



Full wwPDB EM Validation Report ⓘ

Nov 24, 2024 – 03:35 AM JST

PDB ID : 8IC2
EMDB ID : EMD-35352
Title : Respiratory complex CI:CIII2, type I, PERK -/- mouse under cold temperature
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-02-10
Resolution : 6.30 Å(reported)

This is a Full wwPDB EM Validation 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.dev113
Mogul : 1.8.5 (274361), 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 : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

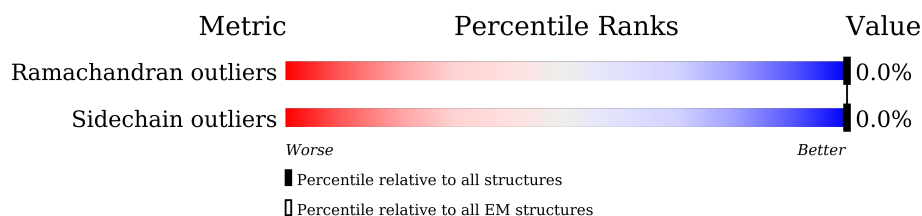
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.30 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	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 ≥ 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	115	 5% 79% 21%
2	B	224	 67% 30%
3	C	263	 75% 25%
4	D	463	 7% 91% 8%
5	E	248	 20% 83% 15%
6	F	464	 24% 89% 9%
7	G	727	 13% 92% 6%
8	H	318	 98%
9	I	212	 80% 18%

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Mol	Chain	Length	Quality of chain
10	J	172	
11	K	98	
12	L	607	
13	M	459	
14	N	345	
15	O	355	
16	P	377	
17	Q	175	
18	R	116	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	131	
23	X	172	
24	Y	143	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	
29	d	120	
30	e	106	
31	f	57	
32	g	151	
33	h	189	

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Mol	Chain	Length	Quality of chain
34	i	128	
35	j	105	
36	k	104	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	104	
45	AA	480	
45	Aa	480	
46	AB	453	
46	Ab	453	
47	AC	381	
47	Ac	381	
48	AD	325	
48	Ad	325	
49	AE	274	
49	AI	274	
49	Ae	274	
50	AF	111	
50	Af	111	
51	AG	82	

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Mol	Chain	Length	Quality of chain
51	Ag	82	<div>84%</div> <div>93%7%</div>
52	AH	89	<div>72%</div> <div>70%28%</div>
52	Ah	89	<div>71%</div> <div>71%28%</div>
53	AJ	64	<div>64%</div> <div>64%36%</div>
53	Aj	64	<div>64%</div> <div>64%36%</div>
54	AK	56	<div>77%</div> <div>77%23%</div>
54	Ak	56	<div>79%</div> <div>80%20%</div>

2 Entry composition

There are 70 unique types of molecules in this entry. The entry contains 97017 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-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	91	Total	C	N	O	S	0	0
			737	511	102	118	6		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	156	Total	C	N	O	S	0	0
			1247	796	223	214	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	198	Total	C	N	O	S	0	0
			1641	1060	279	299	3		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	427	Total	C	N	O	S	0	0
			3443	2201	592	626	24		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	210	Total	C	N	O	S	0	0
			1635	1039	275	310	11		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	424	Total	C	N	O	S	0	0
			3273	2062	586	603	22		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	687	Total	C	N	O	S	0	0
			5287	3316	918	1012	41		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	317	Total	C	N	O	S	0	0
			2531	1701	383	425	22		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	173	Total	C	N	O	S	0	0
			1389	875	239	263	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	155	Total	C	N	O	S	0	0
			1178	797	167	199	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	96	Total	C	N	O	S	0	0
			721	468	110	134	9		

- 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
			4798	3181	746	826	45		

- 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
			3630	2407	567	616	40		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	344	Total	C	N	O	S	0	0
			2694	1790	416	451	37		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	318	Total	C	N	O	S	0	0
			2588	1662	426	490	10		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	339	Total	C	N	O	S	0	0
			2720	1759	476	478	7		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	118	Total	C	N	O	S	0	0
			957	608	165	180	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	83	Total	C	N	O	S	0	0
			660	411	120	126	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	83	Total	C	N	O	S	0	0
			667	419	126	119	3		

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	75	Total	C	N	O	S	0	0
			604	388	89	122	5		
20	U	87	Total	C	N	O	S	0	0
			700	450	103	142	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	112	Total	C	N	O	S	0	0
			915	596	152	164	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	114	Total	C	N	O	S	0	0
			970	619	180	165	6		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	169	Total	C	N	O	S	0	0
			1385	882	248	245	10		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	139	Total	C	N	O	S	0	0
			1030	657	174	191	8		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	139	Total	C	N	O	S	0	0
			1152	741	204	199	8		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	67	Total	C	N	O	S	0	0
			548	356	97	91	4		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	79	Total	C	N	O	S	0	0
			620	408	98	110	4		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	47	Total	C	N	O	S	0	0
			389	255	67	66	1		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	120	Total	C	N	O	S	0	0
			996	651	171	165	9		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	103	Total	C	N	O	S	0	0
			859	544	157	150	8		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	51	Total	C	N	O	S	0	0
			439	284	79	74	2		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	99	Total	C	N	O	S	0	0
			835	541	134	156	4		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	138	Total	C	N	O	S	0	0
			1162	762	194	203	3		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	91	Total	C	N	O	S	0	0
			765	500	131	131	3		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	67	Total	C	N	O	S	0	0
			574	376	95	102	1		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	69	Total	C	N	O	S	0	0
			560	370	97	91	2		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	155	Total	C	N	O	S	0	0
			1304	840	218	235	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	126	Total	C	N	O	S	0	0
			1050	676	189	185			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	177	Total	C	N	O	S	0	0
			1534	981	275	267	11		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	121	Total	C	N	O	S	0	0
			1038	654	196	180	8		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	167	Total	C	N	O	S	0	0
			1415	891	254	262	8		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	122	Total	C	N	O	S	0	0
			1020	655	180	181	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	51	Total	C	N	O	S	0	0
			418	266	78	73	1		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	s	29	Total	C	N	O	0	0
			238	151	39	48		

- Molecule 45 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AA	403	Total	C	N	O	S	0	0
			3157	1971	562	608	16		

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Mol	Chain	Residues	Atoms					AltConf	Trace
45	Aa	400	Total	C	N	O	S	0	0
			3131	1957	554	604	16		

- Molecule 46 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AB	413	Total	C	N	O	S	0	0
			3097	1949	542	597	9		
46	Ab	417	Total	C	N	O	S	0	0
			3128	1965	550	604	9		

- Molecule 47 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	AC	373	Total	C	N	O	S	0	0
			2988	2018	461	489	20		
47	Ac	369	Total	C	N	O	S	0	0
			2956	1995	457	484	20		

- Molecule 48 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AD	238	Total	C	N	O	S	0	0
			1896	1211	326	345	14		
48	Ad	240	Total	C	N	O	S	0	0
			1912	1221	328	349	14		

- Molecule 49 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AE	181	Total	C	N	O	S	0	0
			1397	885	243	263	6		
49	AI	48	Total	C	N	O		0	0
			328	210	61	57			
49	Ae	186	Total	C	N	O	S	0	0
			1436	907	251	271	7		

- Molecule 50 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	AF	97	Total	C	N	O	S	0	0
			855	546	152	154	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
50	Af	98	Total	C	N	O	S	0	0
			864	552	154	155	3		

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AG	75	Total	C	N	O	S	0	0
			634	413	115	105	1		
51	Ag	76	Total	C	N	O	S	0	0
			643	418	116	108	1		

- Molecule 52 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AH	64	Total	C	N	O	S	0	0
			527	321	98	103	5		
52	Ah	64	Total	C	N	O	S	0	0
			527	321	98	103	5		

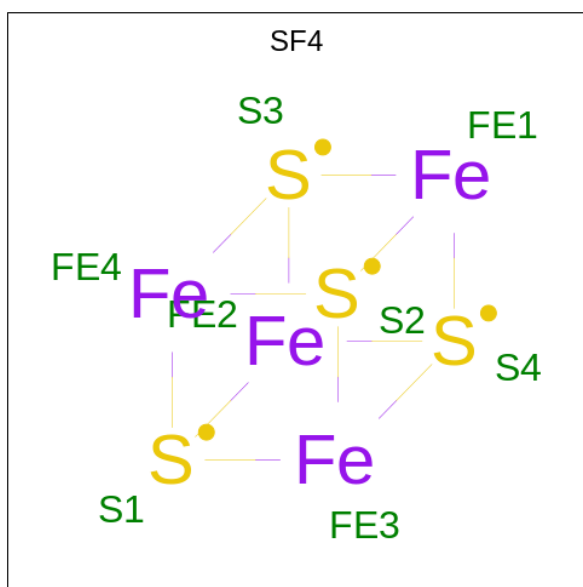
- Molecule 53 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AJ	41	Total	C	N	O		0	0
			332	216	57	59			
53	Aj	41	Total	C	N	O		0	0
			332	216	57	59			

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 10.

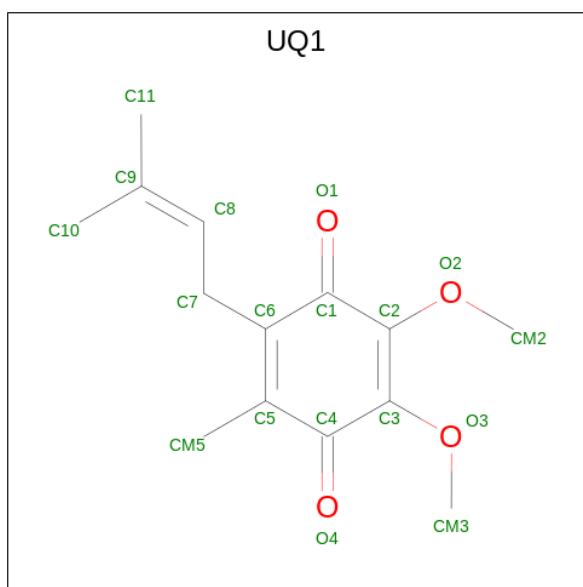
Mol	Chain	Residues	Atoms					AltConf	Trace
54	AK	43	Total	C	N	O	S	0	0
			355	235	64	55	1		
54	Ak	45	Total	C	N	O	S	0	0
			365	242	64	58	1		

- Molecule 55 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



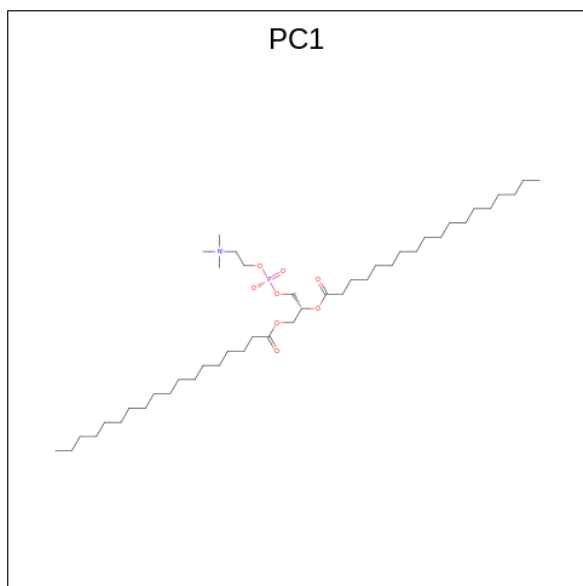
Mol	Chain	Residues	Atoms			AltConf
55	B	1	Total	Fe	S	0
			8	4	4	
55	F	1	Total	Fe	S	0
			8	4	4	
55	G	1	Total	Fe	S	0
			8	4	4	
55	G	1	Total	Fe	S	0
			8	4	4	
55	I	1	Total	Fe	S	0
			8	4	4	
55	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 56 is UBIQUINONE-1 (three-letter code: UQ1) (formula: $C_{14}H_{18}O_4$) (labeled as "Ligand of Interest" by depositor).



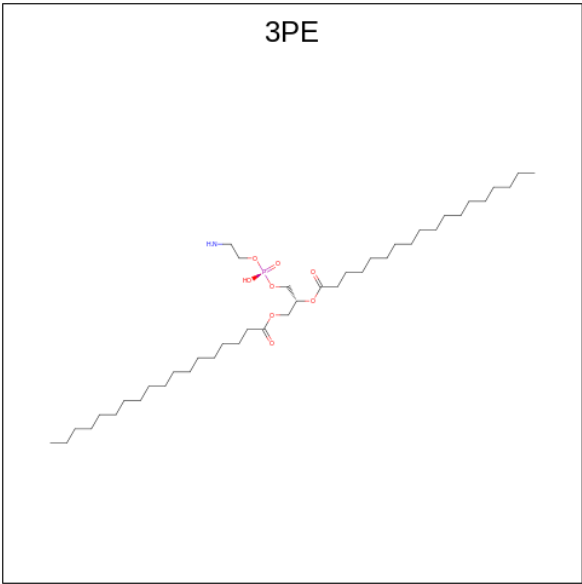
Mol	Chain	Residues	Atoms			AltConf
56	B	1	Total	C	O	0
			18	14	4	

- Molecule 57 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
57	B	1	Total	C	N	O	P	0
			35	25	1	8	1	
57	I	1	Total	C	N	O	P	0
			43	33	1	8	1	

- Molecule 58 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: C₄₁H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



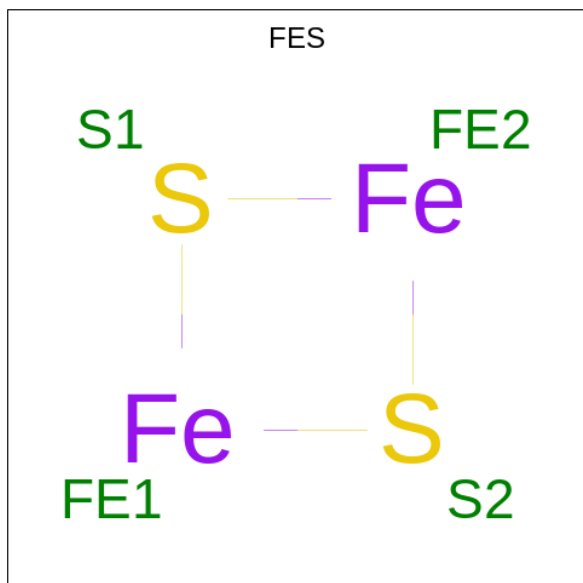
Mol	Chain	Residues	Atoms					AltConf
58	D	1	Total	C	N	O	P	0
			38	28	1	8	1	
58	H	1	Total	C	N	O	P	0
			46	36	1	8	1	
58	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
58	J	1	Total	C	N	O	P	0
			46	36	1	8	1	
58	L	1	Total	C	N	O	P	0
			40	30	1	8	1	
58	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
58	L	1	Total	C	N	O	P	0
			44	34	1	8	1	
58	M	1	Total	C	N	O	P	0
			37	27	1	8	1	
58	M	1	Total	C	N	O	P	0
			49	39	1	8	1	
58	i	1	Total	C	N	O	P	0
			40	30	1	8	1	
58	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
58	Ac	1	Total	C	N	O	P	0
			23	13	1	8	1	

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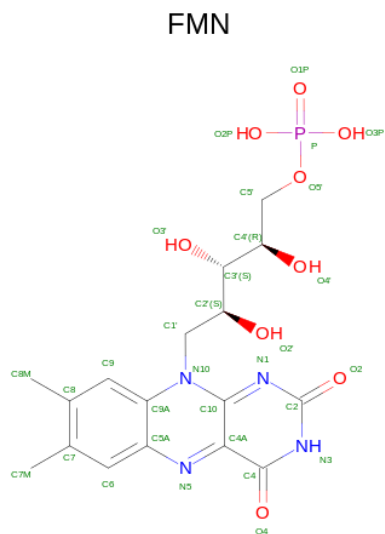
Mol	Chain	Residues	Atoms					AltConf
58	Ac	1	Total	C	N	O	P	0
			35	25	1	8	1	
58	Ag	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 59 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



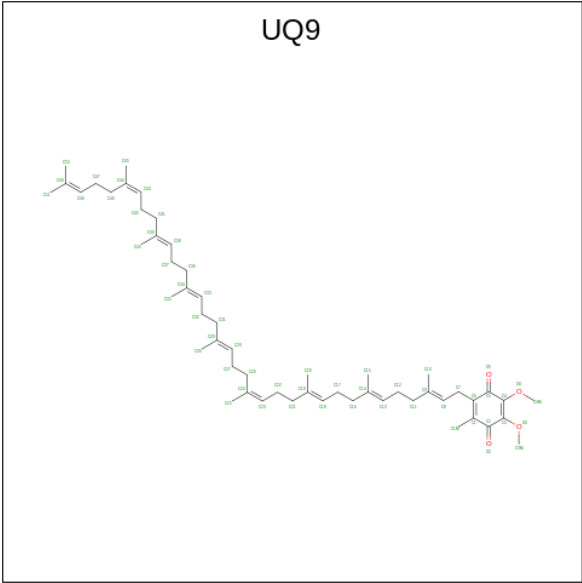
Mol	Chain	Residues	Atoms			AltConf
59	E	1	Total	Fe	S	0
			4	2	2	
59	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 60 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$) (labeled as "Ligand of Interest" by depositor).



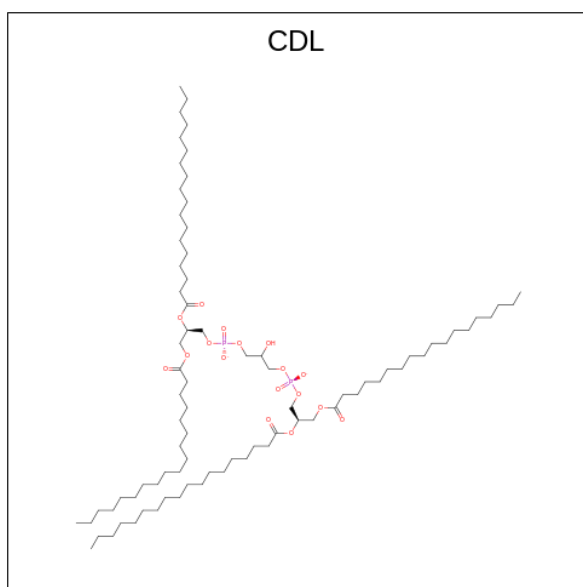
Mol	Chain	Residues	Atoms					AltConf
60	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 61 is Ubiquinone-9 (three-letter code: UQ9) (formula: C₅₄H₈₂O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
61	H	1	Total	C	O	0
			35	31	4	

- Molecule 62 is CARDIOLIPIN (three-letter code: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).

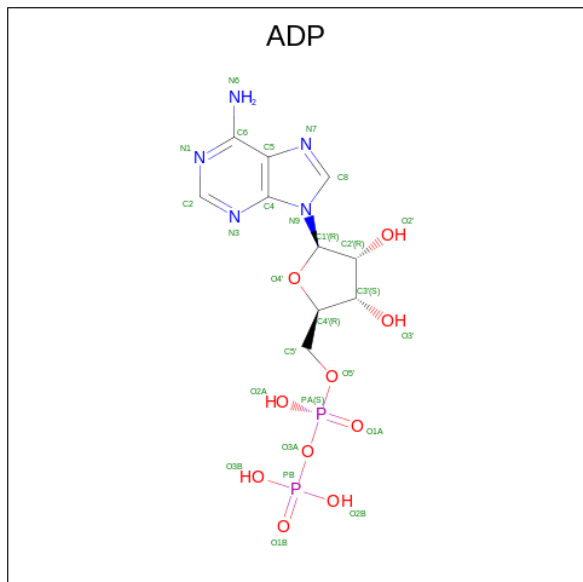


Mol	Chain	Residues	Atoms				AltConf
62	L	1	Total	C	O	P	0
			73	54	17	2	
62	M	1	Total	C	O	P	0
			82	63	17	2	
62	Y	1	Total	C	O	P	0
			71	52	17	2	
62	d	1	Total	C	O	P	0
			65	46	17	2	
62	h	1	Total	C	O	P	0
			68	49	17	2	
62	q	1	Total	C	O	P	0
			57	38	17	2	
62	Aa	1	Total	C	O	P	0
			46	27	17	2	
62	Ag	1	Total	C	O	P	0
			42	23	17	2	
62	Ag	1	Total	C	O	P	0
			56	37	17	2	

- Molecule 63 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

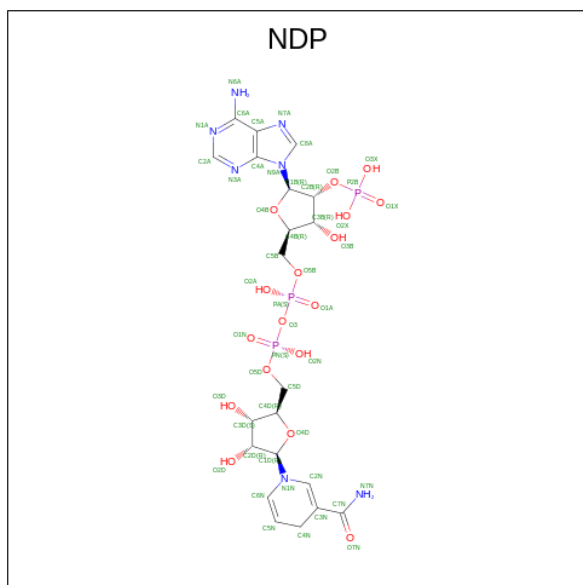
Mol	Chain	Residues	Atoms		AltConf
63	L	1	Total	Zn	0
			1	1	
63	R	1	Total	Zn	0
			1	1	

- Molecule 64 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



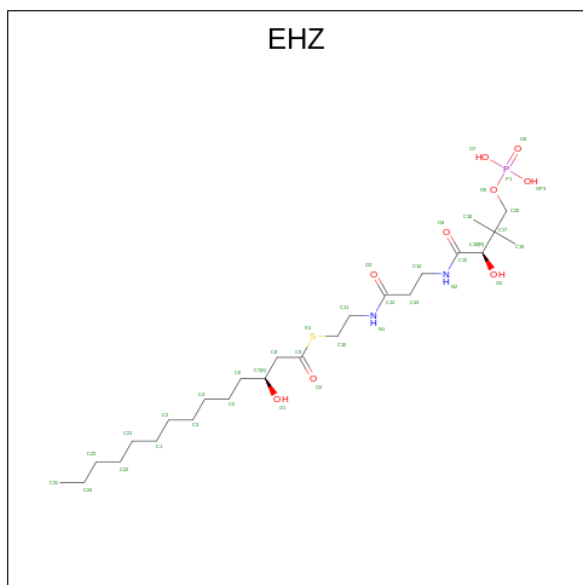
Mol	Chain	Residues	Atoms					AltConf
64	O	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 65 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



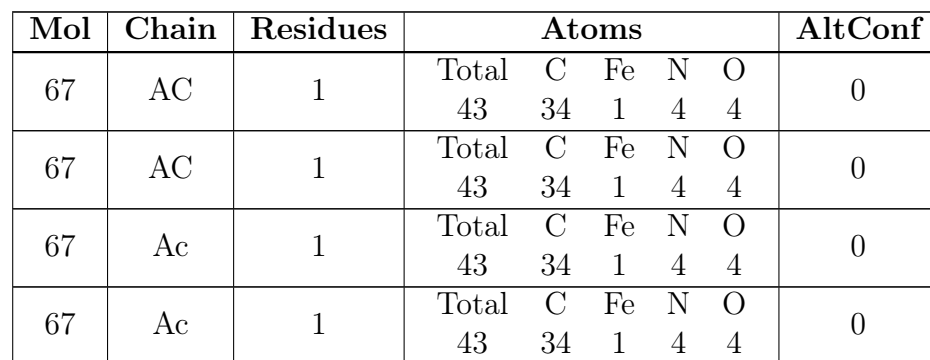
Mol	Chain	Residues	Atoms					AltConf
65	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 66 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: C₂₅H₄₉N₂O₉PS) (labeled as "Ligand of Interest" by depositor).

