,57,99	0.30	0	63,69,111	0.34	0
45	SF4	3	802	3	0,12,12	-	-	-		
51	3PE	L	1002	-	30,30,50	0.41	0	33,35,55	0.78	2 (6%)
53	CDL	V	203	-	93,93,99	0.25	0	99,105,111	0.27	0
53	CDL	N	402	-	89,89,99	0.29	0	95,101,111	0.40	0
45	SF4	1	501	1	0,12,12	-	-	-		
51	3PE	V	202	-	36,36,50	0.35	0	39,41,55	0.31	0
51	3PE	6	203	-	50,50,50	0.30	0	53,55,55	0.32	0
48	FES	2	300	2	0,4,4	-	-	-		
54	ZMP	X	101	17	24,30,36	0.84	1 (4%)	29,37,45	0.94	1 (3%)
56	NDP	d	401	-	45,52,52	0.52	0	53,80,80	0.62	1 (1%)
57	AMP	k	501	-	22,25,25	0.88	1 (4%)	25,38,38	1.19	2 (8%)
51	3PE	4	502	-	39,39,50	0.33	0	42,44,55	0.35	0
51	3PE	o	501	-	30,30,50	0.37	0	33,35,55	0.37	0
52	PC1	M	502	-	53,53,53	0.28	0	59,61,61	0.37	0
46	FMN	1	502	-	33,33,33	1.10	2 (6%)	48,50,50	1.29	8 (16%)
54	ZMP	g	201	-	27,33,36	0.66	1 (3%)	32,40,45	1.22	3 (9%)
45	SF4	3	801	3	0,12,12	-	-	-		
58	MYR	s	201	37	14,14,15	0.19	0	13,13,15	0.21	0
51	3PE	i	201	-	50,50,50	0.30	0	53,55,55	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
53	CDL	M	504	-	99,99,99	0.28	0	105,111,111	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	970	4	501	-	-	4/8/41/41	0/5/5/5
53	CDL	L	1004	-	1/1/9/9	28/95/95/110	-
52	PC1	L	1003	-	-	16/57/57/57	-
52	PC1	M	503	-	-	21/57/57/57	-
45	SF4	6	201	6	-	-	0/6/5/5
45	SF4	9	403	7	-	-	0/6/5/5
51	3PE	N	401	-	-	18/54/54/54	-
51	3PE	L	1001	-	-	9/54/54/54	-
51	3PE	J	201	-	-	13/54/54/54	-
51	3PE	V	201	-	-	3/27/27/54	-
51	3PE	A	201	-	-	13/54/54/54	-
51	3PE	M	501	-	-	11/47/47/54	-
47	NAI	1	503	-	-	8/25/72/72	0/5/5/5
53	CDL	L	1005	-	1/1/9/9	34/110/110/110	-
51	3PE	J	202	-	-	17/43/43/54	-
53	CDL	W	201	-	-	21/110/110/110	-
52	PC1	6	202	-	-	11/49/49/57	-
48	FES	3	803	3	-	-	0/1/1/1
52	PC1	9	401	-	-	17/57/57/57	-
45	SF4	9	402	7	-	-	0/6/5/5
53	CDL	x	101	-	2/2/9/9	15/85/85/110	-
53	CDL	h	201	-	-	20/68/68/110	-
45	SF4	3	802	3	-	-	0/6/5/5
51	3PE	L	1002	-	-	12/34/34/54	-
53	CDL	V	203	-	-	25/104/104/110	-
53	CDL	N	402	-	-	29/100/100/110	-
45	SF4	1	501	1	-	-	0/6/5/5
51	3PE	V	202	-	-	9/40/40/54	-
51	3PE	6	203	-	-	10/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	FES	2	300	2	-	-	0/1/1/1
54	ZMP	X	101	17	-	12/35/37/43	-
56	NDP	d	401	-	-	6/30/77/77	0/5/5/5
57	AMP	k	501	-	-	3/6/26/26	0/3/3/3
51	3PE	4	502	-	-	9/43/43/54	-
51	3PE	o	501	-	-	5/34/34/54	-
52	PC1	M	502	-	-	10/57/57/57	-
46	FMN	1	502	-	-	5/18/18/18	0/3/3/3
54	ZMP	g	201	-	-	7/38/40/43	-
58	MYR	s	201	37	-	0/11/12/13	-
45	SF4	3	801	3	-	-	0/6/5/5
51	3PE	i	201	-	-	13/54/54/54	-
53	CDL	M	504	-	1/1/9/9	29/110/110/110	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	1	502	FMN	C4A-N5	3.52	1.37	1.30
54	X	101	ZMP	C9-C10	2.93	1.53	1.50
57	k	501	AMP	C5-C4	2.37	1.47	1.40
54	g	201	ZMP	C9-C10	2.30	1.53	1.50
46	1	502	FMN	C10-N1	2.12	1.37	1.33

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	1	503	NAI	O5B-PA-O1A	-9.67	71.29	109.07
47	1	503	NAI	O2A-PA-O1A	-8.08	72.31	112.24
46	1	502	FMN	C4-N3-C2	-3.43	119.30	125.64
57	k	501	AMP	N3-C2-N1	-3.21	123.67	128.68
54	g	201	ZMP	O1-C10-C9	-3.03	120.41	123.99

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
53	L	1004	CDL	CB4
53	L	1005	CDL	CB4
53	M	504	CDL	CB4
53	x	101	CDL	CA4

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Mol	Chain	Res	Type	Atom
53	x	101	CDL	CB4

5 of 463 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	1	502	FMN	N10-C1'-C2'-O2'
46	1	502	FMN	N10-C1'-C2'-C3'
46	1	502	FMN	C5'-O5'-P-O1P
46	1	502	FMN	C5'-O5'-P-O2P
46	1	502	FMN	C5'-O5'-P-O3P

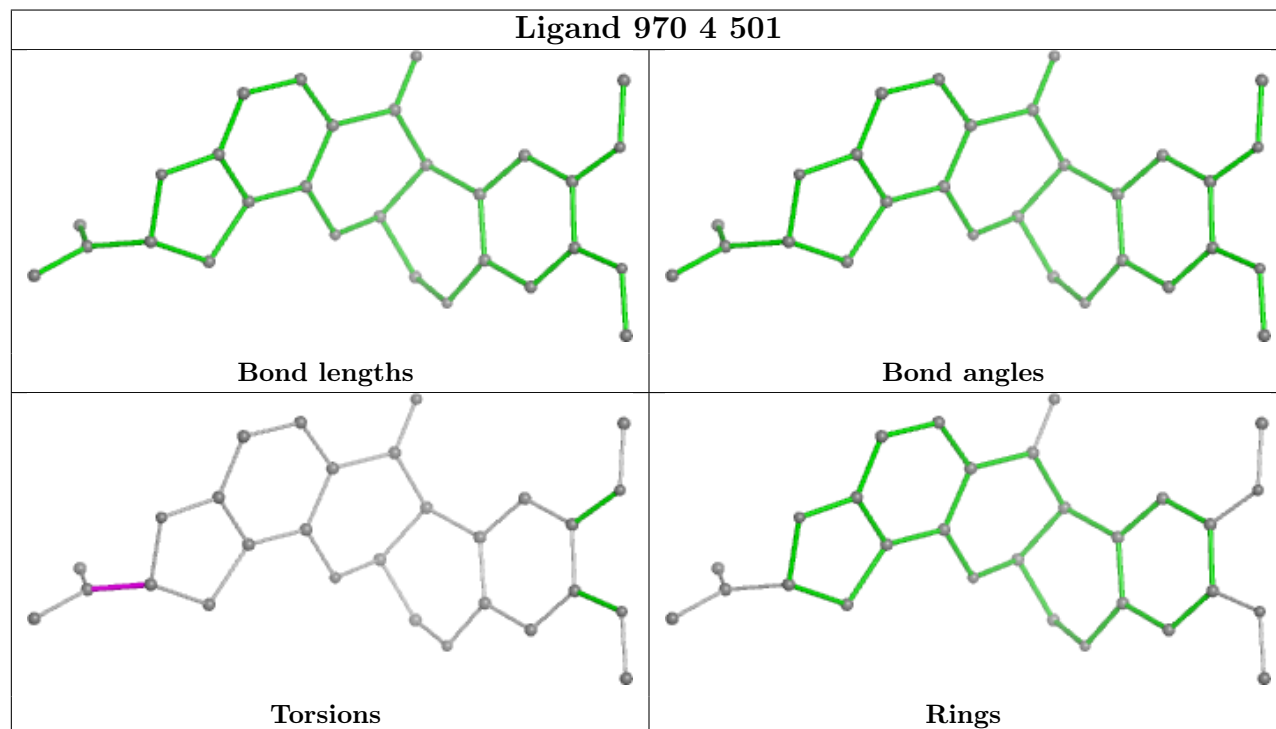
There are no ring outliers.

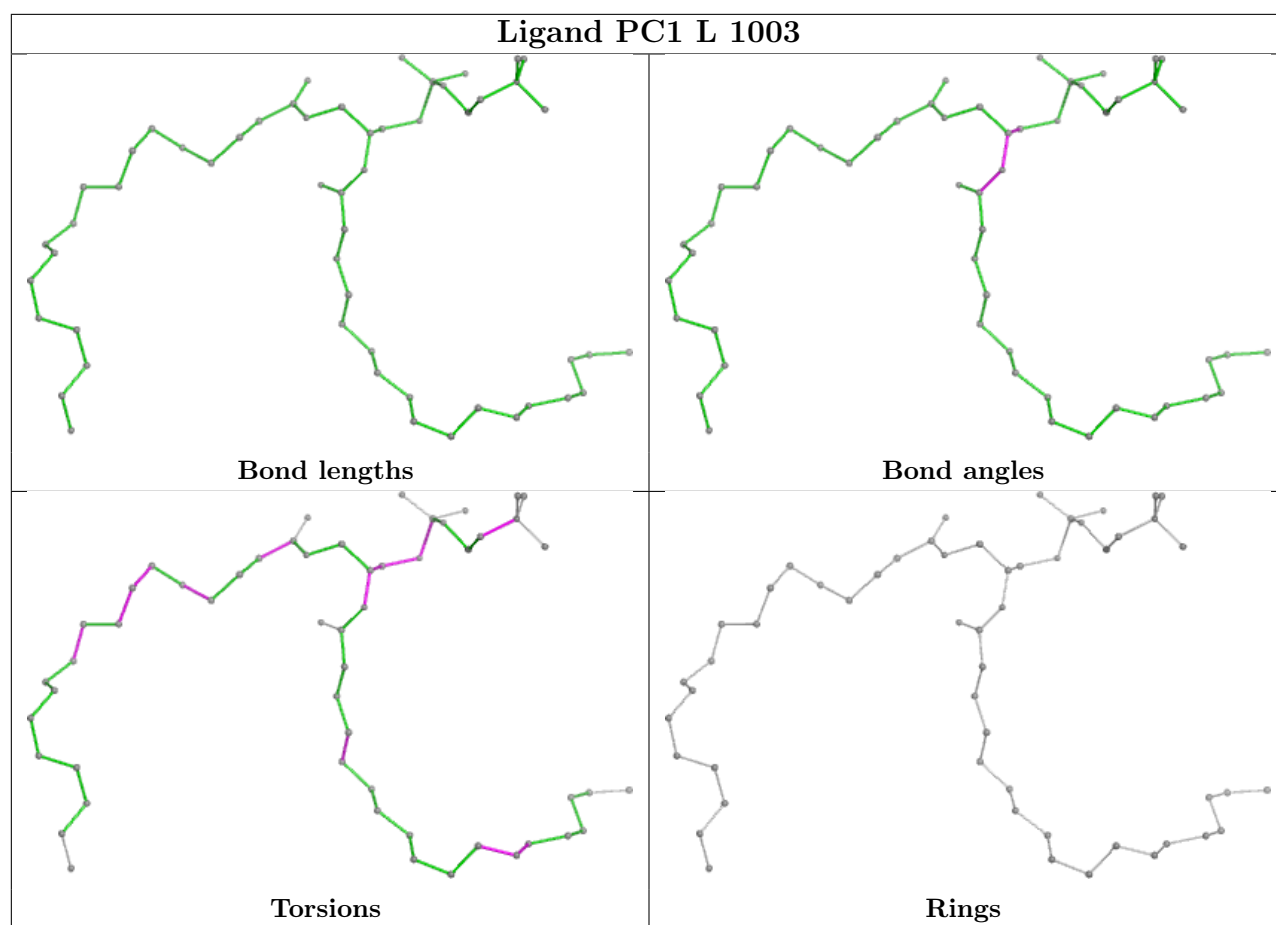
24 monomers are involved in 59 short contacts:

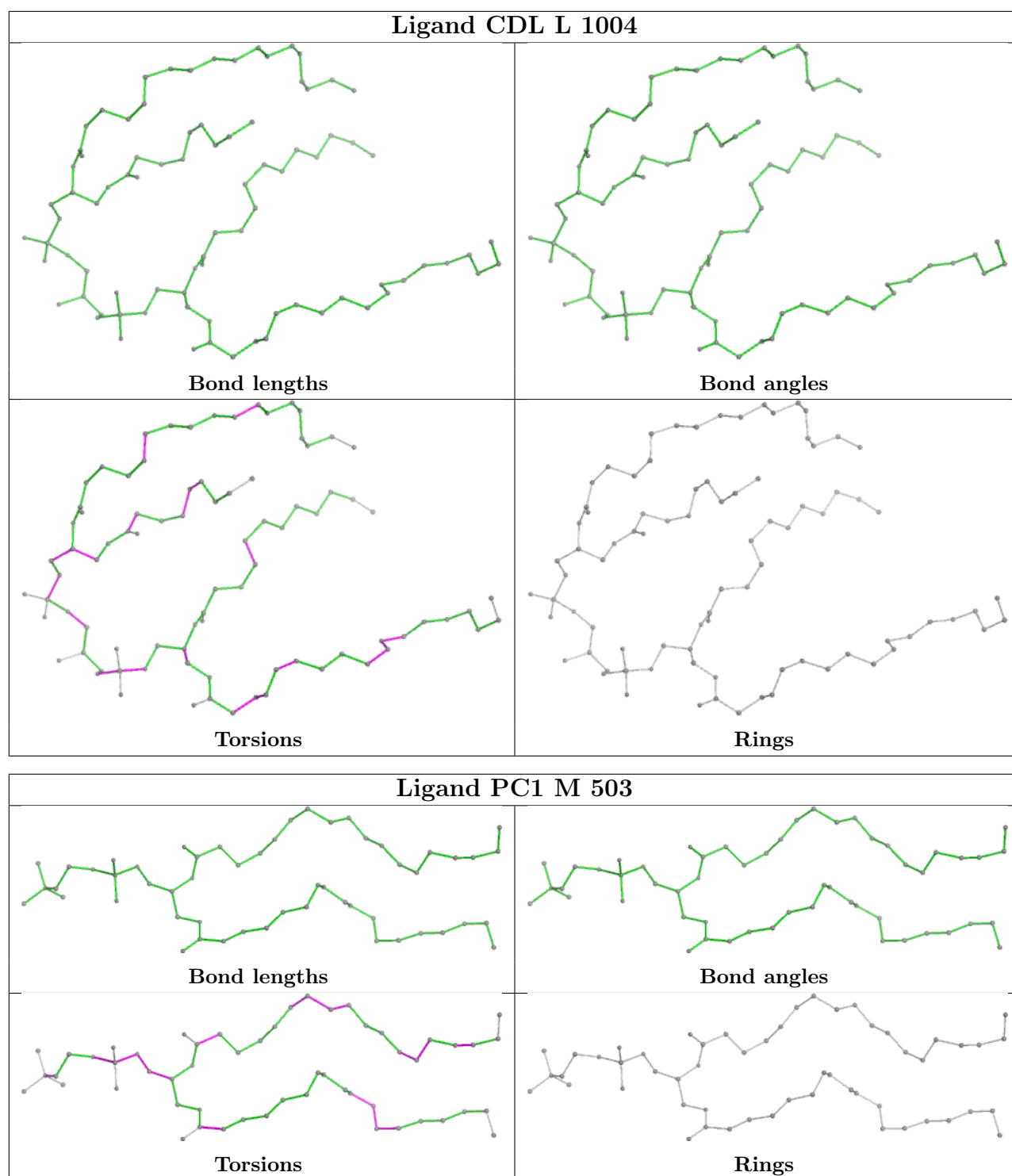
Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	L	1003	PC1	5	0
53	L	1004	CDL	4	0
52	M	503	PC1	2	0
45	6	201	SF4	1	0
51	L	1001	3PE	1	0
51	J	201	3PE	1	0
51	M	501	3PE	1	0
47	1	503	NAI	2	0
53	L	1005	CDL	8	0
51	J	202	3PE	1	0
52	6	202	PC1	1	0
53	W	201	CDL	7	0
52	9	401	PC1	4	0
53	V	203	CDL	4	0
53	N	402	CDL	7	0
45	1	501	SF4	3	0
51	V	202	3PE	1	0
51	6	203	3PE	3	0
48	2	300	FES	1	0
54	X	101	ZMP	1	0
51	4	502	3PE	1	0
52	M	502	PC1	6	0
45	3	801	SF4	1	0
53	M	504	CDL	3	0

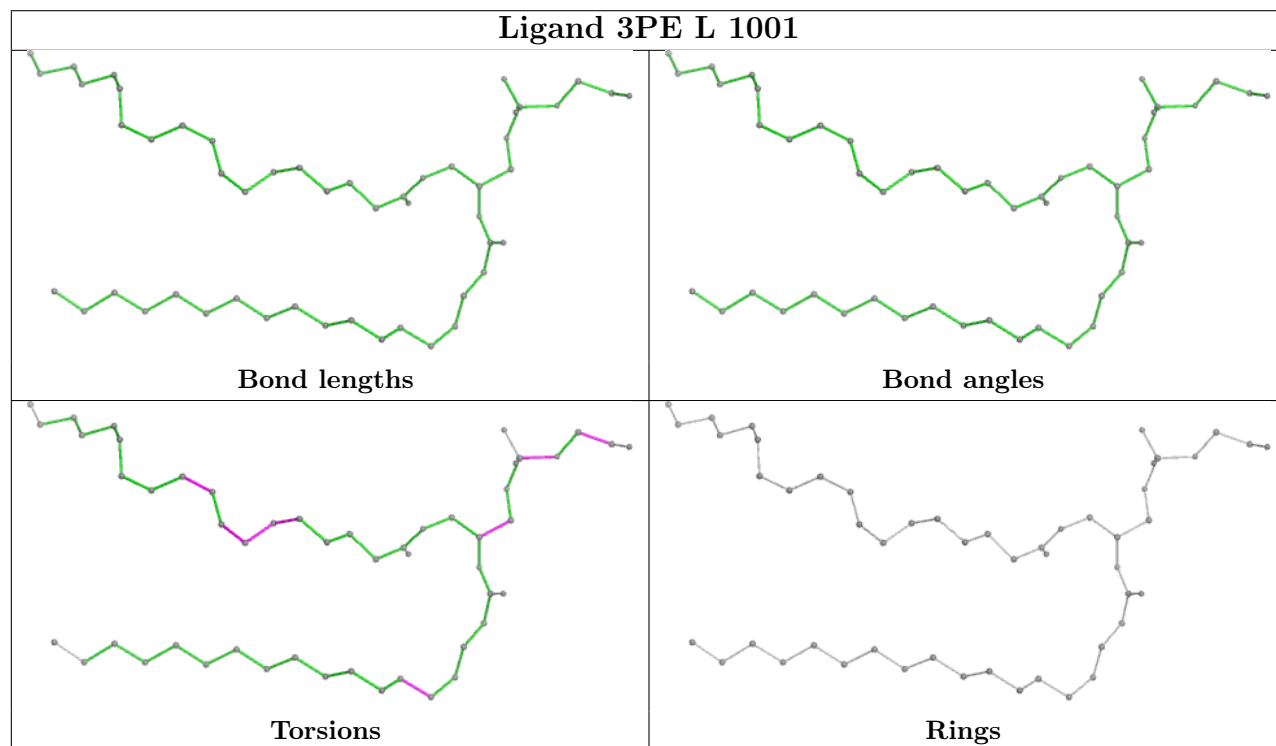
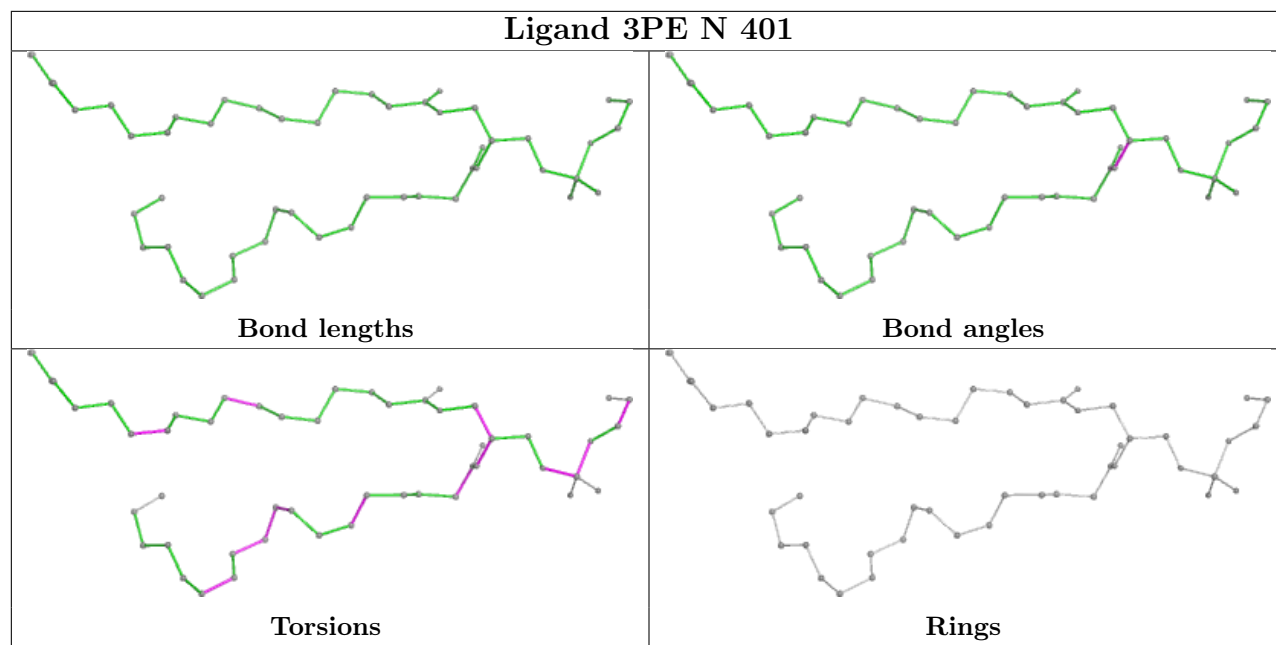
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

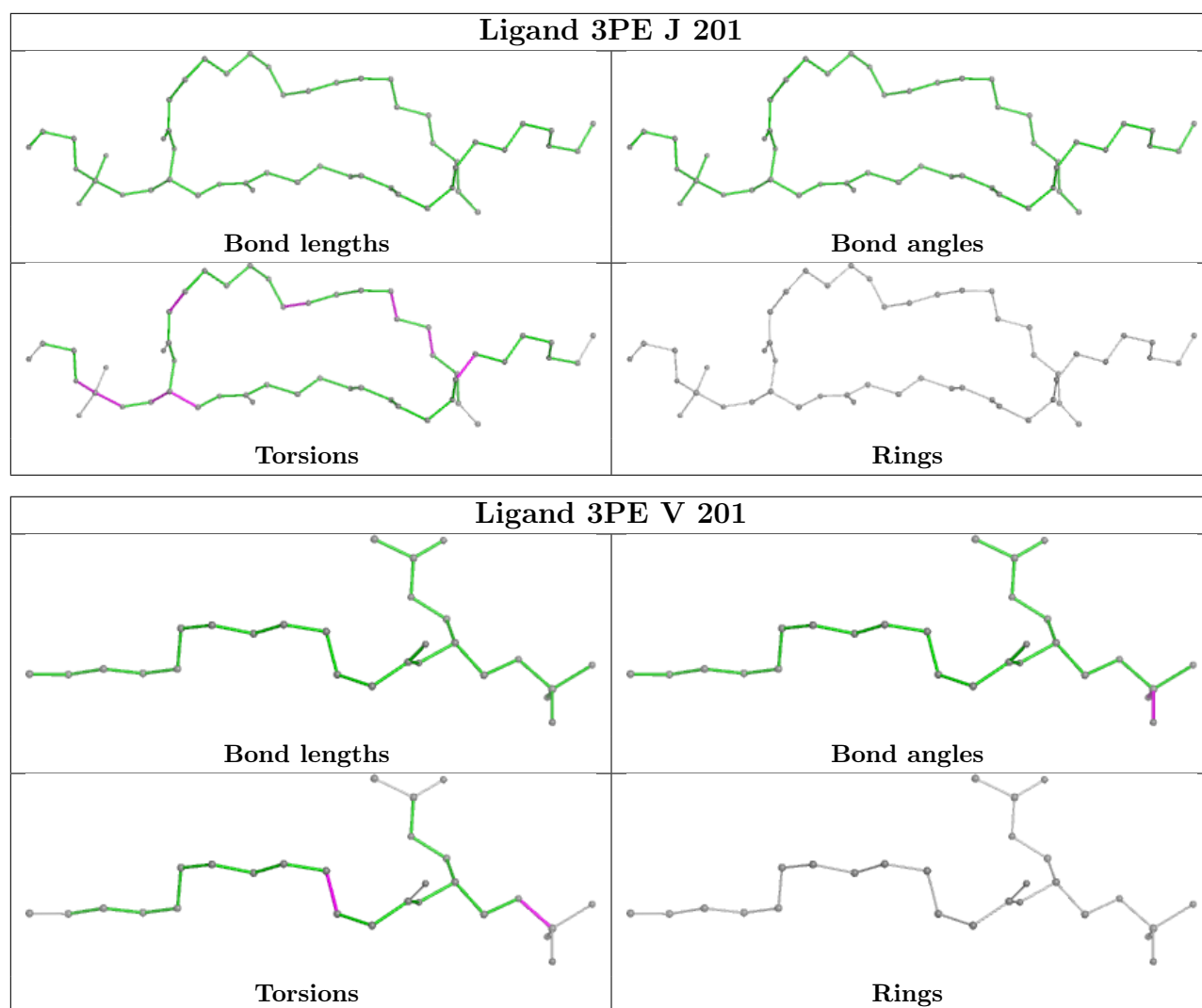
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

