



wwPDB EM Validation Summary Report ⓘ

Dec 7, 2022 – 02:58 PM JST

PDB ID : 7V33
EMDB ID : EMD-31651
Title : Active state complex I from rotenone-NADH dataset
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-08-10
Resolution : 2.60 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:

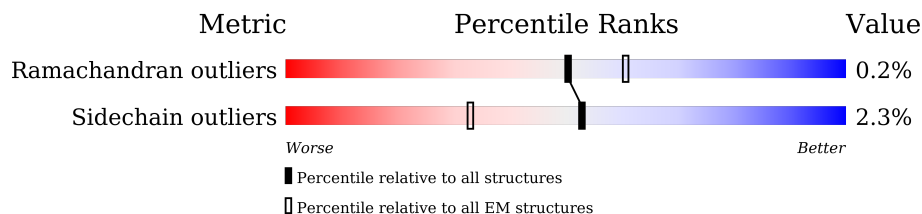
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 2.60 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	433	
2	B	176	
3	C	156	
4	E	115	
5	F	86	
6	G	88	
6	X	88	
7	H	112	
8	I	112	

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Mol	Chain	Length	Quality of chain
9	J	342	97%
10	K	43	7% 95% 5%
11	L	125	99%
12	M	690	99%
13	N	144	97%
14	O	217	98%
15	P	208	99%
16	Q	430	98%
17	S	70	100%
18	T	96	5% 97%
19	U	83	95% 5%
20	V	140	96%
21	W	142	98%
22	Y	67	9% 97%
23	Z	80	14% 96%
24	a	138	99%
25	b	126	6% 76% 22%
26	c	156	97%
27	d	175	6% 100%
28	e	104	7% 96%
29	f	49	22% 100%
30	g	122	99%
31	h	105	97%
32	i	347	99%
33	j	115	97%

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Mol	Chain	Length	Quality of chain
34	k	98	 98%
35	l	606	 98%
36	m	175	 10% 98%
37	n	56	 16% 98%
38	o	128	 98%
39	p	178	 97%
40	r	459	 98%
41	s	318	 100%
42	u	171	 95% 5%
43	v	125	 14% 96%
44	w	320	 97%

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 68246 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
			Total	C	N	O	S		
1	A	433	3330	2103	593	614	20	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	115	971	619	179	168	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	86	684	431	129	122	2	0	0

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	88	693	447	102	139	5	0	0
6	X	88	696	449	103	139	5	0	0

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

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

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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

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

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

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	690	5293	3319	923	1012	39	0	0

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

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

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

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

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

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

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

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

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

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

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

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

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

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

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

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

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	W	142	1161	749	197	206	9	0	0

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

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

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

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

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

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

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	f	49	377	246	65	66	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	g	122	1005	653	174	172	6	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	l	606	4797	3181	743	822	51	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	m	175	1276	850	187	226	13	0	0

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

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

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

4.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	p	178	1534	982	279	265	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	r	459	3624	2406	572	608	38	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	v	124	1036	646	196	185	9	0	0

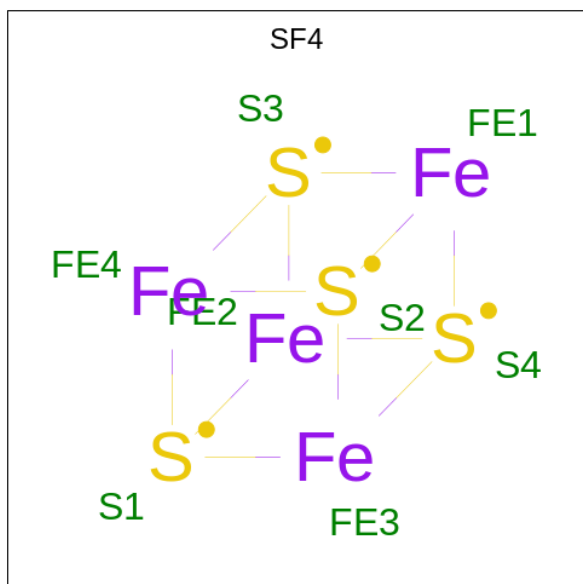
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	1	MYR	-	acetylation	UNP F1SCH1

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

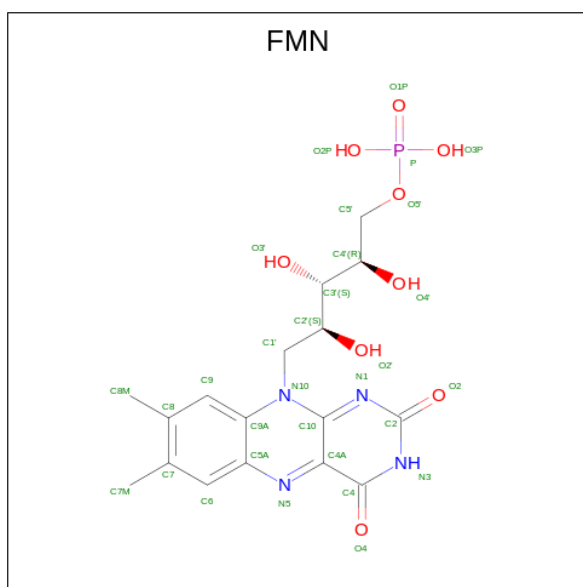
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	w	320	2586	1646	439	491	10	0	0

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



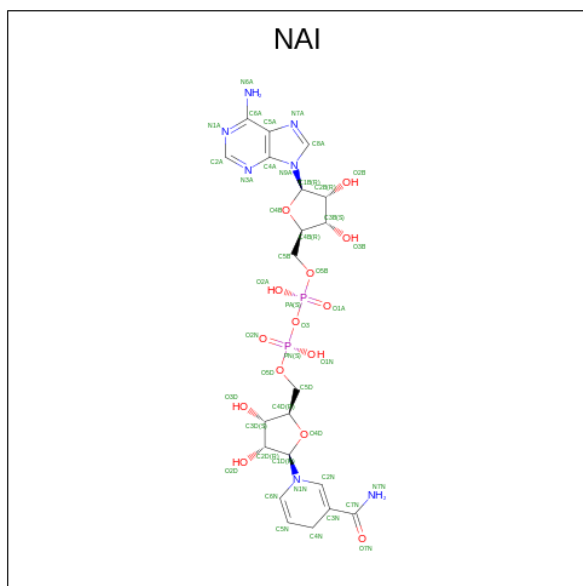
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	A	1	8	4	4	0
45	B	1	16	8	8	0
45	B	1	16	8	8	0
45	C	1	8	4	4	0
45	M	1	16	8	8	0
45	M	1	16	8	8	0

- Molecule 46 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by depositor).



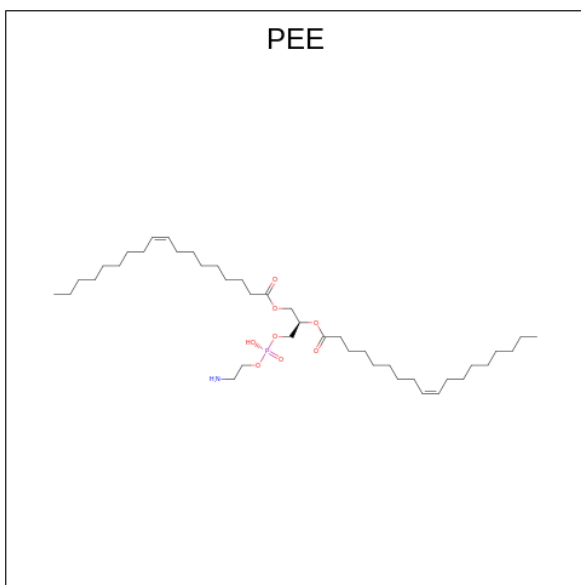
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	A	1	31	17	4	9	1	0

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



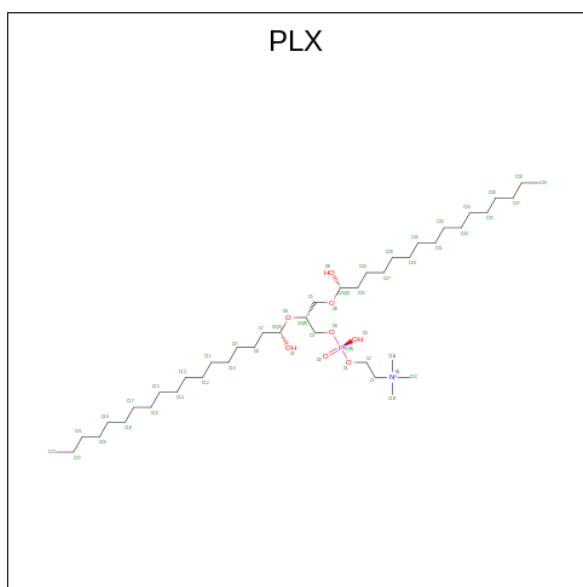
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
47	A	1	44	21	7	14	2	0

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



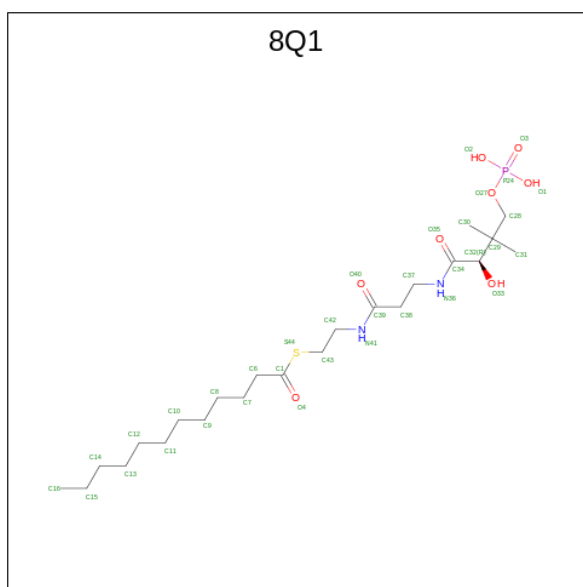
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
48	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	C	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	U	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	V	1	Total	N				0
			1	1				
48	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	j	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	l	1	Total	C	N	O	P	0
			143	113	3	24	3	
48	l	1	Total	C	N	O	P	0
			143	113	3	24	3	
48	l	1	Total	C	N	O	P	0
			143	113	3	24	3	
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-TRIOXOL (three-letter code: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



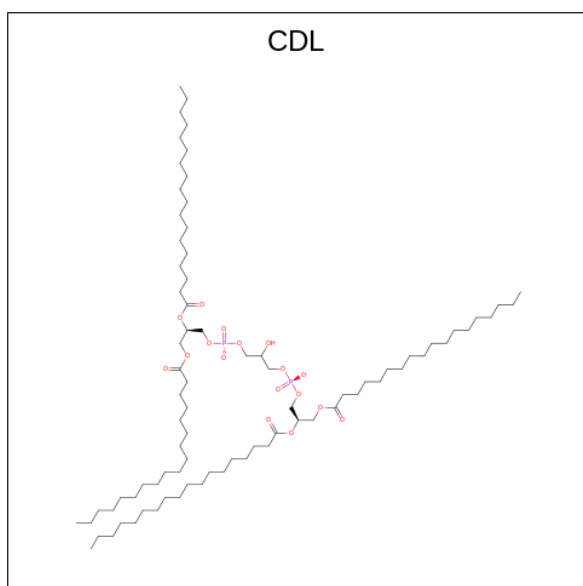
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
49	C	1	Total 52	42	1	8	1	0
49	J	1	Total 52	42	1	8	1	0
49	a	1	Total 52	42	1	8	1	0
49	g	1	Total 52	42	1	8	1	0
49	j	1	Total 52	42	1	8	1	0
49	r	1	Total 104	84	2	16	2	0
49	r	1	Total 104	84	2	16	2	0

- Molecule 50 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: C₂₃H₄₅N₂O₈PS) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 51 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



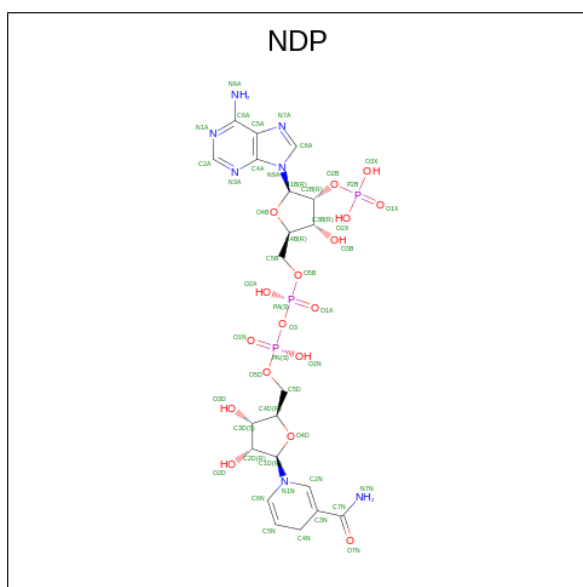
Mol	Chain	Residues	Atoms			AltConf	
			Total	C	O		P
51	I	1	51	32	17	2	0

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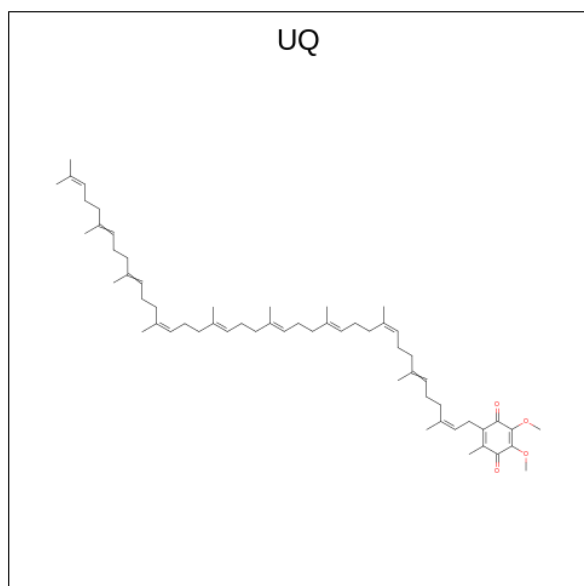
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
51	V	1	Total 94	C 75	O 17	P 2	0
51	a	1	Total 100	C 81	O 17	P 2	0
51	i	1	Total 100	C 81	O 17	P 2	0
51	k	1	Total 78	C 59	O 17	P 2	0
51	l	1	Total 199	C 161	O 34	P 4	0
51	l	1	Total 199	C 161	O 34	P 4	0
51	m	1	Total 89	C 70	O 17	P 2	0
51	o	1	Total 100	C 81	O 17	P 2	0
51	r	1	Total 99	C 80	O 17	P 2	0
51	u	1	Total 55	C 36	O 17	P 2	0

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



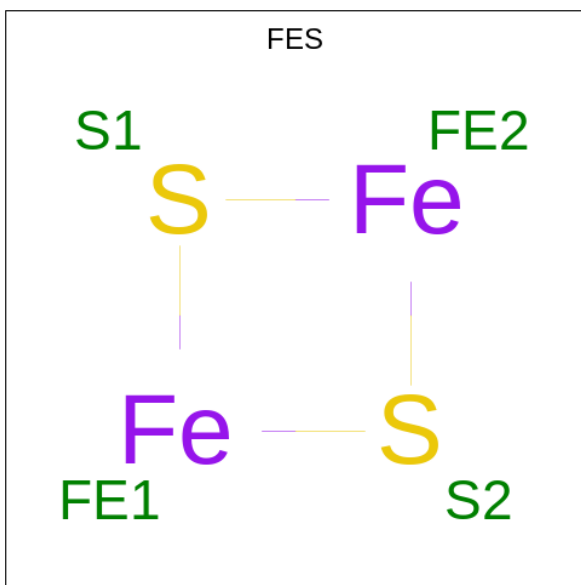
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
52	J	1	48	21	7	17	3	0

- Molecule 53 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula: C₅₉H₉₀O₄) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 54 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).

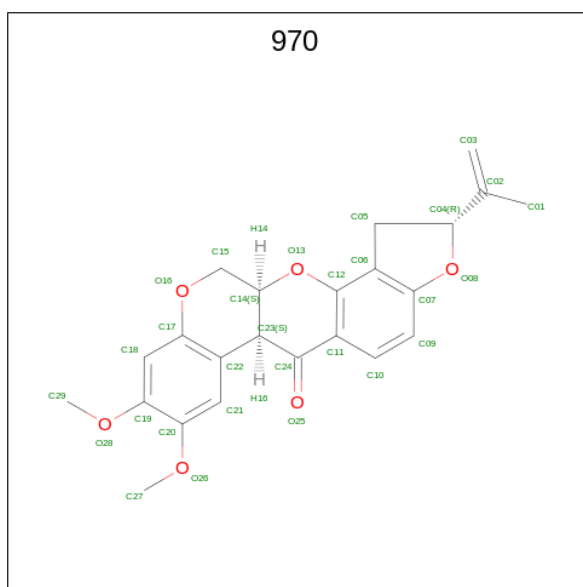


Mol	Chain	Residues	Atoms			AltConf
54	M	1	Total	Fe	S	0
			4	2	2	
54	O	1	Total	Fe	S	0
			4	2	2	

- Molecule 55 is MAGNESIUM ION (three-letter code: 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 (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 (three-letter code: 970) (formula: C₂₃H₂₂O₆) (labeled as "Ligand of Interest" by depositor).

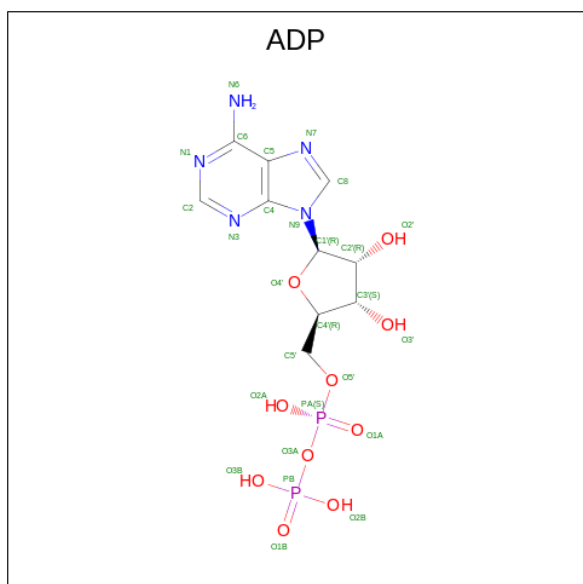


Mol	Chain	Residues	Atoms		AltConf	
56	Q	1	Total	C	O	0
			29	23	6	

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 58 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

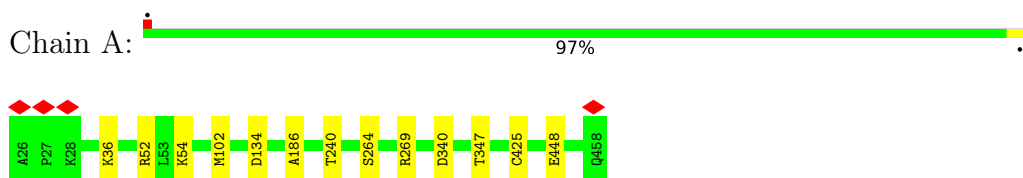


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	w	1	27	10	5	10	2	0

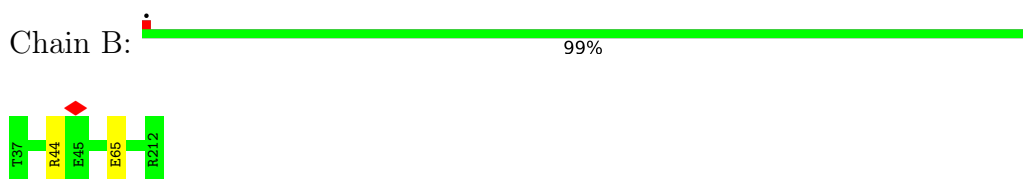
3 Residue-property plots [i](#)

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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

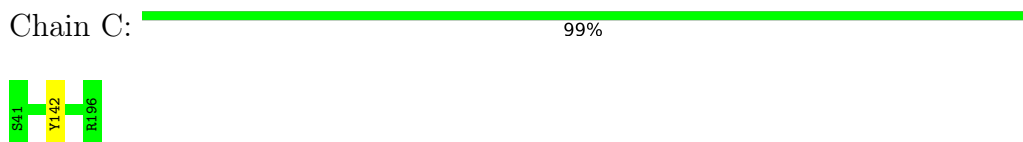
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



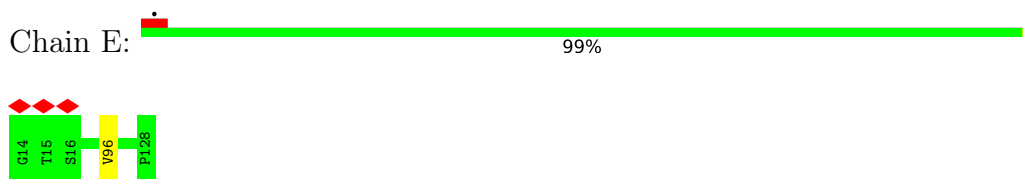
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