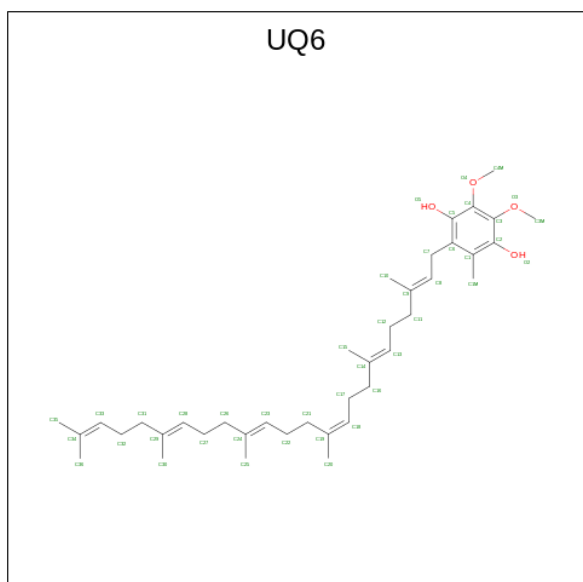


Mol	Chain	Residues	Atoms						AltConf
66	W	1	Total	C	N	O	P	S	0
			32	19	2	9	1	1	
66	n	1	Total	C	N	O	P	S	0
			32	19	2	9	1	1	

- Molecule 67 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄) (labeled as "Ligand of Interest" by depositor).

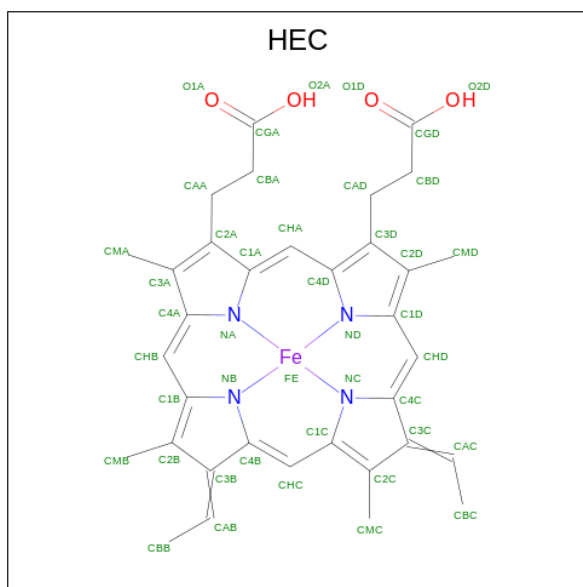


- Molecule 68 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXAENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (three-letter code: UQ6) (formula: C₃₉H₆₀O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
68	AC	1	Total 28	C 24	O 4	0
68	Ac	1	Total 23	C 19	O 4	0

- Molecule 69 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$) (labeled as "Ligand of Interest" by depositor).



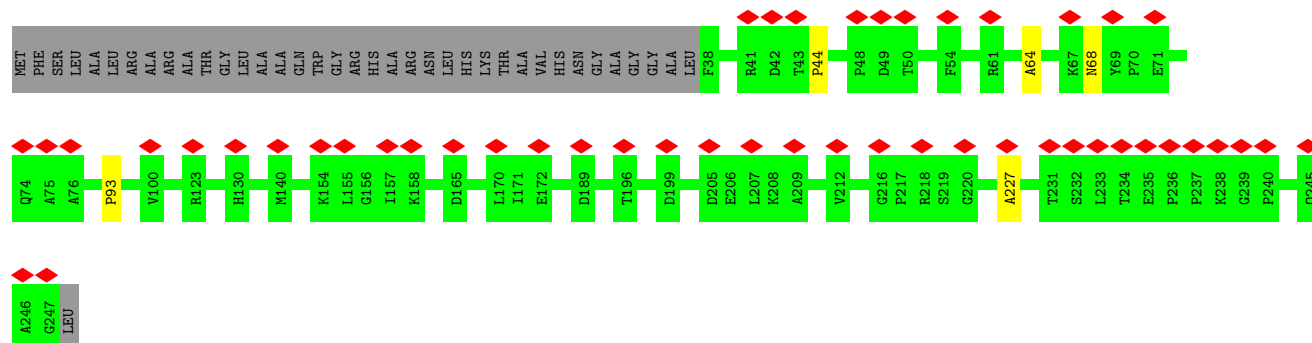
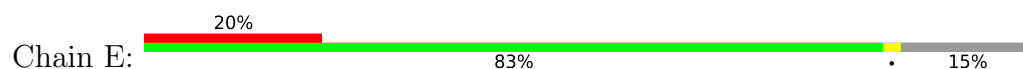
Mol	Chain	Residues	Atoms					AltConf
69	AD	1	Total 43	C 34	Fe 1	N 4	O 4	0
69	Ad	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 70 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).

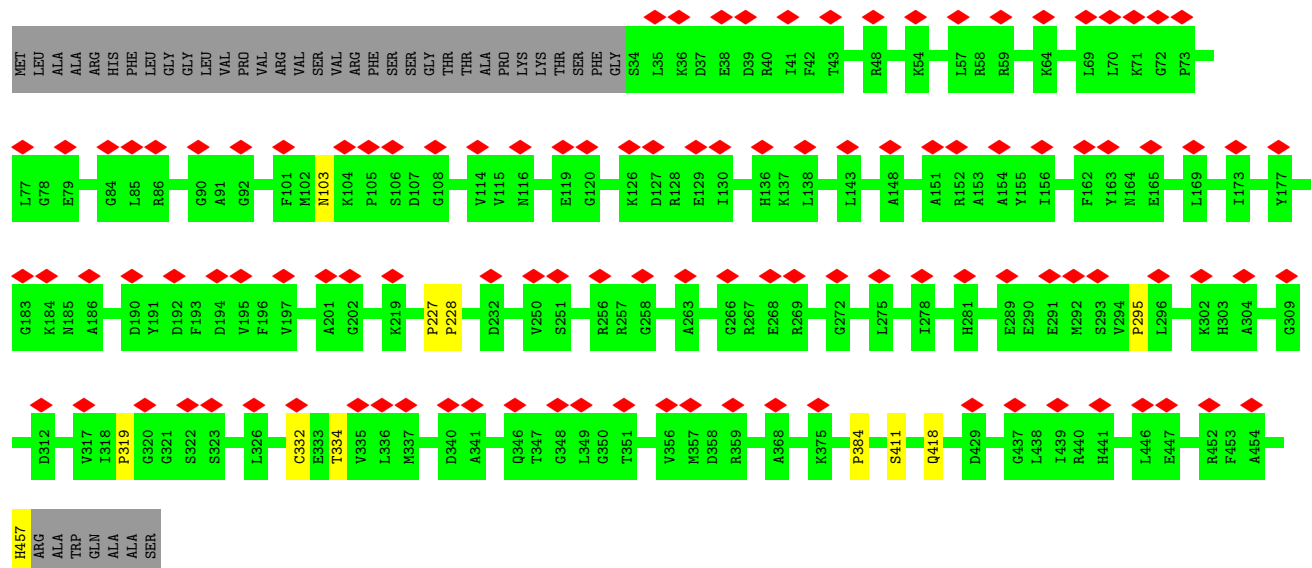
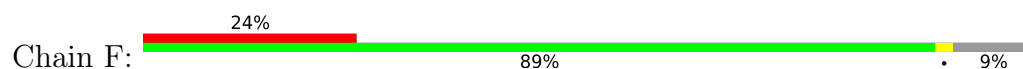




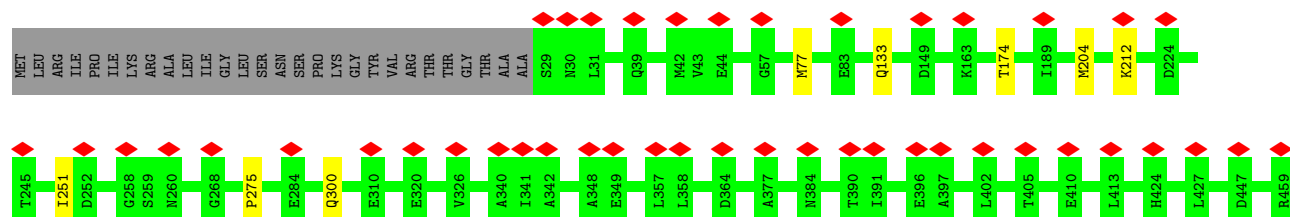
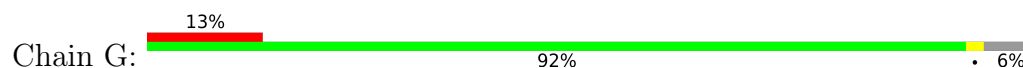
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

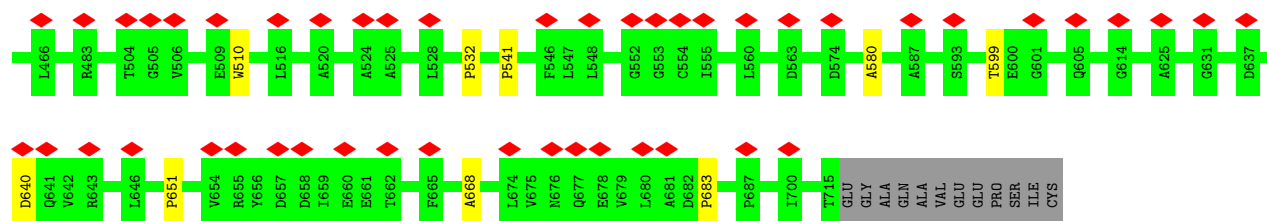


- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



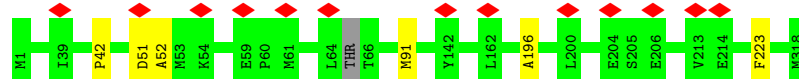
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial





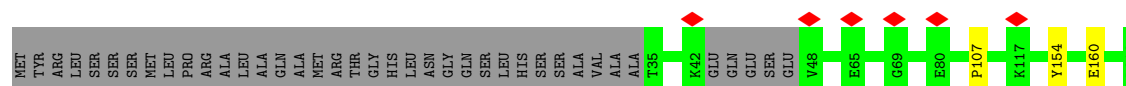
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H: 98%



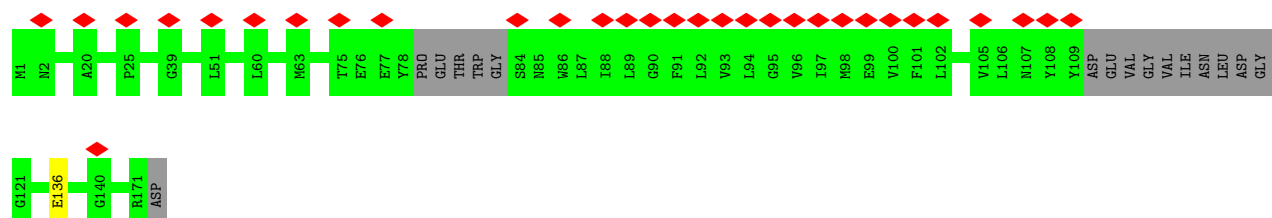
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I: 80% 18%



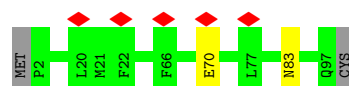
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J: 18% 90% 10%



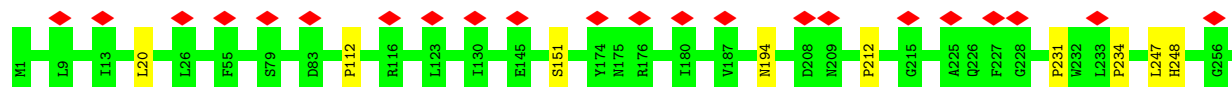
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

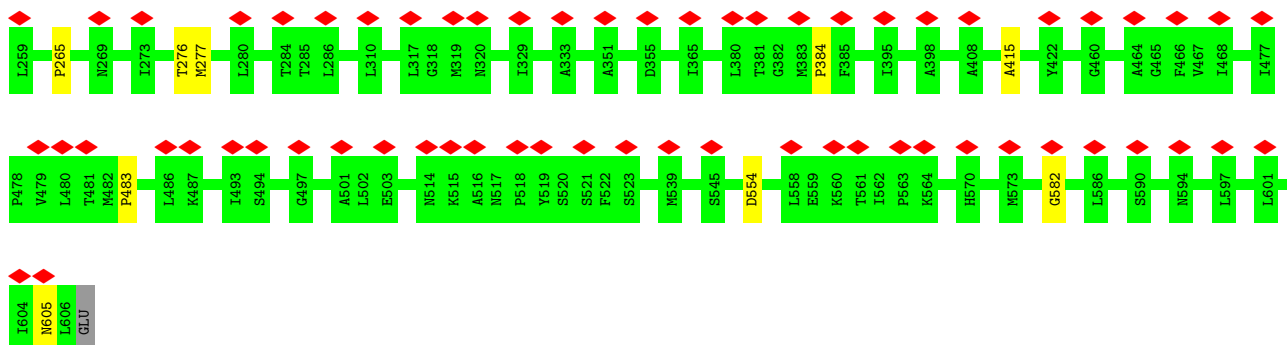
Chain K: 5% 96%



- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

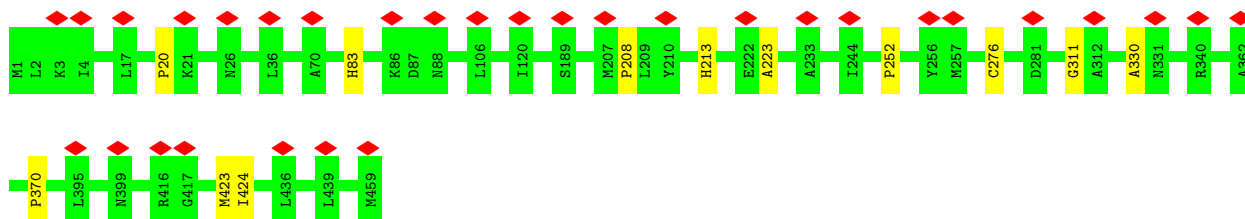
Chain L: 14% 97%





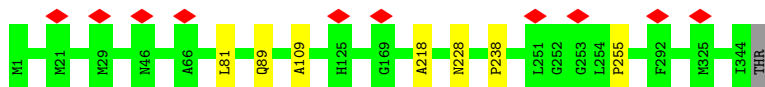
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M: 7% 97% .



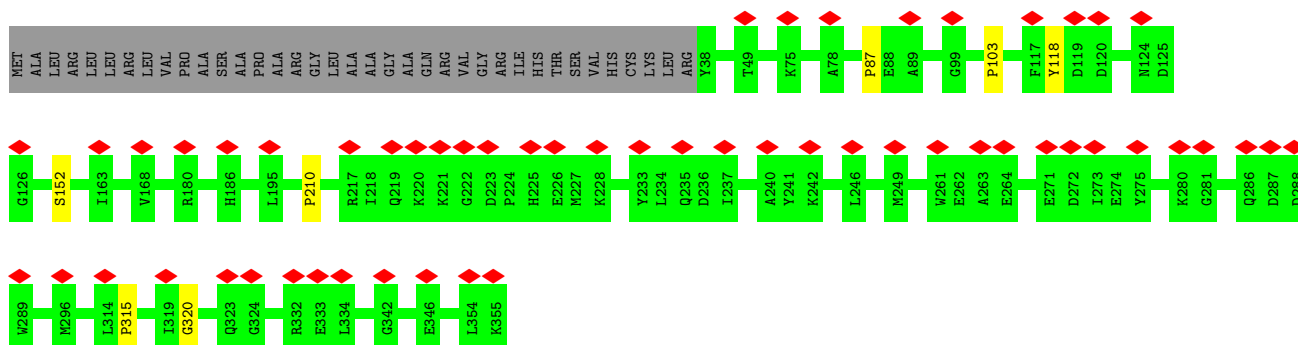
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N: 98% .



- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

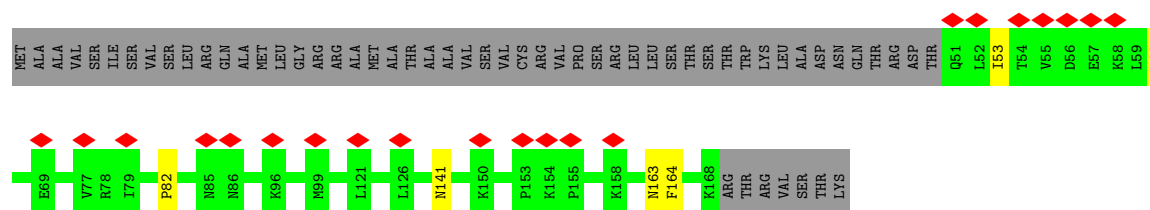
Chain O: 16% 88% 10% .



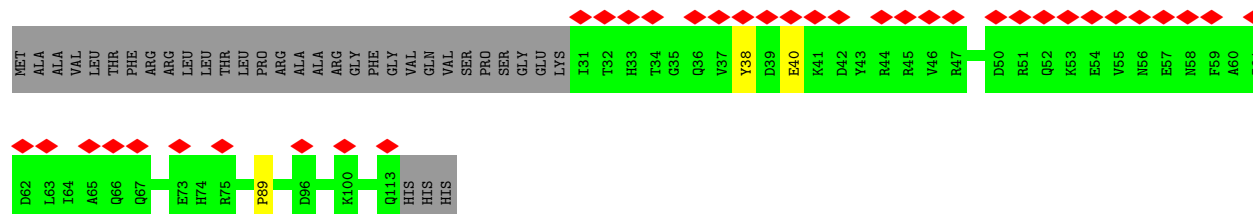
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P: 18% 88% 10% .

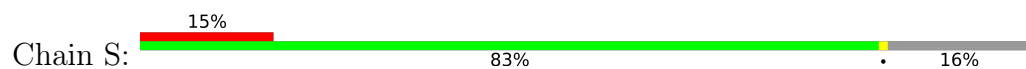
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



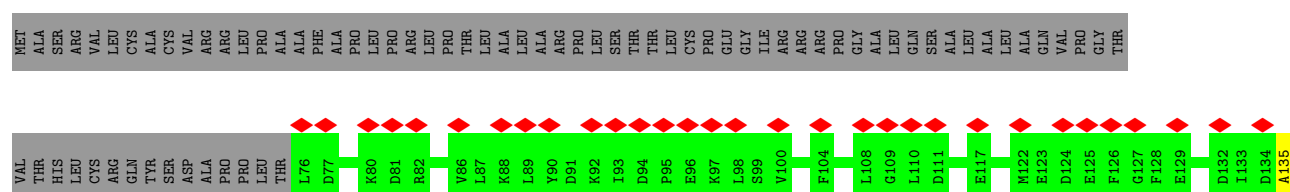
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

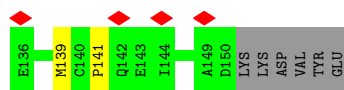


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

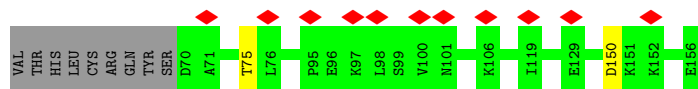


- Molecule 20: Acyl carrier protein, mitochondrial

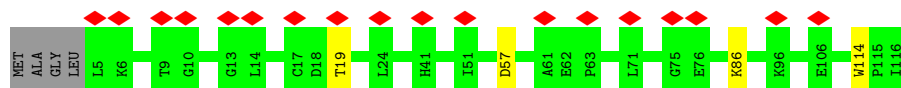




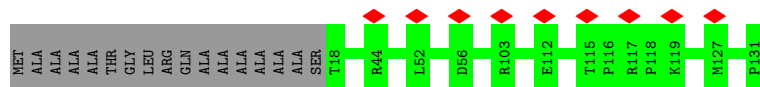
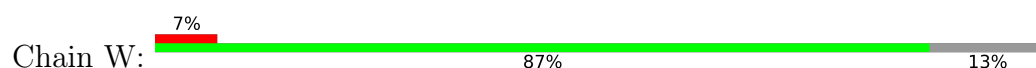
- Molecule 20: Acyl carrier protein, mitochondrial



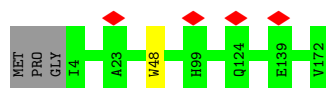
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



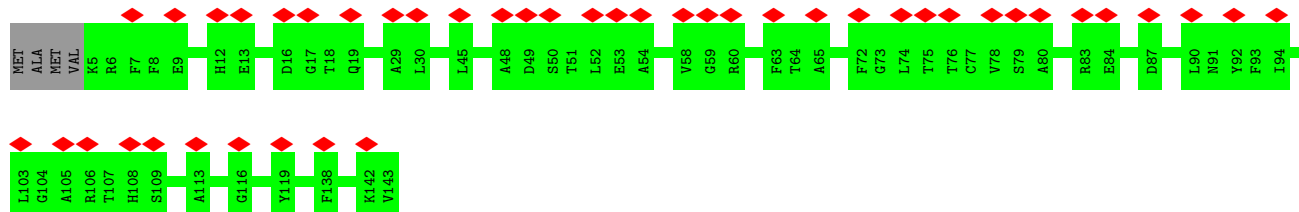
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



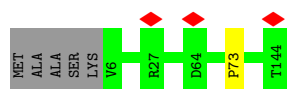
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



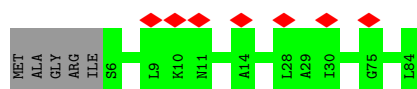
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



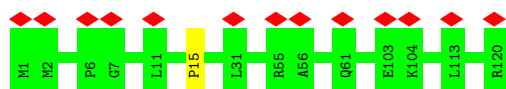
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



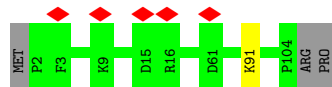
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