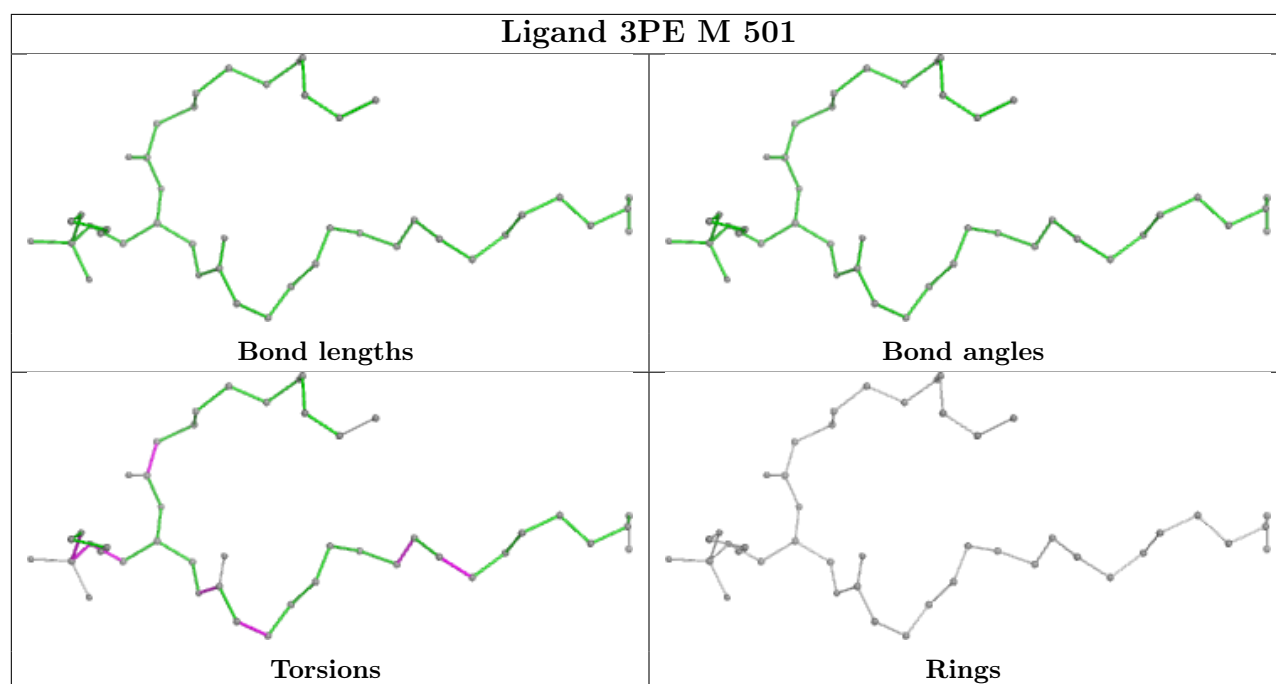
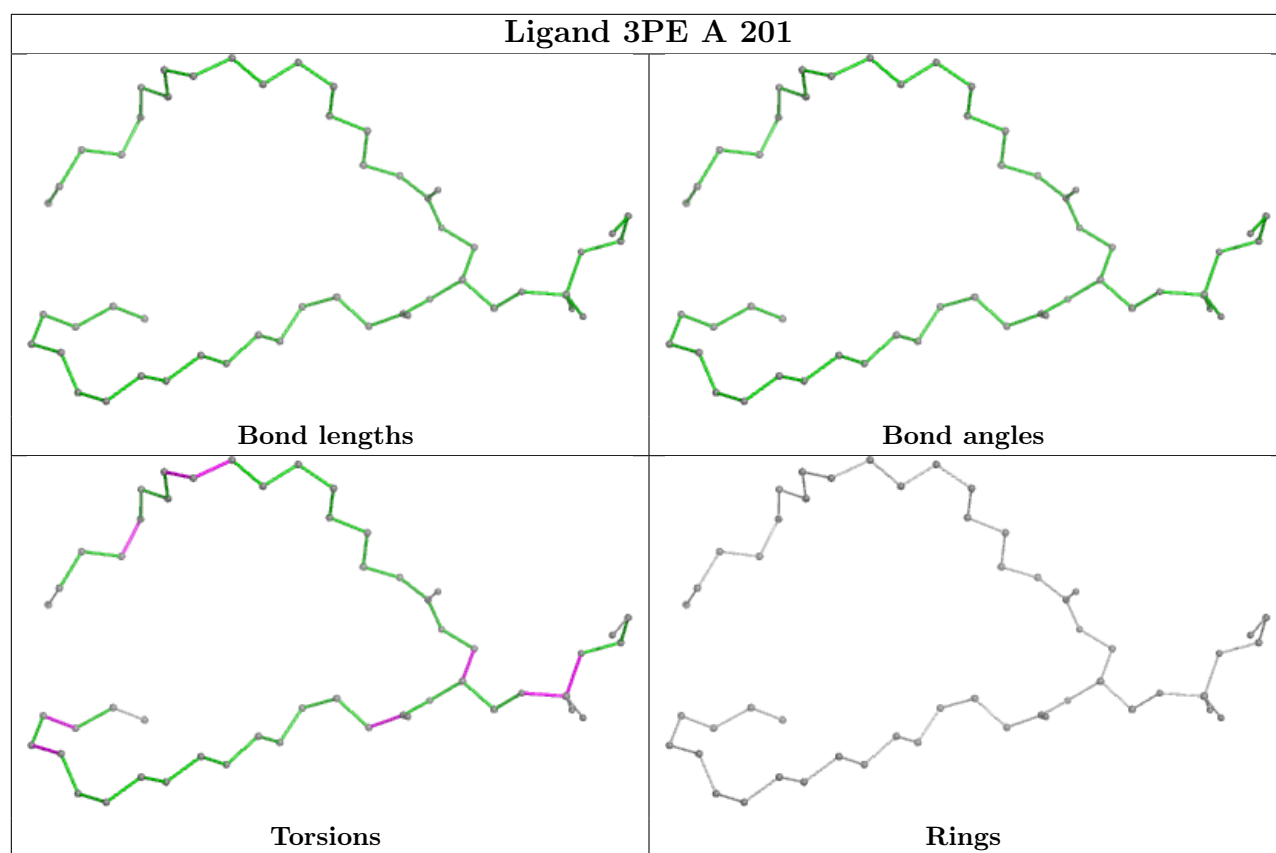


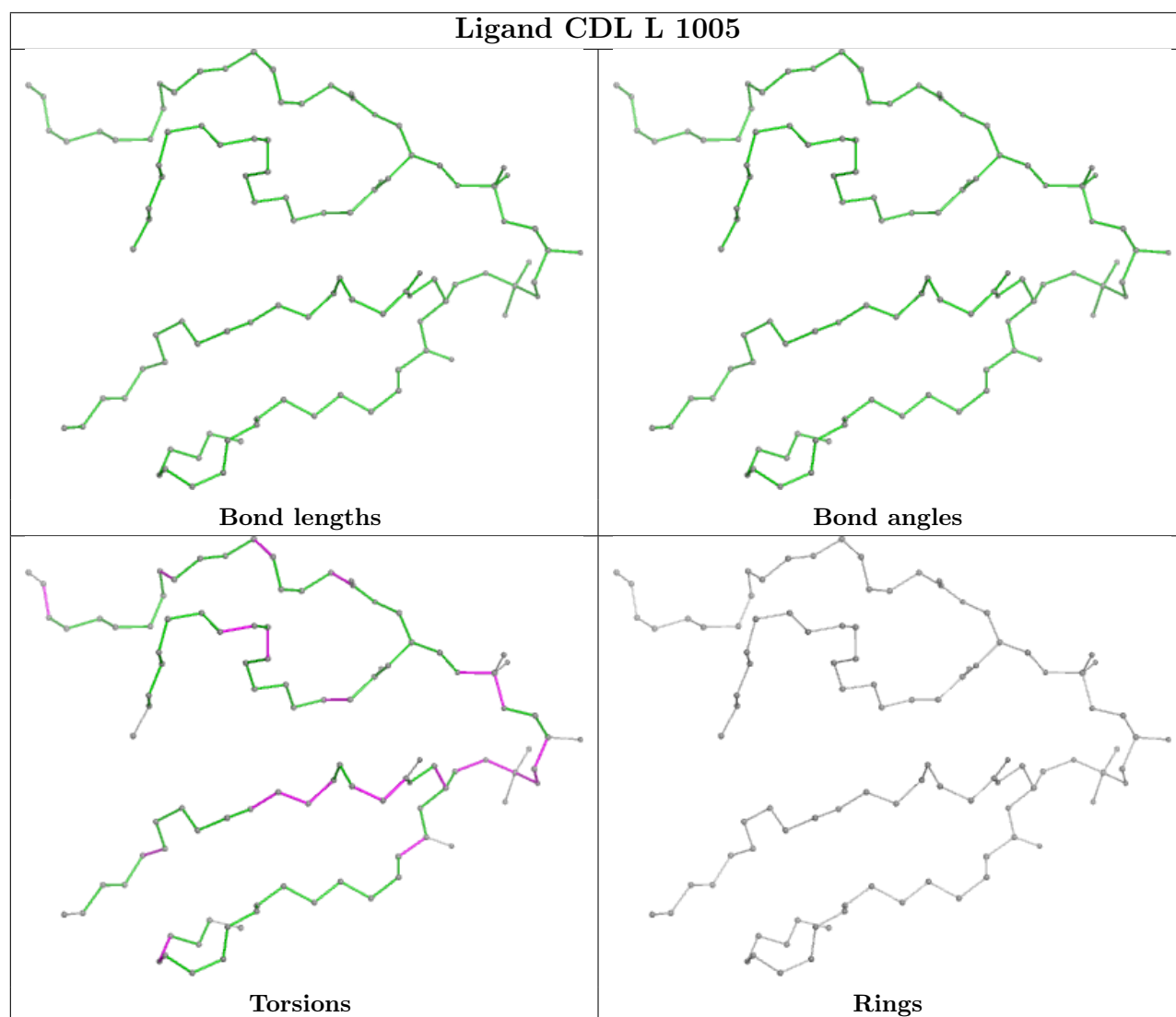
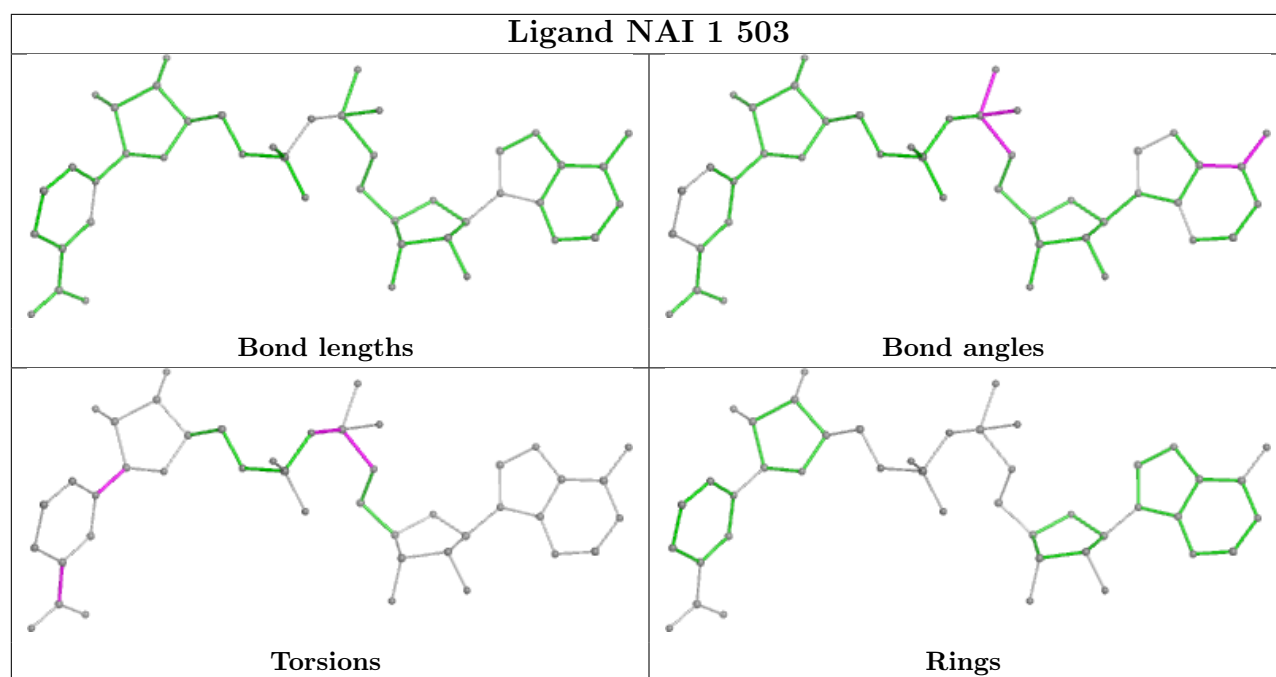