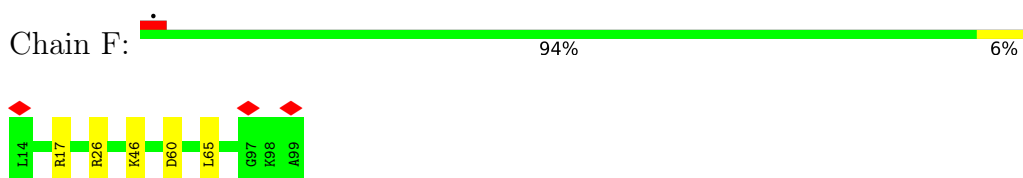
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



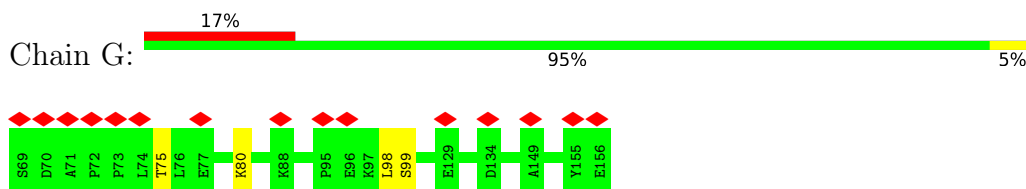
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



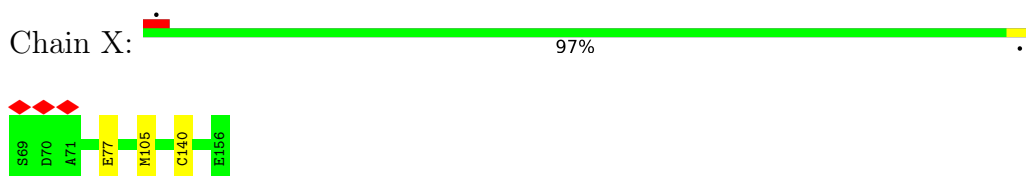
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



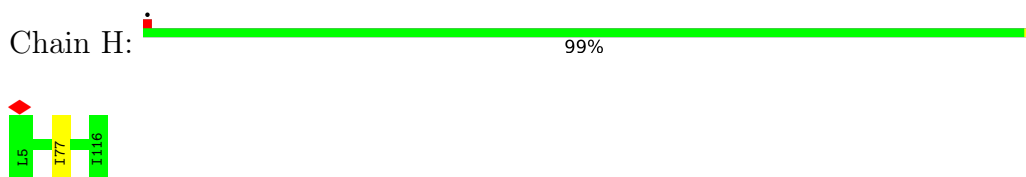
- Molecule 6: Acyl carrier protein, mitochondrial



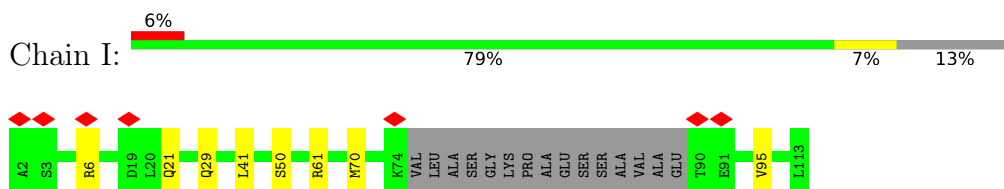
- Molecule 6: Acyl carrier protein, mitochondrial



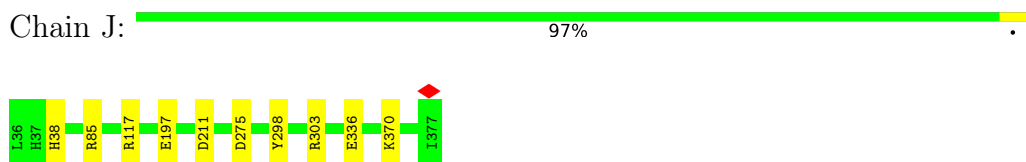
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



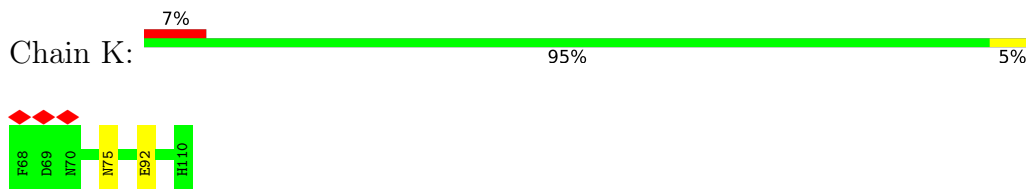
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



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

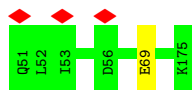


- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

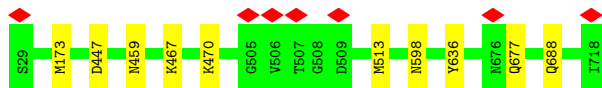


- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

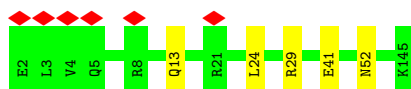




- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



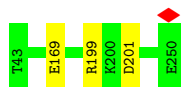
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



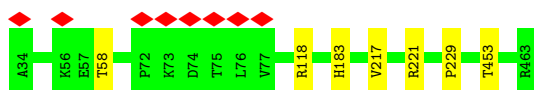
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



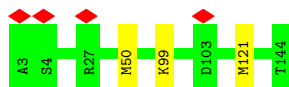
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



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



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

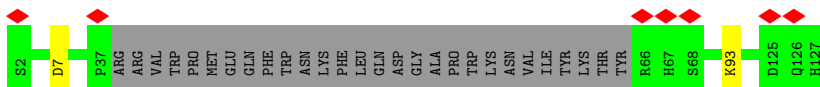
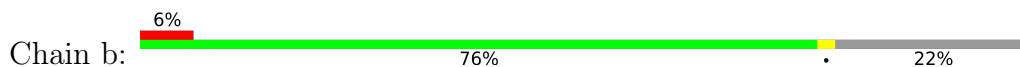


- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial





- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



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



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



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



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



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



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

Chain h:  97%



- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

Chain i:  99%



- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

Chain j:  97%



- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

Chain k:  98%



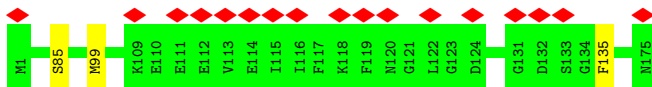
- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

Chain l:  98%



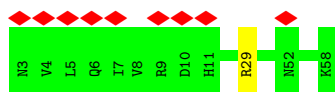
- Molecule 36: NADH-ubiquinone oxidoreductase chain 6

Chain m:  10% 98%

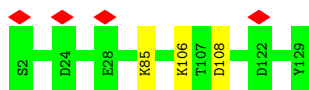


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain n:  16% 98%



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



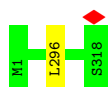
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 40: NADH-ubiquinone oxidoreductase chain 4



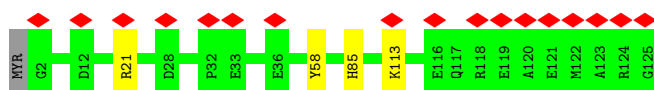
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1



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

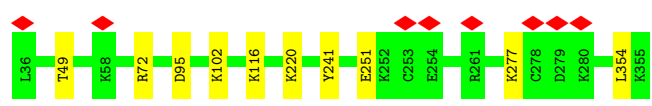


- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



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

Chain w:  97%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	326044	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
Maximum map value	0.248	Depositor
Minimum map value	-0.137	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0271	Depositor
Map size (Å)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, 970, MG, NDP, ZN, 8Q1, PEE, CDL, PLX, SF4, FES, UQ, 2MR, FMN, NAI

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	0.31	0/3406	0.50	0/4603
2	B	0.34	0/1443	0.53	0/1952
3	C	0.37	0/1279	0.52	0/1730
4	E	0.30	0/995	0.54	0/1340
5	F	0.29	0/695	0.54	0/936
6	G	0.28	0/705	0.49	0/956
6	X	0.28	0/708	0.49	0/959
7	H	0.28	0/929	0.49	0/1258
8	I	0.30	0/798	0.57	0/1079
9	J	0.31	0/2828	0.52	0/3834
10	K	0.30	0/377	0.53	0/509
11	L	0.30	0/1039	0.50	0/1403
12	M	0.31	0/5381	0.55	0/7291
13	N	0.32	0/1245	0.55	0/1694
14	O	0.29	0/1711	0.50	0/2328
15	P	0.35	0/1789	0.56	0/2436
16	Q	0.37	0/3538	0.55	0/4796
17	S	0.30	0/581	0.53	0/781
18	T	0.31	0/755	0.54	0/1018
19	U	0.28	0/664	0.46	0/912
20	V	0.34	1/1042 (0.1%)	0.50	0/1411
21	W	0.32	0/1192	0.53	0/1610
22	Y	0.29	0/610	0.50	0/836
23	Z	0.28	0/660	0.48	0/892
24	a	0.32	0/1184	0.51	0/1603
25	b	0.29	0/844	0.49	0/1149
26	c	0.32	0/1371	0.52	0/1875
27	d	0.31	0/1494	0.52	0/2015
28	e	0.29	0/891	0.50	0/1210
29	f	0.29	0/385	0.45	0/522
30	g	0.32	0/1036	0.49	0/1401
31	h	0.29	0/889	0.52	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.31	0/2773	0.50	0/3768
33	j	0.29	0/938	0.44	0/1281
34	k	0.29	0/759	0.49	0/1029
35	l	0.30	0/4926	0.47	0/6700
36	m	0.32	0/1307	0.50	0/1777
37	n	0.26	0/491	0.51	0/663
38	o	0.30	0/1092	0.49	0/1481
39	p	0.30	0/1590	0.50	0/2155
40	r	0.30	0/3715	0.49	0/5067
41	s	0.32	0/2581	0.51	0/3529
42	u	0.29	0/1436	0.49	0/1938
43	v	0.28	0/1060	0.52	0/1421
44	w	0.30	0/2646	0.49	0/3584
All	All	0.31	1/67778 (0.0%)	0.51	0/91922

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	V	95	CYS	CB-SG	-5.21	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	414 (96%)	15 (4%)	2 (0%)	29	52
2	B	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
3	C	154/156 (99%)	144 (94%)	10 (6%)	0	100	100
4	E	113/115 (98%)	108 (96%)	4 (4%)	1 (1%)	17	35
5	F	84/86 (98%)	81 (96%)	2 (2%)	1 (1%)	13	27
6	G	86/88 (98%)	80 (93%)	6 (7%)	0	100	100
6	X	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
7	H	110/112 (98%)	105 (96%)	4 (4%)	1 (1%)	17	35
8	I	93/112 (83%)	84 (90%)	7 (8%)	2 (2%)	6	12
9	J	340/342 (99%)	329 (97%)	10 (3%)	1 (0%)	41	64
10	K	41/43 (95%)	39 (95%)	1 (2%)	1 (2%)	6	10
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	665 (97%)	23 (3%)	0	100	100
13	N	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	O	215/217 (99%)	204 (95%)	10 (5%)	1 (0%)	29	52
15	P	206/208 (99%)	198 (96%)	8 (4%)	0	100	100
16	Q	427/430 (99%)	410 (96%)	16 (4%)	1 (0%)	47	71
17	S	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
18	T	94/96 (98%)	93 (99%)	1 (1%)	0	100	100
19	U	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
20	V	138/140 (99%)	134 (97%)	4 (3%)	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%)	73 (94%)	5 (6%)	0	100	100
24	a	136/138 (99%)	129 (95%)	7 (5%)	0	100	100
25	b	94/126 (75%)	88 (94%)	6 (6%)	0	100	100
26	c	154/156 (99%)	143 (93%)	10 (6%)	1 (1%)	25	47
27	d	173/175 (99%)	170 (98%)	3 (2%)	0	100	100
28	e	102/104 (98%)	97 (95%)	5 (5%)	0	100	100
29	f	47/49 (96%)	42 (89%)	5 (11%)	0	100	100
30	g	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
31	h	103/105 (98%)	97 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	i	345/347 (99%)	332 (96%)	12 (4%)	1 (0%)	41	64
33	j	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
34	k	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
35	l	604/606 (100%)	587 (97%)	17 (3%)	0	100	100
36	m	173/175 (99%)	154 (89%)	19 (11%)	0	100	100
37	n	54/56 (96%)	54 (100%)	0	0	100	100
38	o	126/128 (98%)	119 (94%)	7 (6%)	0	100	100
39	p	176/178 (99%)	171 (97%)	4 (2%)	1 (1%)	25	47
40	r	457/459 (100%)	451 (99%)	6 (1%)	0	100	100
41	s	316/318 (99%)	305 (96%)	11 (4%)	0	100	100
42	u	169/171 (99%)	163 (96%)	5 (3%)	1 (1%)	25	47
43	v	122/125 (98%)	117 (96%)	4 (3%)	1 (1%)	19	39
44	w	318/320 (99%)	309 (97%)	9 (3%)	0	100	100
All	All	8175/8314 (98%)	7857 (96%)	302 (4%)	16 (0%)	50	71

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	60	ASP
10	K	75	ASN
1	A	264	SER
8	I	29	GLN
9	J	38	HIS

5.3.2 Protein sidechains [i](#)

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%)	335 (97%)	11 (3%)	39	65
2	B	151/151 (100%)	149 (99%)	2 (1%)	69	86
3	C	132/132 (100%)	131 (99%)	1 (1%)	81	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	E	107/107 (100%)	107 (100%)	0	100	100
5	F	74/76 (97%)	70 (95%)	4 (5%)	22	44
6	G	76/81 (94%)	72 (95%)	4 (5%)	22	45
6	X	77/81 (95%)	74 (96%)	3 (4%)	32	58
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	81 (93%)	6 (7%)	15	31
9	J	296/296 (100%)	287 (97%)	9 (3%)	41	67
10	K	42/42 (100%)	41 (98%)	1 (2%)	49	74
11	L	113/113 (100%)	112 (99%)	1 (1%)	78	91
12	M	579/580 (100%)	569 (98%)	10 (2%)	60	81
13	N	130/130 (100%)	125 (96%)	5 (4%)	33	59
14	O	183/183 (100%)	180 (98%)	3 (2%)	62	82
15	P	190/190 (100%)	187 (98%)	3 (2%)	62	82
16	Q	370/370 (100%)	365 (99%)	5 (1%)	67	85
17	S	57/58 (98%)	57 (100%)	0	100	100
18	T	79/79 (100%)	76 (96%)	3 (4%)	33	59
19	U	69/69 (100%)	65 (94%)	4 (6%)	20	40
20	V	101/101 (100%)	96 (95%)	5 (5%)	24	47
21	W	121/123 (98%)	118 (98%)	3 (2%)	47	73
22	Y	62/62 (100%)	60 (97%)	2 (3%)	39	65
23	Z	62/62 (100%)	59 (95%)	3 (5%)	25	49
24	a	121/121 (100%)	119 (98%)	2 (2%)	60	81
25	b	90/119 (76%)	88 (98%)	2 (2%)	52	76
26	c	141/141 (100%)	137 (97%)	4 (3%)	43	69
27	d	155/155 (100%)	155 (100%)	0	100	100
28	e	96/96 (100%)	92 (96%)	4 (4%)	30	55
29	f	35/45 (78%)	35 (100%)	0	100	100
30	g	108/109 (99%)	107 (99%)	1 (1%)	78	91
31	h	93/93 (100%)	90 (97%)	3 (3%)	39	65
32	i	311/311 (100%)	307 (99%)	4 (1%)	69	86
33	j	100/100 (100%)	96 (96%)	4 (4%)	31	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	k	85/85 (100%)	83 (98%)	2 (2%)	49	74
35	l	536/540 (99%)	524 (98%)	12 (2%)	52	76
36	m	127/141 (90%)	124 (98%)	3 (2%)	49	74
37	n	53/53 (100%)	52 (98%)	1 (2%)	57	79
38	o	113/113 (100%)	110 (97%)	3 (3%)	44	71
39	p	159/159 (100%)	155 (98%)	4 (2%)	47	73
40	r	409/410 (100%)	399 (98%)	10 (2%)	49	74
41	s	275/275 (100%)	274 (100%)	1 (0%)	91	97
42	u	153/153 (100%)	146 (95%)	7 (5%)	27	51
43	v	106/111 (96%)	103 (97%)	3 (3%)	43	69
44	w	282/283 (100%)	272 (96%)	10 (4%)	36	62
All	All	7151/7241 (99%)	6983 (98%)	168 (2%)	53	75

5 of 168 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	l	176	ARG
40	r	243	MET
35	l	373	LEU
38	o	85	LYS
42	u	92	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
18	T	123	HIS
32	i	171	ASN
40	r	304	GLN
32	i	144	GLN
32	i	273	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	6.11	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	5.59	1.46	1.34
16	Q	118	2MR	CQ2-NH2	-2.05	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	12.39	130.84	119.48
16	Q	118	2MR	CD-NE-CZ	4.45	131.74	123.41
16	Q	118	2MR	CQ2-NH2-CZ	3.23	131.01	123.86