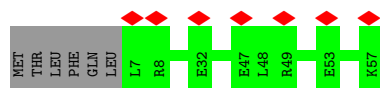
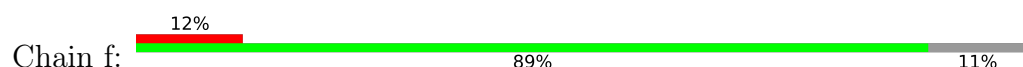
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



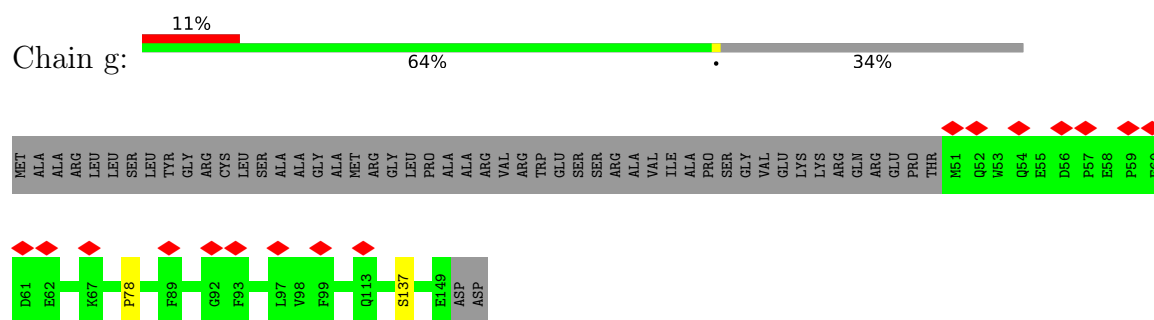
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



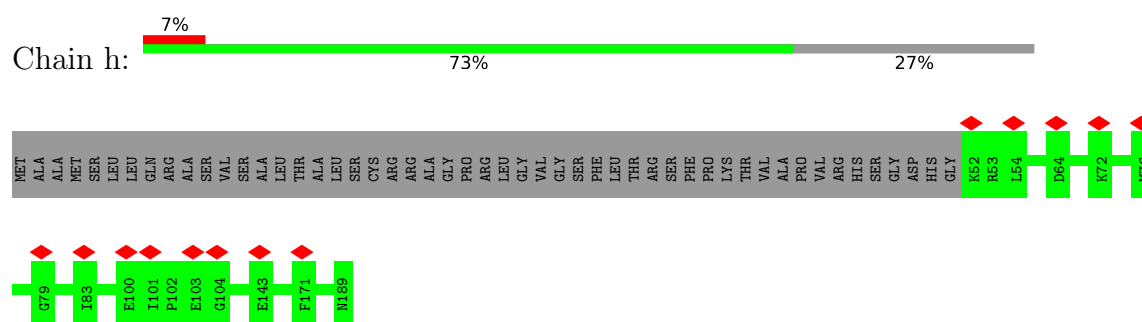
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



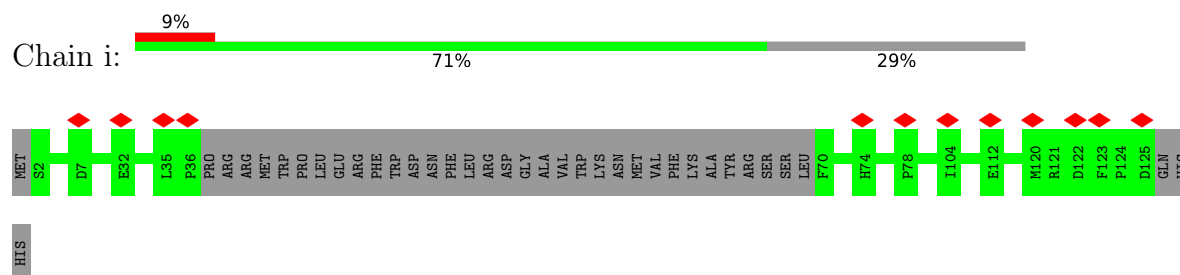
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



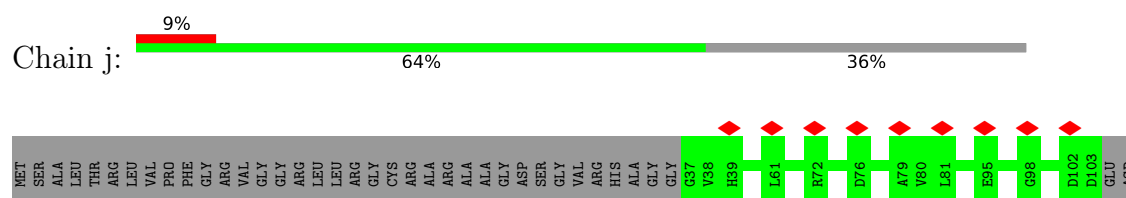
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



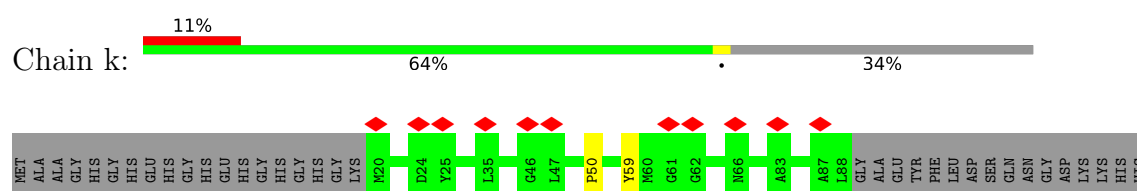
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



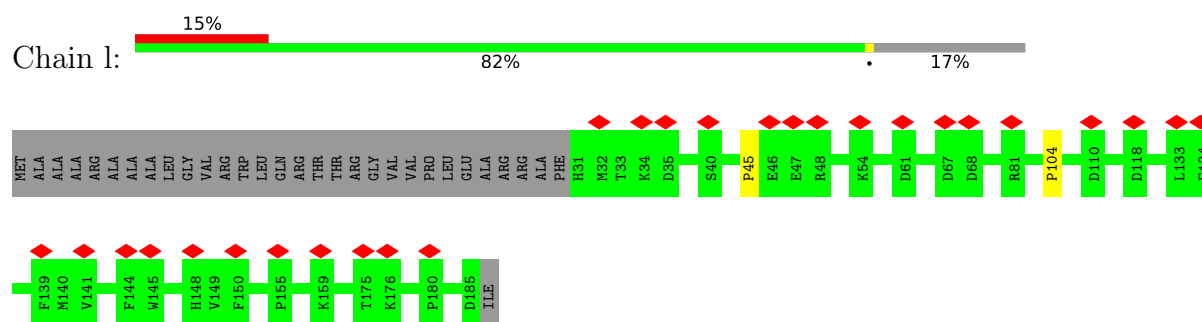
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



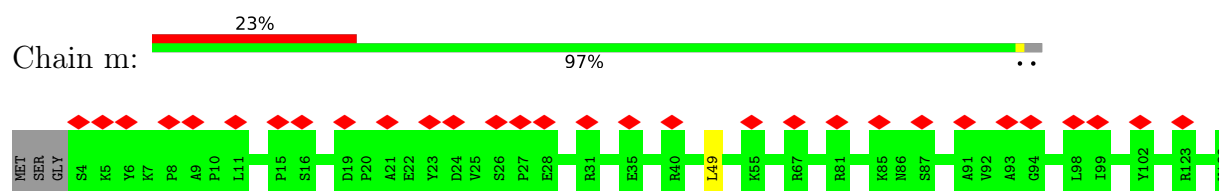
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



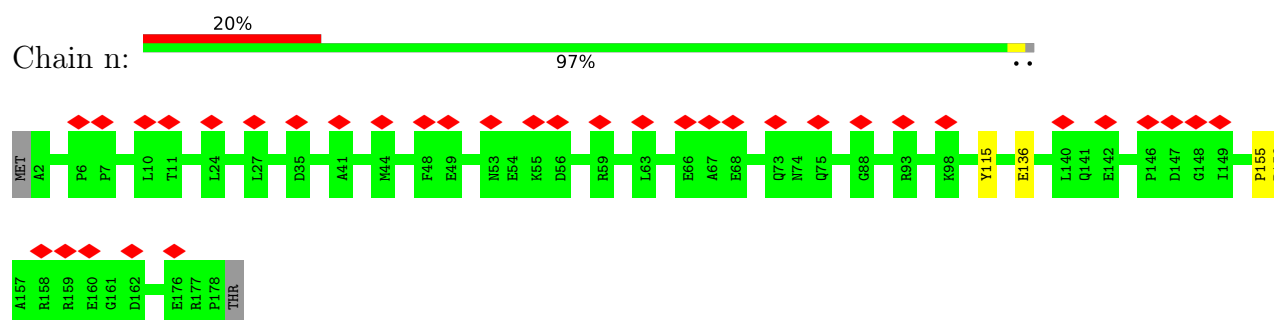
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



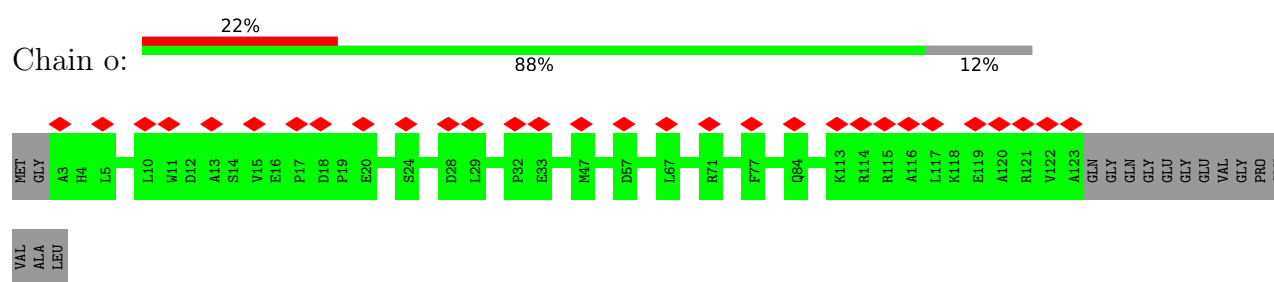
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

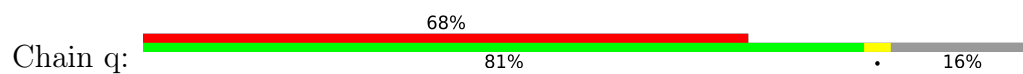


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

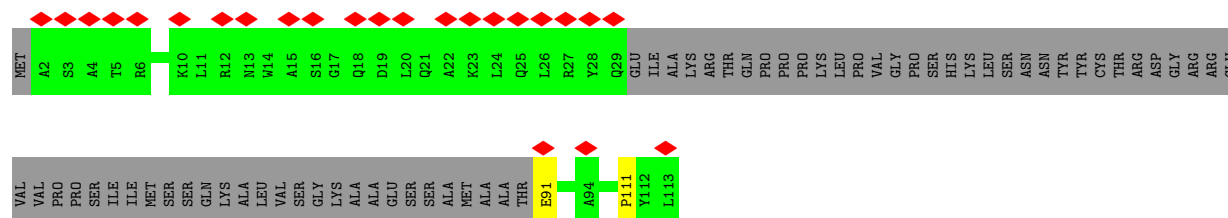
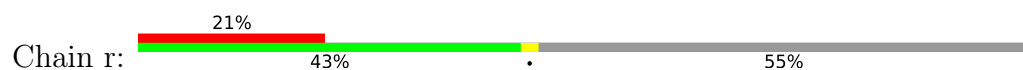


- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

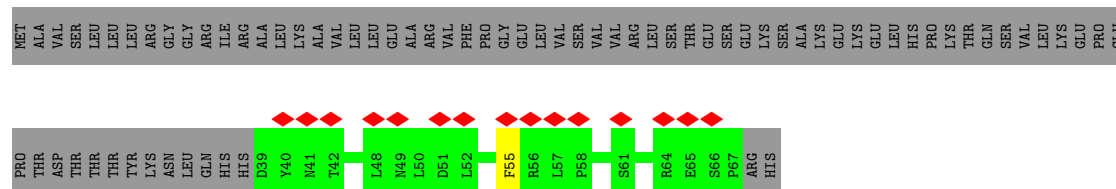




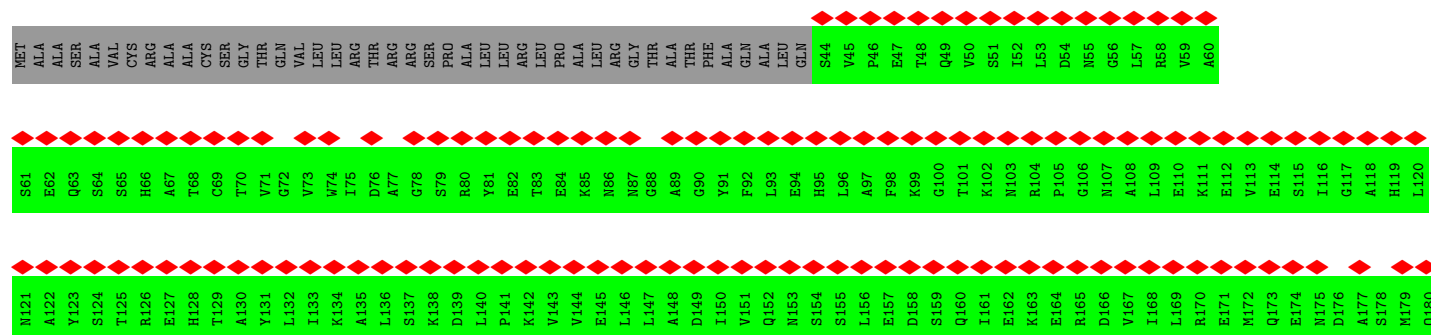
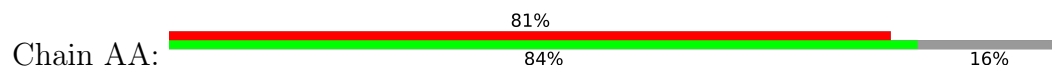
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

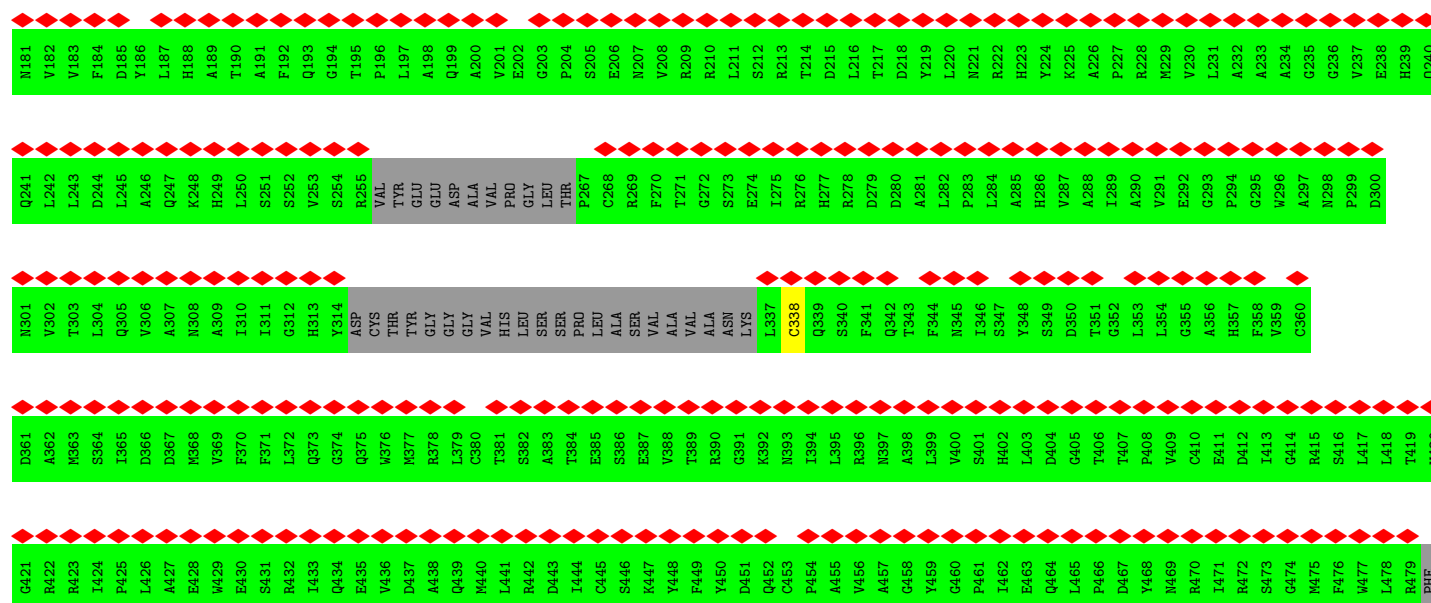


- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



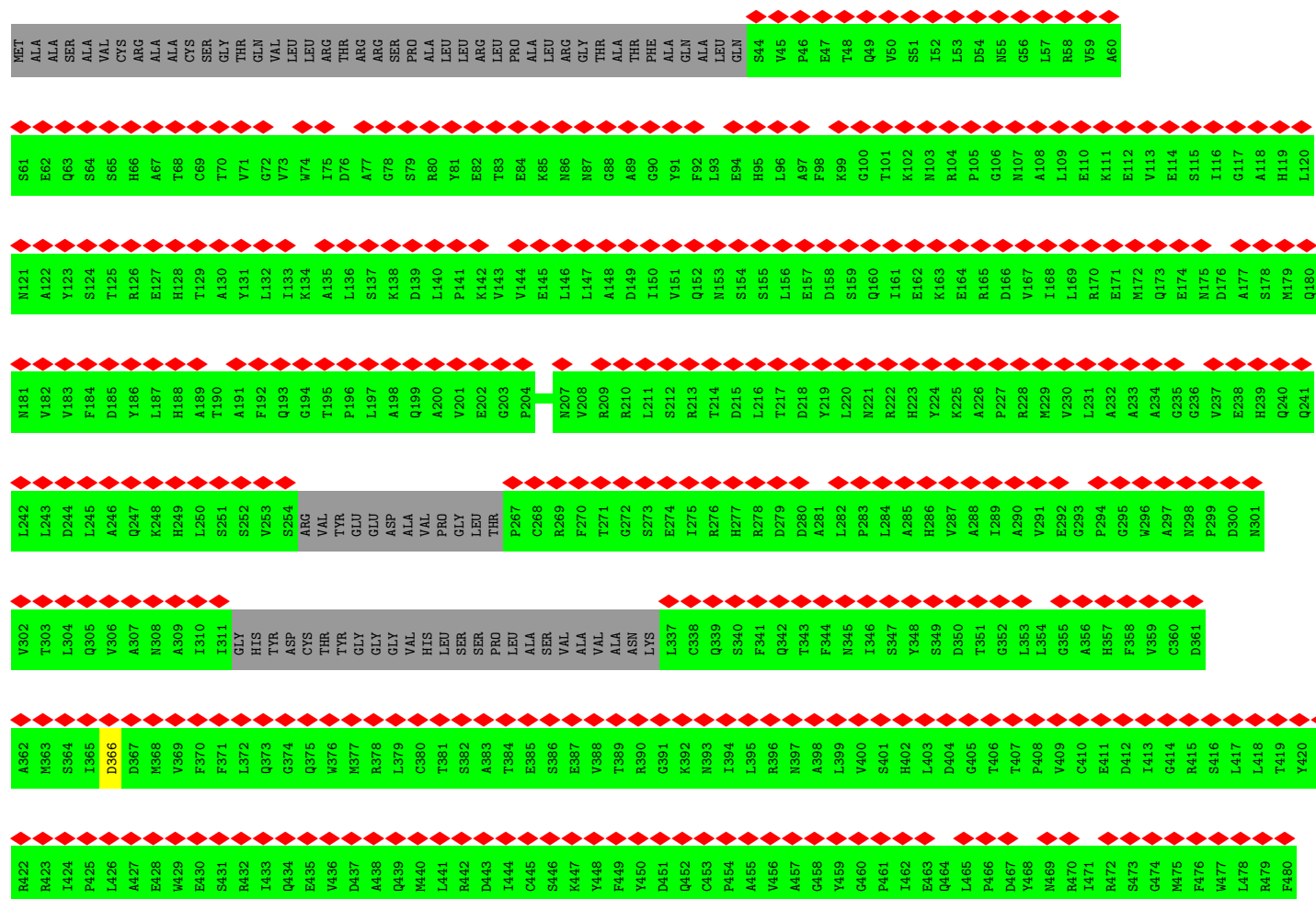
- Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial





• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain Aa:



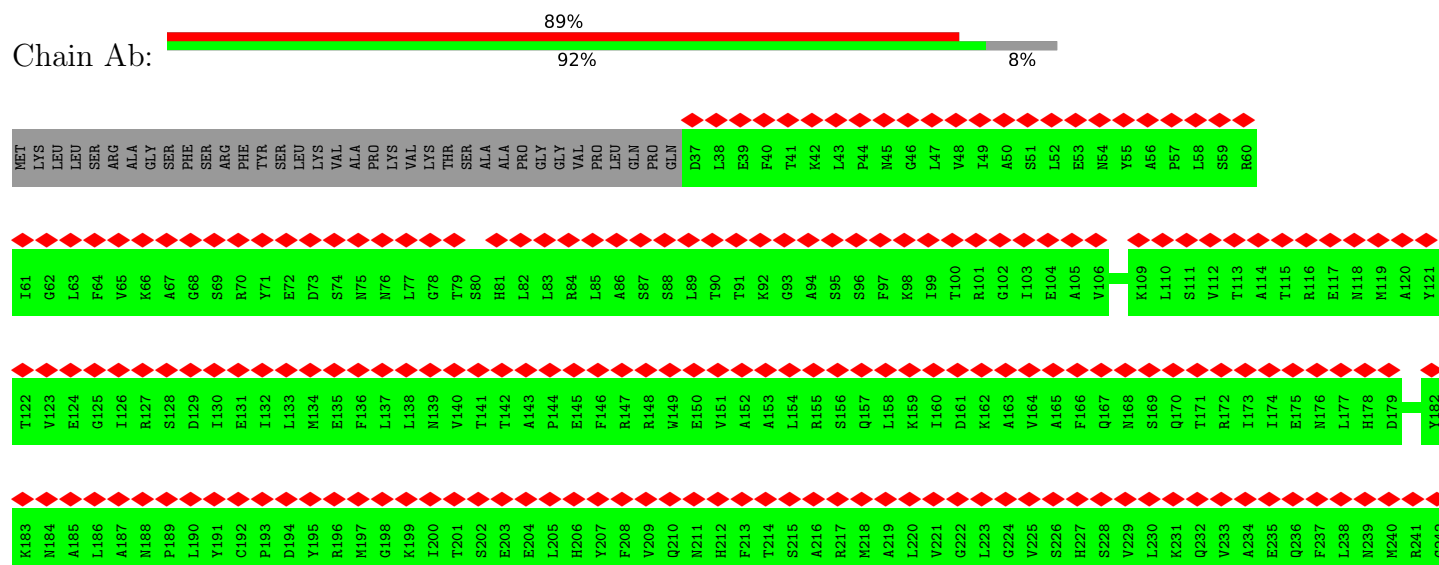
• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain AB:



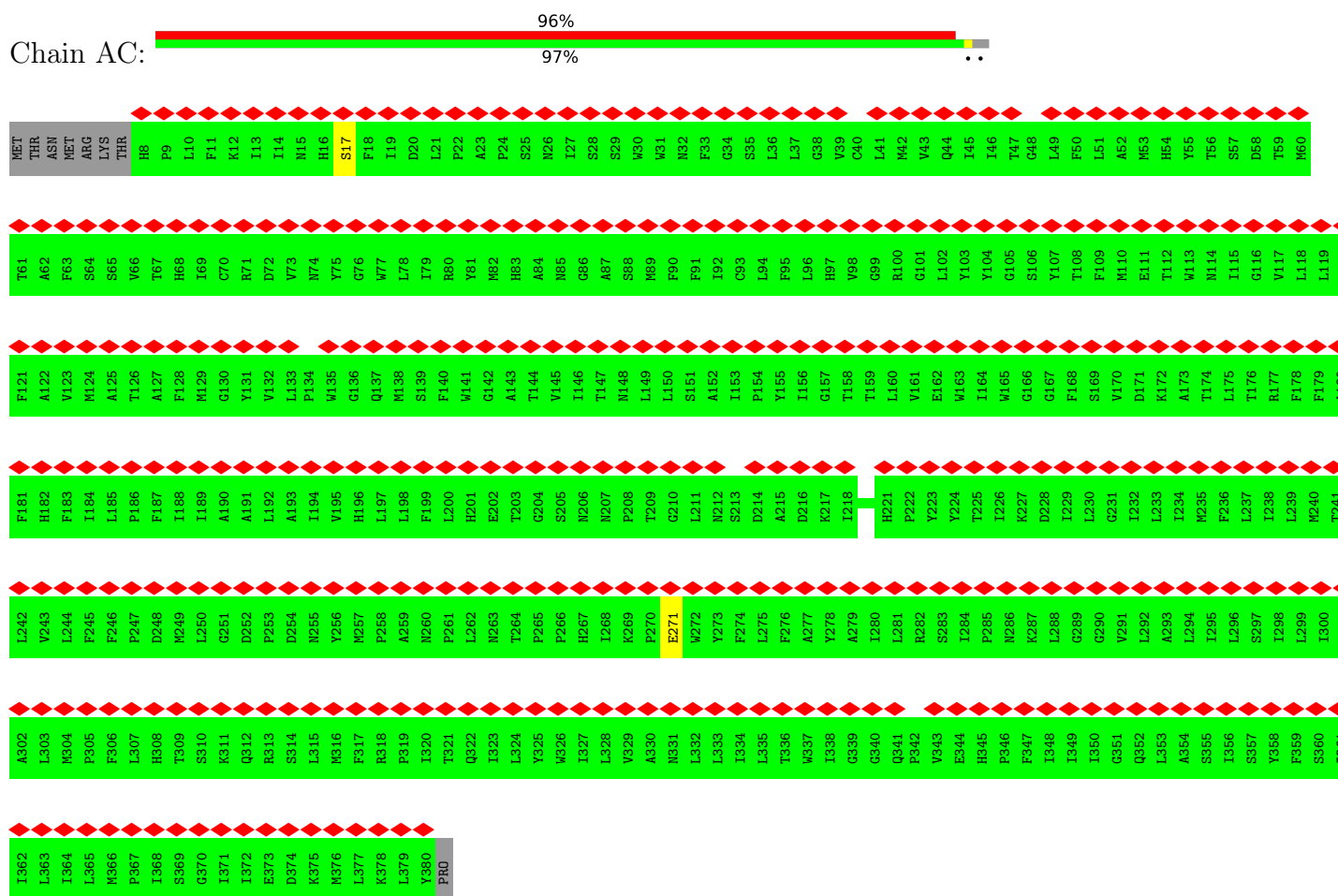
• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain Ab:

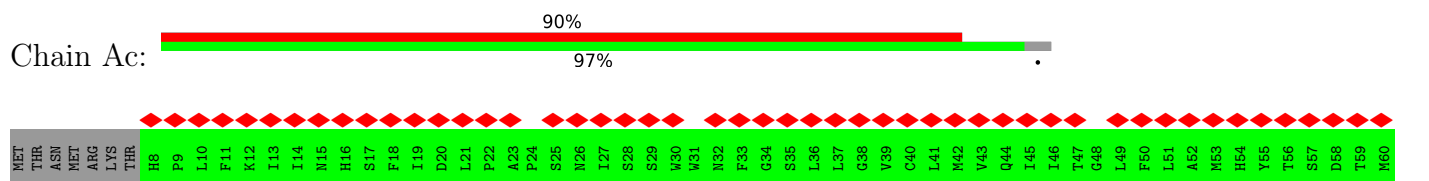


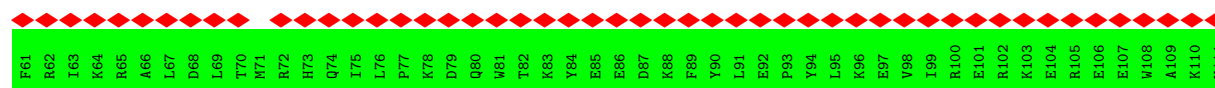


• Molecule 47: Cytochrome b

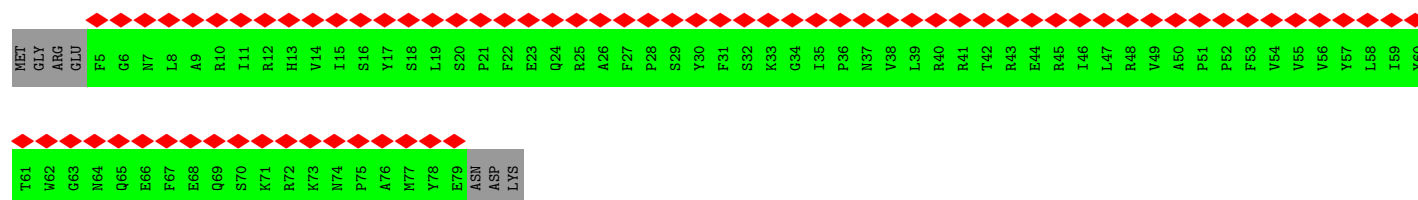


• Molecule 47: Cytochrome b

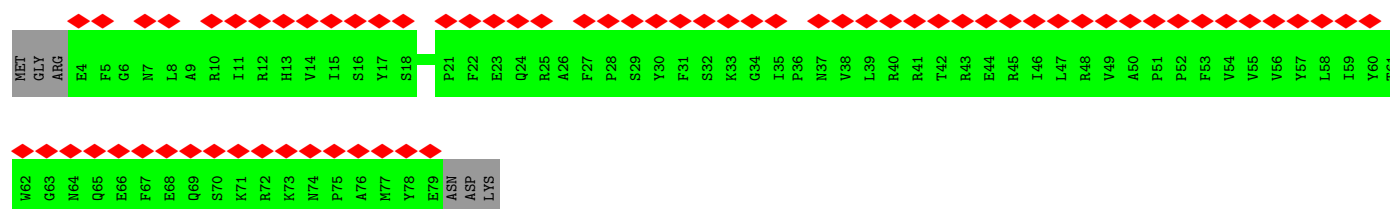
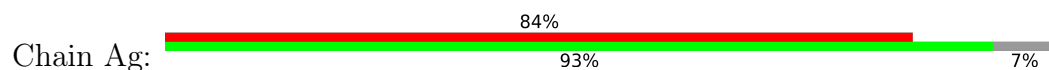




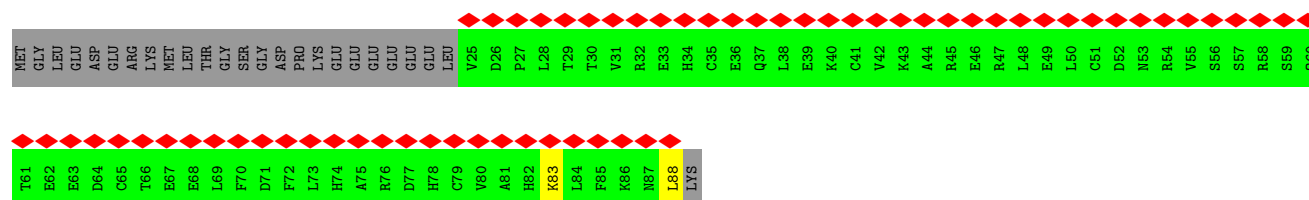
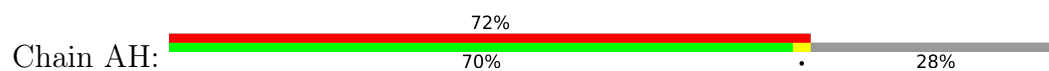
• Molecule 51: Cytochrome b-c1 complex subunit 8



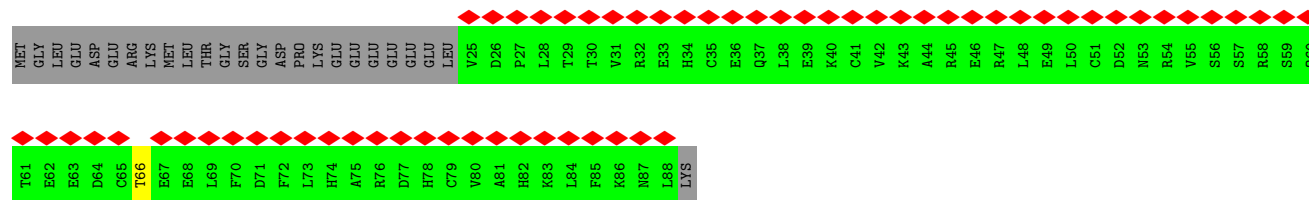
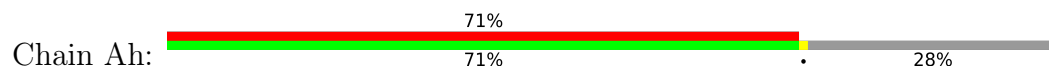
• Molecule 51: Cytochrome b-c1 complex subunit 8



• Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

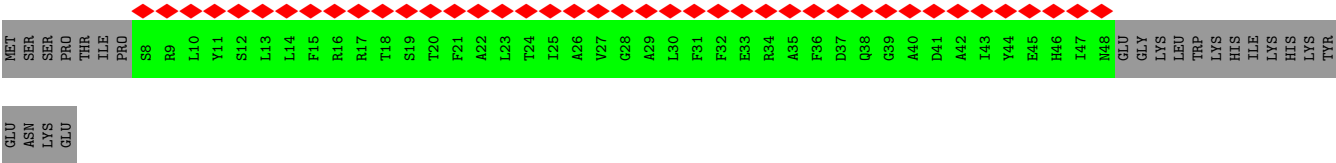


• Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

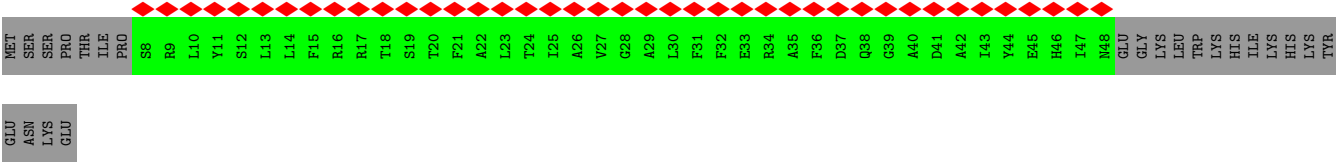


• Molecule 53: Cytochrome b-c1 complex subunit 9

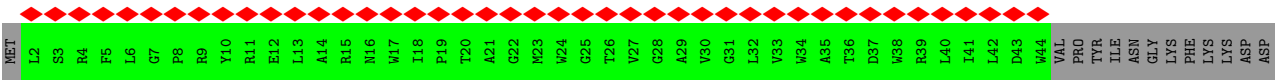
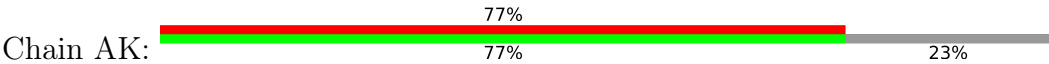




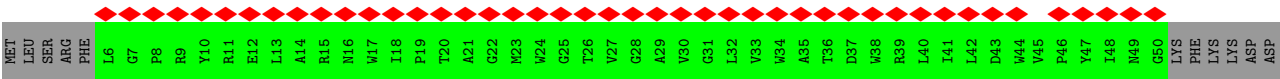
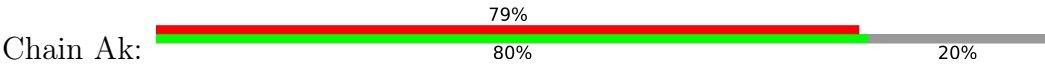
● Molecule 53: Cytochrome b-c1 complex subunit 9



● Molecule 54: Cytochrome b-c1 complex subunit 10



● Molecule 54: Cytochrome b-c1 complex subunit 10



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27478	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.2	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0082	Depositor
Map size (\AA)	424.96, 424.96, 424.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UQ6, UQ9, CDL, HEM, HEC, 3PE, PC1, FES, FMN, U10, ZN, NDP, EHZ, SF4, ADP, UQ1

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	0.42	0/755	0.56	0/1029
2	B	0.62	2/1278 (0.2%)	0.78	1/1730 (0.1%)
3	C	0.55	0/1687	0.79	1/2297 (0.0%)
4	D	0.60	2/3532 (0.1%)	0.83	6/4782 (0.1%)
5	E	0.58	3/1675 (0.2%)	0.68	3/2282 (0.1%)
6	F	0.59	4/3347 (0.1%)	0.78	9/4522 (0.2%)
7	G	0.62	4/5374 (0.1%)	0.93	16/7281 (0.2%)
8	H	0.55	1/2607 (0.0%)	0.71	5/3561 (0.1%)
9	I	0.61	1/1418 (0.1%)	0.87	2/1915 (0.1%)
10	J	0.39	0/1205	0.59	1/1633 (0.1%)
11	K	0.57	0/732	0.79	2/994 (0.2%)
12	L	0.67	5/4921 (0.1%)	0.90	19/6696 (0.3%)
13	M	0.69	4/3717 (0.1%)	0.90	10/5062 (0.2%)
14	N	0.67	2/2756 (0.1%)	0.85	7/3751 (0.2%)
15	O	0.63	4/2655 (0.2%)	0.74	8/3601 (0.2%)
16	P	0.56	2/2793 (0.1%)	0.71	6/3787 (0.2%)
17	Q	0.58	2/980 (0.2%)	0.80	4/1324 (0.3%)
18	R	0.81	2/671 (0.3%)	0.85	2/903 (0.2%)
19	S	0.66	1/678 (0.1%)	0.90	1/915 (0.1%)
20	T	0.76	1/613 (0.2%)	0.90	4/826 (0.5%)
20	U	0.61	0/712	0.79	2/962 (0.2%)
21	V	0.57	0/937	0.85	4/1270 (0.3%)
22	W	0.47	0/993	0.54	0/1335
23	X	0.48	0/1422	0.70	0/1921
24	Y	0.52	0/1054	0.59	0/1429
25	Z	0.56	1/1183 (0.1%)	0.69	0/1597
26	a	0.57	0/561	0.81	2/755 (0.3%)
27	b	0.45	0/643	0.53	0/884
28	c	0.46	0/400	0.76	1/544 (0.2%)
29	d	0.61	1/1028 (0.1%)	0.63	2/1387 (0.1%)
30	e	0.51	1/881 (0.1%)	0.64	1/1173 (0.1%)
31	f	0.40	0/451	0.44	0/607

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	g	0.63	1/863 (0.1%)	0.92	3/1175 (0.3%)
33	h	0.52	0/1197	0.74	0/1621
34	i	0.56	0/790	0.74	0/1074
35	j	0.51	0/599	0.69	0/820
36	k	0.82	1/578 (0.2%)	0.94	3/782 (0.4%)
37	l	0.69	2/1359 (0.1%)	0.76	1/1855 (0.1%)
38	m	0.55	0/1079	0.75	0/1463
39	n	0.64	1/1589 (0.1%)	0.74	2/2152 (0.1%)
40	o	0.50	0/1063	0.63	0/1427
41	p	0.53	0/1448	0.71	1/1957 (0.1%)
42	q	0.76	2/1054 (0.2%)	0.95	4/1431 (0.3%)
43	r	0.87	2/426 (0.5%)	1.17	2/573 (0.3%)
44	s	0.30	0/244	0.71	1/331 (0.3%)
45	AA	0.35	0/3218	0.58	1/4362 (0.0%)
45	Aa	0.33	0/3191	0.60	1/4326 (0.0%)
46	AB	0.33	0/3146	0.56	0/4252
46	Ab	0.32	0/3178	0.55	0/4296
47	AC	0.36	1/3089 (0.0%)	0.55	1/4221 (0.0%)
47	Ac	0.37	1/3054 (0.0%)	0.54	0/4170
48	AD	0.33	0/1955	0.54	0/2655
48	Ad	0.33	0/1971	0.50	0/2677
49	AE	0.45	0/1428	0.60	1/1934 (0.1%)
49	AI	0.34	0/331	0.53	0/451
49	Ae	0.45	0/1467	0.59	1/1985 (0.1%)
50	AF	0.32	0/875	0.52	0/1173
50	Af	0.32	0/884	0.43	0/1184
51	AG	0.37	0/653	0.56	0/883
51	Ag	0.36	0/662	0.56	0/895
52	AH	0.31	0/534	0.68	2/717 (0.3%)
52	Ah	0.36	0/534	0.58	1/717 (0.1%)
53	AJ	0.35	0/339	0.48	0/457
53	Aj	0.35	0/339	0.48	0/457
54	AK	0.32	0/368	0.46	0/504
54	Ak	0.28	0/379	0.42	0/522
All	All	0.54	54/97543 (0.1%)	0.73	144/132254 (0.1%)

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	89	PRO	N-CD	-15.21	1.26	1.47
12	L	265	PRO	N-CD	13.75	1.67	1.47
36	k	50	PRO	N-CD	-13.70	1.28	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	q	139	PRO	N-CD	-13.58	1.28	1.47
14	N	255	PRO	N-CD	-13.52	1.28	1.47
16	P	371	PRO	N-CD	12.83	1.65	1.47
7	G	532	PRO	N-CD	-12.65	1.30	1.47
15	O	315	PRO	N-CD	-12.22	1.30	1.47
20	T	141	PRO	N-CD	11.70	1.64	1.47
15	O	210	PRO	N-CD	-11.38	1.31	1.47
6	F	295	PRO	N-CD	-11.26	1.32	1.47
12	L	234	PRO	N-CD	11.11	1.63	1.47
8	H	42	PRO	N-CD	10.77	1.62	1.47
13	M	370	PRO	N-CD	-10.70	1.32	1.47
5	E	227	ALA	C-O	10.04	1.42	1.23
6	F	227	PRO	N-CD	9.86	1.61	1.47
32	g	78	PRO	N-CD	-9.68	1.34	1.47
5	E	44	PRO	N-CD	-9.61	1.34	1.47
16	P	290	PRO	N-CD	9.54	1.61	1.47
7	G	275	PRO	N-CD	-9.53	1.34	1.47
43	r	91	GLU	N-CA	9.46	1.65	1.46
29	d	15	PRO	N-CD	-9.44	1.34	1.47
6	F	319	PRO	N-CD	8.99	1.60	1.47
9	I	107	PRO	N-CD	8.47	1.59	1.47
13	M	20	PRO	N-CD	8.44	1.59	1.47
4	D	163	PRO	N-CD	-8.33	1.36	1.47
12	L	212	PRO	N-CD	-8.33	1.36	1.47
39	n	155	PRO	N-CD	8.12	1.59	1.47
19	S	63	PRO	N-CD	-8.03	1.36	1.47
25	Z	73	PRO	N-CD	8.02	1.59	1.47
4	D	352	PRO	N-CD	-7.93	1.36	1.47
47	AC	271	GLU	C-N	7.82	1.52	1.34
47	Ac	271	GLU	C-N	7.76	1.51	1.34
43	r	111	PRO	N-CD	-7.54	1.37	1.47
30	e	91	LYS	C-N	7.49	1.51	1.34
37	l	104	PRO	N-CD	-7.23	1.37	1.47
13	M	208	PRO	N-CD	7.16	1.57	1.47
14	N	238	PRO	N-CD	-6.99	1.38	1.47
7	G	541	PRO	N-CD	-6.89	1.38	1.47
2	B	153	PRO	N-CD	-6.37	1.39	1.47
6	F	384	PRO	N-CD	-6.25	1.39	1.47
12	L	384	PRO	N-CD	6.24	1.56	1.47
12	L	112	PRO	N-CD	5.95	1.56	1.47
5	E	93	PRO	N-CD	-5.94	1.39	1.47
37	l	45	PRO	N-CD	-5.81	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	87	PRO	N-CD	-5.77	1.39	1.47
2	B	88	SER	C-N	-5.75	1.20	1.34
13	M	252	PRO	N-CD	-5.61	1.40	1.47
7	G	683	PRO	N-CD	-5.47	1.40	1.47
15	O	103	PRO	N-CD	-5.43	1.40	1.47
17	Q	53	ILE	C-O	5.36	1.33	1.23
42	q	126	PRO	N-CD	5.26	1.55	1.47
17	Q	82	PRO	N-CD	-5.03	1.40	1.47
18	R	40	GLU	N-CA	5.03	1.56	1.46