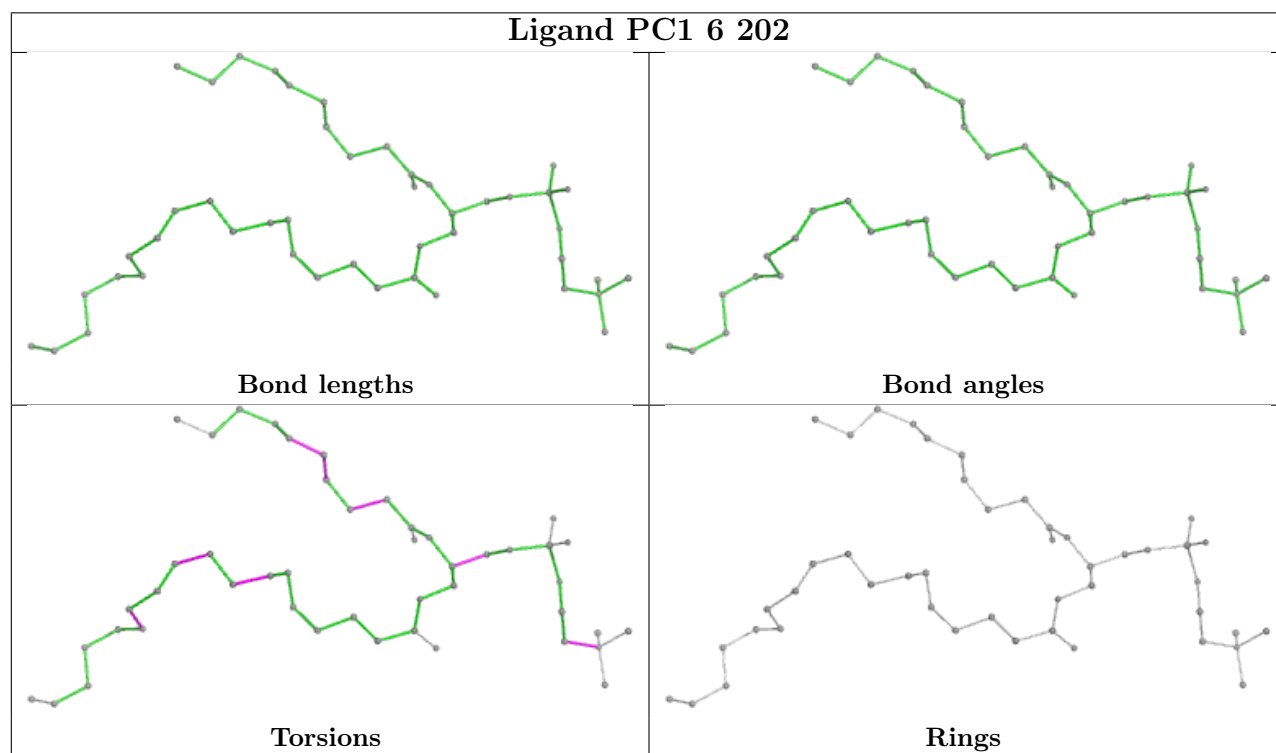
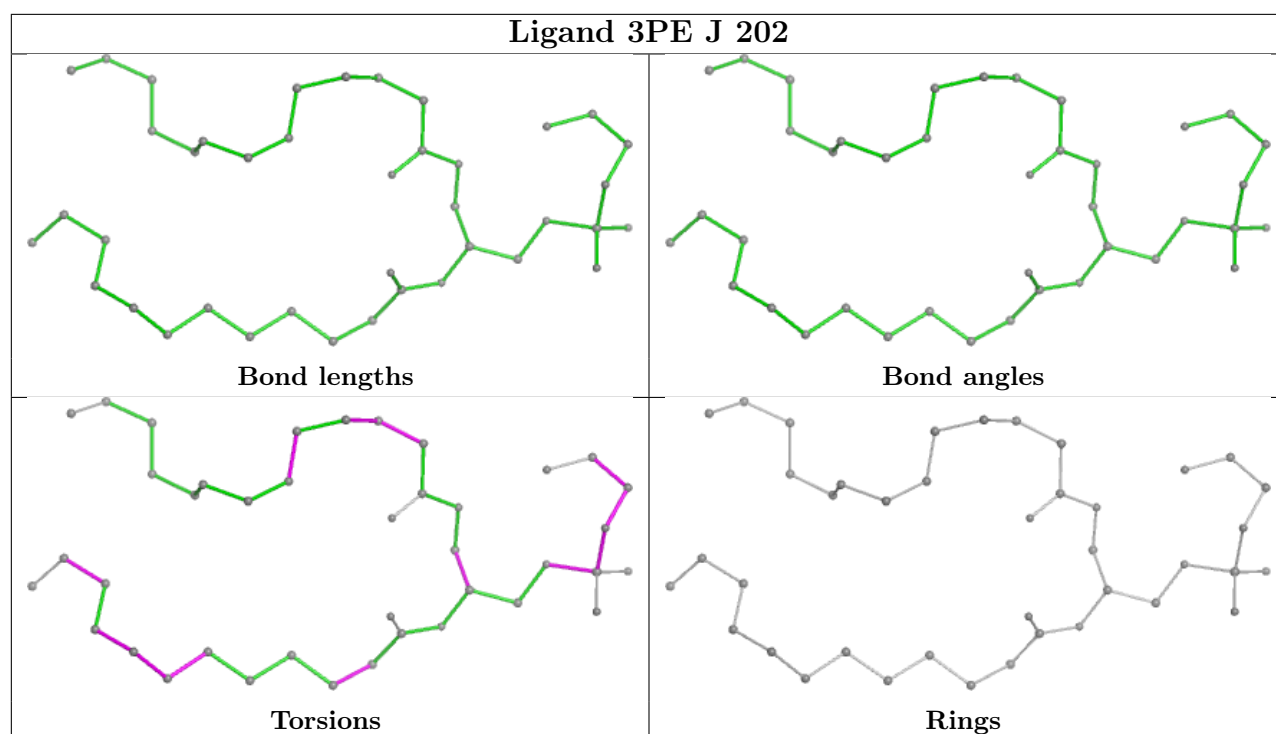