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.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 47 ligands modelled in this entry, 1 is modelled with single atom and 2 are monoatomic - leaving 44 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
48	PEE	l	704	-	49,49,50	1.16	6 (12%)	52,54,55	0.95	2 (3%)
45	SF4	B	302	2	0,12,12	-	-	-		
53	UQ	J	402	-	33,33,63	3.42	9 (27%)	40,43,79	2.87	13 (32%)
46	FMN	A	502	-	33,33,33	1.12	2 (6%)	48,50,50	1.27	9 (18%)
51	CDL	V	201	-	93,93,99	1.12	8 (8%)	99,105,111	0.86	4 (4%)
45	SF4	B	301	2	0,12,12	-	-	-		
49	PLX	J	403	-	51,51,51	1.12	2 (3%)	55,59,59	0.62	1 (1%)
51	CDL	o	201	-	99,99,99	1.07	9 (9%)	105,111,111	0.88	5 (4%)
48	PEE	C	302	-	46,46,50	1.19	6 (13%)	49,51,55	0.99	2 (4%)
50	8Q1	X	201	-	31,34,34	2.10	6 (19%)	40,43,43	1.69	11 (27%)
48	PEE	W	201	-	40,40,50	1.14	5 (12%)	43,45,55	1.02	2 (4%)
49	PLX	C	303	-	51,51,51	0.62	0	55,59,59	0.74	1 (1%)
51	CDL	l	702	-	99,99,99	0.91	4 (4%)	105,111,111	1.10	7 (6%)
48	PEE	j	201	-	40,40,50	1.16	4 (10%)	43,45,55	1.04	2 (4%)
53	UQ	s	401	-	38,38,63	3.55	10 (26%)	46,49,79	2.84	16 (34%)
47	NAI	A	503	-	42,48,48	4.93	18 (42%)	47,73,73	1.30	6 (12%)
45	SF4	A	501	1	0,12,12	-	-	-		
49	PLX	r	503	-	51,51,51	1.13	3 (5%)	55,59,59	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
51	CDL	a	201	-	99,99,99	1.08	8 (8%)	105,111,111	0.89	4 (3%)
51	CDL	i	401	-	99,99,99	0.93	4 (4%)	105,111,111	1.01	4 (3%)
52	NDP	J	401	-	45,52,52	0.96	2 (4%)	53,80,80	1.08	3 (5%)
54	FES	M	803	12	0,4,4	-	-	-		
45	SF4	C	301	3	0,12,12	-	-	-		
48	PEE	l	705	-	45,45,50	1.22	5 (11%)	48,50,55	0.98	2 (4%)
54	FES	O	301	14	0,4,4	-	-	-		
51	CDL	k	101	-	77,77,99	1.18	6 (7%)	83,89,111	0.94	4 (4%)
58	ADP	w	401	-	24,29,29	3.12	6 (25%)	29,45,45	1.36	3 (10%)
51	CDL	m	201	-	88,88,99	0.97	4 (4%)	94,100,111	1.10	6 (6%)
51	CDL	r	504	-	98,98,99	1.07	8 (8%)	104,110,111	0.86	4 (3%)
48	PEE	B	303	-	50,50,50	1.15	6 (12%)	53,55,55	0.99	2 (3%)
49	PLX	g	201	-	51,51,51	1.12	3 (5%)	55,59,59	0.67	1 (1%)
51	CDL	l	701	-	98,98,99	0.92	4 (4%)	104,110,111	1.09	8 (7%)
48	PEE	l	703	-	46,46,50	1.19	6 (13%)	49,51,55	1.03	3 (6%)
51	CDL	I	201	-	50,50,99	1.28	4 (8%)	56,62,111	1.35	6 (10%)
51	CDL	u	201	-	54,54,99	1.22	4 (7%)	60,66,111	1.25	5 (8%)
49	PLX	a	202	-	51,51,51	1.15	4 (7%)	55,59,59	0.62	1 (1%)
56	970	Q	501	-	33,33,33	4.84	14 (42%)	48,50,50	2.41	21 (43%)
45	SF4	M	802	12	0,12,12	-	-	-		
49	PLX	r	502	-	51,51,51	1.14	5 (9%)	55,59,59	0.62	1 (1%)
45	SF4	M	801	12	0,12,12	-	-	-		
50	8Q1	G	201	-	31,34,34	2.12	6 (19%)	40,43,43	1.81	12 (30%)
48	PEE	U	101	-	50,50,50	1.15	5 (10%)	53,55,55	0.93	2 (3%)
49	PLX	j	202	-	51,51,51	1.13	4 (7%)	55,59,59	0.59	1 (1%)
48	PEE	r	501	-	50,50,50	1.15	6 (12%)	53,55,55	0.95	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
48	PEE	l	704	-	-	22/53/53/54	-
45	SF4	B	302	2	-	-	0/6/5/5
53	UQ	J	402	-	-	14/27/51/87	0/1/1/1
46	FMN	A	502	-	-	7/18/18/18	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	CDL	V	201	-	-	58/104/104/110	-
45	SF4	B	301	2	-	-	0/6/5/5
49	PLX	J	403	-	-	27/55/55/55	-
51	CDL	o	201	-	-	56/110/110/110	-
48	PEE	C	302	-	-	28/50/50/54	-
50	8Q1	X	201	-	-	27/41/41/41	-
48	PEE	W	201	-	-	23/44/44/54	-
49	PLX	C	303	-	-	20/55/55/55	-
51	CDL	l	702	-	-	40/110/110/110	-
48	PEE	j	201	-	-	17/44/44/54	-
53	UQ	s	401	-	-	13/33/57/87	0/1/1/1
47	NAI	A	503	-	-	6/25/72/72	0/5/5/5
49	PLX	r	503	-	-	37/55/55/55	-
51	CDL	a	201	-	-	60/110/110/110	-
51	CDL	i	401	-	-	35/110/110/110	-
52	NDP	J	401	-	-	8/30/77/77	0/5/5/5
45	SF4	A	501	1	-	-	0/6/5/5
54	FES	M	803	12	-	-	0/1/1/1
45	SF4	C	301	3	-	-	0/6/5/5
48	PEE	l	705	-	-	22/49/49/54	-
54	FES	O	301	14	-	-	0/1/1/1
51	CDL	k	101	-	-	41/88/88/110	-
58	ADP	w	401	-	-	6/12/32/32	0/3/3/3
51	CDL	m	201	-	-	35/99/99/110	-
51	CDL	r	504	-	-	58/109/109/110	-
48	PEE	B	303	-	-	26/54/54/54	-
49	PLX	g	201	-	-	36/55/55/55	-
51	CDL	l	701	-	-	39/109/109/110	-
48	PEE	l	703	-	-	26/50/50/54	-
51	CDL	I	201	-	-	28/61/61/110	-
51	CDL	u	201	-	-	19/65/65/110	-
49	PLX	a	202	-	-	34/55/55/55	-
56	970	Q	501	-	-	7/8/41/41	0/5/5/5
45	SF4	M	802	12	-	-	0/6/5/5
49	PLX	r	502	-	-	30/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	8Q1	G	201	-	-	17/41/41/41	-
45	SF4	M	801	12	-	-	0/6/5/5
48	PEE	U	101	-	-	30/54/54/54	-
49	PLX	j	202	-	-	33/55/55/55	-
48	PEE	r	501	-	-	34/54/54/54	-

The worst 5 of 206 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Q	501	970	O16-C17	19.03	1.58	1.37
47	A	503	NAI	O4B-C1B	16.13	1.63	1.41
47	A	503	NAI	C2B-C1B	-15.48	1.30	1.53
56	Q	501	970	C14-C23	-11.88	1.41	1.52
47	A	503	NAI	C3D-C4D	-10.45	1.26	1.53

The worst 5 of 176 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	J	402	UQ	C7-C8-C9	-8.19	113.16	126.79
53	s	401	UQ	C7-C8-C9	-7.84	113.74	126.79
56	Q	501	970	O08-C07-C06	-7.63	108.35	113.00
53	J	402	UQ	C12-C13-C14	-6.42	112.19	127.66
53	J	402	UQ	C17-C18-C19	-6.32	112.44	127.66

There are no chirality outliers.

5 of 1019 torsion outliers are listed below:

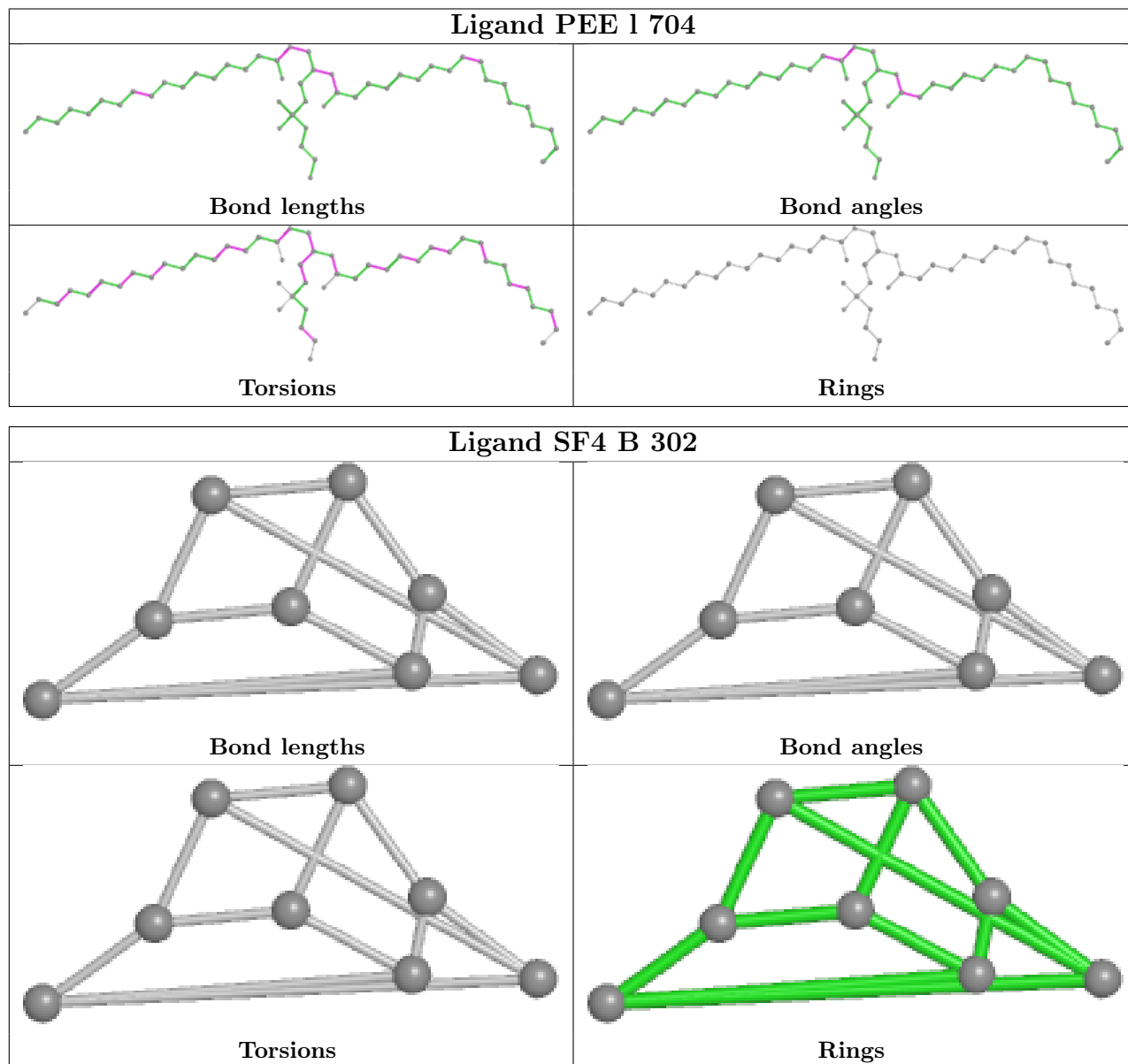
Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
46	A	502	FMN	C3'-C4'-C5'-O5'
46	A	502	FMN	O4'-C4'-C5'-O5'
47	A	503	NAI	C5B-O5B-PA-O1A

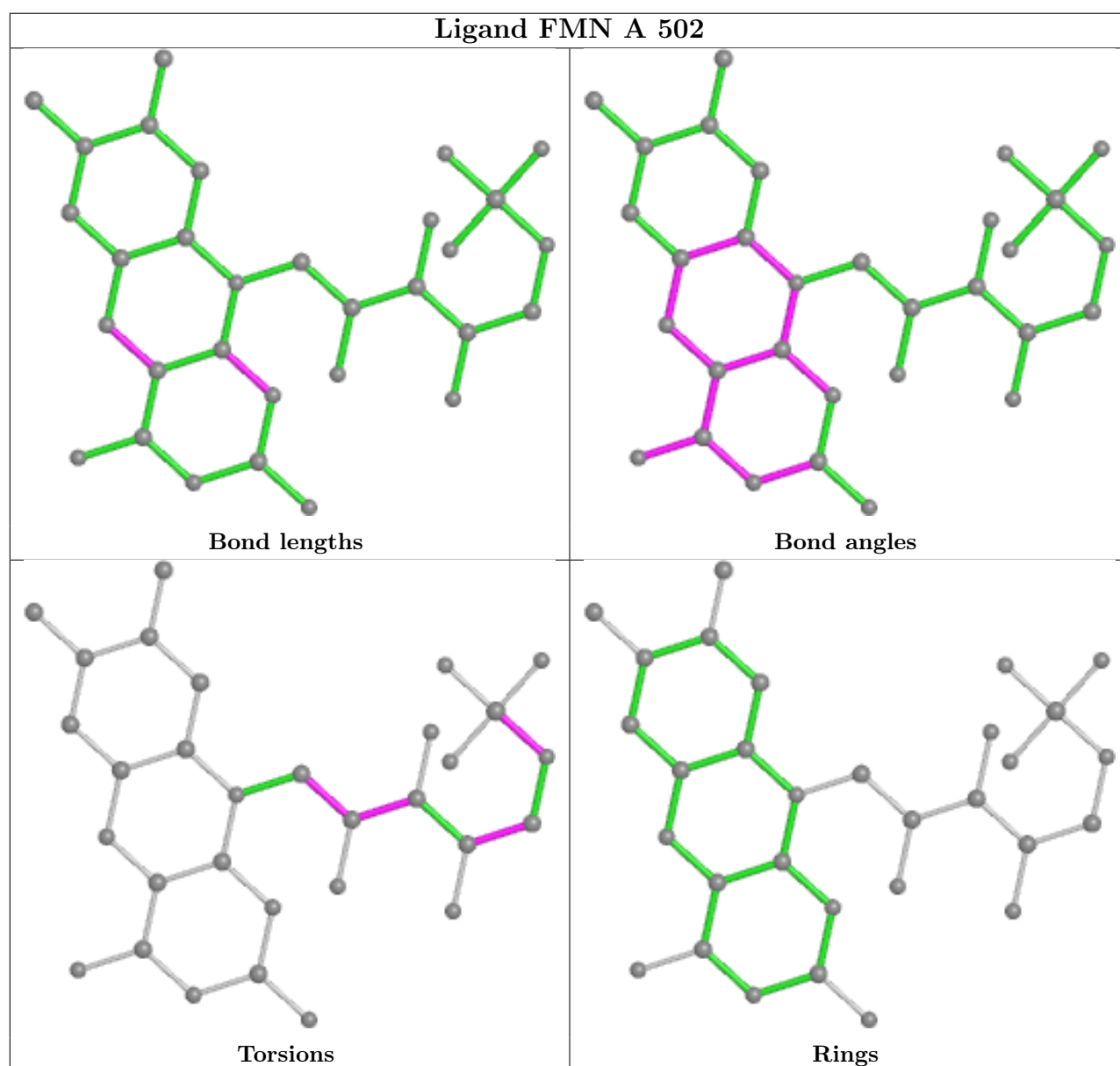
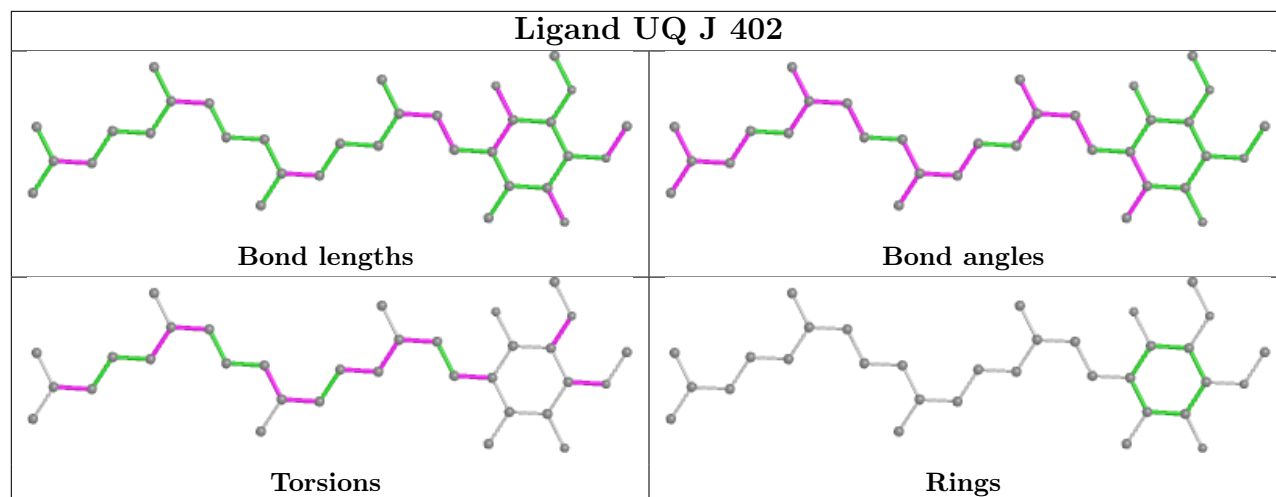
There are no ring outliers.

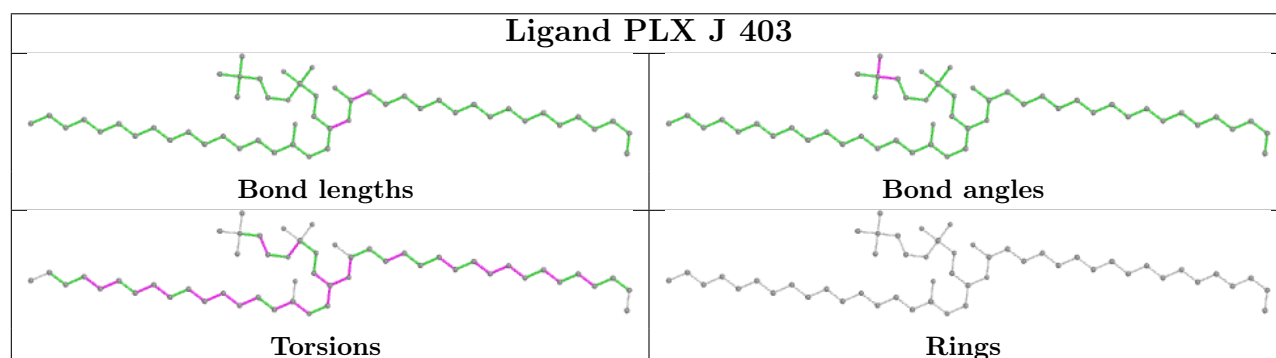
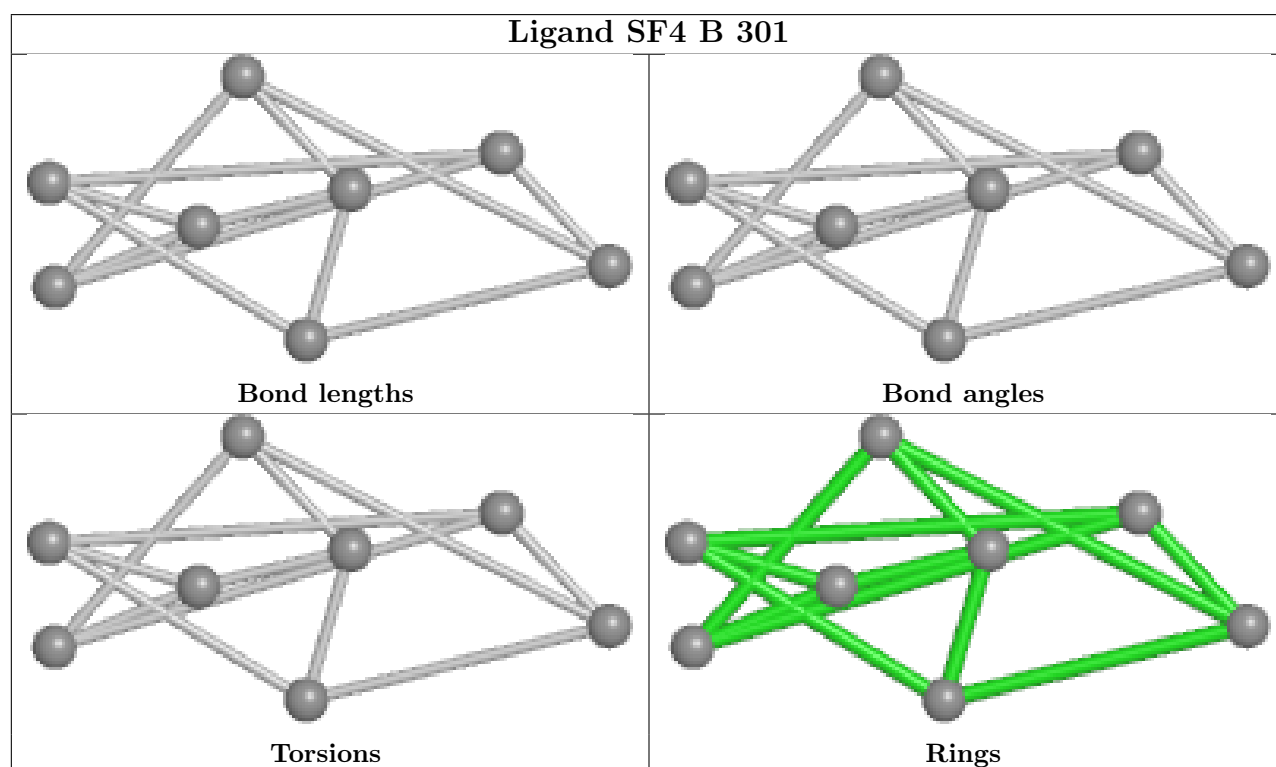
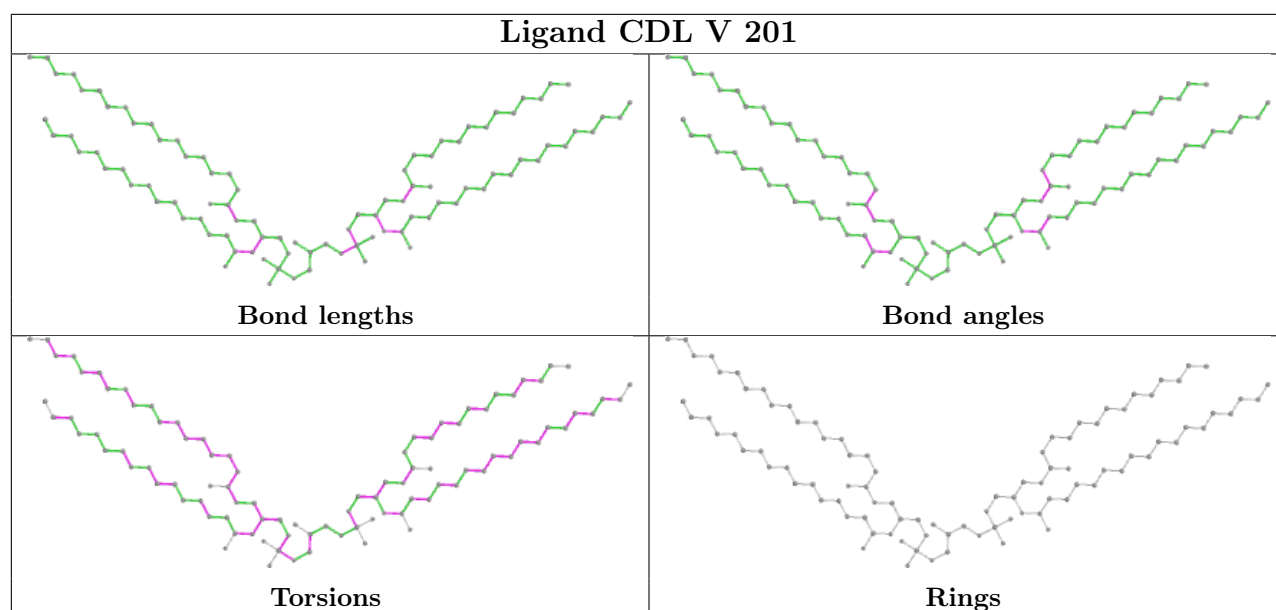
No monomer is involved in short contacts.