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	r	91	GLU	N-CA-CB	13.66	135.18	110.60
26	a	3	PHE	CB-CA-C	-10.41	89.59	110.40
36	k	50	PRO	CA-N-CD	9.93	125.61	111.70
14	N	255	PRO	CA-N-CD	9.86	125.50	111.70
42	q	139	PRO	CA-N-CD	9.59	125.12	111.70
4	D	142	VAL	N-CA-CB	9.53	132.46	111.50
45	Aa	366	ASP	CB-CG-OD1	9.43	126.79	118.30
6	F	334	THR	N-CA-CB	8.92	127.25	110.30
15	O	315	PRO	CA-N-CD	8.77	123.98	111.70
7	G	532	PRO	CA-N-CD	8.56	123.69	111.70
7	G	174	THR	N-CA-C	-8.13	89.04	111.00
36	k	50	PRO	N-CA-CB	-8.13	93.54	103.30
15	O	210	PRO	CA-N-CD	7.79	122.60	111.70
6	F	295	PRO	CA-N-CD	7.70	122.47	111.70
17	Q	60	ASP	N-CA-C	-7.66	90.32	111.00
6	F	411	SER	N-CA-CB	7.52	121.78	110.50
12	L	265	PRO	CA-N-CD	-7.43	101.09	111.50
7	G	204	MET	N-CA-C	-7.24	91.45	111.00
15	O	210	PRO	N-CA-CB	-7.23	94.62	103.30
14	N	255	PRO	N-CA-CB	-7.14	94.73	103.30
16	P	371	PRO	N-CA-CB	7.13	111.86	103.30
6	F	332	CYS	N-CA-C	7.05	130.04	111.00
32	g	78	PRO	CA-N-CD	7.01	121.52	111.70
12	L	265	PRO	N-CA-CB	7.00	111.70	103.30
45	AA	338	CYS	CA-CB-SG	-6.98	101.44	114.00
16	P	369	THR	N-CA-CB	6.93	123.47	110.30
28	c	47	SER	N-CA-CB	6.87	120.80	110.50
4	D	142	VAL	N-CA-C	-6.84	92.53	111.00
5	E	44	PRO	CA-N-CD	6.79	121.21	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	213	HIS	CB-CA-C	-6.78	96.84	110.40
7	G	275	PRO	CA-N-CD	6.62	120.97	111.70
15	O	320	GLY	N-CA-C	-6.61	96.57	113.10
29	d	15	PRO	CA-N-CD	6.59	120.92	111.70
7	G	300	GLN	N-CA-CB	6.58	122.44	110.60
16	P	106	LEU	N-CA-C	6.57	128.73	111.00
5	E	64	ALA	N-CA-CB	6.54	119.26	110.10
36	k	59	TYR	N-CA-CB	-6.52	98.86	110.60
39	n	115	TYR	N-CA-CB	6.42	122.15	110.60
42	q	139	PRO	N-CA-CB	-6.37	95.59	102.60
8	H	52	ALA	N-CA-CB	6.36	119.01	110.10
16	P	371	PRO	CA-N-CD	-6.33	102.64	111.50
4	D	427	PRO	N-CA-C	-6.32	95.66	112.10
8	H	196	ALA	N-CA-C	6.31	128.04	111.00
9	I	154	TYR	N-CA-CB	-6.31	99.24	110.60
13	M	370	PRO	N-CA-C	6.29	128.46	112.10
13	M	424	ILE	N-CA-C	-6.28	94.03	111.00
13	M	370	PRO	CA-N-CD	6.23	120.42	111.70
14	N	255	PRO	N-CA-C	6.22	128.28	112.10
4	D	140	ASP	CB-CA-C	-6.17	98.07	110.40
32	g	137	SER	N-CA-CB	-6.15	101.28	110.50
14	N	81	LEU	N-CA-C	-6.15	94.40	111.00
20	T	141	PRO	CA-N-CD	-6.10	102.97	111.50
7	G	133	GLN	N-CA-CB	6.08	121.55	110.60
7	G	212	LYS	N-CA-C	-6.06	94.63	111.00
12	L	231	PRO	N-CA-C	6.05	127.82	112.10
20	U	75	THR	N-CA-CB	6.03	121.77	110.30
20	T	141	PRO	N-CA-CB	6.03	110.53	103.30
15	O	315	PRO	N-CA-CB	-6.01	95.99	102.60
14	N	218	ALA	N-CA-CB	5.97	118.45	110.10
42	q	69	ASN	N-CA-CB	5.96	121.32	110.60
12	L	276	THR	N-CA-CB	5.95	121.61	110.30
12	L	234	PRO	CA-N-CD	-5.95	103.17	111.50
12	L	554	ASP	N-CA-CB	5.92	121.25	110.60
12	L	605	ASN	N-CA-CB	5.89	121.20	110.60
52	AH	83	LYS	N-CA-CB	5.88	121.19	110.60
12	L	483	PRO	N-CA-C	-5.88	96.81	112.10
19	S	63	PRO	CA-N-CD	5.86	119.90	111.70
10	J	136	GLU	C-N-CA	-5.86	110.00	122.30
7	G	251	ILE	N-CA-C	5.84	126.76	111.00
6	F	103	ASN	N-CA-CB	5.82	121.08	110.60
5	E	68	ASN	N-CA-CB	5.82	121.07	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	T	135	ALA	N-CA-CB	5.76	118.16	110.10
11	K	83	ASN	N-CA-CB	5.74	120.93	110.60
13	M	223	ALA	N-CA-CB	5.72	118.11	110.10
20	U	150	ASP	CB-CA-C	5.72	121.83	110.40
29	d	15	PRO	N-CA-CB	-5.71	96.32	102.60
7	G	510	TRP	N-CA-CB	5.69	120.84	110.60
8	H	223	PHE	CB-CA-C	-5.67	99.06	110.40
17	Q	141	ASN	N-CA-CB	5.65	120.77	110.60
7	G	599	THR	N-CA-C	5.63	126.21	111.00
47	AC	17	SER	N-CA-CB	-5.63	102.05	110.50
14	N	89	GLN	N-CA-CB	-5.63	100.46	110.60
21	V	57	ASP	N-CA-CB	5.62	120.72	110.60
15	O	118	TYR	N-CA-CB	-5.57	100.58	110.60
12	L	415	ALA	N-CA-CB	5.56	117.89	110.10
17	Q	163	ASN	CB-CA-C	-5.54	99.32	110.40
7	G	580	ALA	N-CA-CB	5.53	117.84	110.10
15	O	118	TYR	N-CA-C	5.53	125.94	111.00
13	M	311	GLY	N-CA-C	-5.52	99.31	113.10
3	C	125	PHE	N-CA-CB	-5.51	100.68	110.60
49	AE	221	GLY	N-CA-C	5.50	126.85	113.10
49	Ae	221	GLY	N-CA-C	5.50	126.85	113.10
21	V	19	THR	N-CA-CB	5.48	120.72	110.30
9	I	160	GLU	N-CA-CB	-5.48	100.73	110.60
44	s	55	PHE	N-CA-C	5.46	125.75	111.00
16	P	367	GLU	CB-CA-C	-5.45	99.50	110.40
39	n	136	GLU	CB-CA-C	5.45	121.30	110.40
12	L	582	GLY	N-CA-C	-5.44	99.49	113.10
2	B	195	PRO	N-CA-C	-5.43	97.99	112.10
18	R	38	TYR	N-CA-C	-5.42	96.37	111.00
6	F	457	HIS	N-CA-CB	-5.41	100.86	110.60
21	V	114	TRP	N-CA-CB	5.41	120.34	110.60
15	O	152	SER	N-CA-CB	5.41	118.61	110.50
7	G	651	PRO	CB-CA-C	-5.40	98.49	112.00
43	r	111	PRO	CA-N-CD	5.40	119.26	111.70
42	q	67	GLU	CB-CA-C	-5.39	99.62	110.40
8	H	91	MET	N-CA-C	-5.37	96.49	111.00
4	D	140	ASP	N-CA-C	-5.37	96.50	111.00
52	AH	88	LEU	N-CA-CB	5.36	121.12	110.40
12	L	194	ASN	N-CA-C	5.35	125.45	111.00
13	M	276	CYS	N-CA-CB	5.33	120.19	110.60
12	L	151	SER	N-CA-CB	5.31	118.46	110.50
6	F	295	PRO	N-CA-CB	-5.30	96.77	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	418	GLN	N-CA-CB	5.30	120.14	110.60
41	p	94	ARG	NE-CZ-NH1	5.24	122.92	120.30
12	L	277	MET	CB-CA-C	-5.24	99.92	110.40
13	M	330	ALA	N-CA-CB	5.24	117.44	110.10
11	K	70	GLU	N-CA-CB	5.23	120.02	110.60
8	H	51	ASP	CB-CA-C	-5.23	99.94	110.40
12	L	212	PRO	CA-N-CD	5.21	118.99	111.70
13	M	423	MET	N-CA-C	-5.21	96.94	111.00
7	G	640	ASP	N-CA-CB	5.21	119.97	110.60
12	L	248	HIS	CB-CA-C	5.21	120.81	110.40
12	L	212	PRO	N-CA-C	5.19	125.59	112.10
12	L	234	PRO	N-CA-CB	5.16	109.49	103.30
37	l	104	PRO	CA-N-CD	5.16	118.92	111.70
18	R	89	PRO	CA-N-CD	5.15	118.91	111.70
12	L	247	LEU	N-CA-CB	5.14	120.69	110.40
17	Q	164	PHE	N-CA-CB	5.13	119.83	110.60
52	Ah	66	THR	N-CA-C	-5.13	97.16	111.00
16	P	368	GLU	N-CA-CB	5.11	119.79	110.60
26	a	4	GLU	N-CA-C	5.11	124.79	111.00
13	M	83	HIS	N-CA-C	-5.10	97.24	111.00
32	g	78	PRO	N-CA-CB	-5.09	97.00	102.60
6	F	228	PRO	N-CA-C	-5.09	98.87	112.10
30	e	91	LYS	C-N-CA	-5.06	109.04	121.70
7	G	77	MET	N-CA-C	-5.05	97.36	111.00
7	G	668	ALA	N-CA-CB	5.05	117.17	110.10
21	V	86	LYS	N-CA-CB	5.04	119.67	110.60
7	G	532	PRO	N-CA-CB	-5.03	97.06	102.60
4	D	352	PRO	CA-N-CD	5.03	118.74	111.70
12	L	20	LEU	CB-CA-C	-5.02	100.67	110.20
14	N	228	ASN	N-CA-CB	5.01	119.61	110.60
20	T	139	MET	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	87/115 (76%)	83 (95%)	4 (5%)	0	100	100
2	B	154/224 (69%)	142 (92%)	11 (7%)	1 (1%)	22	60
3	C	196/263 (74%)	187 (95%)	9 (5%)	0	100	100
4	D	423/463 (91%)	392 (93%)	31 (7%)	0	100	100
5	E	208/248 (84%)	193 (93%)	15 (7%)	0	100	100
6	F	422/464 (91%)	403 (96%)	19 (4%)	0	100	100
7	G	685/727 (94%)	632 (92%)	53 (8%)	0	100	100
8	H	313/318 (98%)	295 (94%)	18 (6%)	0	100	100
9	I	169/212 (80%)	169 (100%)	0	0	100	100
10	J	149/172 (87%)	136 (91%)	13 (9%)	0	100	100
11	K	94/98 (96%)	92 (98%)	2 (2%)	0	100	100
12	L	604/607 (100%)	576 (95%)	28 (5%)	0	100	100
13	M	457/459 (100%)	439 (96%)	18 (4%)	0	100	100
14	N	342/345 (99%)	331 (97%)	10 (3%)	1 (0%)	37	72
15	O	316/355 (89%)	302 (96%)	14 (4%)	0	100	100
16	P	337/377 (89%)	314 (93%)	23 (7%)	0	100	100
17	Q	116/175 (66%)	114 (98%)	2 (2%)	0	100	100
18	R	81/116 (70%)	75 (93%)	6 (7%)	0	100	100
19	S	81/99 (82%)	77 (95%)	4 (5%)	0	100	100
20	T	73/156 (47%)	72 (99%)	1 (1%)	0	100	100
20	U	85/156 (54%)	83 (98%)	2 (2%)	0	100	100
21	V	110/116 (95%)	107 (97%)	3 (3%)	0	100	100
22	W	112/131 (86%)	111 (99%)	1 (1%)	0	100	100
23	X	167/172 (97%)	153 (92%)	14 (8%)	0	100	100
24	Y	137/143 (96%)	133 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Z	137/144 (95%)	132 (96%)	5 (4%)	0	100	100
26	a	65/70 (93%)	61 (94%)	4 (6%)	0	100	100
27	b	77/84 (92%)	69 (90%)	8 (10%)	0	100	100
28	c	45/76 (59%)	44 (98%)	1 (2%)	0	100	100
29	d	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
30	e	101/106 (95%)	95 (94%)	6 (6%)	0	100	100
31	f	49/57 (86%)	49 (100%)	0	0	100	100
32	g	97/151 (64%)	91 (94%)	6 (6%)	0	100	100
33	h	136/189 (72%)	130 (96%)	6 (4%)	0	100	100
34	i	87/128 (68%)	80 (92%)	7 (8%)	0	100	100
35	j	65/105 (62%)	61 (94%)	4 (6%)	0	100	100
36	k	67/104 (64%)	64 (96%)	3 (4%)	0	100	100
37	l	153/186 (82%)	141 (92%)	12 (8%)	0	100	100
38	m	124/129 (96%)	117 (94%)	7 (6%)	0	100	100
39	n	175/179 (98%)	165 (94%)	9 (5%)	1 (1%)	22	60
40	o	119/137 (87%)	116 (98%)	3 (2%)	0	100	100
41	p	165/176 (94%)	148 (90%)	17 (10%)	0	100	100
42	q	118/145 (81%)	115 (98%)	3 (2%)	0	100	100
43	r	47/113 (42%)	43 (92%)	4 (8%)	0	100	100
44	s	27/104 (26%)	27 (100%)	0	0	100	100
45	AA	397/480 (83%)	385 (97%)	12 (3%)	0	100	100
45	Aa	394/480 (82%)	385 (98%)	9 (2%)	0	100	100
46	AB	409/453 (90%)	397 (97%)	12 (3%)	0	100	100
46	Ab	415/453 (92%)	406 (98%)	9 (2%)	0	100	100
47	AC	371/381 (97%)	365 (98%)	6 (2%)	0	100	100
47	Ac	365/381 (96%)	361 (99%)	4 (1%)	0	100	100
48	AD	236/325 (73%)	230 (98%)	6 (2%)	0	100	100
48	Ad	238/325 (73%)	229 (96%)	9 (4%)	0	100	100
49	AE	175/274 (64%)	164 (94%)	11 (6%)	0	100	100
49	AI	40/274 (15%)	38 (95%)	2 (5%)	0	100	100
49	Ae	180/274 (66%)	167 (93%)	13 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	AF	95/111 (86%)	95 (100%)	0	0	100	100
50	Af	96/111 (86%)	96 (100%)	0	0	100	100
51	AG	73/82 (89%)	73 (100%)	0	0	100	100
51	Ag	74/82 (90%)	74 (100%)	0	0	100	100
52	AH	62/89 (70%)	60 (97%)	2 (3%)	0	100	100
52	Ah	62/89 (70%)	60 (97%)	2 (3%)	0	100	100
53	AJ	39/64 (61%)	39 (100%)	0	0	100	100
53	Aj	39/64 (61%)	39 (100%)	0	0	100	100
54	AK	41/56 (73%)	39 (95%)	2 (5%)	0	100	100
54	Ak	43/56 (77%)	40 (93%)	3 (7%)	0	100	100
All	All	11734/14118 (83%)	11218 (96%)	513 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	N	109	ALA
2	B	195	PRO
39	n	156	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	83/104 (80%)	83 (100%)	0	100	100
2	B	132/185 (71%)	130 (98%)	2 (2%)	60	75
3	C	180/227 (79%)	180 (100%)	0	100	100
4	D	369/395 (93%)	369 (100%)	0	100	100
5	E	182/206 (88%)	182 (100%)	0	100	100
6	F	340/370 (92%)	340 (100%)	0	100	100
7	G	579/610 (95%)	579 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	279/280 (100%)	279 (100%)	0	100	100
9	I	147/178 (83%)	147 (100%)	0	100	100
10	J	124/138 (90%)	124 (100%)	0	100	100
11	K	86/88 (98%)	86 (100%)	0	100	100
12	L	549/550 (100%)	549 (100%)	0	100	100
13	M	415/415 (100%)	415 (100%)	0	100	100
14	N	307/308 (100%)	307 (100%)	0	100	100
15	O	282/309 (91%)	282 (100%)	0	100	100
16	P	296/325 (91%)	296 (100%)	0	100	100
17	Q	105/153 (69%)	105 (100%)	0	100	100
18	R	70/96 (73%)	70 (100%)	0	100	100
19	S	74/80 (92%)	74 (100%)	0	100	100
20	T	69/135 (51%)	69 (100%)	0	100	100
20	U	80/135 (59%)	80 (100%)	0	100	100
21	V	100/102 (98%)	100 (100%)	0	100	100
22	W	108/114 (95%)	108 (100%)	0	100	100
23	X	152/154 (99%)	151 (99%)	1 (1%)	81	87
24	Y	104/107 (97%)	104 (100%)	0	100	100
25	Z	120/123 (98%)	120 (100%)	0	100	100
26	a	57/60 (95%)	57 (100%)	0	100	100
27	b	70/73 (96%)	70 (100%)	0	100	100
28	c	41/67 (61%)	41 (100%)	0	100	100
29	d	107/107 (100%)	107 (100%)	0	100	100
30	e	91/94 (97%)	91 (100%)	0	100	100
31	f	47/53 (89%)	47 (100%)	0	100	100
32	g	90/129 (70%)	90 (100%)	0	100	100
33	h	123/162 (76%)	123 (100%)	0	100	100
34	i	86/120 (72%)	86 (100%)	0	100	100
35	j	62/87 (71%)	62 (100%)	0	100	100
36	k	54/78 (69%)	54 (100%)	0	100	100
37	l	140/161 (87%)	140 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	m	112/114 (98%)	111 (99%)	1 (1%)	75	83
39	n	162/164 (99%)	162 (100%)	0	100	100
40	o	111/121 (92%)	111 (100%)	0	100	100
41	p	152/158 (96%)	152 (100%)	0	100	100
42	q	110/131 (84%)	110 (100%)	0	100	100
43	r	44/96 (46%)	44 (100%)	0	100	100
44	s	28/95 (30%)	28 (100%)	0	100	100
45	AA	341/398 (86%)	341 (100%)	0	100	100
45	Aa	339/398 (85%)	339 (100%)	0	100	100
46	AB	324/356 (91%)	324 (100%)	0	100	100
46	Ab	327/356 (92%)	327 (100%)	0	100	100
47	AC	325/333 (98%)	325 (100%)	0	100	100
47	Ac	322/333 (97%)	322 (100%)	0	100	100
48	AD	203/260 (78%)	203 (100%)	0	100	100
48	Ad	205/260 (79%)	205 (100%)	0	100	100
49	AE	152/224 (68%)	152 (100%)	0	100	100
49	AI	33/224 (15%)	33 (100%)	0	100	100
49	Ae	156/224 (70%)	156 (100%)	0	100	100
50	AF	89/99 (90%)	89 (100%)	0	100	100
50	Af	90/99 (91%)	90 (100%)	0	100	100
51	AG	68/74 (92%)	68 (100%)	0	100	100
51	Ag	69/74 (93%)	69 (100%)	0	100	100
52	AH	61/83 (74%)	61 (100%)	0	100	100
52	Ah	61/83 (74%)	61 (100%)	0	100	100
53	AJ	33/55 (60%)	33 (100%)	0	100	100
53	Aj	33/55 (60%)	33 (100%)	0	100	100
54	AK	34/46 (74%)	34 (100%)	0	100	100
54	Ak	35/46 (76%)	35 (100%)	0	100	100
All	All	10319/12037 (86%)	10315 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	95	PHE
2	B	170	TYR
23	X	48	TRP
38	m	49	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (202) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	106	HIS
2	B	151	GLN
2	B	209	GLN
3	C	54	HIS
3	C	73	GLN
3	C	88	HIS
3	C	123	ASN
3	C	179	ASN
3	C	180	HIS
3	C	195	HIS
3	C	227	GLN
3	C	235	ASN
4	D	60	HIS
4	D	88	HIS
4	D	92	HIS
4	D	117	HIS
4	D	131	GLN
4	D	147	ASN
4	D	182	ASN
4	D	233	HIS
4	D	339	GLN
4	D	346	GLN
4	D	381	HIS
5	E	245	GLN
6	F	168	ASN
6	F	270	ASN
6	F	283	ASN
6	F	303	HIS
6	F	346	GLN
6	F	441	HIS
7	G	59	GLN
7	G	74	ASN
7	G	140	GLN
7	G	164	ASN
7	G	205	GLN

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Mol	Chain	Res	Type
7	G	359	ASN
7	G	365	ASN
7	G	388	ASN
7	G	406	ASN
7	G	444	HIS
7	G	495	ASN
7	G	540	ASN
7	G	571	HIS
7	G	605	GLN
7	G	666	GLN
8	H	5	ASN
8	H	32	GLN
8	H	47	GLN
8	H	124	ASN
8	H	169	GLN
8	H	171	HIS
8	H	258	ASN
8	H	292	ASN
11	K	7	ASN
12	L	2	ASN
12	L	25	ASN
12	L	58	ASN
12	L	135	ASN
12	L	136	ASN
12	L	139	GLN
12	L	170	GLN
12	L	199	GLN
12	L	209	ASN
12	L	226	GLN
12	L	264	HIS
12	L	321	GLN
12	L	328	HIS
12	L	332	HIS
12	L	354	GLN
12	L	400	ASN
12	L	446	ASN
12	L	452	ASN
12	L	579	ASN
13	M	26	ASN
13	M	51	ASN
13	M	81	GLN
13	M	92	GLN

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Mol	Chain	Res	Type
13	M	170	HIS
13	M	175	ASN
13	M	184	HIS
13	M	192	ASN
13	M	213	HIS
13	M	279	GLN
13	M	293	HIS
13	M	304	GLN
13	M	349	GLN
13	M	374	ASN
13	M	390	ASN
13	M	415	GLN
13	M	421	ASN
14	N	120	GLN
14	N	134	GLN
14	N	204	ASN
14	N	273	ASN
14	N	310	ASN
15	O	54	HIS
15	O	80	GLN
15	O	132	GLN
15	O	175	ASN
15	O	219	GLN
15	O	292	HIS
15	O	299	GLN
15	O	306	ASN
15	O	323	GLN
16	P	71	ASN
16	P	79	GLN
16	P	154	GLN
16	P	166	HIS
16	P	219	ASN
16	P	238	GLN
16	P	269	ASN
16	P	275	HIS
16	P	341	GLN
16	P	356	HIS
17	Q	51	GLN
17	Q	88	GLN
18	R	52	GLN
18	R	56	ASN
19	S	48	HIS

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Mol	Chain	Res	Type
21	V	41	HIS
21	V	50	GLN
22	W	54	GLN
22	W	105	HIS
23	X	30	HIS
23	X	77	HIS
23	X	151	ASN
24	Y	21	HIS
24	Y	91	ASN
25	Z	76	GLN
26	a	31	ASN
27	b	69	HIS
27	b	71	GLN
27	b	83	ASN
29	d	59	HIS
29	d	88	HIS
33	h	170	GLN
34	i	74	HIS
34	i	83	HIS
35	j	41	GLN
36	k	39	GLN
36	k	66	ASN
37	l	91	GLN
37	l	106	HIS
38	m	75	ASN
38	m	79	ASN
39	n	12	HIS
39	n	14	GLN
39	n	33	HIS
39	n	53	ASN
39	n	76	HIS
40	o	54	GLN
40	o	61	HIS
41	p	67	GLN
41	p	91	GLN
41	p	100	GLN
41	p	124	ASN
42	q	13	GLN
42	q	31	ASN
42	q	54	GLN
42	q	87	HIS
42	q	91	HIS