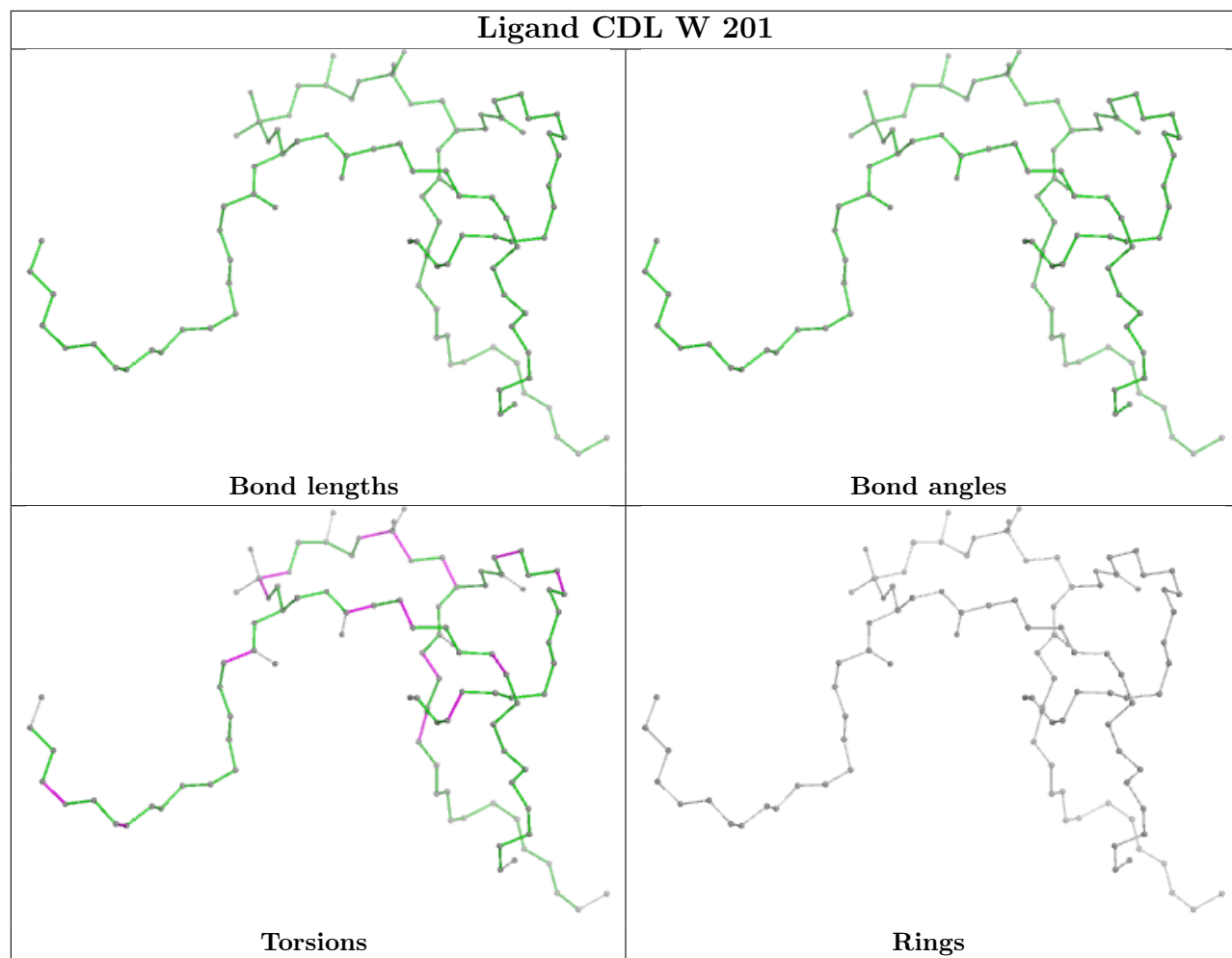


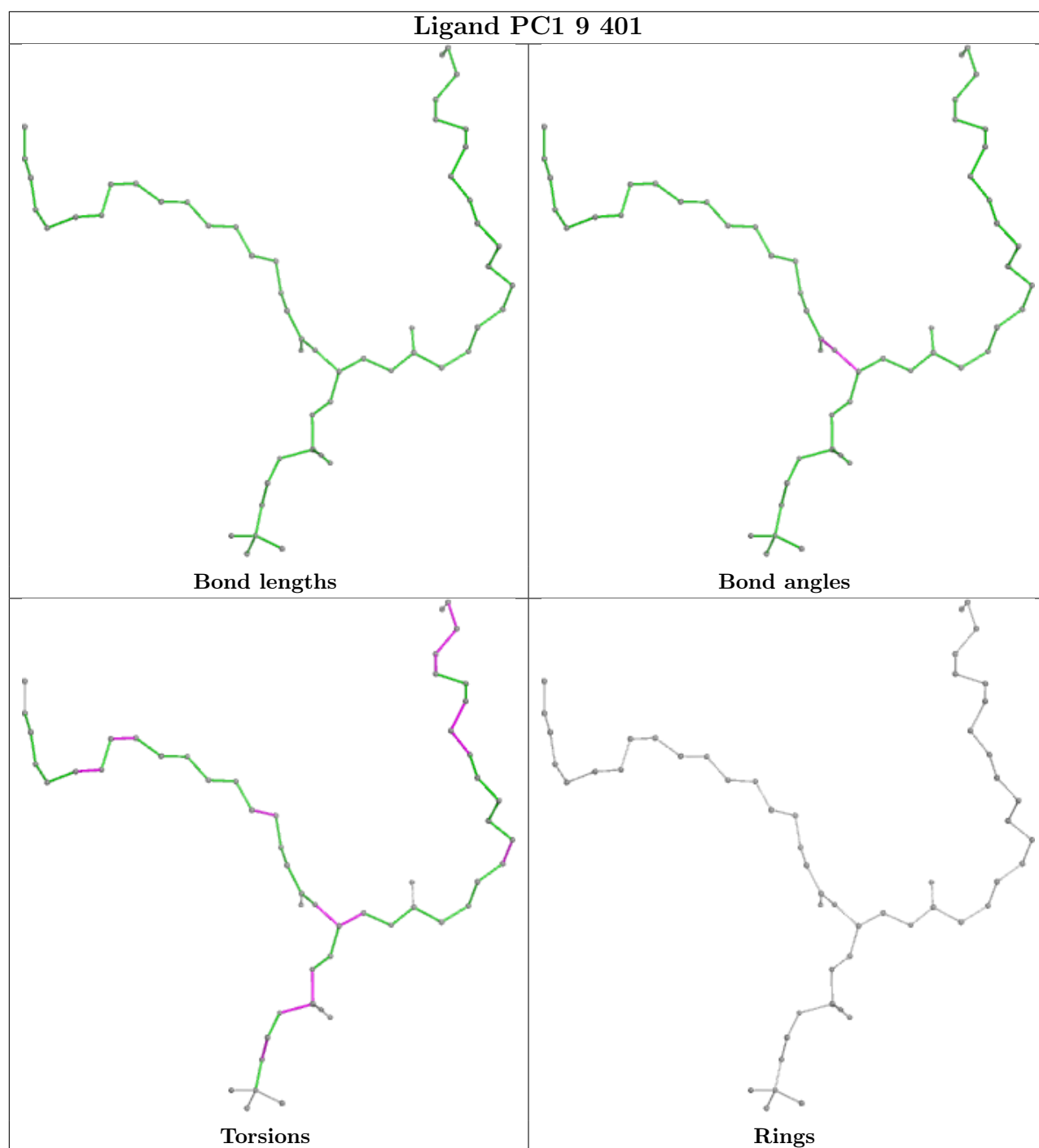


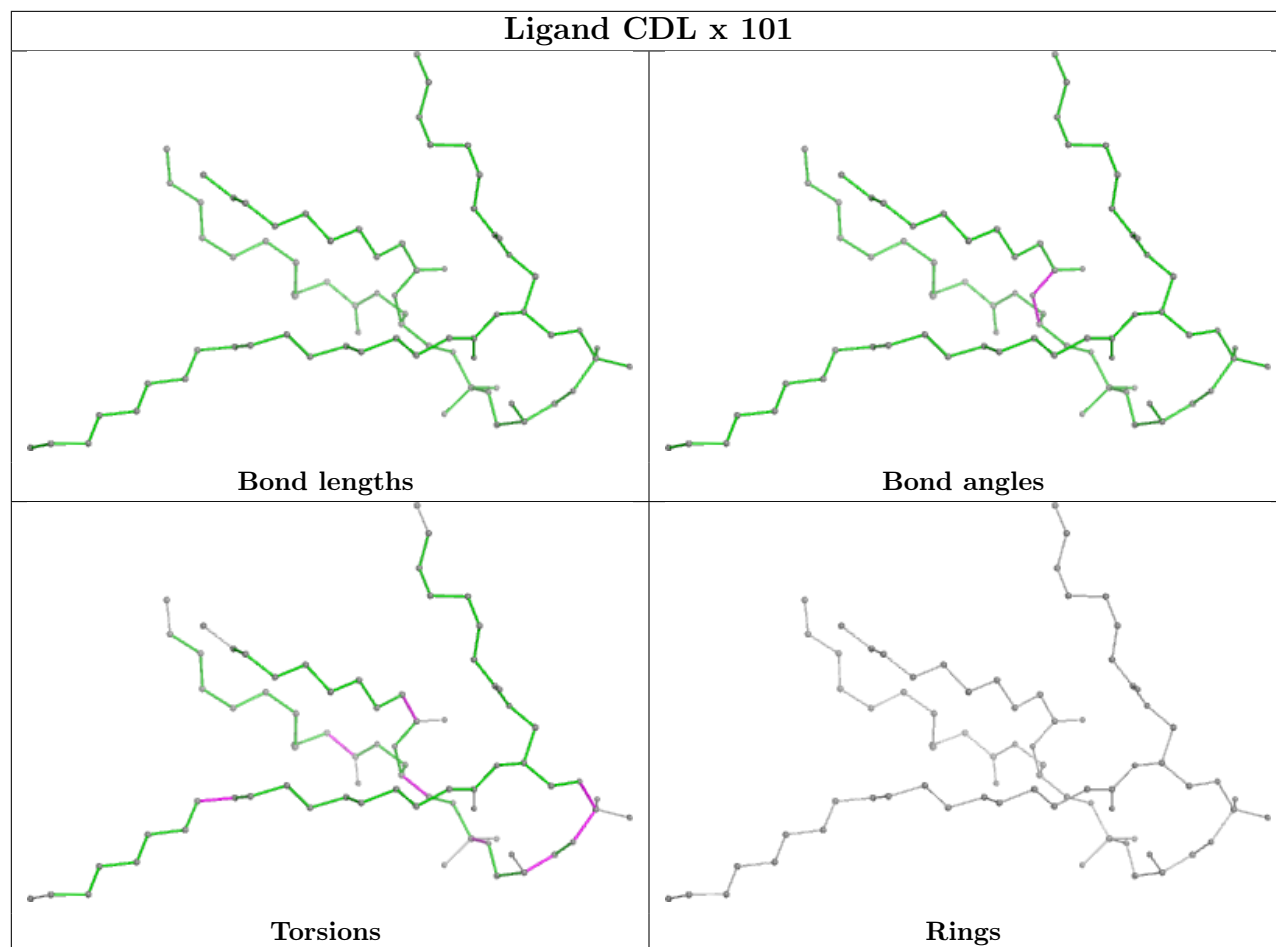


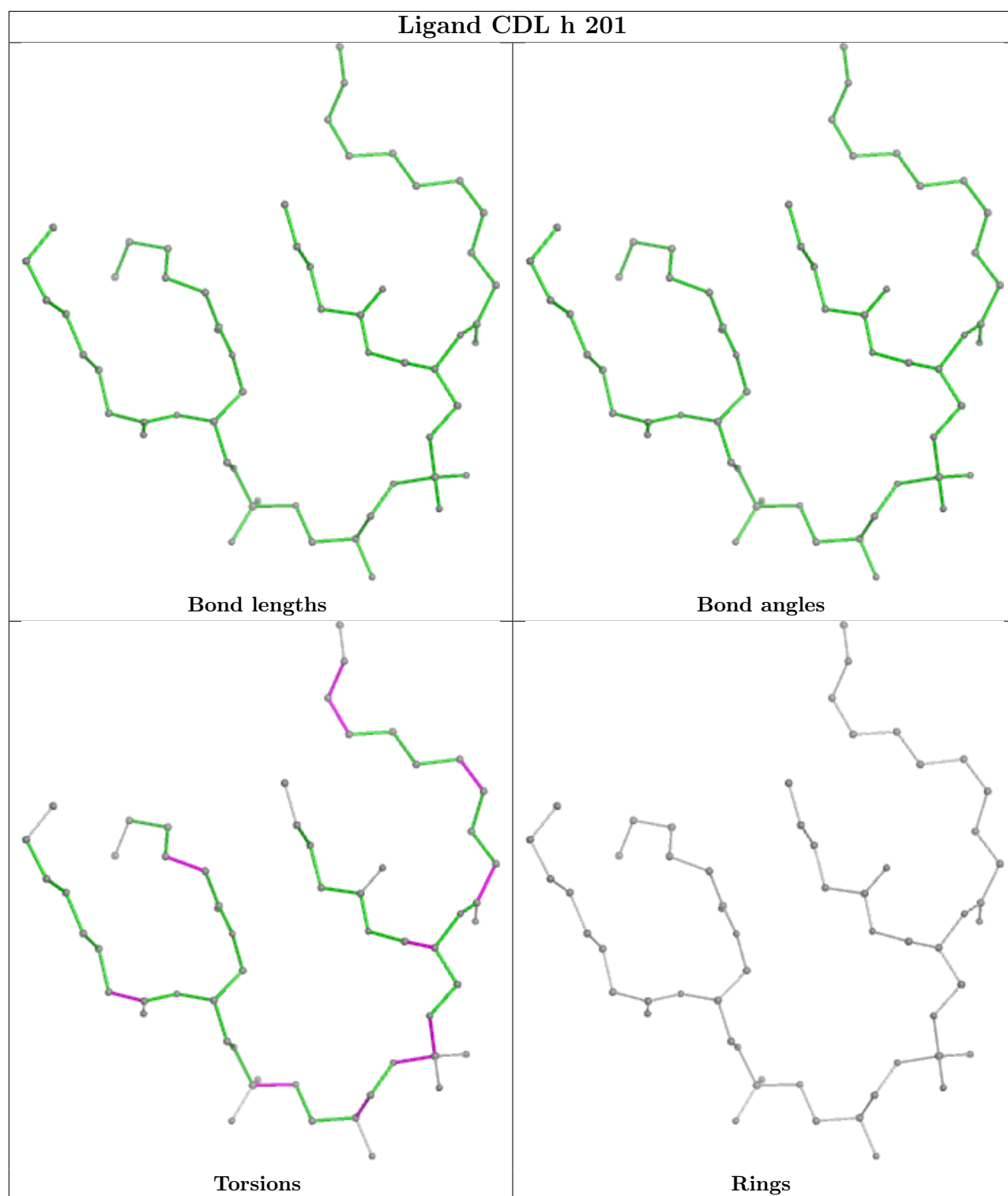