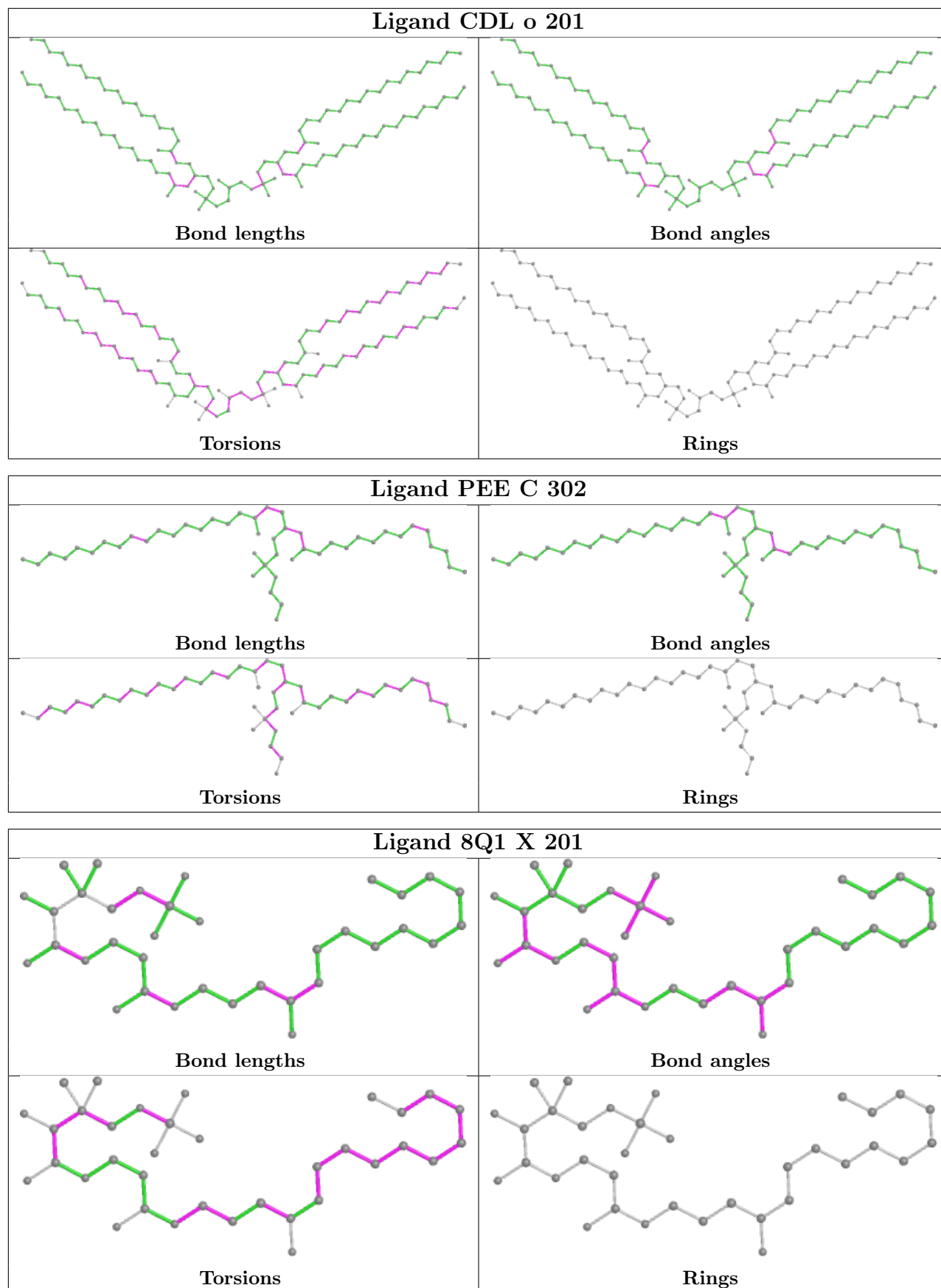
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

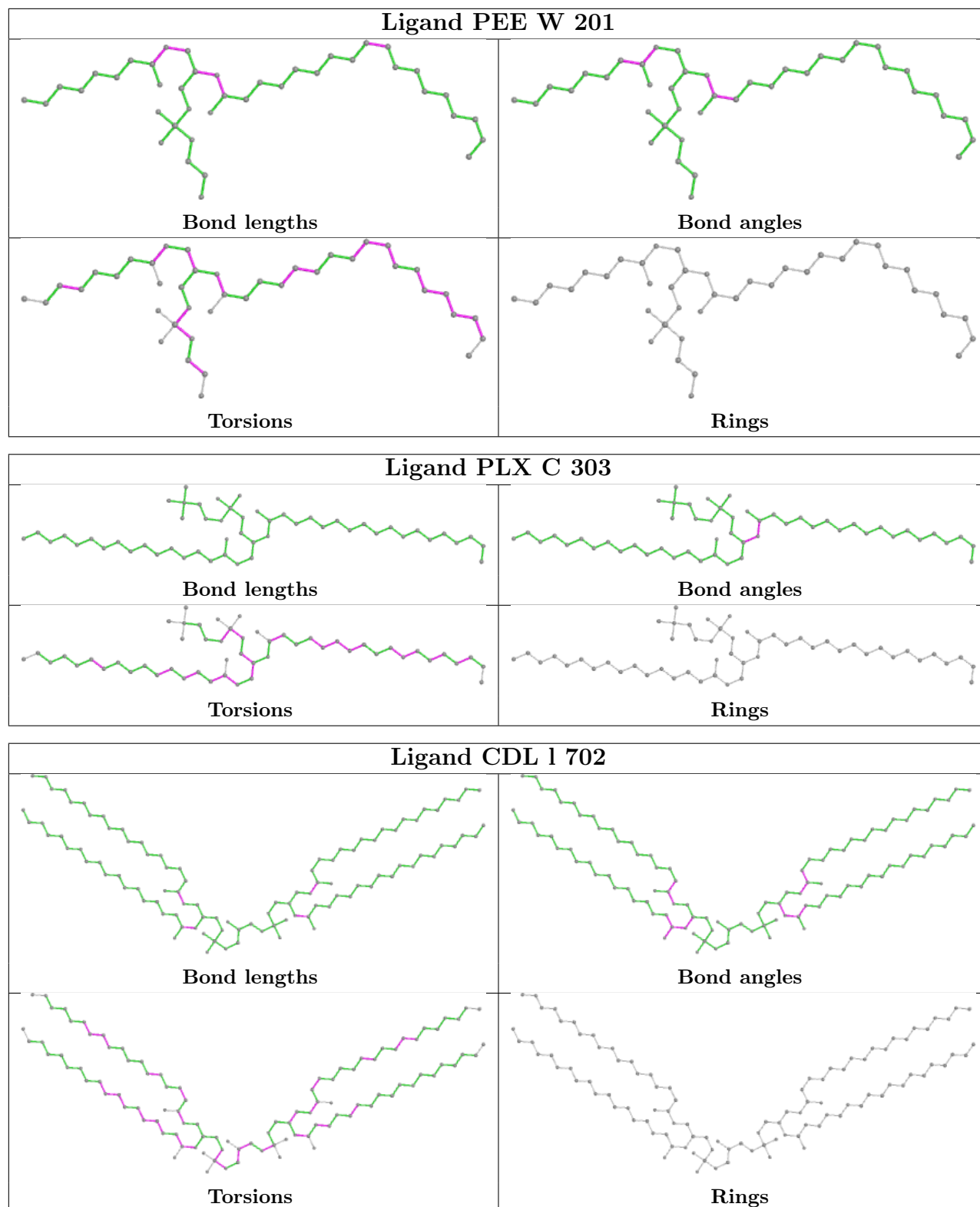
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

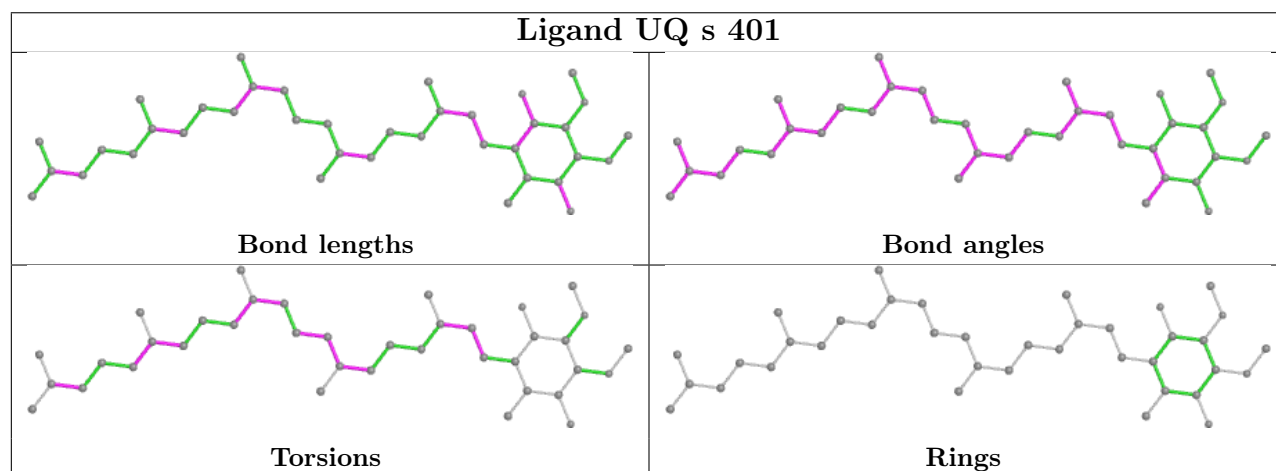
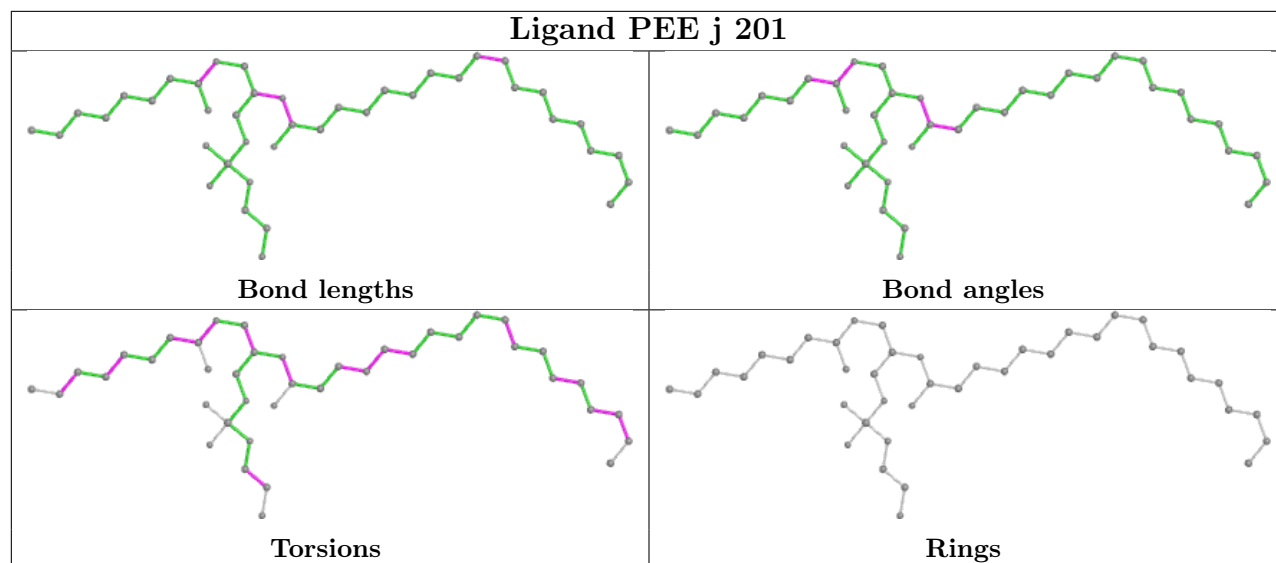


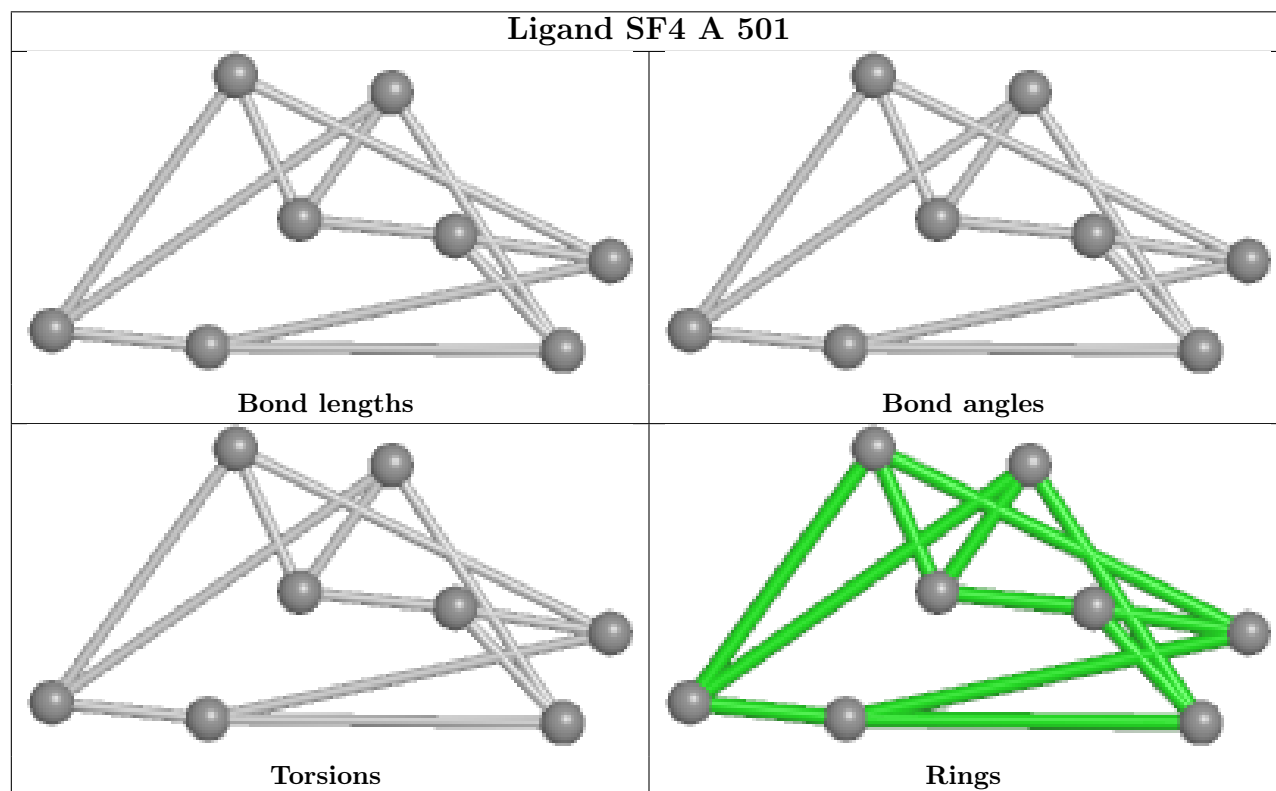
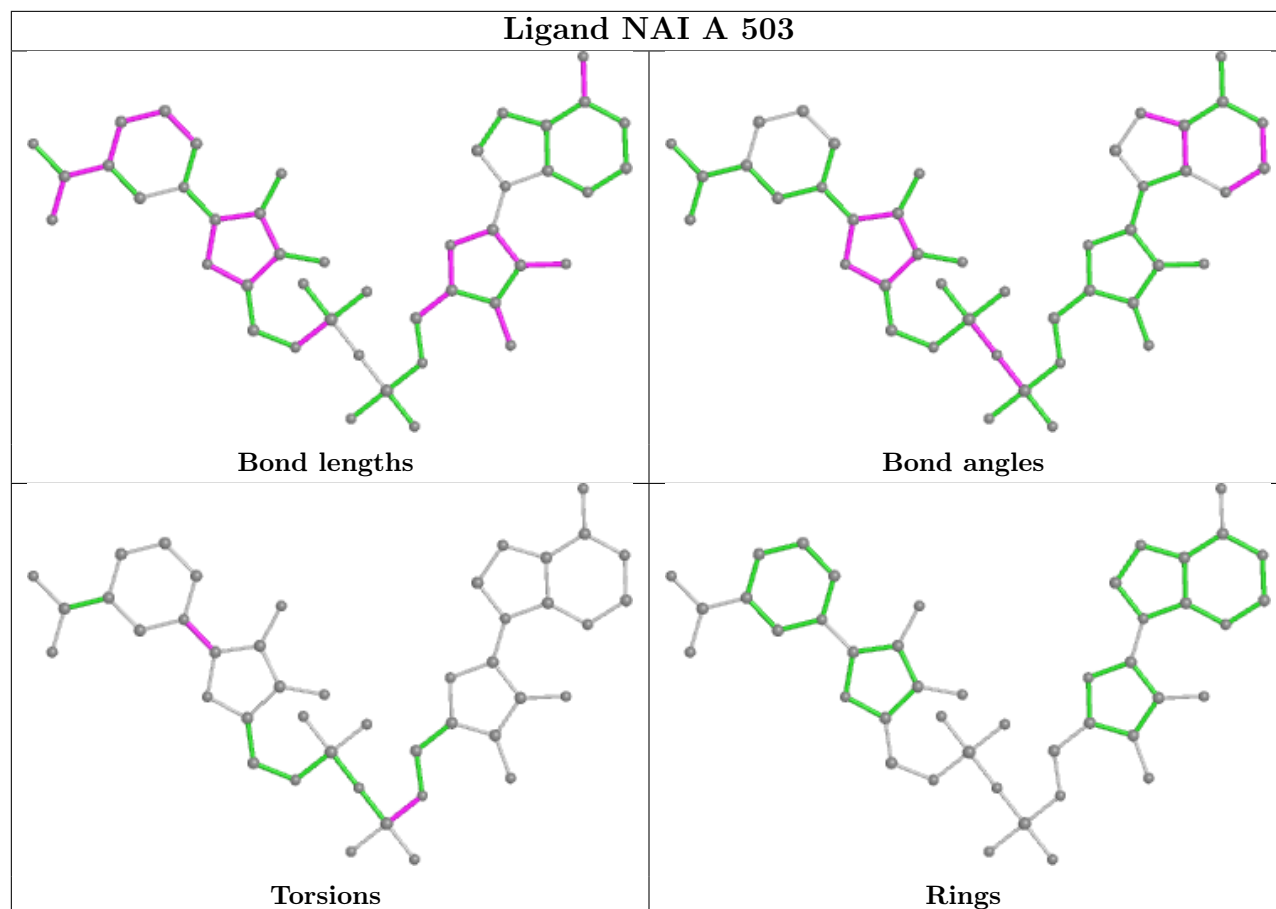