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Mol	Chain	Res	Type
43	r	21	GLN
43	r	110	GLN
45	AA	55	ASN
45	AA	87	ASN
45	AA	173	GLN
45	AA	181	ASN
45	AA	193	GLN
45	AA	207	ASN
45	AA	342	GLN
45	AA	469	ASN
46	AB	167	GLN
46	AB	415	GLN
47	AC	312	GLN
47	AC	341	GLN
48	AD	115	GLN
49	AE	219	HIS
49	AE	242	HIS
51	AG	7	ASN
52	AH	37	GLN
52	AH	87	ASN
45	Aa	160	GLN
45	Aa	173	GLN
45	Aa	181	ASN
45	Aa	193	GLN
45	Aa	207	ASN
45	Aa	402	HIS
46	Ab	284	ASN
46	Ab	298	HIS
46	Ab	415	GLN
47	Ac	148	ASN
47	Ac	312	GLN
47	Ac	341	GLN
48	Ad	115	GLN
49	Ae	219	HIS
49	Ae	242	HIS
50	Af	73	HIS
50	Af	80	GLN
51	Ag	13	HIS
52	Ah	37	GLN
52	Ah	78	HIS
52	Ah	82	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 51 ligands modelled in this entry, 2 are monoatomic - leaving 49 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$
67	HEM	AC	402	47	41,50,50	1.35	4 (9%)	45,82,82	1.96	9 (20%)
65	NDP	P	401	-	45,52,52	0.96	2 (4%)	53,80,80	1.17	4 (7%)
62	CDL	M	503	-	81,81,99	1.01	4 (4%)	87,93,111	1.14	6 (6%)
62	CDL	d	201	-	64,64,99	1.13	4 (6%)	70,76,111	1.20	6 (8%)
55	SF4	G	802	7	0,12,12	-	-	-	-	-
58	3PE	M	502	-	48,48,50	0.93	2 (4%)	51,53,55	1.14	3 (5%)
62	CDL	Aa	501	-	45,45,99	0.43	0	51,57,111	0.36	0
67	HEM	AC	401	47	41,50,50	1.24	4 (9%)	45,82,82	1.68	8 (17%)
62	CDL	h	201	-	67,67,99	1.10	4 (5%)	73,79,111	1.15	6 (8%)
67	HEM	Ac	403	47	41,50,50	1.26	3 (7%)	45,82,82	1.69	9 (20%)
58	3PE	i	201	-	39,39,50	1.03	2 (5%)	42,44,55	1.14	3 (7%)
61	UQ9	H	401	-	35,35,58	0.79	2 (5%)	42,45,73	0.50	0
55	SF4	I	303	9	0,12,12	-	-	-	-	-
64	ADP	O	401	-	24,29,29	0.94	1 (4%)	29,45,45	1.37	4 (13%)
62	CDL	L	703	-	72,72,99	1.06	4 (5%)	78,84,111	1.14	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
62	CDL	q	201	-	56,56,99	1.21	4 (7%)	62,68,111	1.21	5 (8%)
66	EHZ	W	201	-	27,31,37	1.89	7 (25%)	37,41,47	1.86	11 (29%)
57	PC1	B	303	-	34,34,53	1.15	2 (5%)	40,42,61	1.16	4 (10%)
58	3PE	L	701	-	39,39,50	1.02	2 (5%)	42,44,55	1.06	2 (4%)
59	FES	E	301	5	0,4,4	-	-	-	-	-
70	U10	Ac	405	-	23,23,63	1.24	3 (13%)	28,31,79	2.08	7 (25%)
58	3PE	M	501	-	36,36,50	1.08	2 (5%)	39,41,55	1.05	3 (7%)
58	3PE	D	501	-	37,37,50	1.06	2 (5%)	40,42,55	1.08	3 (7%)
58	3PE	m	201	-	40,40,50	1.01	2 (5%)	43,45,55	1.15	3 (6%)
62	CDL	Ag	101	-	41,41,99	0.45	0	47,53,111	0.36	0
58	3PE	Ac	401	-	22,22,50	0.47	0	25,27,55	0.74	1 (4%)
58	3PE	Ac	404	-	34,34,50	0.32	0	37,39,55	0.41	0
67	HEM	Ac	402	47	41,50,50	1.22	4 (9%)	45,82,82	1.69	8 (17%)
58	3PE	L	705	-	43,43,50	0.99	2 (4%)	46,48,55	1.08	3 (6%)
58	3PE	H	403	-	50,50,50	0.91	2 (4%)	53,55,55	1.01	2 (3%)
55	SF4	B	301	2	0,12,12	-	-	-	-	-
58	3PE	Ag	103	-	50,50,50	0.31	0	53,55,55	0.29	0
56	UQ1	B	302	-	18,18,18	2.00	2 (11%)	22,25,25	1.18	3 (13%)
68	UQ6	Ac	406	-	23,23,43	2.77	6 (26%)	27,31,55	1.96	5 (18%)
55	SF4	G	801	7	0,12,12	-	-	-	-	-
62	CDL	Ag	102	-	55,55,99	0.39	0	61,67,111	0.33	0
68	UQ6	AC	403	-	28,28,43	2.42	6 (21%)	33,37,55	2.03	9 (27%)
58	3PE	L	702	-	48,48,50	0.92	2 (4%)	51,53,55	1.10	3 (5%)
62	CDL	Y	201	-	70,70,99	1.08	4 (5%)	76,82,111	1.16	7 (9%)
66	EHZ	n	201	-	27,31,37	1.91	7 (25%)	37,41,47	1.56	4 (10%)
60	FMN	F	501	-	33,33,33	1.39	5 (15%)	48,50,50	1.23	7 (14%)
57	PC1	I	301	-	42,42,53	1.04	2 (4%)	48,50,61	1.04	3 (6%)
55	SF4	I	302	9	0,12,12	-	-	-	-	-
69	HEC	AD	401	48	32,50,50	2.17	3 (9%)	24,82,82	1.64	5 (20%)
55	SF4	F	502	6	0,12,12	-	-	-	-	-
59	FES	G	803	7	0,4,4	-	-	-	-	-
58	3PE	H	402	-	45,45,50	0.97	2 (4%)	48,50,55	0.97	2 (4%)
58	3PE	J	201	-	45,45,50	0.97	2 (4%)	48,50,55	1.06	3 (6%)
69	HEC	Ad	401	48	32,50,50	2.15	3 (9%)	24,82,82	1.64	4 (16%)

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
67	HEM	AC	402	47	-	7/12/54/54	-
65	NDP	P	401	-	-	4/30/77/77	0/5/5/5
62	CDL	M	503	-	-	24/92/92/110	-
62	CDL	d	201	-	-	27/75/75/110	-
55	SF4	G	802	7	-	-	0/6/5/5
58	3PE	M	502	-	-	14/52/52/54	-
62	CDL	Aa	501	-	-	17/56/56/110	-
67	HEM	AC	401	47	-	7/12/54/54	-
62	CDL	h	201	-	-	19/78/78/110	-
67	HEM	Ac	403	47	-	6/12/54/54	-
58	3PE	i	201	-	-	9/43/43/54	-
61	UQ9	H	401	-	-	17/30/54/81	0/1/1/1
64	ADP	O	401	-	-	2/12/32/32	0/3/3/3
66	EHZ	W	201	-	-	21/39/39/45	-
62	CDL	L	703	-	-	20/83/83/110	-
62	CDL	q	201	-	-	20/67/67/110	-
55	SF4	I	303	9	-	-	0/6/5/5
57	PC1	B	303	-	-	11/38/38/57	-
58	3PE	L	701	-	-	9/43/43/54	-
59	FES	E	301	5	-	-	0/1/1/1
70	U10	Ac	405	-	-	6/15/39/87	0/1/1/1
58	3PE	M	501	-	-	10/40/40/54	-
58	3PE	D	501	-	-	10/41/41/54	-
58	3PE	m	201	-	-	11/44/44/54	-
62	CDL	Ag	101	-	-	14/52/52/110	-
58	3PE	Ac	401	-	-	7/26/26/54	-
58	3PE	Ac	404	-	-	13/38/38/54	-
67	HEM	Ac	402	47	-	7/12/54/54	-
58	3PE	L	705	-	-	13/47/47/54	-
58	3PE	H	403	-	-	11/54/54/54	-
55	SF4	B	301	2	-	-	0/6/5/5
58	3PE	Ag	103	-	-	10/54/54/54	-
56	UQ1	B	302	-	-	0/9/33/33	0/1/1/1
68	UQ6	Ac	406	-	-	2/15/15/39	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	CDL	Ag	102	-	-	13/66/66/110	-
68	UQ6	AC	403	-	-	4/21/21/39	0/1/1/1
55	SF4	G	801	7	-	-	0/6/5/5
58	3PE	L	702	-	-	13/52/52/54	-
62	CDL	Y	201	-	-	16/81/81/110	-
66	EHZ	n	201	-	-	21/39/39/45	-
60	FMN	F	501	-	-	1/18/18/18	0/3/3/3
57	PC1	I	301	-	-	9/46/46/57	-
55	SF4	I	302	9	-	-	0/6/5/5
69	HEC	AD	401	48	-	0/10/54/54	-
55	SF4	F	502	6	-	-	0/6/5/5
59	FES	G	803	7	-	-	0/1/1/1
58	3PE	H	402	-	-	13/49/49/54	-
58	3PE	J	201	-	-	13/49/49/54	-
69	HEC	Ad	401	48	-	0/10/54/54	-

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	AC	403	UQ6	C5-C4	8.00	1.52	1.39
56	B	302	UQ1	C6-C5	7.58	1.49	1.35
69	Ad	401	HEC	C3C-C2C	-6.41	1.34	1.40
69	AD	401	HEC	C3C-C2C	-6.40	1.34	1.40
69	AD	401	HEC	C2B-C3B	-6.15	1.34	1.40
69	Ad	401	HEC	C2B-C3B	-6.01	1.34	1.40
68	Ac	406	UQ6	C2-C3	5.95	1.49	1.39
68	Ac	406	UQ6	C5-C4	5.92	1.49	1.39
68	Ac	406	UQ6	C5-C6	5.81	1.49	1.40
66	n	201	EHZ	C12-N1	5.51	1.45	1.33
69	Ad	401	HEC	C3D-C2D	5.47	1.53	1.37
69	AD	401	HEC	C3D-C2D	5.41	1.53	1.37
66	W	201	EHZ	C15-N2	5.39	1.45	1.33
68	AC	403	UQ6	C6-C1	5.34	1.49	1.40
66	n	201	EHZ	C15-N2	5.29	1.45	1.33
68	AC	403	UQ6	C5-C6	5.23	1.48	1.40
66	W	201	EHZ	C12-N1	5.18	1.45	1.33
68	Ac	406	UQ6	C6-C1	5.01	1.48	1.40
60	F	501	FMN	C9A-C5A	4.92	1.49	1.41
68	Ac	406	UQ6	C4-C3	4.73	1.49	1.39
62	Y	201	CDL	OA8-CA7	4.30	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	M	501	3PE	O31-C31	4.30	1.45	1.33
58	J	201	3PE	O31-C31	4.29	1.45	1.33
68	Ac	406	UQ6	C2-C1	4.27	1.49	1.40
62	q	201	CDL	OA8-CA7	4.27	1.45	1.33
58	D	501	3PE	O31-C31	4.26	1.45	1.33
62	L	703	CDL	OB8-CB7	4.26	1.45	1.33
58	L	705	3PE	O31-C31	4.26	1.45	1.33
62	q	201	CDL	OB8-CB7	4.26	1.45	1.33
58	M	502	3PE	O31-C31	4.26	1.45	1.33
57	I	301	PC1	O31-C31	4.25	1.45	1.33
58	i	201	3PE	O31-C31	4.25	1.45	1.33
62	d	201	CDL	OB8-CB7	4.24	1.45	1.33
57	B	303	PC1	O31-C31	4.23	1.45	1.33
62	M	503	CDL	OA8-CA7	4.23	1.45	1.33
58	m	201	3PE	O31-C31	4.20	1.45	1.33
58	H	403	3PE	O31-C31	4.20	1.45	1.33
62	M	503	CDL	OB8-CB7	4.19	1.45	1.33
58	H	402	3PE	O31-C31	4.19	1.45	1.33
62	d	201	CDL	OA8-CA7	4.19	1.45	1.33
62	h	201	CDL	OB8-CB7	4.17	1.45	1.33
62	h	201	CDL	OA8-CA7	4.16	1.45	1.33
58	L	701	3PE	O21-C21	4.15	1.46	1.34
58	L	702	3PE	O31-C31	4.13	1.45	1.33
68	AC	403	UQ6	C2-C1	4.13	1.48	1.40
62	M	503	CDL	OB6-CB5	4.11	1.45	1.34
58	L	701	3PE	O31-C31	4.10	1.45	1.33
62	h	201	CDL	OB6-CB5	4.10	1.45	1.34
62	L	703	CDL	OA8-CA7	4.10	1.45	1.33
58	H	402	3PE	O21-C21	4.09	1.45	1.34
62	Y	201	CDL	OB8-CB7	4.08	1.45	1.33
62	d	201	CDL	OB6-CB5	4.08	1.45	1.34
62	h	201	CDL	OA6-CA5	4.08	1.45	1.34
62	q	201	CDL	OB6-CB5	4.07	1.45	1.34
58	M	501	3PE	O21-C21	4.07	1.45	1.34
58	H	403	3PE	O21-C21	4.06	1.45	1.34
58	i	201	3PE	O21-C21	4.06	1.45	1.34
62	M	503	CDL	OA6-CA5	4.05	1.45	1.34
62	L	703	CDL	OB6-CB5	4.05	1.45	1.34
57	I	301	PC1	O21-C21	4.04	1.45	1.34
62	Y	201	CDL	OB6-CB5	4.04	1.45	1.34
57	B	303	PC1	O21-C21	4.04	1.45	1.34
62	Y	201	CDL	OA6-CA5	4.04	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	q	201	CDL	OA6-CA5	4.03	1.45	1.34
58	J	201	3PE	O21-C21	4.02	1.45	1.34
58	m	201	3PE	O21-C21	4.01	1.45	1.34
58	D	501	3PE	O21-C21	4.00	1.45	1.34
58	L	705	3PE	O21-C21	4.00	1.45	1.34
58	M	502	3PE	O21-C21	3.99	1.45	1.34
58	L	702	3PE	O21-C21	3.98	1.45	1.34
62	d	201	CDL	OA6-CA5	3.94	1.45	1.34
62	L	703	CDL	OA6-CA5	3.89	1.45	1.34
67	Ac	403	HEM	C4D-ND	-3.76	1.33	1.40
67	AC	401	HEM	C4D-ND	-3.65	1.34	1.40
67	Ac	402	HEM	C4D-ND	-3.60	1.34	1.40
68	AC	403	UQ6	C2-C3	3.54	1.45	1.39
67	AC	402	HEM	C1B-NB	-3.47	1.34	1.40
67	AC	402	HEM	C4D-ND	-3.46	1.34	1.40
68	AC	403	UQ6	C4-C3	3.29	1.46	1.39
65	P	401	NDP	C6N-C5N	3.26	1.39	1.33
67	Ac	403	HEM	C1B-NB	-3.25	1.34	1.40
60	F	501	FMN	C8-C7	3.15	1.48	1.40
67	AC	401	HEM	C1B-NB	-3.07	1.35	1.40
56	B	302	UQ1	C3-C2	3.05	1.48	1.36
67	Ac	402	HEM	C1B-NB	-3.03	1.35	1.40
70	Ac	405	U10	C6-C5	-2.92	1.38	1.46
70	Ac	405	U10	C4-C3	2.89	1.48	1.36
67	AC	402	HEM	FE-NB	2.87	2.11	1.96
61	H	401	UQ9	C3-C2	-2.69	1.41	1.48
67	Ac	403	HEM	C1D-ND	-2.68	1.33	1.38
66	n	201	EHZ	P1-O7	2.67	1.65	1.54
66	n	201	EHZ	C9-S1	2.57	1.82	1.76
66	W	201	EHZ	P1-O7	2.57	1.64	1.54
70	Ac	405	U10	C3-C2	-2.55	1.41	1.48
67	AC	401	HEM	C1D-ND	-2.54	1.33	1.38
60	F	501	FMN	C4-N3	-2.52	1.34	1.38
61	H	401	UQ9	C4-C5	-2.49	1.41	1.48
67	Ac	402	HEM	C1D-ND	-2.46	1.33	1.38
66	W	201	EHZ	O4-C15	-2.45	1.18	1.23
66	W	201	EHZ	O3-C12	-2.42	1.18	1.23
66	n	201	EHZ	O4-C15	-2.39	1.18	1.23
66	W	201	EHZ	C9-S1	2.38	1.81	1.76
64	O	401	ADP	C5-C4	2.34	1.47	1.40
65	P	401	NDP	C5A-C4A	2.33	1.47	1.40
66	n	201	EHZ	O3-C12	-2.27	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	W	201	EHZ	P1-OP3	-2.24	1.46	1.54
60	F	501	FMN	C5A-N5	-2.20	1.35	1.39
66	n	201	EHZ	P1-OP3	-2.17	1.46	1.54
60	F	501	FMN	C4A-N5	2.14	1.34	1.30
67	AC	401	HEM	CHB-C1B	2.09	1.40	1.35
67	AC	402	HEM	CHB-C1B	2.04	1.40	1.35
67	Ac	402	HEM	CHB-C1B	2.03	1.40	1.35