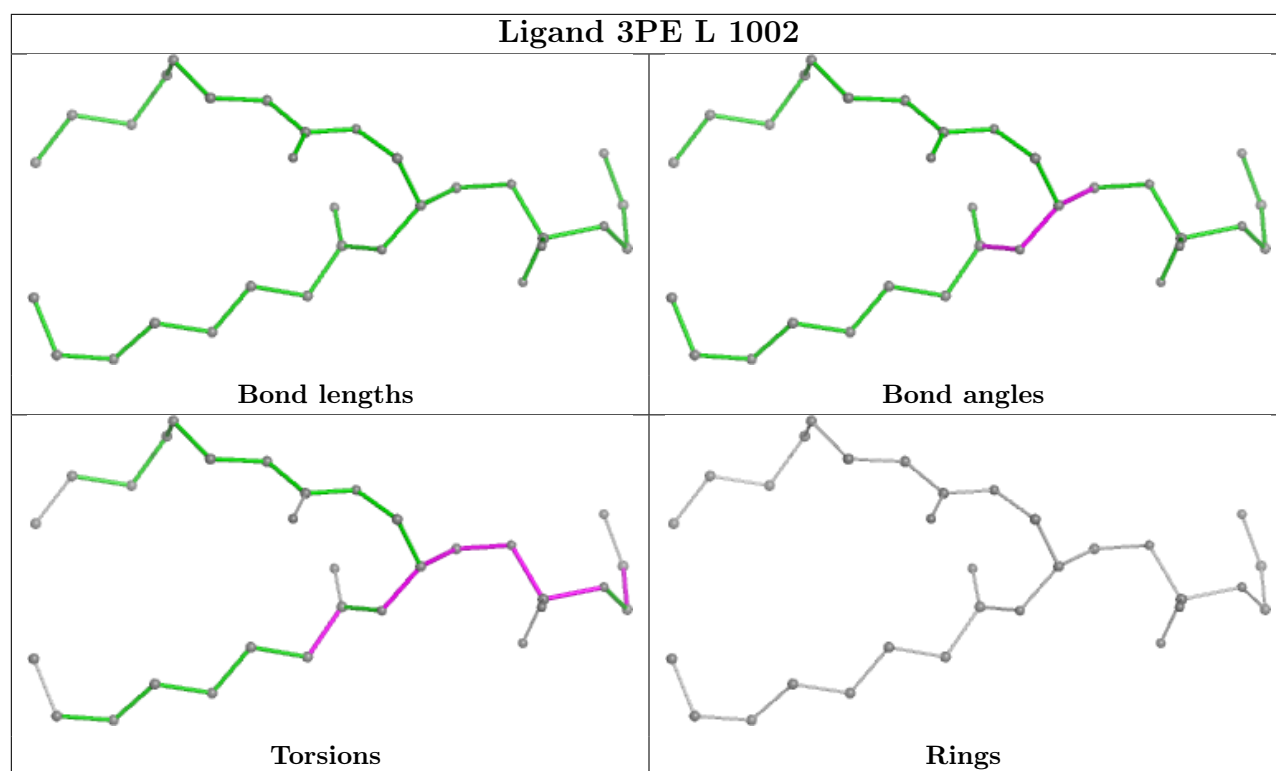


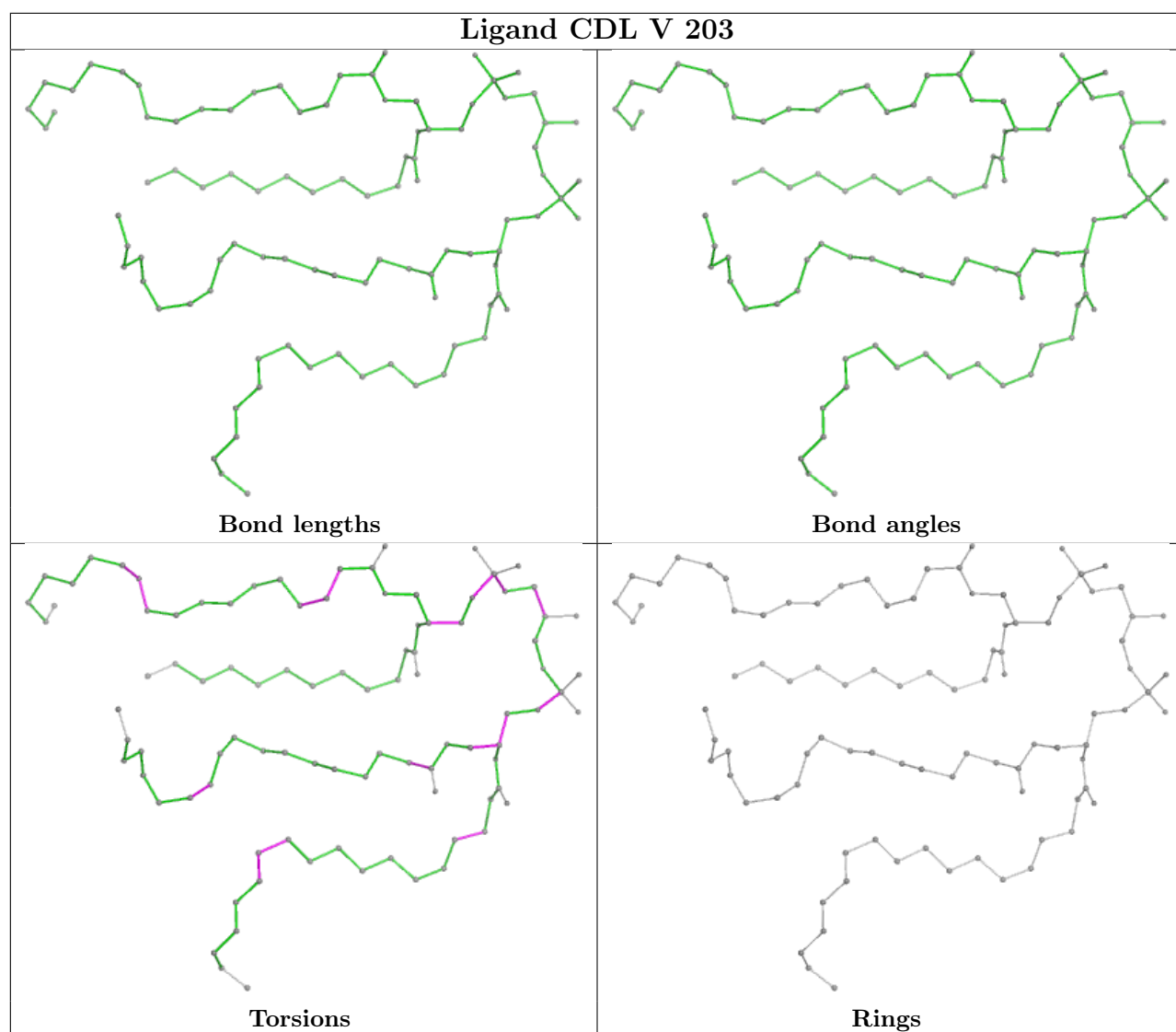


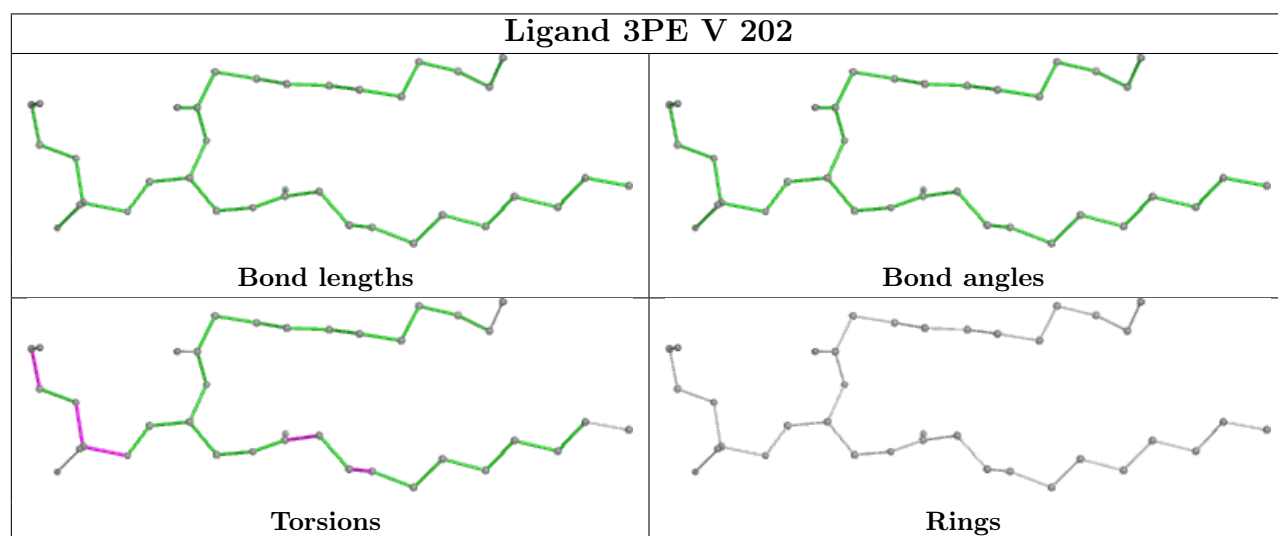
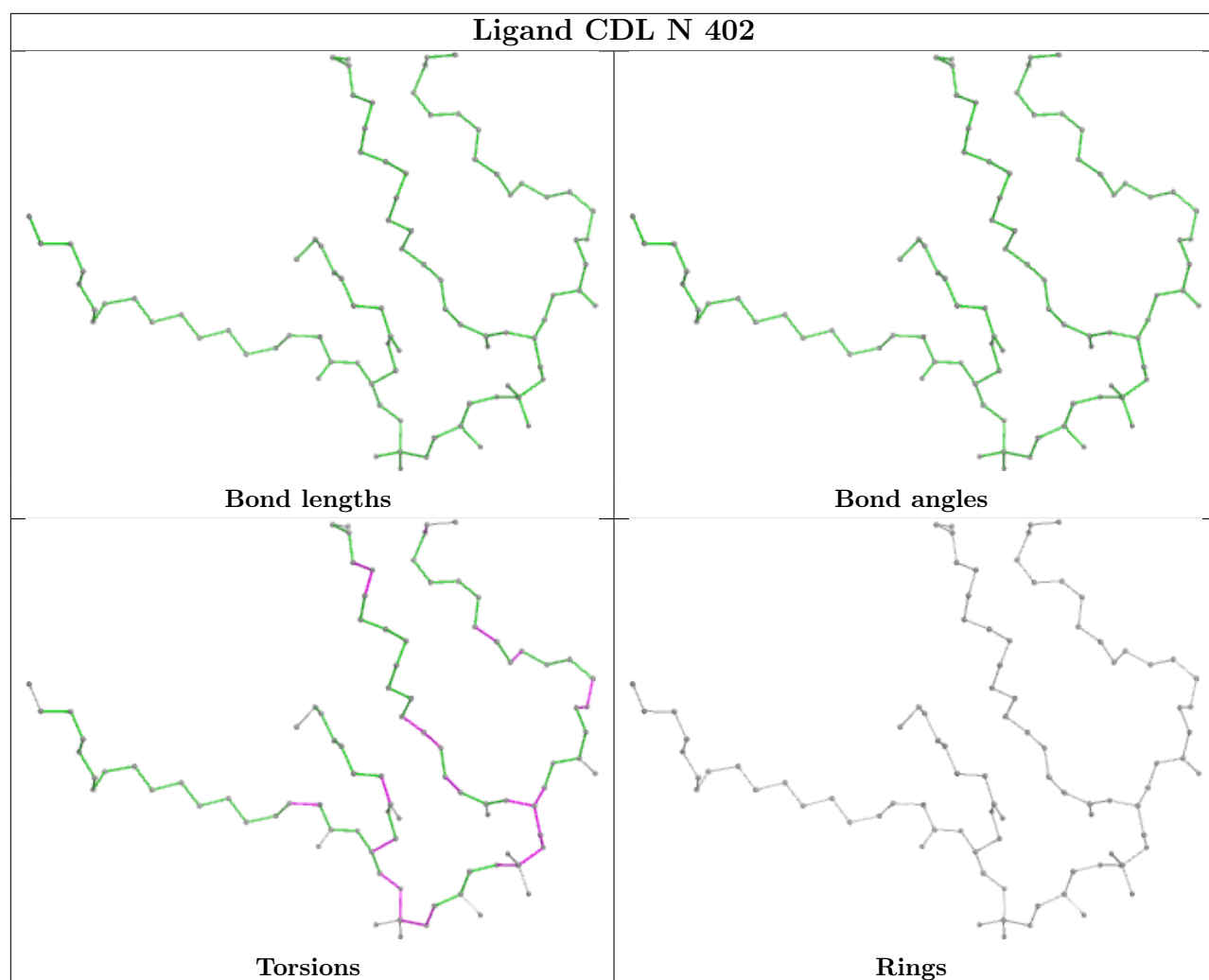