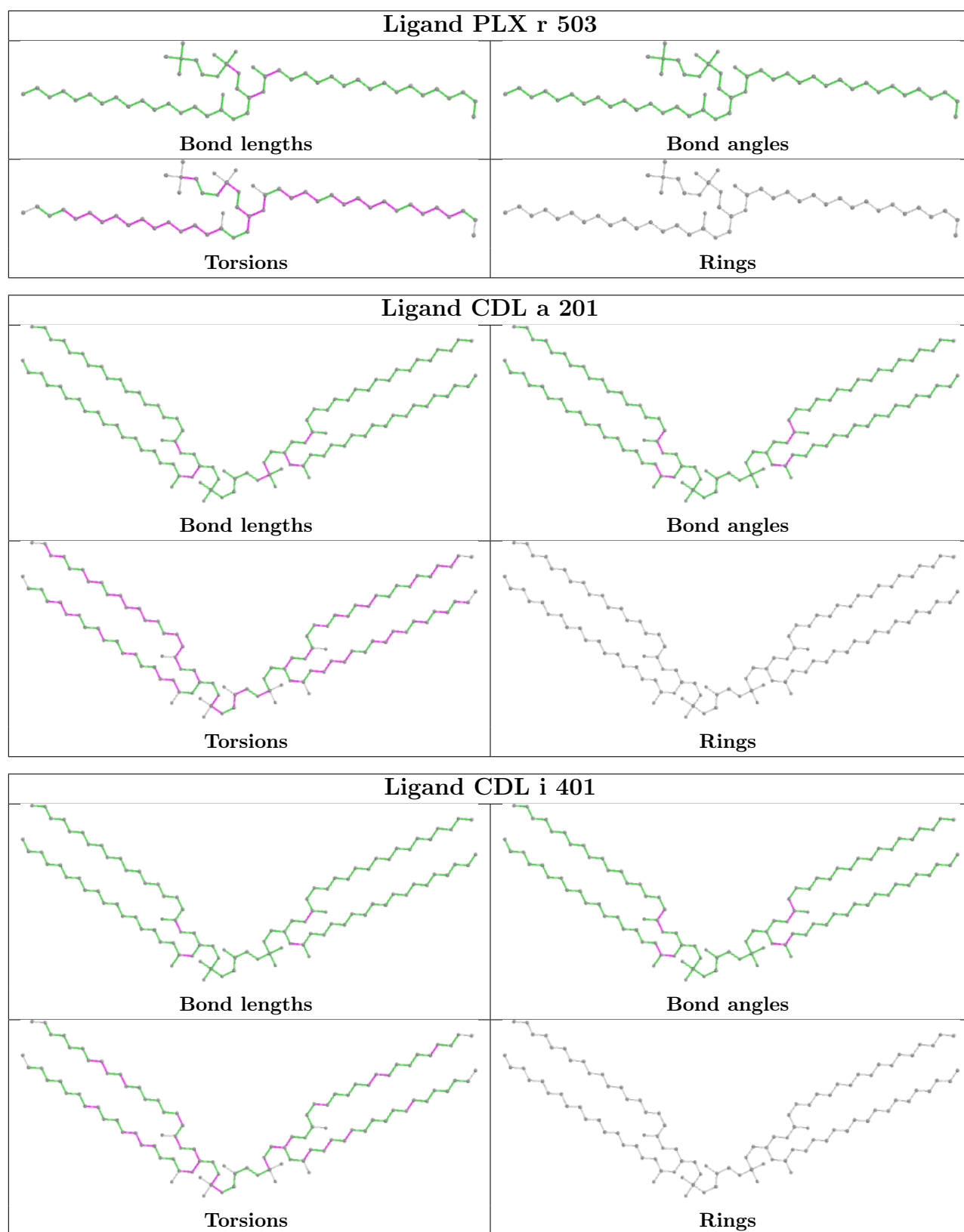


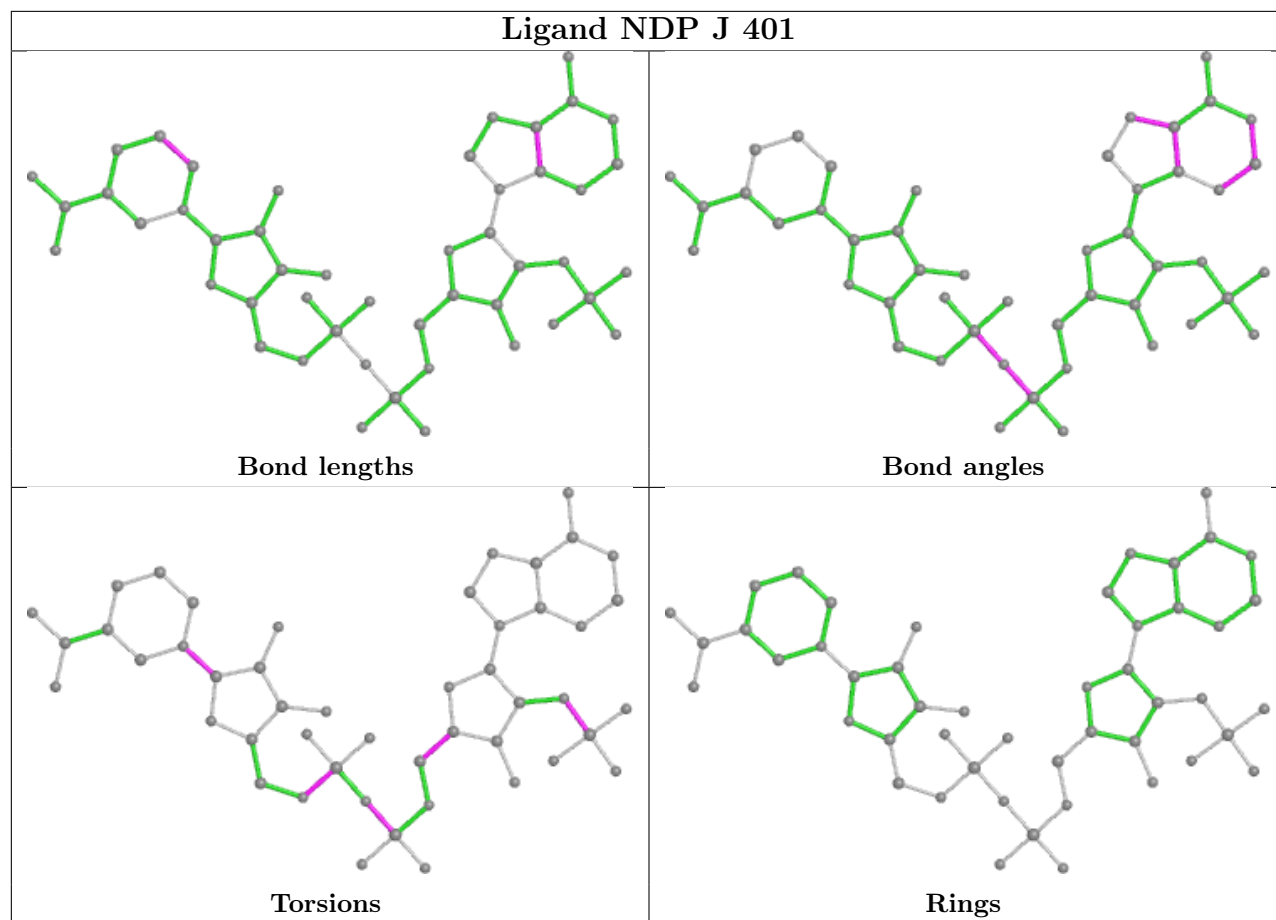


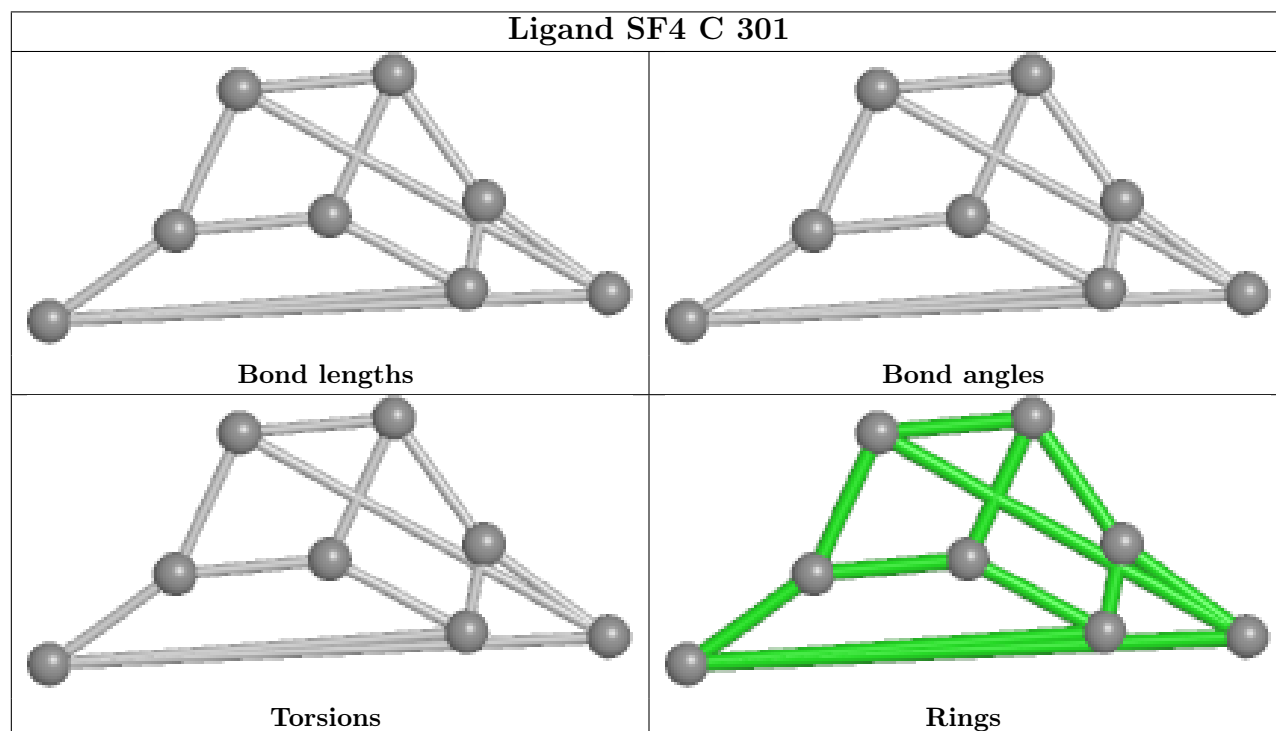
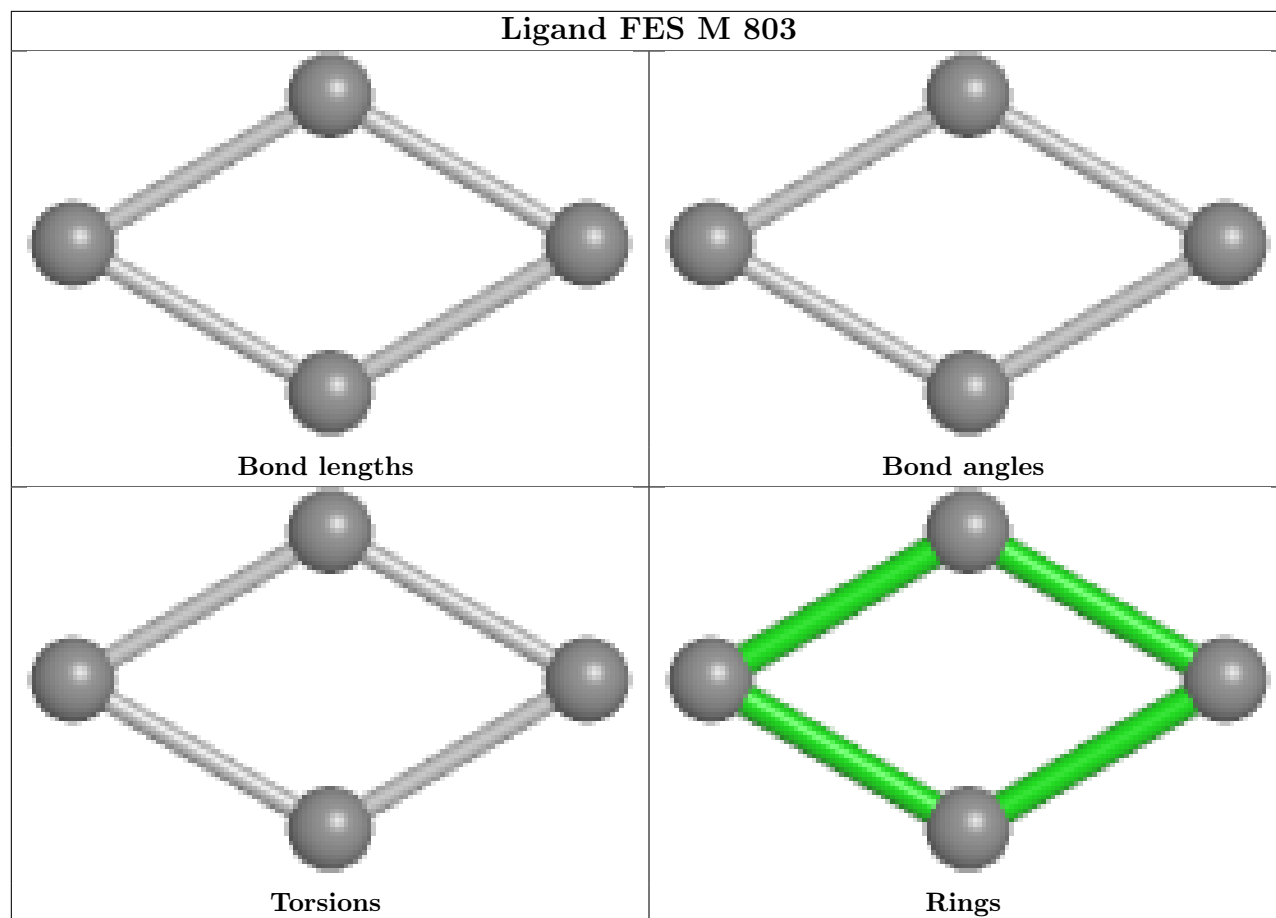


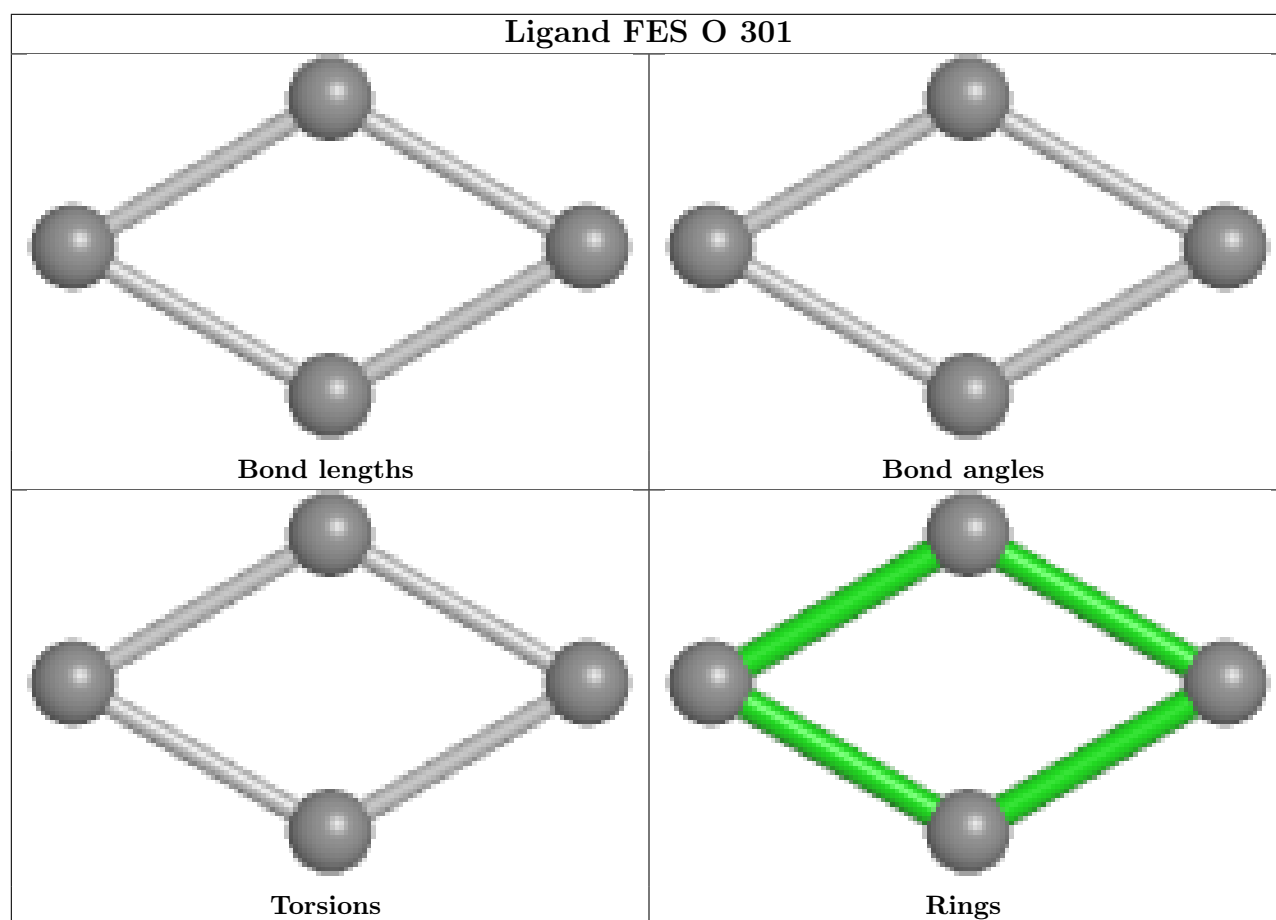
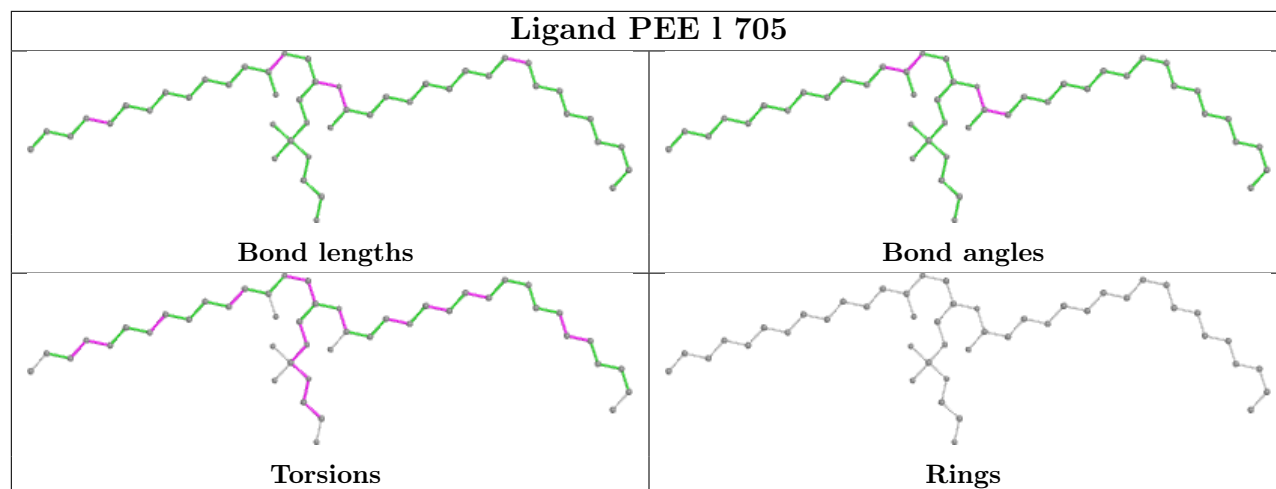