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
70	Ac	405	U10	C6-C1-C2	7.72	125.28	119.18
66	W	201	EHZ	C8-C9-S1	6.35	121.48	113.63
68	Ac	406	UQ6	C4M-O4-C4	5.92	131.00	114.78
68	AC	403	UQ6	C7-C8-C9	-5.78	118.27	127.24
66	n	201	EHZ	C8-C9-S1	5.56	120.50	113.63
67	AC	402	HEM	CHC-C4B-NB	5.38	130.28	124.43
67	AC	402	HEM	CHD-C1D-ND	4.85	129.70	124.43
67	Ac	402	HEM	CHC-C4B-NB	4.75	129.59	124.43
67	AC	401	HEM	CHC-C4B-NB	4.73	129.56	124.43
62	M	503	CDL	OA6-CA5-C11	4.63	121.47	111.50
68	AC	403	UQ6	O4-C4-C3	-4.61	109.72	120.39
68	Ac	406	UQ6	C7-C8-C9	-4.60	120.11	127.24
67	Ac	403	HEM	C4D-ND-C1D	4.28	109.49	105.07
57	B	303	PC1	O21-C21-C22	4.24	120.65	111.50
62	L	703	CDL	OB6-CB5-C51	4.23	120.61	111.50
62	h	201	CDL	OB6-CB5-C51	4.21	120.57	111.50
67	Ac	403	HEM	CHC-C4B-NB	4.19	128.99	124.43
68	AC	403	UQ6	O4-C4-C5	4.14	127.91	119.00
58	M	502	3PE	O21-C21-C22	4.14	120.42	111.50
62	d	201	CDL	OA6-CA5-C11	4.12	120.37	111.50
68	Ac	406	UQ6	C10-C9-C11	4.10	122.16	115.27
70	Ac	405	U10	C1-C6-C5	-4.08	115.74	119.58
62	Y	201	CDL	OA6-CA5-C11	4.07	120.28	111.50
67	AC	402	HEM	C1B-NB-C4B	4.04	109.25	105.07
58	L	701	3PE	O21-C21-C22	4.02	120.17	111.50
58	J	201	3PE	O21-C21-C22	3.97	120.06	111.50
62	d	201	CDL	OB6-CB5-C51	3.97	120.05	111.50
62	M	503	CDL	OB6-CB5-C51	3.96	120.05	111.50
67	Ac	402	HEM	CHB-C1B-NB	3.95	129.26	124.38
58	L	702	3PE	O21-C21-C22	3.92	119.96	111.50
57	I	301	PC1	O21-C21-C22	3.92	119.95	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	Y	201	CDL	OB6-CB5-C51	3.90	119.91	111.50
58	m	201	3PE	O21-C21-C22	3.90	119.91	111.50
67	Ac	403	HEM	CHB-C1B-NB	3.89	129.19	124.38
58	L	705	3PE	O21-C21-C22	3.86	119.83	111.50
62	q	201	CDL	OB6-CB5-C51	3.86	119.82	111.50
62	q	201	CDL	OA6-CA5-C11	3.85	119.80	111.50
67	AC	401	HEM	CHB-C1B-NB	3.84	129.12	124.38
67	AC	402	HEM	CBD-CAD-C3D	-3.82	102.00	112.63
58	i	201	3PE	O21-C21-C22	3.82	119.72	111.50
69	AD	401	HEC	CMC-C2C-C1C	-3.82	122.60	128.46
67	AC	402	HEM	CHA-C4D-ND	3.74	129.01	124.38
69	Ad	401	HEC	CMC-C2C-C1C	-3.72	122.74	128.46
62	h	201	CDL	OA6-CA5-C11	3.64	119.35	111.50
62	L	703	CDL	OA6-CA5-C11	3.63	119.32	111.50
58	H	402	3PE	O21-C21-C22	3.62	119.31	111.50
58	D	501	3PE	O21-C21-C22	3.60	119.27	111.50
58	M	501	3PE	O21-C21-C22	3.59	119.25	111.50
67	AC	402	HEM	CHB-C1B-NB	3.48	128.68	124.38
65	P	401	NDP	PN-O3-PA	-3.42	121.08	132.83
58	H	403	3PE	O21-C21-C22	3.36	118.74	111.50
67	AC	401	HEM	C4D-ND-C1D	3.29	108.47	105.07
70	Ac	405	U10	C4-C3-C2	-3.28	114.23	120.68
64	O	401	ADP	N3-C2-N1	-3.25	123.59	128.68
64	O	401	ADP	PA-O3A-PB	-3.25	121.68	132.83
68	AC	403	UQ6	C10-C9-C11	3.19	120.64	115.27
67	Ac	402	HEM	C4D-ND-C1D	3.19	108.37	105.07
65	P	401	NDP	N3A-C2A-N1A	-3.19	123.70	128.68
67	Ac	402	HEM	C1B-NB-C4B	3.15	108.33	105.07
67	AC	402	HEM	CHD-C1D-C2D	-3.14	120.08	124.98
67	Ac	403	HEM	C1B-NB-C4B	3.11	108.29	105.07
67	Ac	403	HEM	CHD-C1D-ND	3.11	127.81	124.43
66	W	201	EHZ	C13-C12-N1	3.09	121.62	116.42
67	AC	401	HEM	C1B-NB-C4B	3.04	108.21	105.07
66	W	201	EHZ	C14-C13-C12	-3.04	107.29	112.36
68	Ac	406	UQ6	C6-C7-C8	-2.95	107.50	112.17
58	M	502	3PE	O31-C31-C32	2.94	121.12	111.91
58	M	502	3PE	C2-O21-C21	-2.93	110.58	117.79
64	O	401	ADP	C3'-C2'-C1'	2.91	105.36	100.98
66	W	201	EHZ	OP3-P1-O9	-2.90	99.31	110.68
62	d	201	CDL	CA4-OA6-CA5	-2.87	110.72	117.79
66	W	201	EHZ	C7-C8-C9	-2.86	107.36	113.89
58	L	702	3PE	C2-O21-C21	-2.86	110.75	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	AC	401	HEM	CHD-C1D-ND	2.86	127.54	124.43
58	L	705	3PE	O31-C31-C32	2.82	120.74	111.91
58	i	201	3PE	C2-O21-C21	-2.81	110.88	117.79
65	P	401	NDP	C4A-C5A-N7A	-2.79	106.49	109.40
68	AC	403	UQ6	C15-C14-C16	2.78	119.94	115.27
67	Ac	402	HEM	CHD-C1D-ND	2.78	127.45	124.43
62	M	503	CDL	OA8-CA7-C31	2.77	120.61	111.91
62	d	201	CDL	OA8-CA7-C31	2.77	120.60	111.91
69	Ad	401	HEC	CMB-C2B-C1B	-2.76	124.22	128.46
58	m	201	3PE	O31-C31-C32	2.75	120.55	111.91
58	J	201	3PE	C2-O21-C21	-2.75	111.03	117.79
58	m	201	3PE	C2-O21-C21	-2.75	111.03	117.79
69	AD	401	HEC	CMB-C2B-C1B	-2.74	124.26	128.46
62	q	201	CDL	OB8-CB7-C71	2.73	120.46	111.91
58	H	403	3PE	O31-C31-C32	2.68	120.32	111.91
62	Y	201	CDL	OA8-CA7-C31	2.66	120.27	111.91
58	L	702	3PE	O31-C31-C32	2.65	120.24	111.91
57	I	301	PC1	C2-O21-C21	-2.65	111.28	117.79
66	n	201	EHZ	OP3-P1-O9	-2.64	100.33	110.68
60	F	501	FMN	O4-C4-C4A	-2.64	119.60	126.60
60	F	501	FMN	C4A-C10-N1	-2.64	118.61	124.73
62	h	201	CDL	OB8-CB7-C71	2.61	120.11	111.91
62	Y	201	CDL	CA4-OA6-CA5	-2.60	111.39	117.79
58	H	402	3PE	O31-C31-C32	2.59	120.05	111.91
58	J	201	3PE	O31-C31-C32	2.59	120.03	111.91
62	L	703	CDL	CB4-OB6-CB5	-2.57	111.46	117.79
62	Y	201	CDL	OB8-CB7-C71	2.57	119.96	111.91
70	Ac	405	U10	C7-C6-C5	2.57	121.56	118.48
66	n	201	EHZ	C10-S1-C9	2.56	109.85	101.87
70	Ac	405	U10	O4-C4-C5	-2.56	107.90	116.56
58	i	201	3PE	O31-C31-C32	2.55	119.91	111.91
62	L	703	CDL	OA8-CA7-C31	2.53	119.86	111.91
67	AC	401	HEM	CHA-C4D-ND	2.52	127.50	124.38
62	h	201	CDL	OA8-CA7-C31	2.51	119.79	111.91
57	I	301	PC1	O31-C31-C32	2.50	119.75	111.91
58	L	705	3PE	C2-O21-C21	-2.49	111.66	117.79
56	B	302	UQ1	C11-C9-C10	2.49	120.10	114.60
62	q	201	CDL	OA8-CA7-C31	2.49	119.72	111.91
62	L	703	CDL	OB8-CB7-C71	2.49	119.72	111.91
67	Ac	402	HEM	CHA-C4D-ND	2.47	127.44	124.38
64	O	401	ADP	C4-C5-N7	-2.47	106.82	109.40
62	d	201	CDL	OB8-CB7-C71	2.47	119.66	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	Ac	403	HEM	CHB-C1B-C2B	-2.44	119.97	126.72
56	B	302	UQ1	CM5-C5-C6	-2.43	120.44	124.40
69	Ad	401	HEC	CBD-CAD-C3D	-2.42	108.49	112.62
68	AC	403	UQ6	C12-C13-C14	-2.42	121.84	127.66
57	B	303	PC1	O31-C31-C32	2.41	119.48	111.91
58	M	501	3PE	O31-C31-C32	2.41	119.47	111.91
62	L	703	CDL	CA4-OA6-CA5	-2.41	111.86	117.79
58	D	501	3PE	O31-C31-C32	2.39	119.42	111.91
69	AD	401	HEC	CBD-CAD-C3D	-2.39	108.55	112.62
68	Ac	406	UQ6	C16-C14-C15	2.38	119.87	114.60
68	AC	403	UQ6	C3M-O3-C3	2.37	121.28	114.78
66	W	201	EHZ	C5-C6-C7	-2.37	108.03	114.85
68	AC	403	UQ6	C21-C19-C20	2.34	119.78	114.60
69	AD	401	HEC	C1D-C2D-C3D	-2.34	105.37	107.00
69	Ad	401	HEC	C1D-C2D-C3D	-2.32	105.38	107.00
66	n	201	EHZ	C5-C6-C7	-2.32	108.17	114.85
62	M	503	CDL	OB8-CB7-C71	2.30	119.12	111.91
67	Ac	402	HEM	C4B-C3B-C2B	-2.29	105.30	107.11
58	Ac	401	3PE	C2-O21-C21	2.28	123.40	117.79
57	B	303	PC1	C2-O21-C21	-2.28	112.18	117.79
66	W	201	EHZ	C10-S1-C9	2.27	108.94	101.87
58	M	501	3PE	C2-O21-C21	-2.27	112.21	117.79
62	q	201	CDL	CA4-OA6-CA5	-2.27	112.21	117.79
62	Y	201	CDL	CB4-OB6-CB5	-2.26	112.23	117.79
67	AC	401	HEM	C4B-C3B-C2B	-2.26	105.32	107.11
67	AC	402	HEM	CHA-C4D-C3D	-2.24	121.12	125.33
67	AC	401	HEM	CHB-C1B-C2B	-2.24	120.53	126.72
67	Ac	402	HEM	CHB-C1B-C2B	-2.23	120.54	126.72
68	AC	403	UQ6	C17-C18-C19	-2.22	120.16	127.75
62	d	201	CDL	CB4-OB6-CB5	-2.21	112.34	117.79
60	F	501	FMN	C4-C4A-N5	2.21	121.38	118.23
60	F	501	FMN	C10-N1-C2	2.20	121.29	116.90
58	L	701	3PE	O31-C31-C32	2.19	118.78	111.91
62	h	201	CDL	CA4-OA6-CA5	-2.18	112.41	117.79
66	W	201	EHZ	C11-N1-C12	-2.17	118.81	122.84
67	Ac	403	HEM	CHA-C4D-ND	2.17	127.06	124.38
66	W	201	EHZ	O2-C9-S1	-2.13	119.84	122.61
66	W	201	EHZ	O6-P1-O9	2.12	112.43	106.47
66	W	201	EHZ	O3-C12-N1	-2.12	119.01	123.01
60	F	501	FMN	C4A-C4-N3	2.11	118.54	113.19
67	AC	402	HEM	C4D-ND-C1D	2.10	107.24	105.07
62	M	503	CDL	CA4-OA6-CA5	-2.10	112.63	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	F	501	FMN	O2-C2-N1	-2.09	118.37	121.83
65	P	401	NDP	C3D-C2D-C1D	2.08	105.38	101.43
62	M	503	CDL	OA6-CA5-OA7	-2.05	118.75	123.70
69	AD	401	HEC	CAA-CBA-CGA	-2.05	108.02	113.76
62	Y	201	CDL	OB8-CB7-OB9	-2.04	118.44	123.59
67	Ac	403	HEM	CMC-C2C-C3C	2.04	128.49	124.68
70	Ac	405	U10	C3M-O3-C3	2.04	123.69	116.47
67	Ac	403	HEM	CAD-C3D-C4D	2.03	128.21	124.66
57	B	303	PC1	O21-C21-O22	-2.03	118.80	123.70
58	D	501	3PE	C2-O21-C21	-2.03	112.80	117.79
56	B	302	UQ1	C7-C8-C9	-2.01	120.95	127.26
62	h	201	CDL	OA8-CA7-OA9	-2.01	118.53	123.59
70	Ac	405	U10	O4-C4-C3	2.00	131.20	123.64
60	F	501	FMN	C4-N3-C2	-2.00	121.94	125.64

There are no chirality outliers.

All (451) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	B	303	PC1	C1-O11-P-O12
57	B	303	PC1	C1-O11-P-O14
57	B	303	PC1	C1-O11-P-O13
57	B	303	PC1	O22-C21-O21-C2
58	D	501	3PE	C1-O11-P-O14
58	H	402	3PE	C1-O11-P-O12
58	H	402	3PE	C1-O11-P-O14
58	H	402	3PE	C11-O13-P-O12
58	H	402	3PE	C11-O13-P-O14
58	H	402	3PE	O32-C31-O31-C3
58	H	402	3PE	C32-C31-O31-C3
58	H	403	3PE	C1-O11-P-O12
58	H	403	3PE	C1-O11-P-O13
58	H	403	3PE	C1-O11-P-O14
58	H	403	3PE	C11-O13-P-O14
58	J	201	3PE	C1-O11-P-O12
58	J	201	3PE	C1-O11-P-O13
58	J	201	3PE	C1-O11-P-O14
58	L	701	3PE	C1-O11-P-O12
58	L	701	3PE	C22-C21-O21-C2
58	L	702	3PE	C1-O11-P-O12
58	L	702	3PE	C1-O11-P-O14
58	L	702	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
58	L	702	3PE	C11-O13-P-O12
58	L	702	3PE	C11-O13-P-O14
58	L	702	3PE	O22-C21-O21-C2
58	L	702	3PE	C22-C21-O21-C2
58	L	705	3PE	C1-O11-P-O12
58	L	705	3PE	C11-O13-P-O12
58	L	705	3PE	C11-O13-P-O14
58	L	705	3PE	O22-C21-O21-C2
58	L	705	3PE	C22-C21-O21-C2
58	M	501	3PE	C11-O13-P-O12
58	M	502	3PE	C1-O11-P-O14
58	M	502	3PE	C32-C31-O31-C3
58	M	502	3PE	C22-C21-O21-C2
58	i	201	3PE	C1-O11-P-O12
58	i	201	3PE	C1-O11-P-O13
58	i	201	3PE	C1-O11-P-O14
58	i	201	3PE	C2-C1-O11-P
58	i	201	3PE	C22-C21-O21-C2
58	m	201	3PE	C1-O11-P-O14
58	m	201	3PE	C11-O13-P-O12
58	Ac	401	3PE	C11-O13-P-O12
58	Ac	401	3PE	O13-C11-C12-N
58	Ac	404	3PE	O13-C11-C12-N
58	Ag	103	3PE	C1-O11-P-O12
58	Ag	103	3PE	C1-O11-P-O14
58	Ag	103	3PE	C11-O13-P-O11
58	Ag	103	3PE	O13-C11-C12-N
61	H	401	UQ9	C17-C18-C19-C21
61	H	401	UQ9	C17-C18-C19-C20
61	H	401	UQ9	C12-C13-C14-C16
61	H	401	UQ9	C12-C13-C14-C15
61	H	401	UQ9	C9-C11-C12-C13
61	H	401	UQ9	C7-C8-C9-C11
61	H	401	UQ9	C7-C8-C9-C10
61	H	401	UQ9	C6-C7-C8-C9
62	L	703	CDL	CA3-OA5-PA1-OA4
62	L	703	CDL	CB2-OB2-PB2-OB5
62	L	703	CDL	CB3-OB5-PB2-OB3
62	L	703	CDL	C51-CB5-OB6-CB4
62	M	503	CDL	CA2-OA2-PA1-OA3
62	M	503	CDL	CA2-OA2-PA1-OA4
62	M	503	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
62	M	503	CDL	C11-CA5-OA6-CA4
62	M	503	CDL	CB2-OB2-PB2-OB3
62	M	503	CDL	CB2-OB2-PB2-OB4
62	M	503	CDL	CB2-OB2-PB2-OB5
62	M	503	CDL	CB3-OB5-PB2-OB3
62	M	503	CDL	CB3-OB5-PB2-OB4
62	M	503	CDL	C51-CB5-OB6-CB4
62	Y	201	CDL	CA2-OA2-PA1-OA3
62	Y	201	CDL	CA2-OA2-PA1-OA4
62	Y	201	CDL	CA2-OA2-PA1-OA5
62	Y	201	CDL	CB3-OB5-PB2-OB2
62	d	201	CDL	CA2-OA2-PA1-OA3
62	d	201	CDL	CA2-OA2-PA1-OA4
62	d	201	CDL	CA2-OA2-PA1-OA5
62	d	201	CDL	CB2-OB2-PB2-OB4
62	h	201	CDL	CA2-OA2-PA1-OA3
62	h	201	CDL	CA2-OA2-PA1-OA4
62	h	201	CDL	CA2-OA2-PA1-OA5
62	h	201	CDL	CA3-OA5-PA1-OA4
62	h	201	CDL	CB3-OB5-PB2-OB3
62	h	201	CDL	C51-CB5-OB6-CB4
62	q	201	CDL	CA2-OA2-PA1-OA3
62	q	201	CDL	OA7-CA5-OA6-CA4
62	q	201	CDL	C11-CA5-OA6-CA4
62	q	201	CDL	CB2-OB2-PB2-OB3
62	q	201	CDL	CB2-OB2-PB2-OB4
62	q	201	CDL	CB2-OB2-PB2-OB5
62	q	201	CDL	CB3-OB5-PB2-OB2
62	q	201	CDL	CB3-OB5-PB2-OB4
62	Aa	501	CDL	CA2-OA2-PA1-OA3
62	Aa	501	CDL	CA2-OA2-PA1-OA4
62	Aa	501	CDL	CA2-OA2-PA1-OA5
62	Aa	501	CDL	CB2-OB2-PB2-OB4
62	Ag	101	CDL	CA2-OA2-PA1-OA3
62	Ag	101	CDL	CA2-OA2-PA1-OA4
62	Ag	101	CDL	CB2-OB2-PB2-OB3
62	Ag	101	CDL	CB2-OB2-PB2-OB4
62	Ag	101	CDL	CB2-OB2-PB2-OB5
62	Ag	101	CDL	CB3-OB5-PB2-OB2
62	Ag	101	CDL	CB3-OB5-PB2-OB3
62	Ag	101	CDL	CB3-OB5-PB2-OB4
62	Ag	102	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
62	Ag	102	CDL	CB3-OB5-PB2-OB4
65	P	401	NDP	C2B-O2B-P2B-O2X
65	P	401	NDP	C2N-C3N-C7N-N7N
66	W	201	EHZ	O1-C7-C8-C9
66	W	201	EHZ	C6-C7-C8-C9
66	W	201	EHZ	C7-C8-C9-S1
66	W	201	EHZ	S1-C10-C11-N1
66	W	201	EHZ	C11-C10-S1-C9
66	W	201	EHZ	C16-C17-C20-O6
66	W	201	EHZ	C20-O6-P1-O7
66	W	201	EHZ	C20-O6-P1-O9
66	W	201	EHZ	C20-O6-P1-OP3
66	n	201	EHZ	O1-C7-C8-C9
66	n	201	EHZ	C7-C8-C9-S1
66	n	201	EHZ	C10-C11-N1-C12
66	n	201	EHZ	C15-C16-C17-C18
66	n	201	EHZ	C15-C16-C17-C19
66	n	201	EHZ	C15-C16-C17-C20
66	n	201	EHZ	O5-C16-C17-C18
66	n	201	EHZ	O5-C16-C17-C19
66	n	201	EHZ	O5-C16-C17-C20
66	n	201	EHZ	O2-C9-S1-C10
66	n	201	EHZ	C8-C9-S1-C10
66	n	201	EHZ	C20-O6-P1-O7
66	n	201	EHZ	C20-O6-P1-O9
66	n	201	EHZ	C20-O6-P1-OP3
67	AC	401	HEM	C2B-C3B-CAB-CBB
67	AC	402	HEM	C2B-C3B-CAB-CBB
67	AC	402	HEM	C4B-C3B-CAB-CBB
67	Ac	402	HEM	C2B-C3B-CAB-CBB
67	Ac	403	HEM	C2B-C3B-CAB-CBB
67	Ac	403	HEM	C4B-C3B-CAB-CBB
68	AC	403	UQ6	C1-C6-C7-C8
70	Ac	405	U10	C7-C8-C9-C10
70	Ac	405	U10	C7-C8-C9-C11
58	M	502	3PE	O32-C31-O31-C3
58	m	201	3PE	O32-C31-O31-C3
58	m	201	3PE	C32-C31-O31-C3
70	Ac	405	U10	C12-C13-C14-C15
70	Ac	405	U10	C12-C13-C14-C16
57	I	301	PC1	O22-C21-O21-C2
58	D	501	3PE	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
58	L	701	3PE	O22-C21-O21-C2
58	M	502	3PE	O22-C21-O21-C2
62	L	703	CDL	OB7-CB5-OB6-CB4
62	M	503	CDL	OA7-CA5-OA6-CA4
62	h	201	CDL	OB7-CB5-OB6-CB4
58	M	501	3PE	C2-C3-O31-C31
57	B	303	PC1	C22-C21-O21-C2
57	I	301	PC1	C22-C21-O21-C2
58	D	501	3PE	C22-C21-O21-C2
68	AC	403	UQ6	C15-C14-C16-C17
68	Ac	406	UQ6	C12-C11-C9-C10
68	AC	403	UQ6	C13-C14-C16-C17
58	i	201	3PE	C32-C31-O31-C3
58	i	201	3PE	O22-C21-O21-C2
62	M	503	CDL	OB7-CB5-OB6-CB4
58	Ac	404	3PE	C23-C24-C25-C26
58	H	402	3PE	C22-C21-O21-C2
62	L	703	CDL	C11-CA5-OA6-CA4
58	Ac	404	3PE	C2C-C2D-C2E-C2F
58	i	201	3PE	O32-C31-O31-C3
61	H	401	UQ9	C25-C24-C26-C27
61	H	401	UQ9	C23-C24-C26-C27
61	H	401	UQ9	C14-C16-C17-C18
68	AC	403	UQ6	C9-C11-C12-C13
58	H	403	3PE	C32-C31-O31-C3
62	Y	201	CDL	C31-CA7-OA8-CA6
62	Y	201	CDL	C71-CB7-OB8-CB6
62	h	201	CDL	C71-CB7-OB8-CB6
62	q	201	CDL	C31-CA7-OA8-CA6
58	Ac	404	3PE	C2A-C2B-C2C-C2D
58	H	403	3PE	O32-C31-O31-C3
62	h	201	CDL	OB9-CB7-OB8-CB6
68	Ac	406	UQ6	C12-C11-C9-C8
58	H	402	3PE	O22-C21-O21-C2
58	m	201	3PE	C22-C21-O21-C2
62	q	201	CDL	C51-CB5-OB6-CB4
62	Y	201	CDL	OB9-CB7-OB8-CB6
67	AC	401	HEM	C2A-CAA-CBA-CGA
67	Ac	402	HEM	C2A-CAA-CBA-CGA
58	Ag	103	3PE	C32-C33-C34-C35
58	Ac	404	3PE	C21-C22-C23-C24
62	h	201	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
62	d	201	CDL	C54-C55-C56-C57
62	Y	201	CDL	OA9-CA7-OA8-CA6
62	q	201	CDL	OA9-CA7-OA8-CA6
62	d	201	CDL	O1-C1-CB2-OB2
62	L	703	CDL	OA7-CA5-OA6-CA4
62	q	201	CDL	OB7-CB5-OB6-CB4
57	I	301	PC1	C32-C31-O31-C3
62	d	201	CDL	C11-CA5-OA6-CA4
58	H	402	3PE	C1-O11-P-O13
58	H	402	3PE	C11-O13-P-O11
58	H	403	3PE	C11-O13-P-O11
58	L	701	3PE	C1-O11-P-O13
58	L	702	3PE	C1-O11-P-O13
58	L	705	3PE	C1-O11-P-O13
58	L	705	3PE	C11-O13-P-O11
58	M	501	3PE	C1-O11-P-O13
58	M	501	3PE	C11-O13-P-O11
58	M	502	3PE	C1-O11-P-O13
58	M	502	3PE	C11-O13-P-O11
58	Ac	401	3PE	C11-O13-P-O11
58	Ag	103	3PE	C1-O11-P-O13
62	L	703	CDL	CA3-OA5-PA1-OA2
62	L	703	CDL	CB3-OB5-PB2-OB2
62	M	503	CDL	CA3-OA5-PA1-OA2
62	M	503	CDL	CB3-OB5-PB2-OB2
62	d	201	CDL	CA3-OA5-PA1-OA2
62	d	201	CDL	CB2-OB2-PB2-OB5
62	d	201	CDL	CB3-OB5-PB2-OB2
62	h	201	CDL	CB3-OB5-PB2-OB2
62	q	201	CDL	CA3-OA5-PA1-OA2
62	Aa	501	CDL	CB2-OB2-PB2-OB5
62	Aa	501	CDL	CB3-OB5-PB2-OB2
62	Ag	101	CDL	CA2-OA2-PA1-OA5
62	Ag	102	CDL	CB3-OB5-PB2-OB2
62	L	703	CDL	C71-CB7-OB8-CB6
62	d	201	CDL	CA2-C1-CB2-OB2
58	m	201	3PE	O22-C21-O21-C2
58	Ag	103	3PE	C3C-C3D-C3E-C3F
62	L	703	CDL	C11-C12-C13-C14
58	M	501	3PE	C32-C33-C34-C35
62	q	201	CDL	CB6-CB4-OB6-CB5
62	d	201	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
62	L	703	CDL	OB9-CB7-OB8-CB6
58	Ag	103	3PE	C37-C38-C39-C3A
62	M	503	CDL	C62-C63-C64-C65
62	Ag	102	CDL	C74-C75-C76-C77
58	M	501	3PE	C23-C24-C25-C26
62	d	201	CDL	C71-CB7-OB8-CB6
57	I	301	PC1	O32-C31-O31-C3
57	B	303	PC1	C32-C33-C34-C35
58	J	201	3PE	C32-C31-O31-C3
58	M	501	3PE	C32-C31-O31-C3
62	h	201	CDL	C14-C15-C16-C17
62	M	503	CDL	C71-CB7-OB8-CB6
58	Ac	404	3PE	C22-C21-O21-C2
57	B	303	PC1	C23-C24-C25-C26
61	H	401	UQ9	C15-C14-C16-C17
61	H	401	UQ9	C13-C14-C16-C17
61	H	401	UQ9	C12-C11-C9-C8
58	J	201	3PE	O32-C31-O31-C3
62	d	201	CDL	OB9-CB7-OB8-CB6
58	J	201	3PE	O22-C21-O21-C2
62	L	703	CDL	C31-CA7-OA8-CA6
62	d	201	CDL	C31-CA7-OA8-CA6
58	M	501	3PE	O32-C31-O31-C3
58	J	201	3PE	C22-C21-O21-C2
62	Ag	101	CDL	OB5-CB3-CB4-OB6
67	AC	401	HEM	C4B-C3B-CAB-CBB
67	Ac	402	HEM	C4B-C3B-CAB-CBB
61	H	401	UQ9	C12-C11-C9-C10
58	H	402	3PE	C31-C32-C33-C34
58	M	502	3PE	C2-C3-O31-C31
58	L	702	3PE	C24-C25-C26-C27
62	M	503	CDL	OB9-CB7-OB8-CB6
62	d	201	CDL	OA9-CA7-OA8-CA6
58	Ac	404	3PE	O22-C21-O21-C2
58	J	201	3PE	C2A-C2B-C2C-C2D
62	q	201	CDL	CA2-OA2-PA1-OA5
58	i	201	3PE	C27-C28-C29-C2A
62	Ag	102	CDL	C1-CB2-OB2-PB2
58	H	402	3PE	C2E-C2F-C2G-C2H
58	L	705	3PE	C3C-C3D-C3E-C3F
62	L	703	CDL	OA9-CA7-OA8-CA6
66	n	201	EHZ	C5-C6-C7-O1