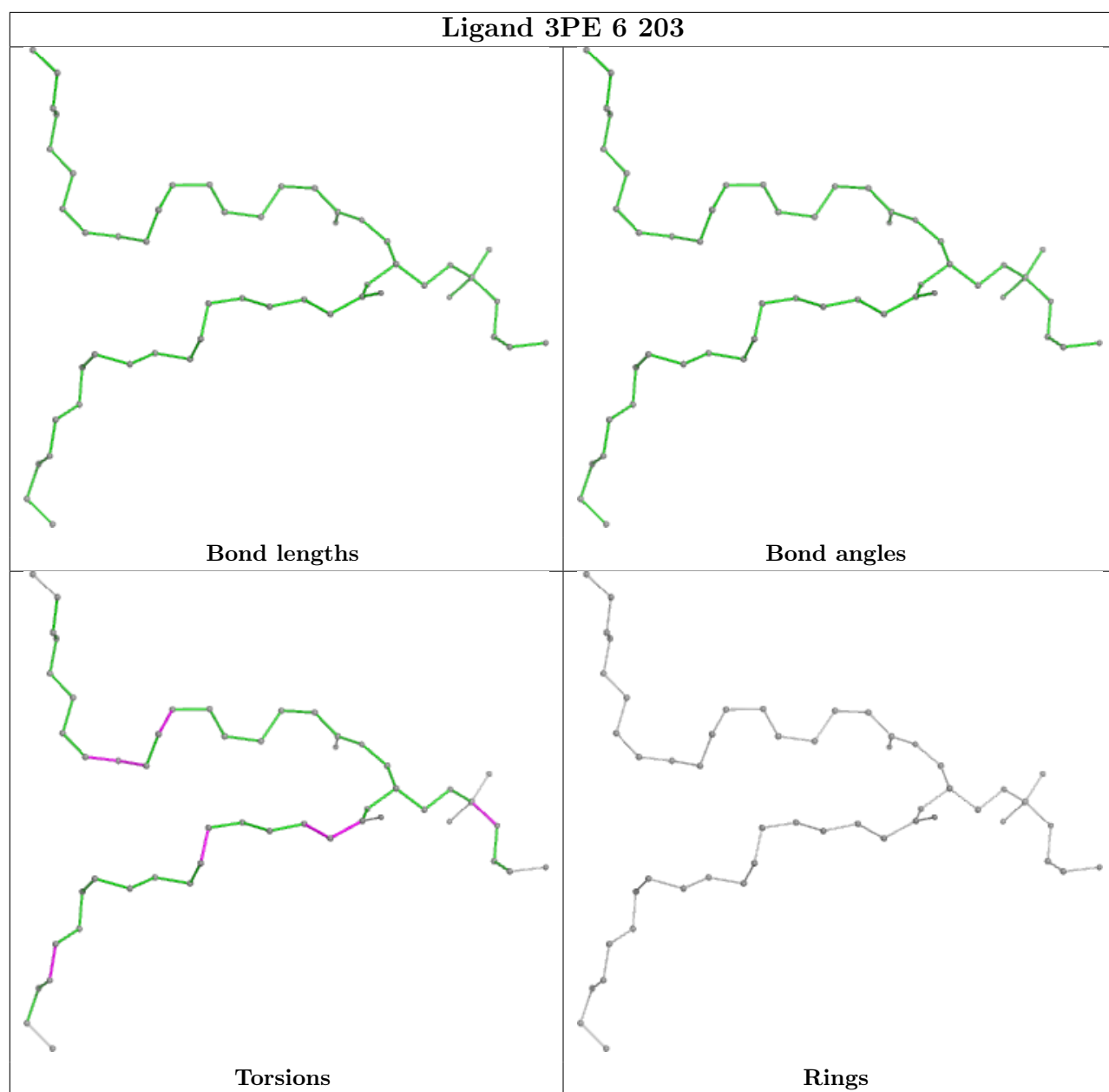


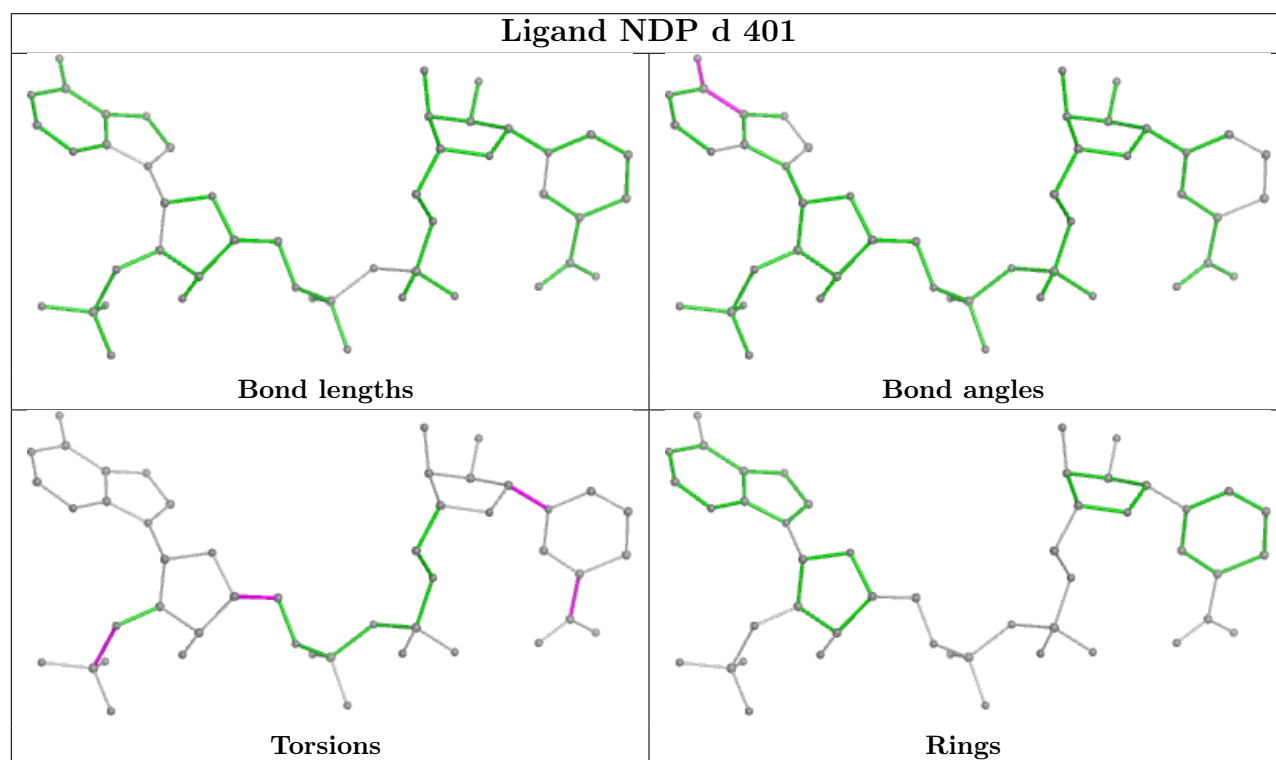
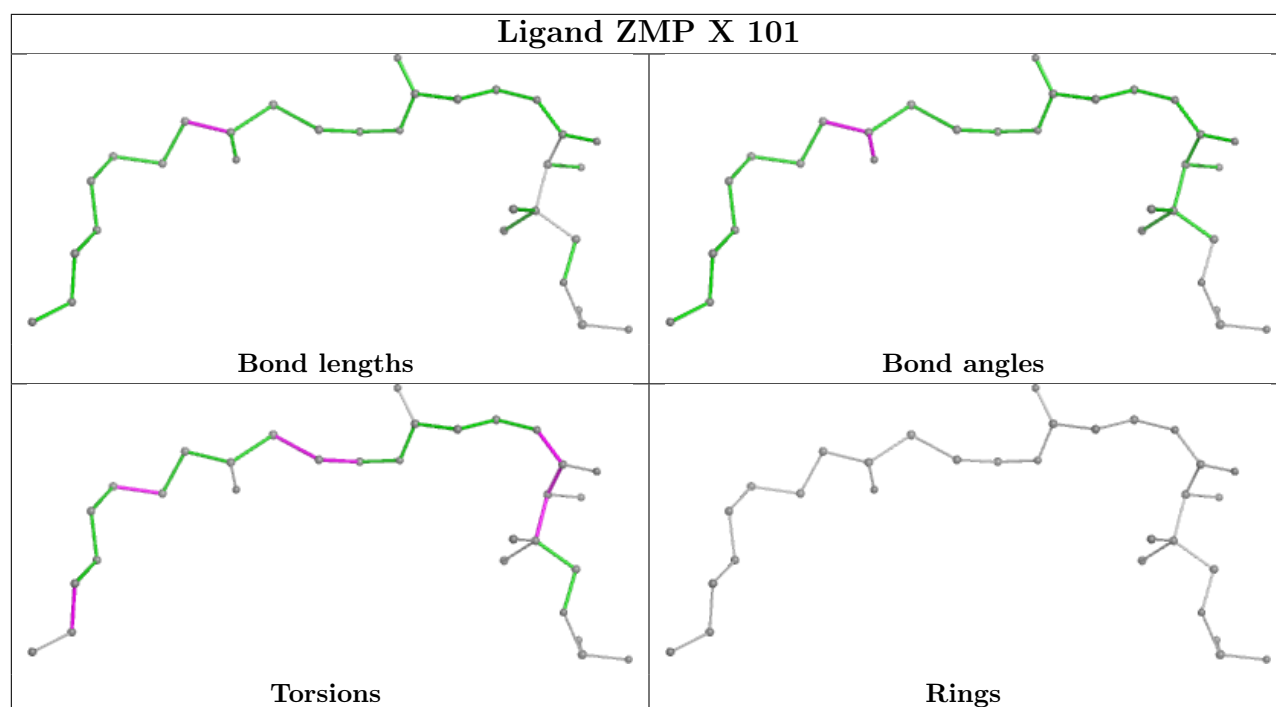


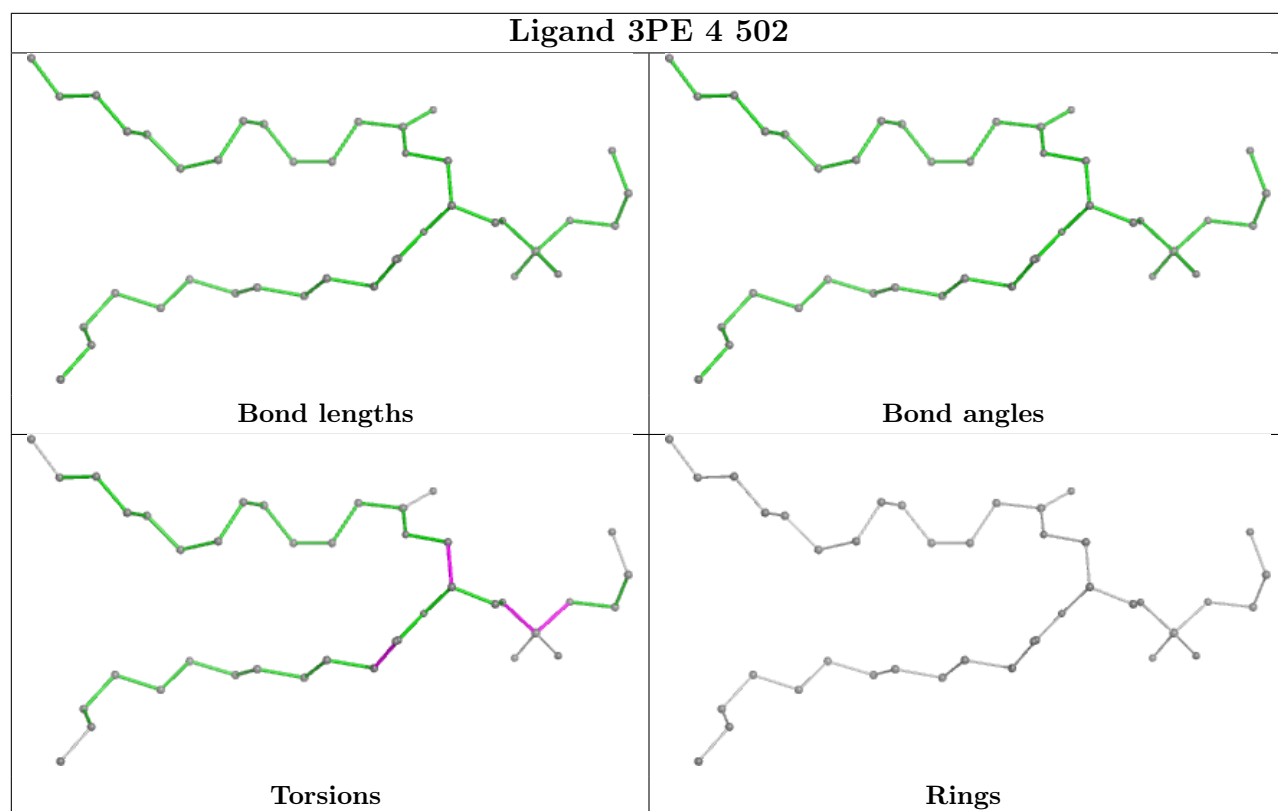
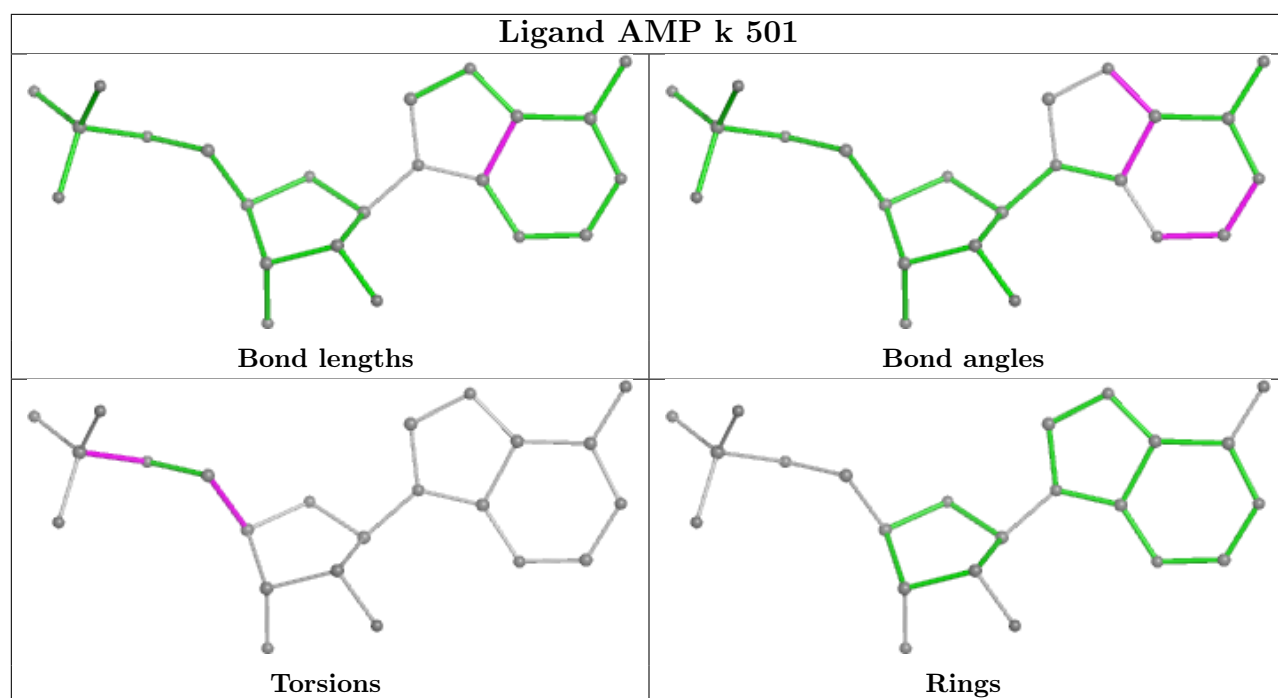