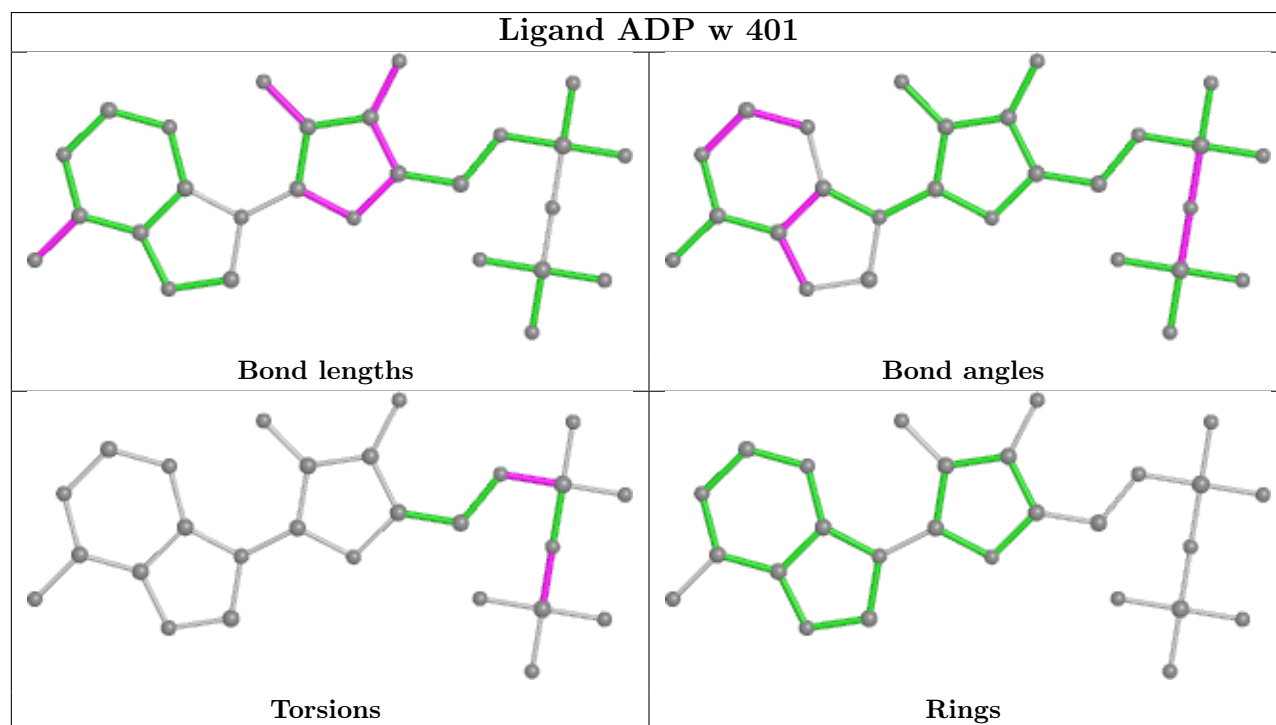
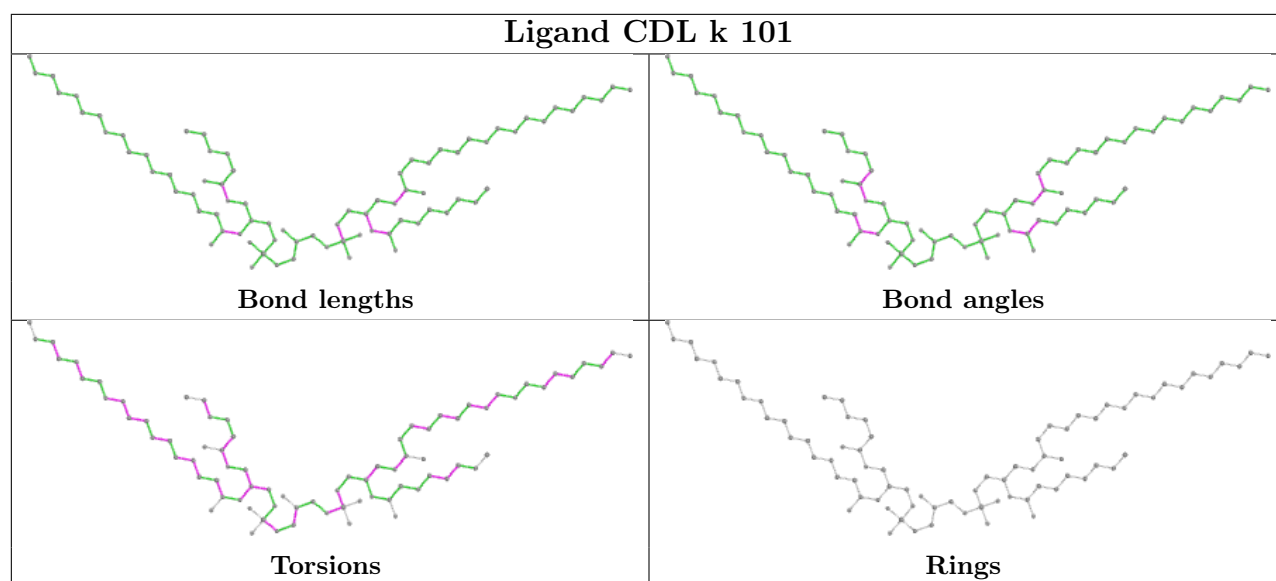


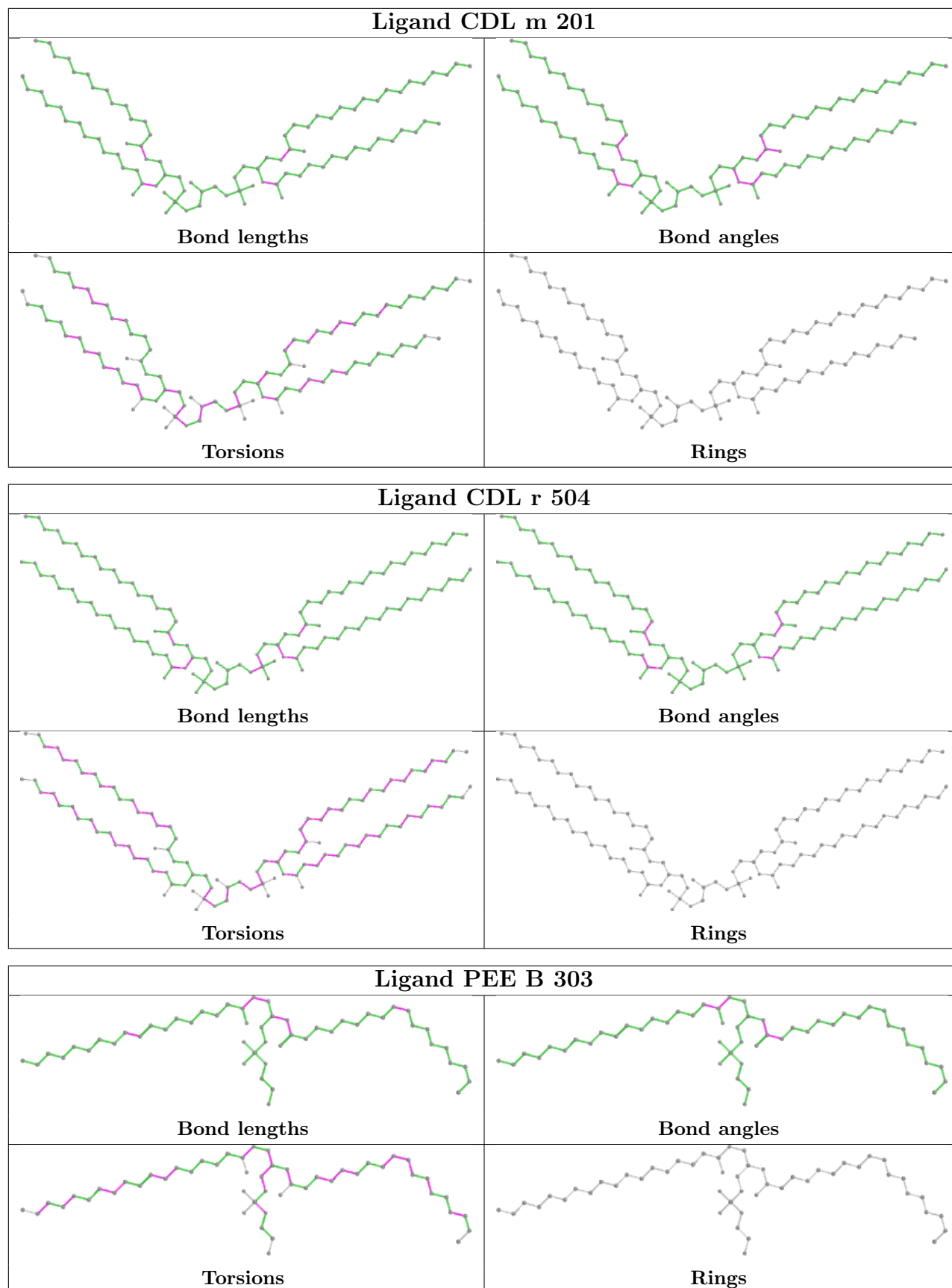


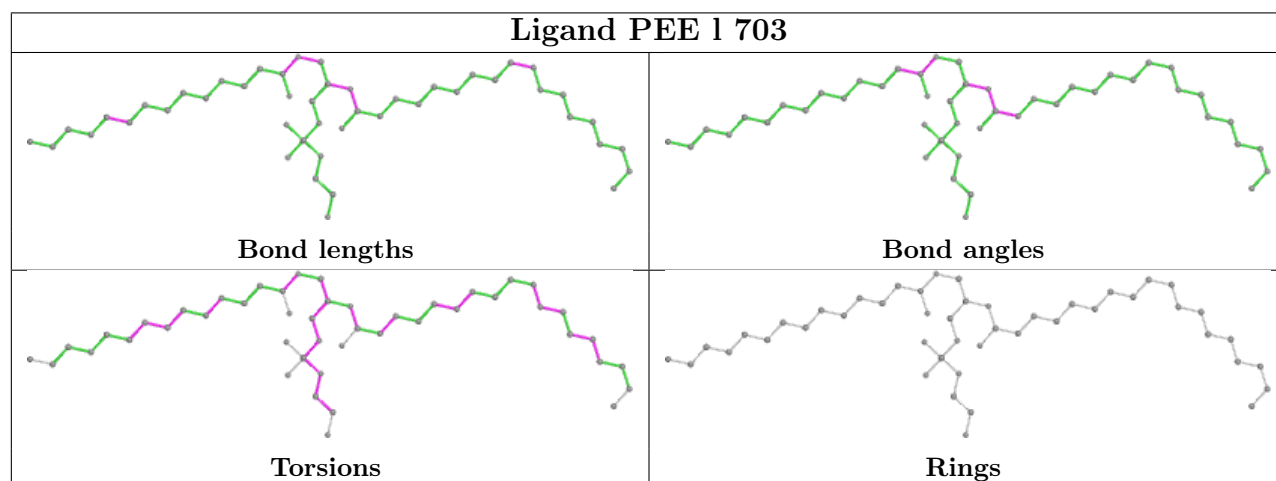
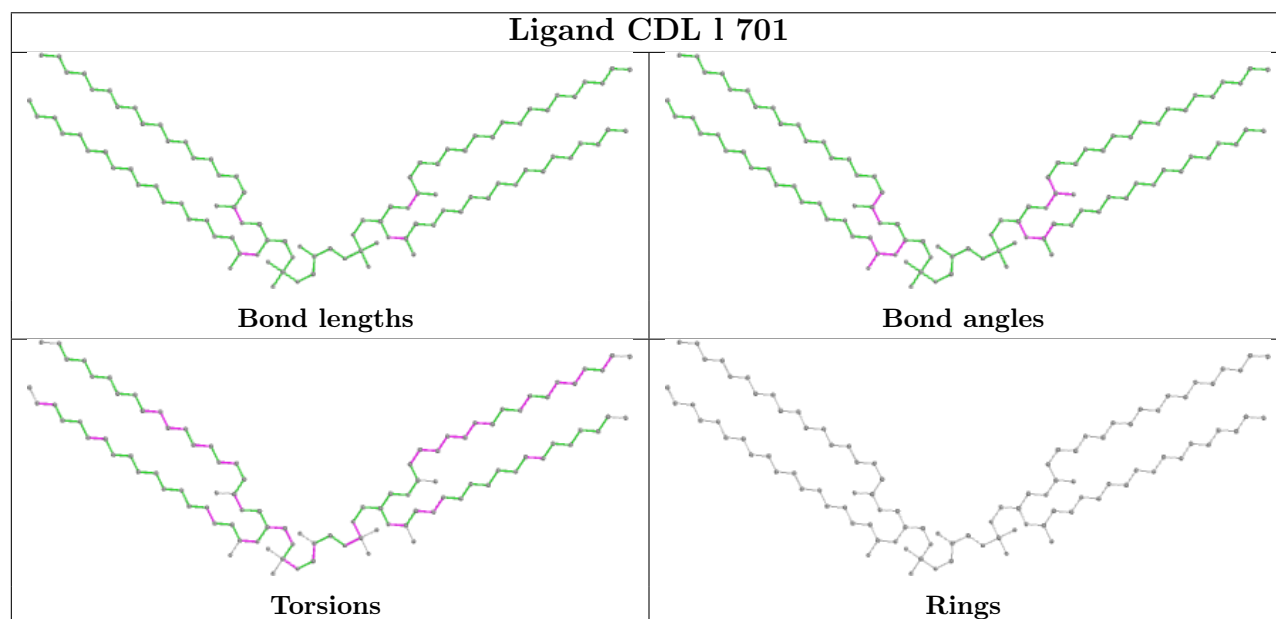
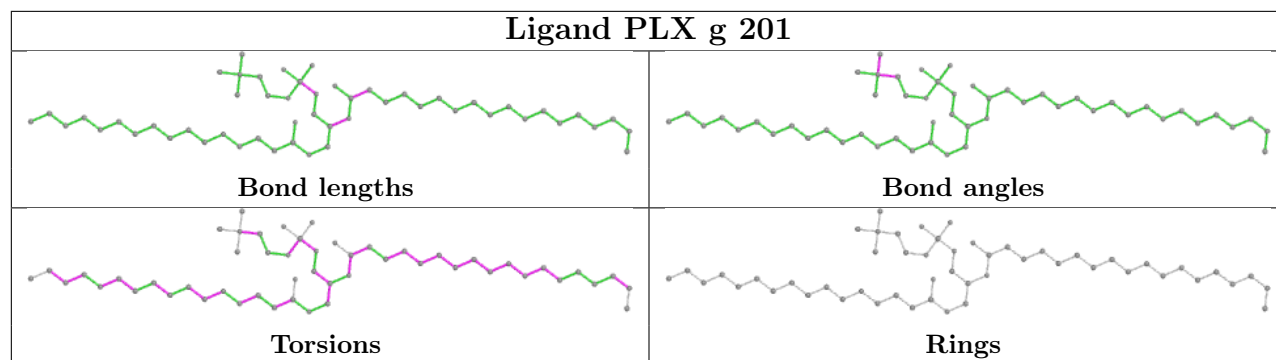


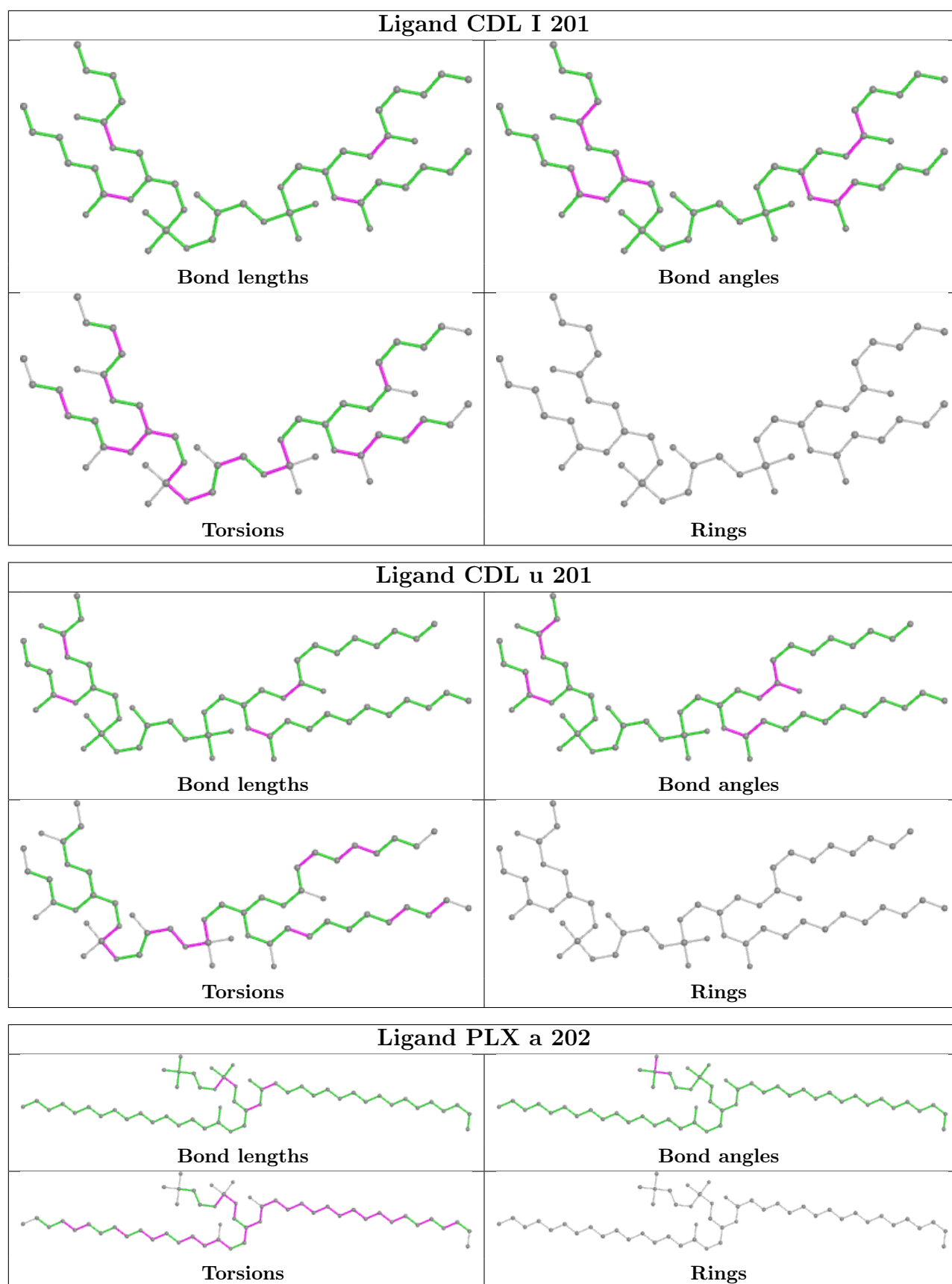


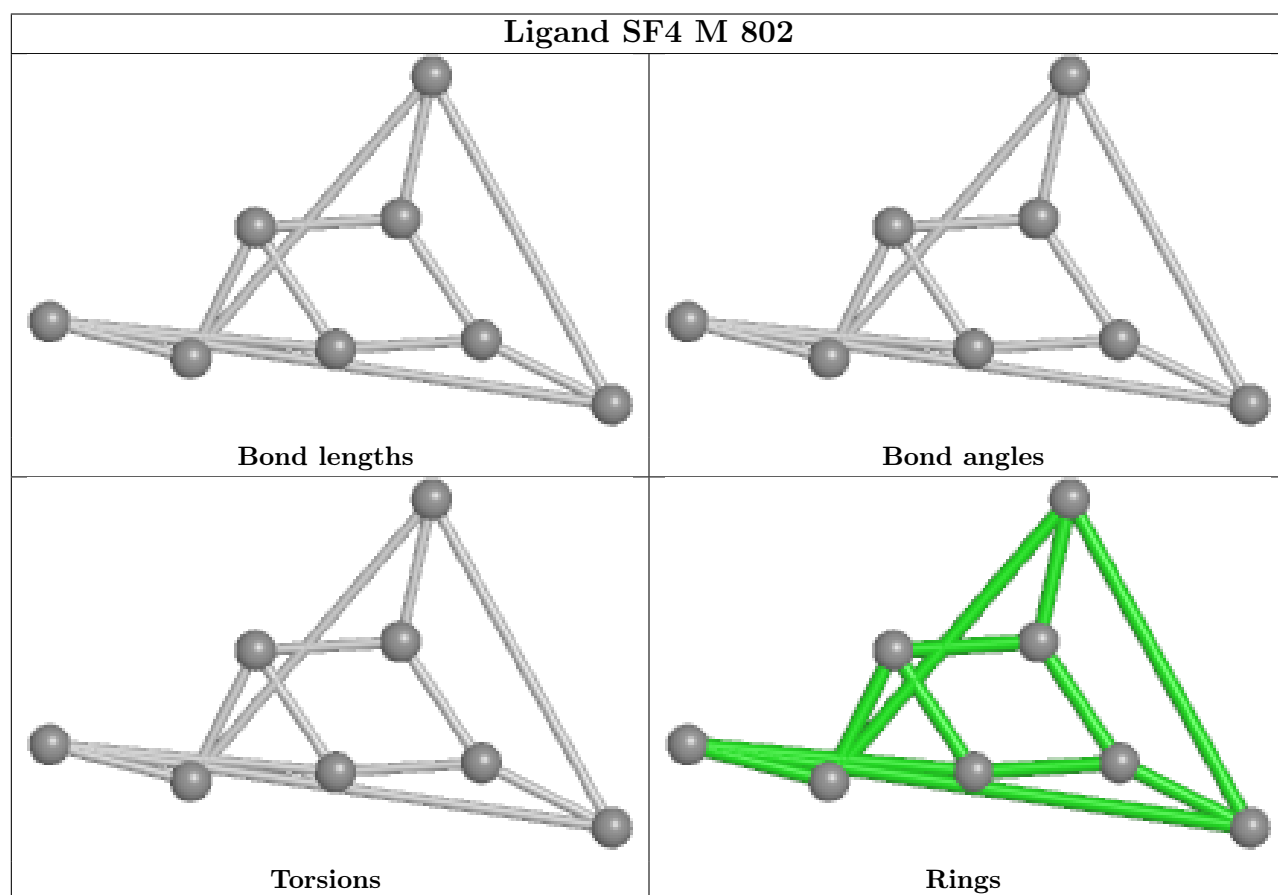
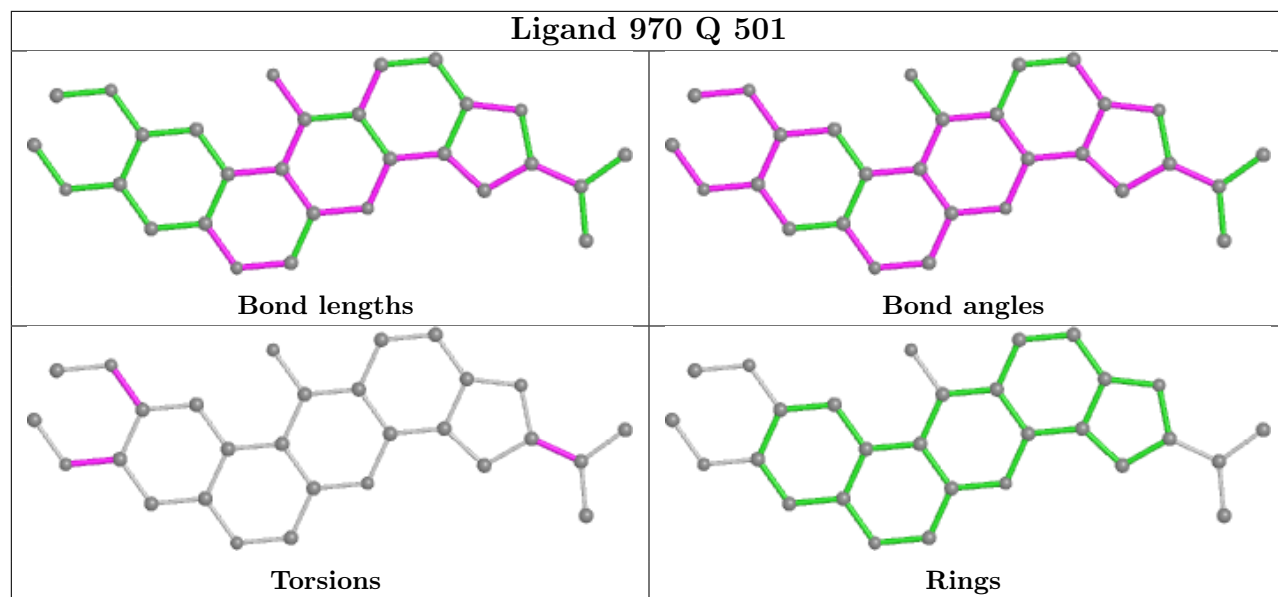


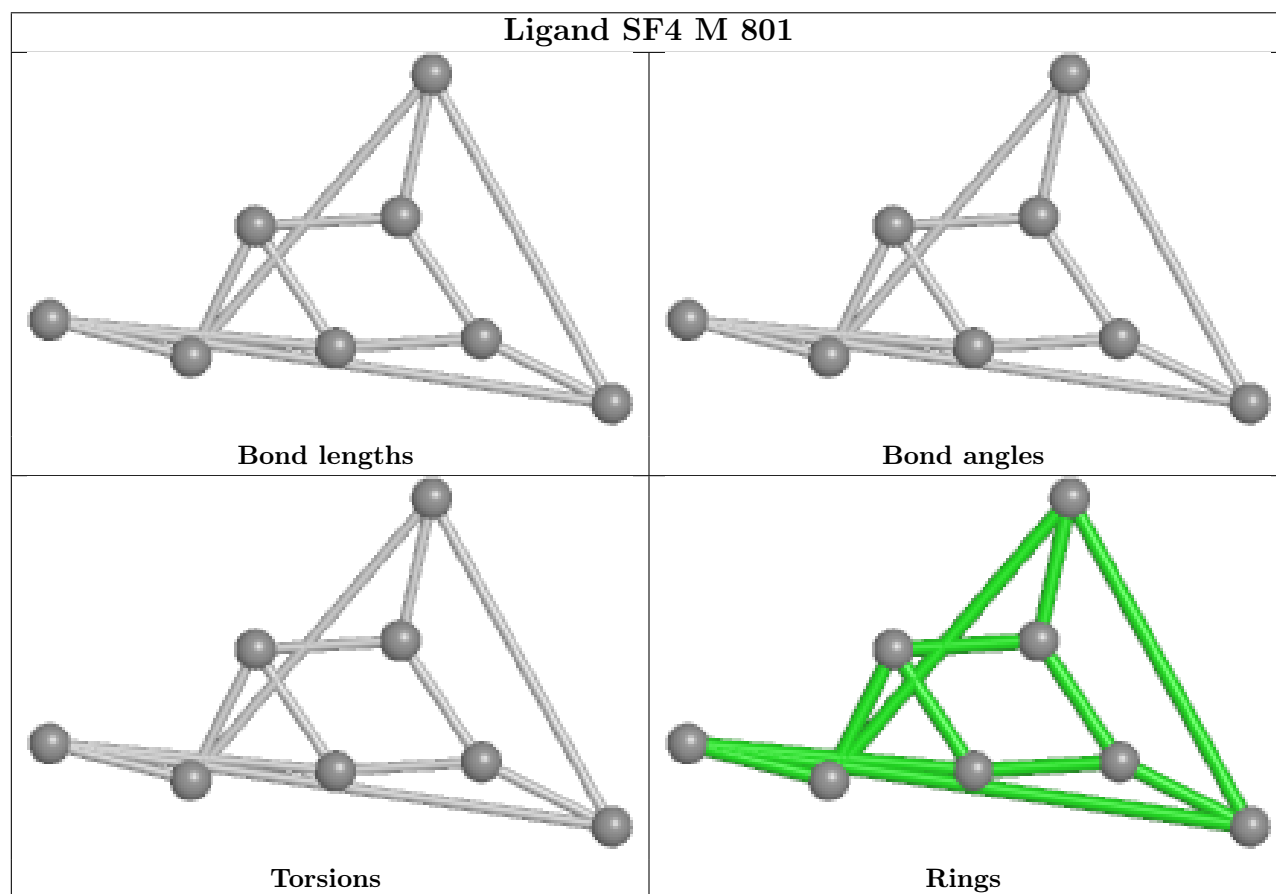
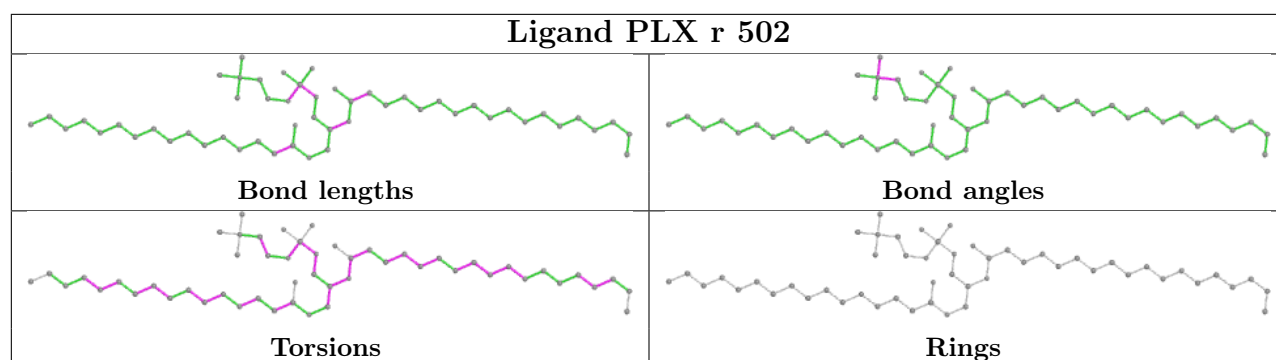


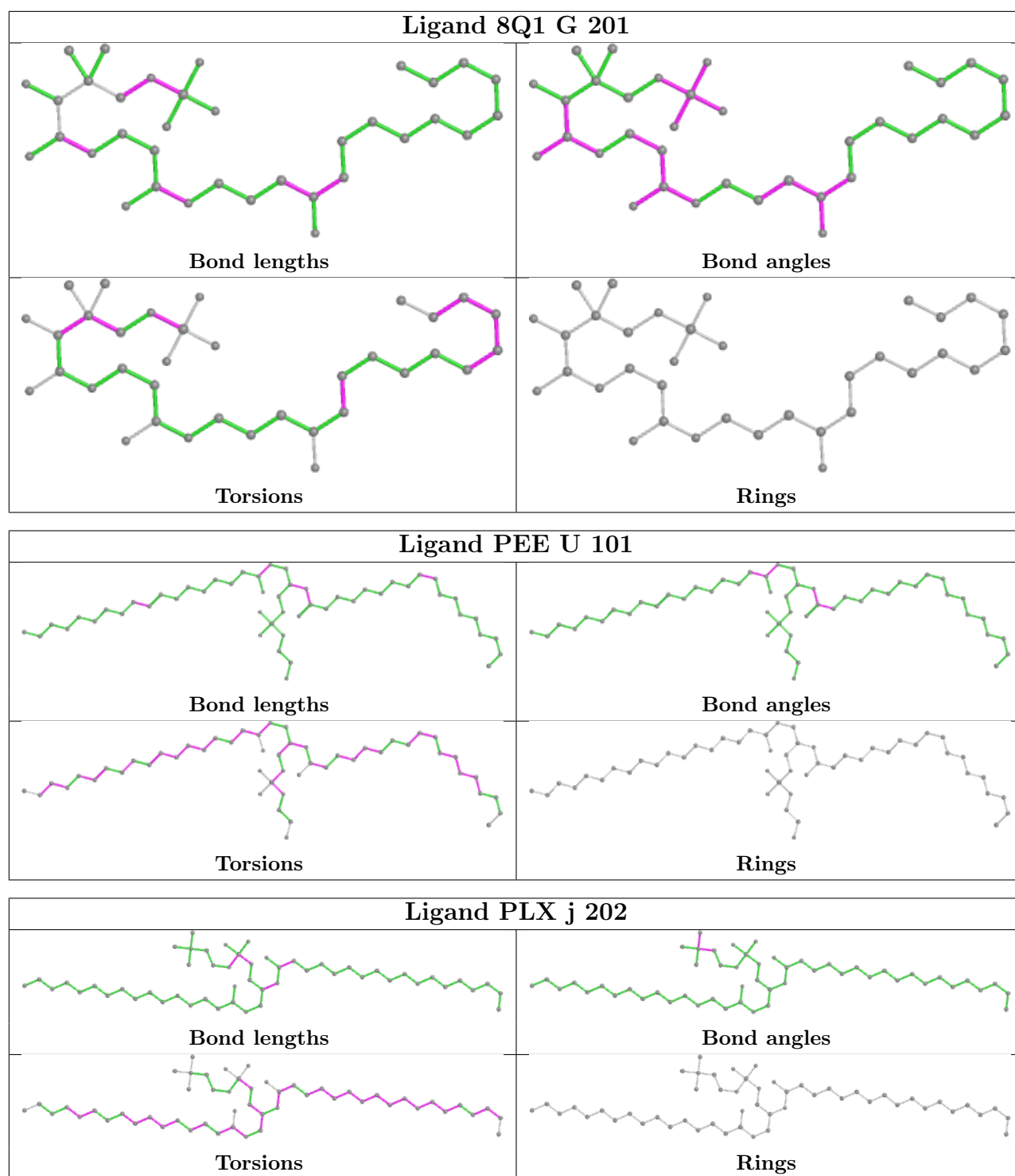


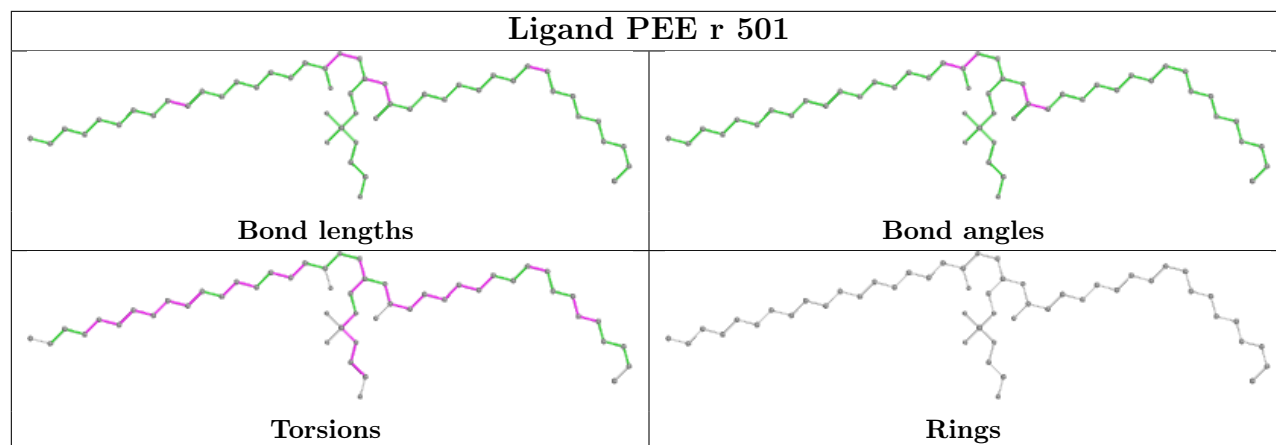












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

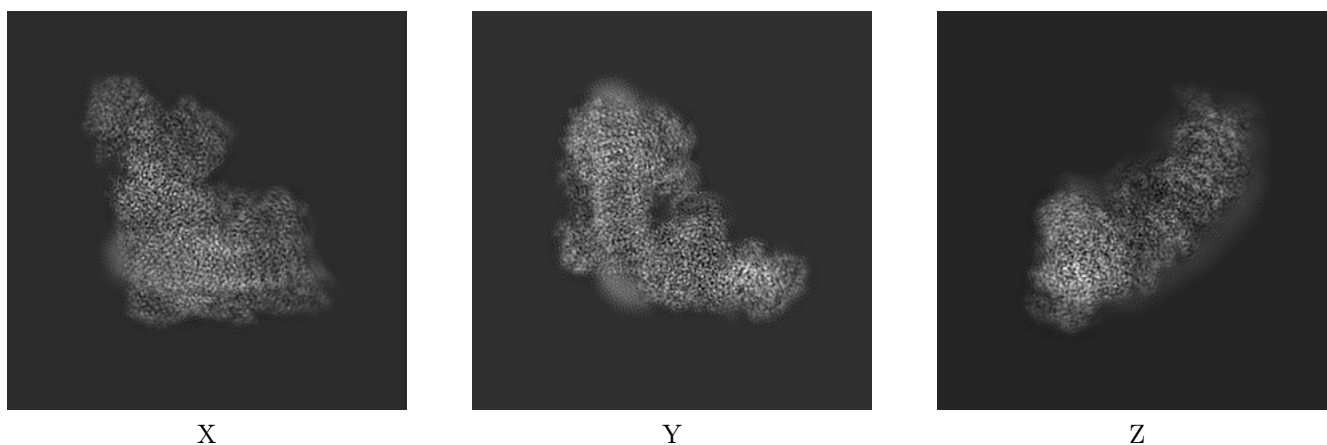
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31651. 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 [i](#)

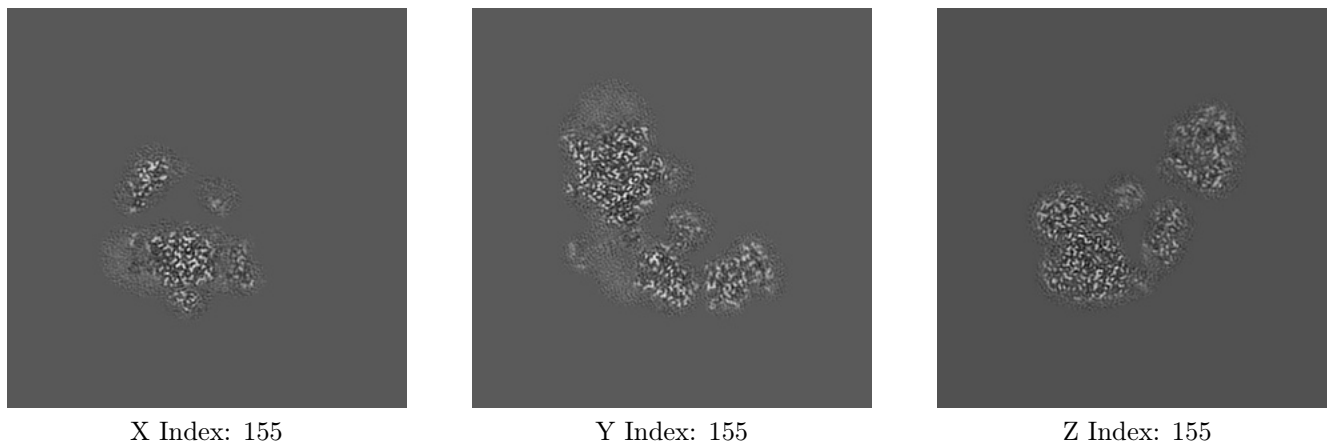
6.1.1 Primary map



The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

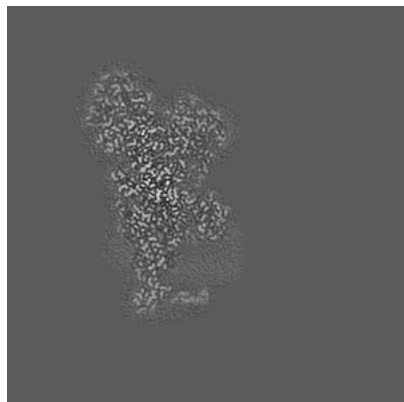
6.2.1 Primary map



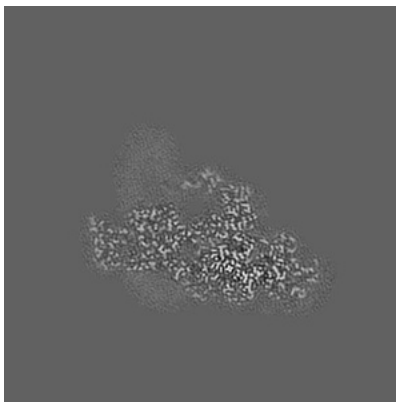
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

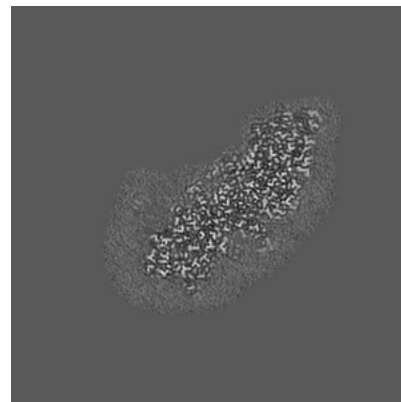
6.3.1 Primary map



X Index: 109



Y Index: 112

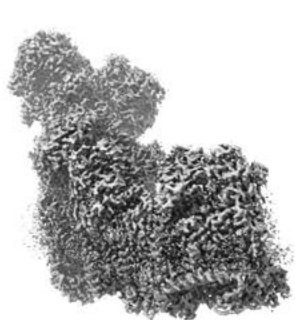


Z Index: 124

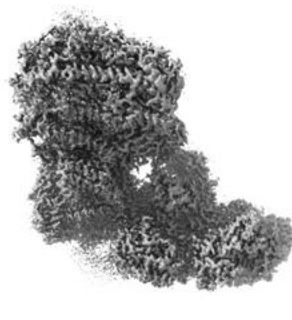
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0271. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