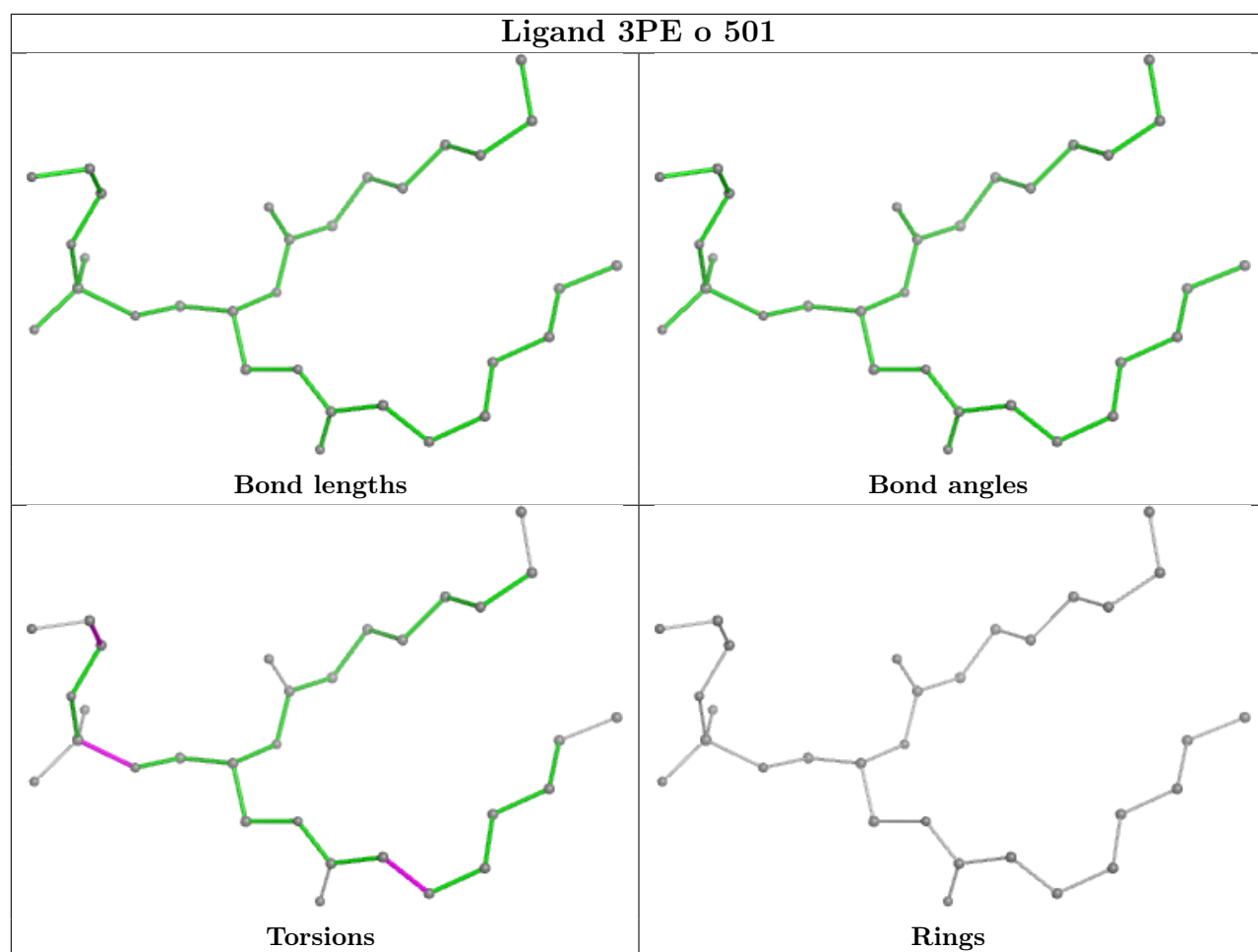


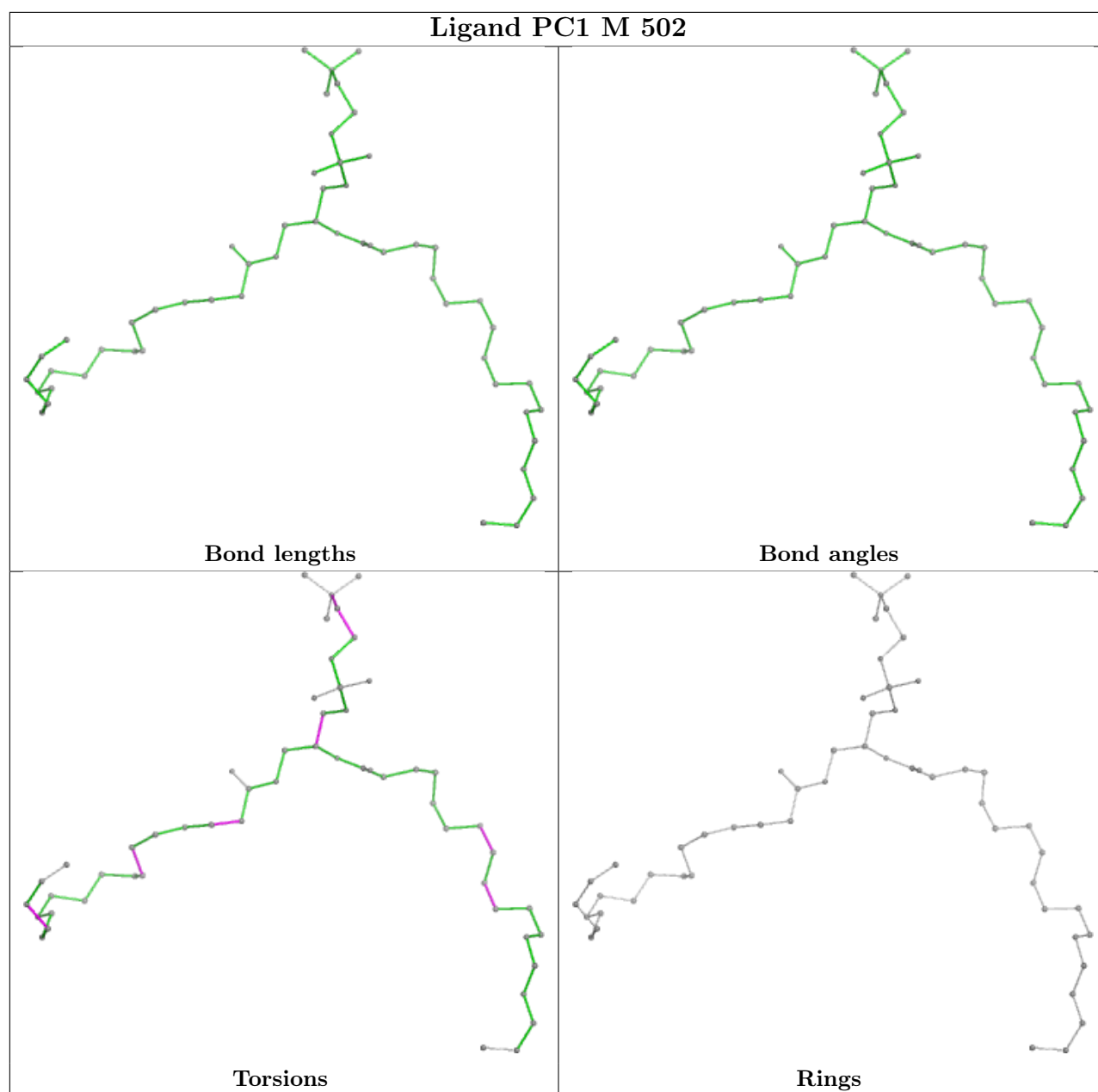


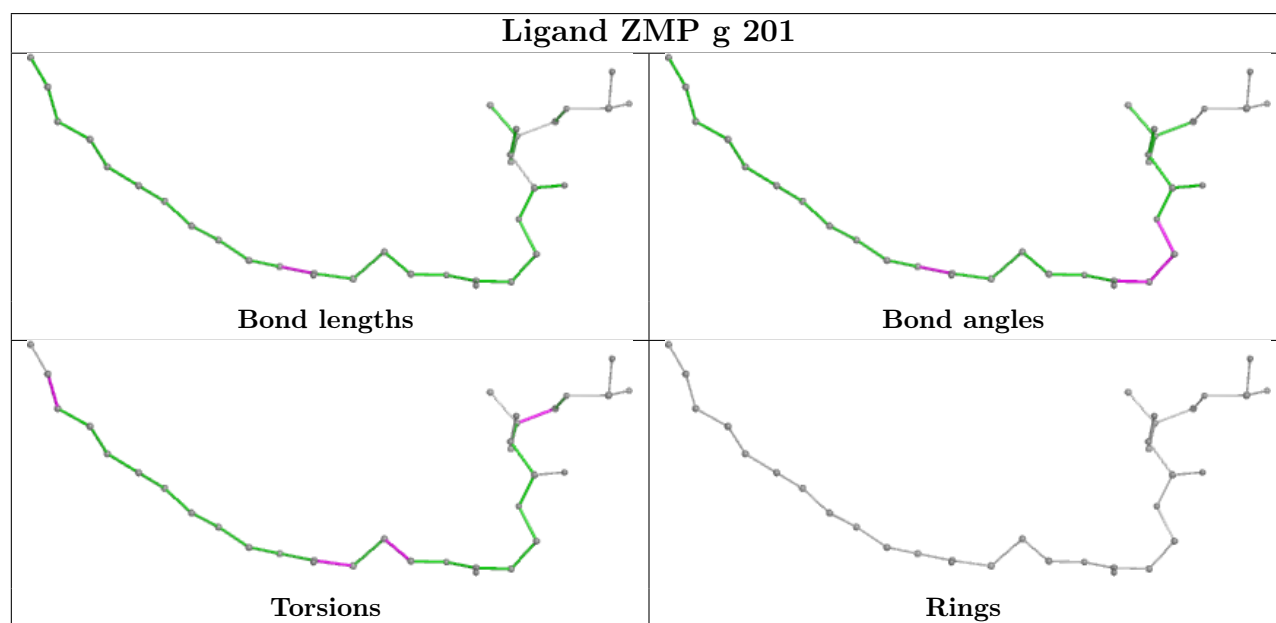
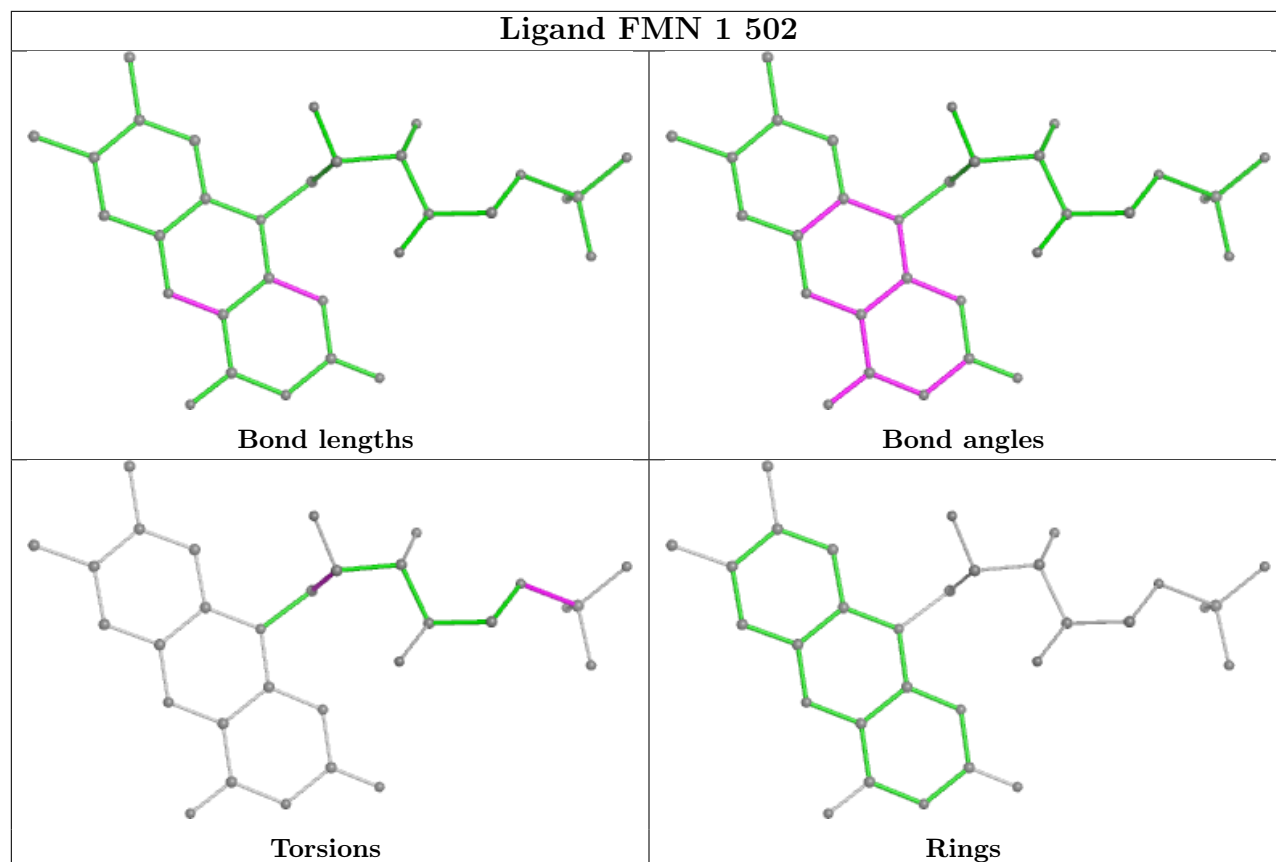


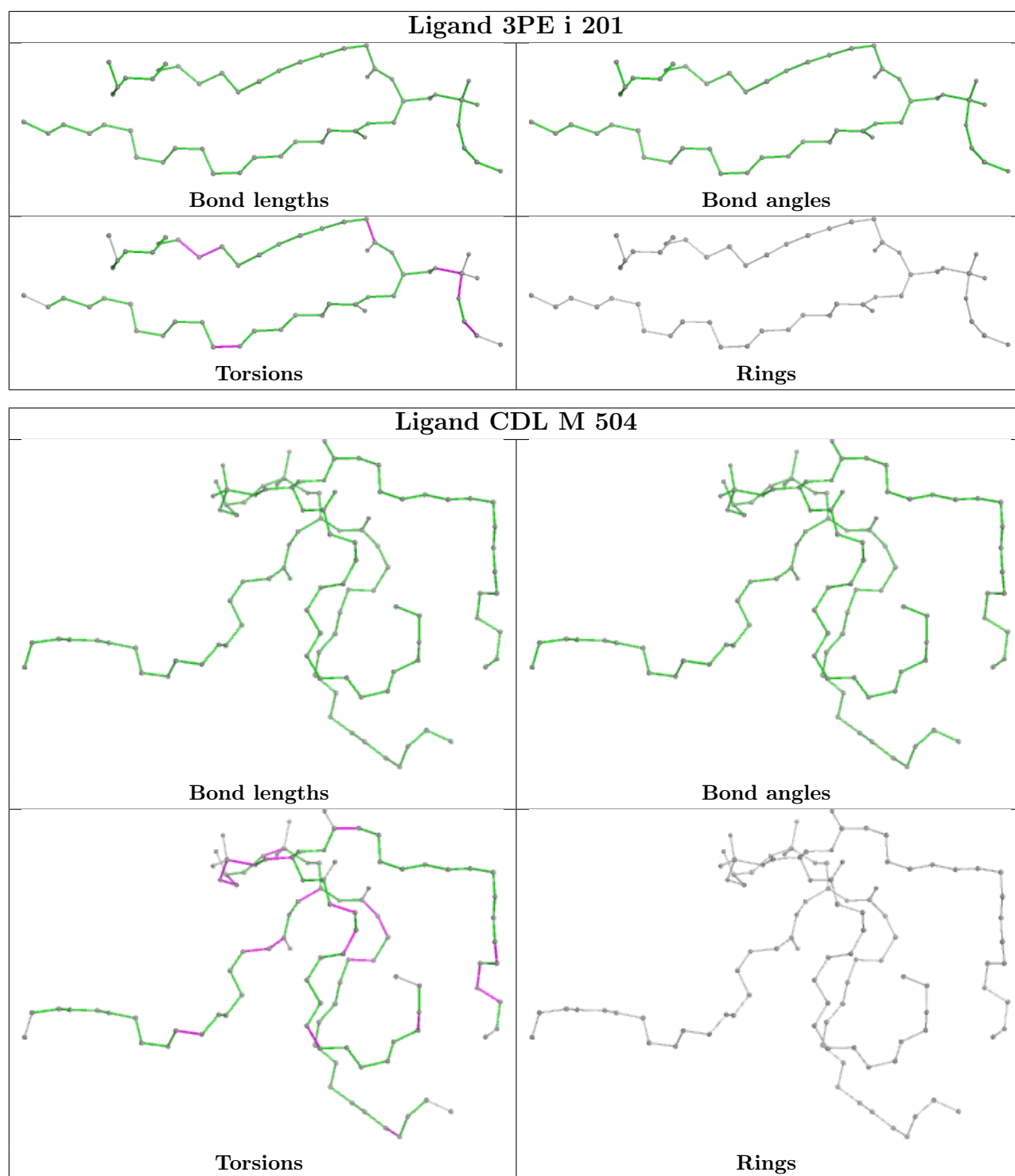












## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11252. 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.