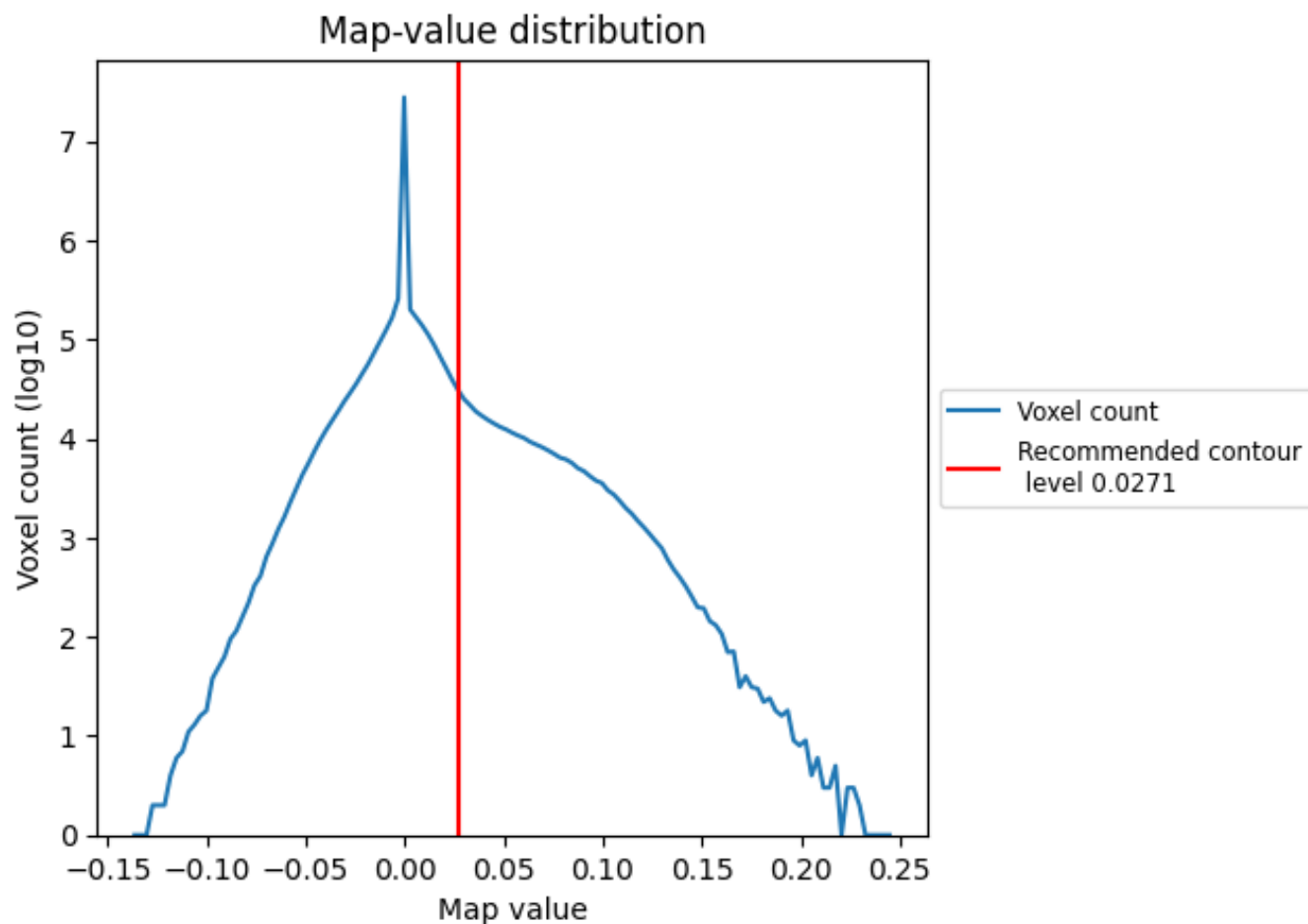
6.5 Mask visualisation

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

7 Map analysis [i](#)

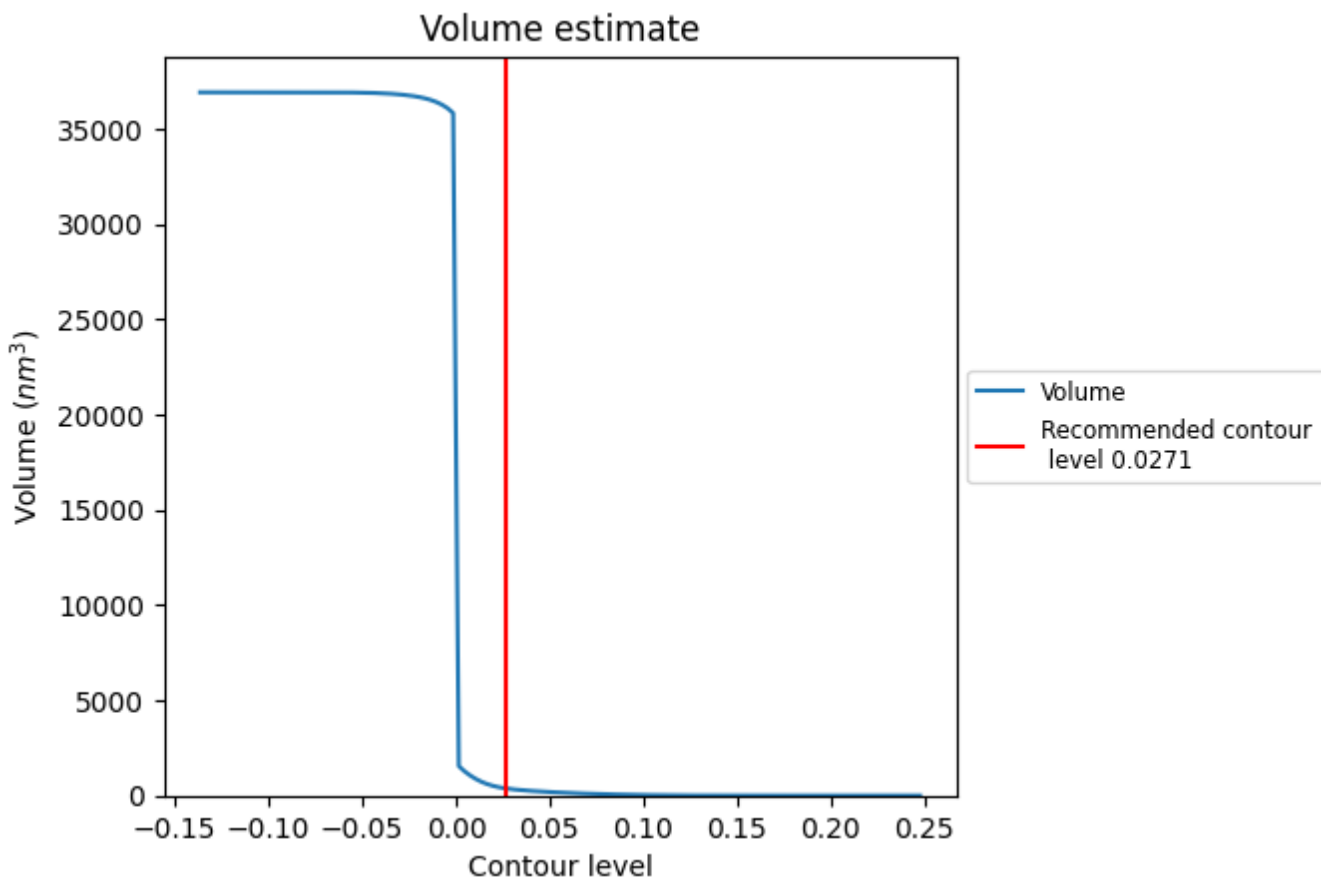
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

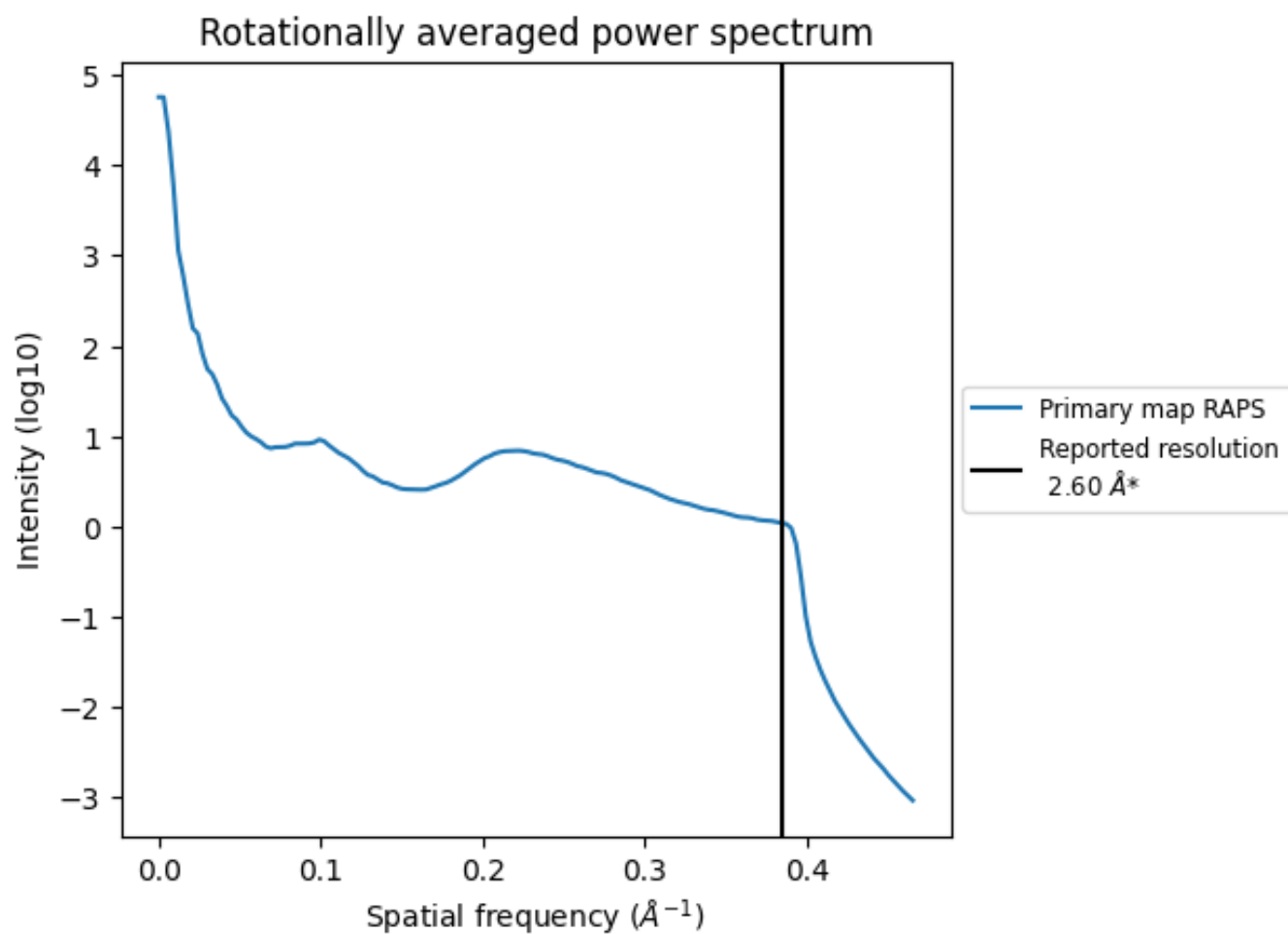
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 371 nm^3 ; this corresponds to an approximate mass of 335 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

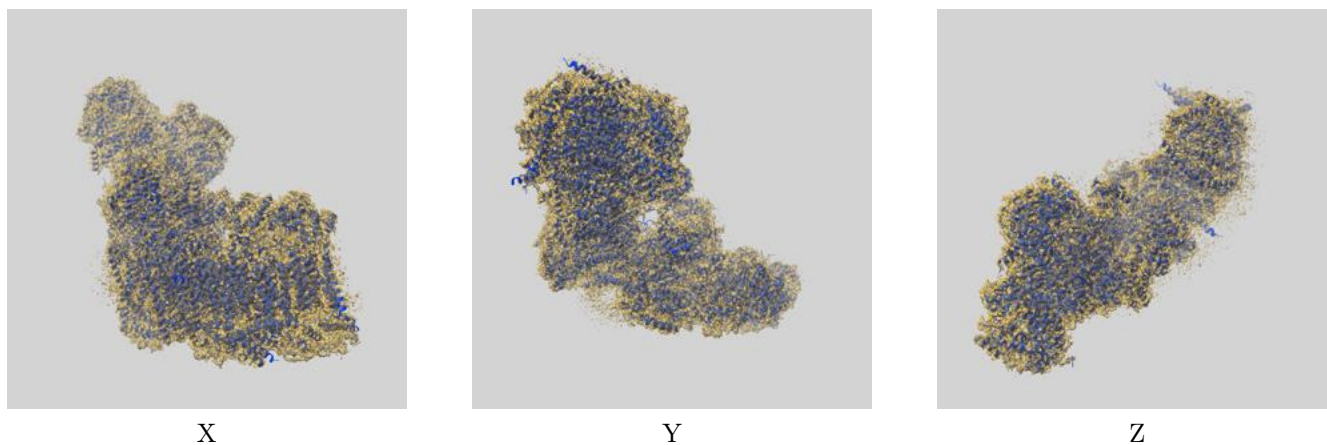
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

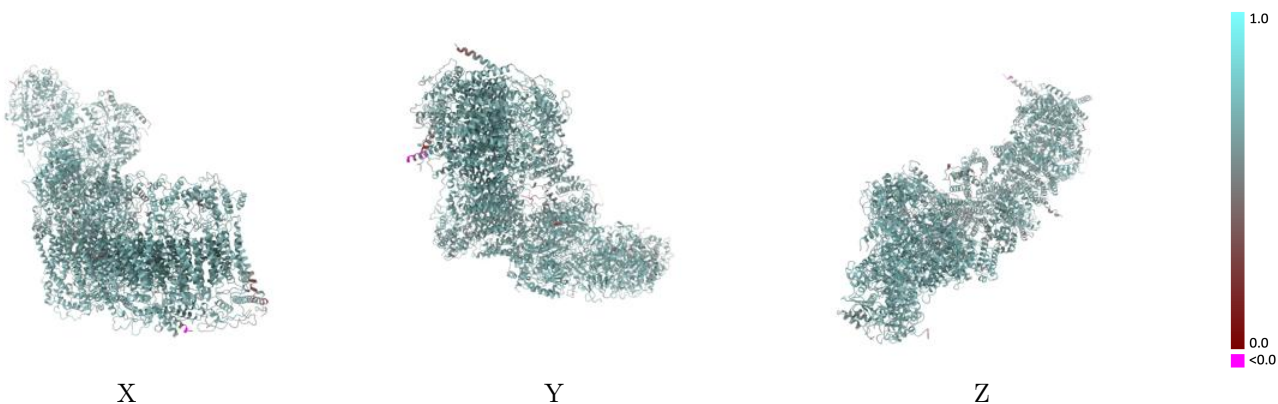
This section contains information regarding the fit between EMDB map EMD-31651 and PDB model 7V33. Per-residue inclusion information can be found in section 3 on page 22.

9.1 Map-model overlay [i](#)



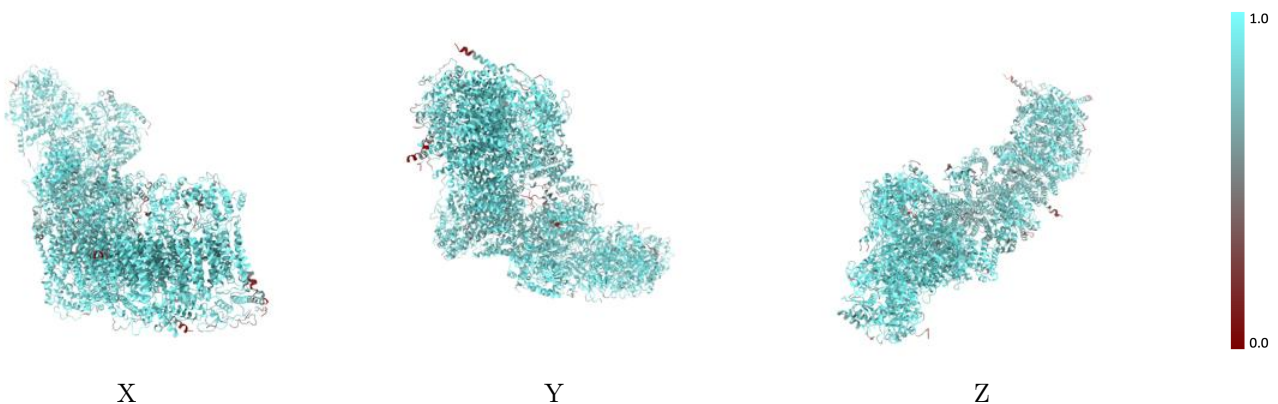
The images above show the 3D surface view of the map at the recommended contour level 0.0271 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



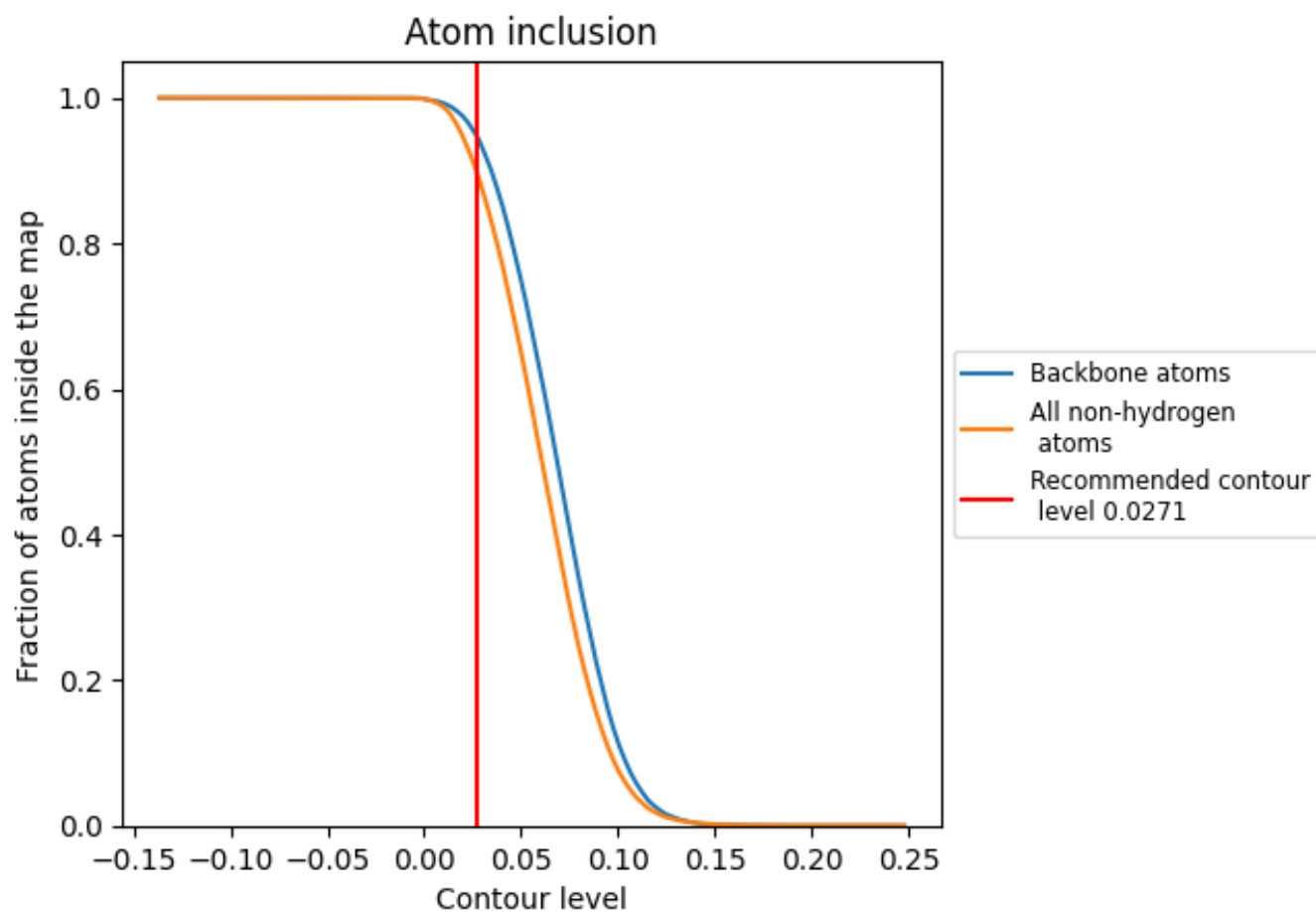
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0271).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary























The table lists the average atom inclusion at the recommended contour level (0.0271) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8986	 0.6490
A	 0.9057	 0.6390
B	 0.9646	 0.6870
C	 0.9602	 0.6870
E	 0.9076	 0.6600
F	 0.8286	 0.5970
G	 0.6925	 0.5290
H	 0.9173	 0.6420
I	 0.8042	 0.6240
J	 0.9202	 0.6570
K	 0.8225	 0.6020
L	 0.9215	 0.6720
M	 0.9308	 0.6570
N	 0.8841	 0.6480
O	 0.8673	 0.6220
P	 0.9681	 0.6890
Q	 0.9610	 0.6850
S	 0.9583	 0.6650
T	 0.8892	 0.6610
U	 0.8721	 0.6430
V	 0.8586	 0.6340
W	 0.8973	 0.6460
X	 0.8083	 0.6030
Y	 0.7733	 0.5930
Z	 0.7360	 0.5720
a	 0.8992	 0.6580
b	 0.8262	 0.6170
c	 0.8600	 0.6320
d	 0.8481	 0.6230
e	 0.8487	 0.6280
f	 0.7507	 0.5920
g	 0.9133	 0.6550
h	 0.8913	 0.6410
i	 0.9447	 0.6770
j	 0.8978	 0.6650



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Chain	Atom inclusion	Q-score
k	 0.9402	 0.6740
l	 0.9105	 0.6560
m	 0.8497	 0.6310
n	 0.7500	 0.5980
o	 0.8255	 0.6290
p	 0.8734	 0.6350
r	 0.9530	 0.6750
s	 0.9613	 0.6780
u	 0.9036	 0.6500
v	 0.7463	 0.5730
w	 0.8638	 0.6270