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Mol	Chain	Res	Type	Atoms
58	H	402	3PE	C3-C2-O21-C21
62	L	703	CDL	C74-C75-C76-C77
58	H	403	3PE	C3E-C3F-C3G-C3H
58	L	702	3PE	C28-C29-C2A-C2B
66	n	201	EHZ	C3-C4-C5-C6
58	Ac	404	3PE	C29-C2A-C2B-C2C
62	Ag	101	CDL	OB5-CB3-CB4-CB6
62	Ag	102	CDL	OB5-CB3-CB4-CB6
62	h	201	CDL	C18-C19-C20-C21
58	D	501	3PE	C24-C25-C26-C27
58	Ac	404	3PE	C2B-C2C-C2D-C2E
66	W	201	EHZ	N2-C15-C16-C17
62	Y	201	CDL	CB2-OB2-PB2-OB5
58	H	403	3PE	C37-C38-C39-C3A
62	Ag	102	CDL	OB5-CB3-CB4-OB6
66	W	201	EHZ	C3-C4-C5-C6
66	W	201	EHZ	C5-C6-C7-O1
66	W	201	EHZ	O2-C9-S1-C10
62	Aa	501	CDL	OB5-CB3-CB4-CB6
66	n	201	EHZ	C5-C6-C7-C8
58	Ac	404	3PE	C32-C31-O31-C3
58	L	701	3PE	C3-C2-O21-C21
62	h	201	CDL	CB3-CB4-OB6-CB5
62	h	201	CDL	CB4-CB3-OB5-PB2
62	Ag	102	CDL	CB4-CB3-OB5-PB2
62	Aa	501	CDL	OB5-CB3-CB4-OB6
58	L	705	3PE	C27-C28-C29-C2A
58	Ac	404	3PE	O32-C31-O31-C3
65	P	401	NDP	PN-O3-PA-O2A
58	D	501	3PE	C1-O11-P-O13
58	m	201	3PE	C1-O11-P-O13
58	m	201	3PE	C11-O13-P-O11
62	h	201	CDL	CA3-OA5-PA1-OA2
65	P	401	NDP	O4D-C1D-N1N-C6N
62	Y	201	CDL	C1-CA2-OA2-PA1
62	q	201	CDL	C1-CA2-OA2-PA1
57	I	301	PC1	C11-C12-N-C13
57	I	301	PC1	C11-C12-N-C15
58	H	403	3PE	C11-O13-P-O12
58	L	701	3PE	C1-O11-P-O14
58	L	705	3PE	C1-O11-P-O14
58	M	501	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
58	M	501	3PE	C1-O11-P-O14
58	M	502	3PE	C1-O11-P-O12
58	M	502	3PE	C11-O13-P-O12
58	M	502	3PE	C11-O13-P-O14
58	m	201	3PE	C11-O13-P-O14
58	Ac	401	3PE	C11-O13-P-O14
58	Ag	103	3PE	C11-O13-P-O12
62	L	703	CDL	CA3-OA5-PA1-OA3
62	L	703	CDL	CB2-OB2-PB2-OB4
62	L	703	CDL	CB3-OB5-PB2-OB4
62	M	503	CDL	CA3-OA5-PA1-OA3
62	Y	201	CDL	CB3-OB5-PB2-OB4
62	d	201	CDL	CA3-OA5-PA1-OA3
62	d	201	CDL	CB3-OB5-PB2-OB3
62	h	201	CDL	CB3-OB5-PB2-OB4
62	q	201	CDL	CA3-OA5-PA1-OA3
62	q	201	CDL	CB3-OB5-PB2-OB3
62	Aa	501	CDL	CB2-OB2-PB2-OB3
62	Aa	501	CDL	CB3-OB5-PB2-OB3
62	Aa	501	CDL	CB3-OB5-PB2-OB4
62	Ag	102	CDL	CB2-OB2-PB2-OB4
66	n	201	EHZ	C6-C7-C8-C9
58	L	705	3PE	C32-C31-O31-C3
62	M	503	CDL	C31-CA7-OA8-CA6
62	d	201	CDL	C51-CB5-OB6-CB4
58	L	701	3PE	C36-C37-C38-C39
58	L	705	3PE	O32-C31-O31-C3
62	M	503	CDL	OA9-CA7-OA8-CA6
58	L	701	3PE	C2-C1-O11-P
58	L	702	3PE	C33-C34-C35-C36
62	L	703	CDL	C32-C33-C34-C35
58	M	502	3PE	C2D-C2E-C2F-C2G
66	W	201	EHZ	O4-C15-C16-O5
66	n	201	EHZ	O4-C15-C16-O5
66	W	201	EHZ	C19-C17-C20-O6
62	d	201	CDL	OB7-CB5-OB6-CB4
58	L	705	3PE	C36-C37-C38-C39
60	F	501	FMN	C5'-O5'-P-O1P
62	M	503	CDL	CB4-CB3-OB5-PB2
62	Ag	102	CDL	C1-CA2-OA2-PA1
57	I	301	PC1	C1-O11-P-O13
62	Y	201	CDL	C55-C56-C57-C58

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Mol	Chain	Res	Type	Atoms
66	n	201	EHZ	C2-C3-C4-C5
58	J	201	3PE	C36-C37-C38-C39
58	Ag	103	3PE	C35-C36-C37-C38
66	W	201	EHZ	C2-C3-C4-C5
61	H	401	UQ9	C20-C19-C21-C22
58	D	501	3PE	C32-C31-O31-C3
62	M	503	CDL	C58-C59-C60-C61
58	D	501	3PE	O32-C31-O31-C3
58	H	403	3PE	C24-C25-C26-C27
61	H	401	UQ9	C18-C19-C21-C22
67	AC	402	HEM	CAA-CBA-CGA-O1A
58	L	702	3PE	C2-C1-O11-P
64	O	401	ADP	C4'-C5'-O5'-PA
67	AC	402	HEM	CAD-CBD-CGD-O1D
70	Ac	405	U10	C12-C11-C9-C10
62	Y	201	CDL	C56-C57-C58-C59
57	B	303	PC1	C1-C2-C3-O31
62	L	703	CDL	CA3-CA4-CA6-OA8
62	M	503	CDL	CB3-CB4-CB6-OB8
67	Ac	403	HEM	CAD-CBD-CGD-O1D
67	AC	402	HEM	CAA-CBA-CGA-O2A
66	n	201	EHZ	C7-C8-C9-O2
58	m	201	3PE	C3-C2-O21-C21
57	I	301	PC1	C11-C12-N-C14
67	AC	401	HEM	CAD-CBD-CGD-O2D
67	Ac	402	HEM	CAD-CBD-CGD-O1D
67	Ac	402	HEM	CAD-CBD-CGD-O2D
67	AC	401	HEM	CAA-CBA-CGA-O2A
67	AC	401	HEM	CAD-CBD-CGD-O1D
67	Ac	402	HEM	CAA-CBA-CGA-O2A
67	Ac	403	HEM	CAD-CBD-CGD-O2D
64	O	401	ADP	O4'-C4'-C5'-O5'
67	AC	401	HEM	CAA-CBA-CGA-O1A
67	AC	402	HEM	CAD-CBD-CGD-O2D
67	Ac	402	HEM	CAA-CBA-CGA-O1A
62	M	503	CDL	C36-C37-C38-C39
70	Ac	405	U10	C12-C11-C9-C8
62	Ag	102	CDL	C72-C73-C74-C75
58	M	502	3PE	C34-C35-C36-C37
67	Ac	403	HEM	CAA-CBA-CGA-O2A
62	Ag	102	CDL	C52-C51-CB5-OB6
58	J	201	3PE	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
57	I	301	PC1	C32-C33-C34-C35
62	Ag	101	CDL	C72-C71-CB7-OB8
62	d	201	CDL	CB4-CB3-OB5-PB2
62	q	201	CDL	CA4-CA3-OA5-PA1
58	J	201	3PE	O21-C2-C3-O31
66	W	201	EHZ	N2-C15-C16-O5
62	Y	201	CDL	OA7-CA5-OA6-CA4
66	W	201	EHZ	C18-C17-C20-O6
62	Aa	501	CDL	C32-C31-CA7-OA8
58	M	502	3PE	C32-C33-C34-C35
58	J	201	3PE	C38-C39-C3A-C3B
67	Ac	403	HEM	CAA-CBA-CGA-O1A
58	D	501	3PE	C32-C33-C34-C35
66	W	201	EHZ	C15-C16-C17-C18
58	J	201	3PE	O11-C1-C2-C3
58	Ac	401	3PE	O31-C31-C32-C33
62	d	201	CDL	C32-C31-CA7-OA8
62	Ag	101	CDL	C72-C71-CB7-OB9
66	W	201	EHZ	O5-C16-C17-C18
62	Y	201	CDL	C11-CA5-OA6-CA4
58	L	702	3PE	C26-C27-C28-C29
57	B	303	PC1	C32-C31-O31-C3
58	D	501	3PE	C34-C35-C36-C37
62	d	201	CDL	C57-C58-C59-C60
67	AC	402	HEM	C2A-CAA-CBA-CGA
62	Aa	501	CDL	C32-C31-CA7-OA9
57	B	303	PC1	O32-C31-O31-C3
62	Aa	501	CDL	CB3-CB4-CB6-OB8
62	d	201	CDL	C1-CB2-OB2-PB2
62	q	201	CDL	CB4-CB3-OB5-PB2
58	m	201	3PE	C1-O11-P-O12
62	Y	201	CDL	CB2-OB2-PB2-OB4
62	h	201	CDL	CA3-OA5-PA1-OA3
62	d	201	CDL	C34-C35-C36-C37
58	Ac	404	3PE	O21-C21-C22-C23
58	L	701	3PE	C22-C23-C24-C25
57	B	303	PC1	C3-C2-O21-C21
58	D	501	3PE	C12-C11-O13-P
66	W	201	EHZ	O4-C15-C16-C17
62	Ag	101	CDL	C32-C31-CA7-OA8
62	d	201	CDL	C56-C57-C58-C59
62	Aa	501	CDL	C12-C11-CA5-OA6

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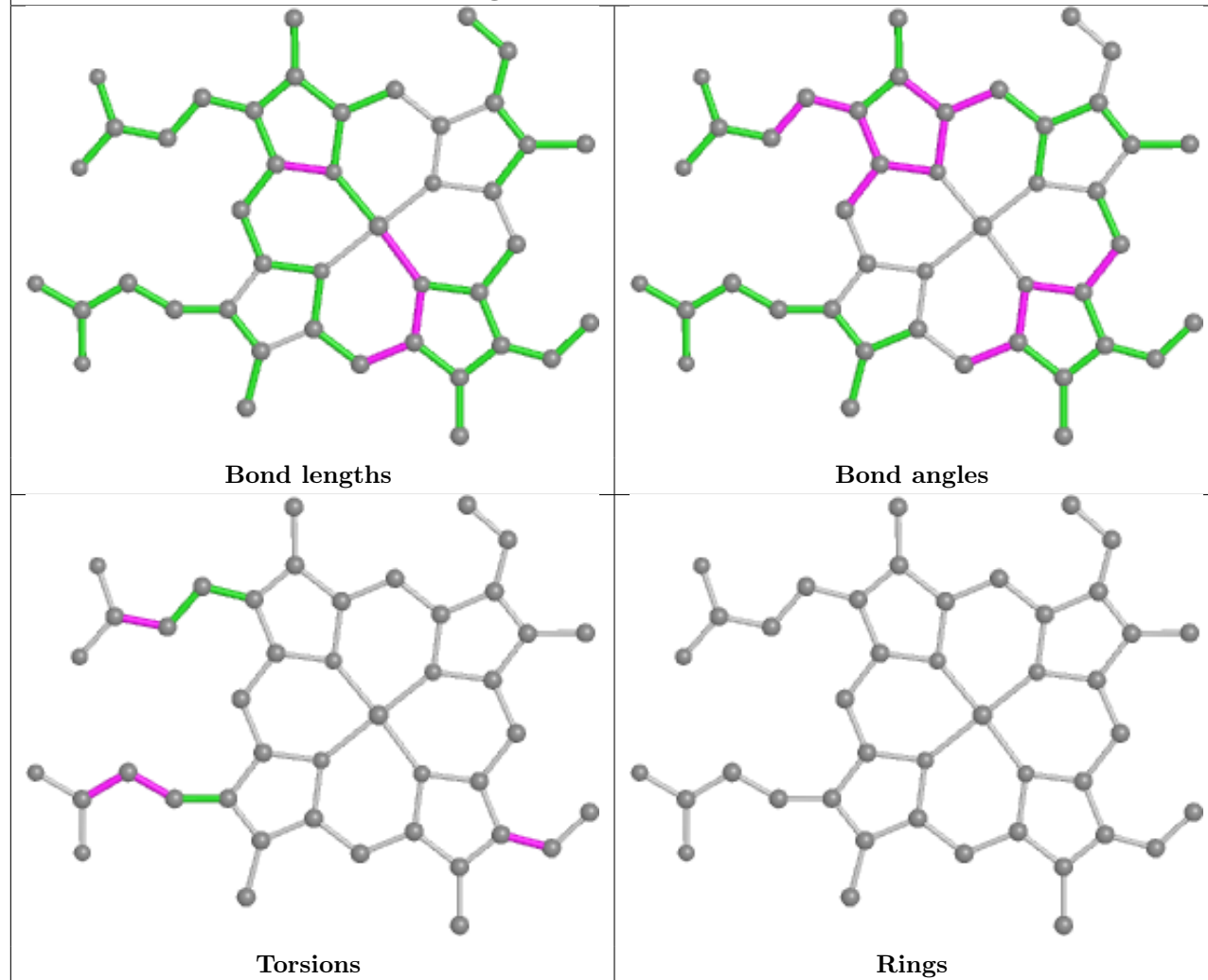
Mol	Chain	Res	Type	Atoms
62	Ag	102	CDL	CB2-C1-CA2-OA2
62	d	201	CDL	C32-C31-CA7-OA9
62	Aa	501	CDL	C12-C11-CA5-OA7
62	h	201	CDL	C11-C12-C13-C14
58	Ac	401	3PE	O21-C21-C22-C23
62	Aa	501	CDL	C72-C71-CB7-OB8
58	Ac	401	3PE	O32-C31-C32-C33
58	Ac	404	3PE	O22-C21-C22-C23

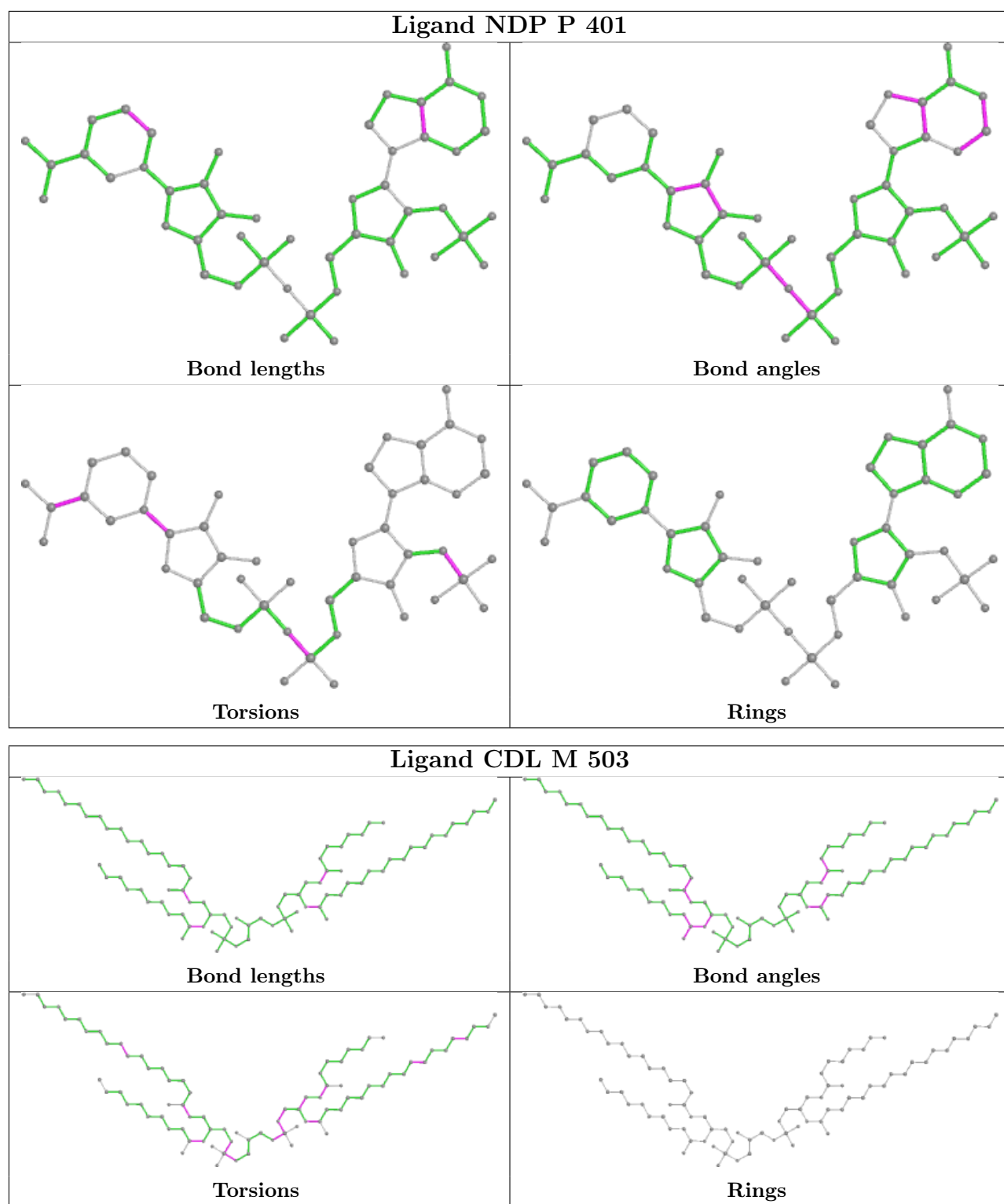
There are no ring outliers.

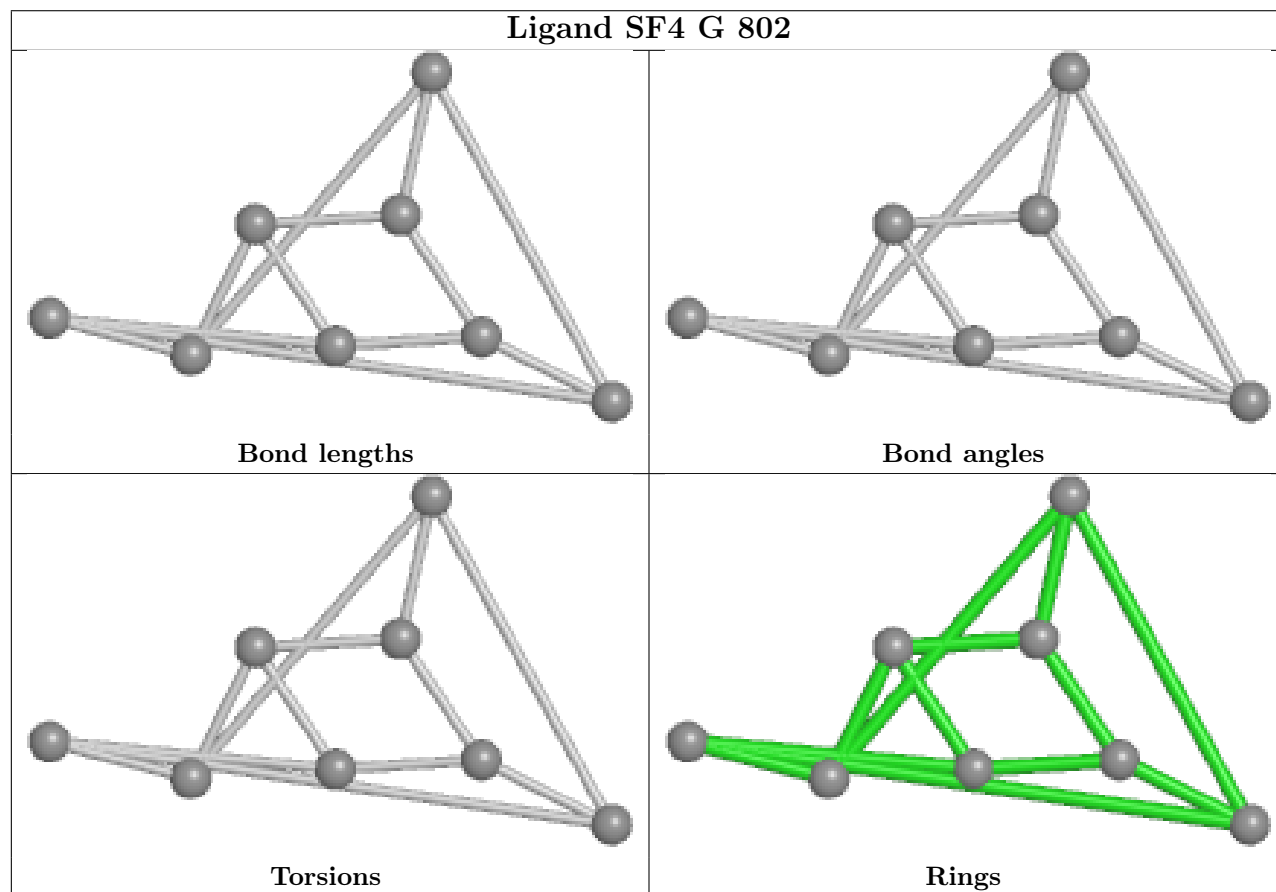
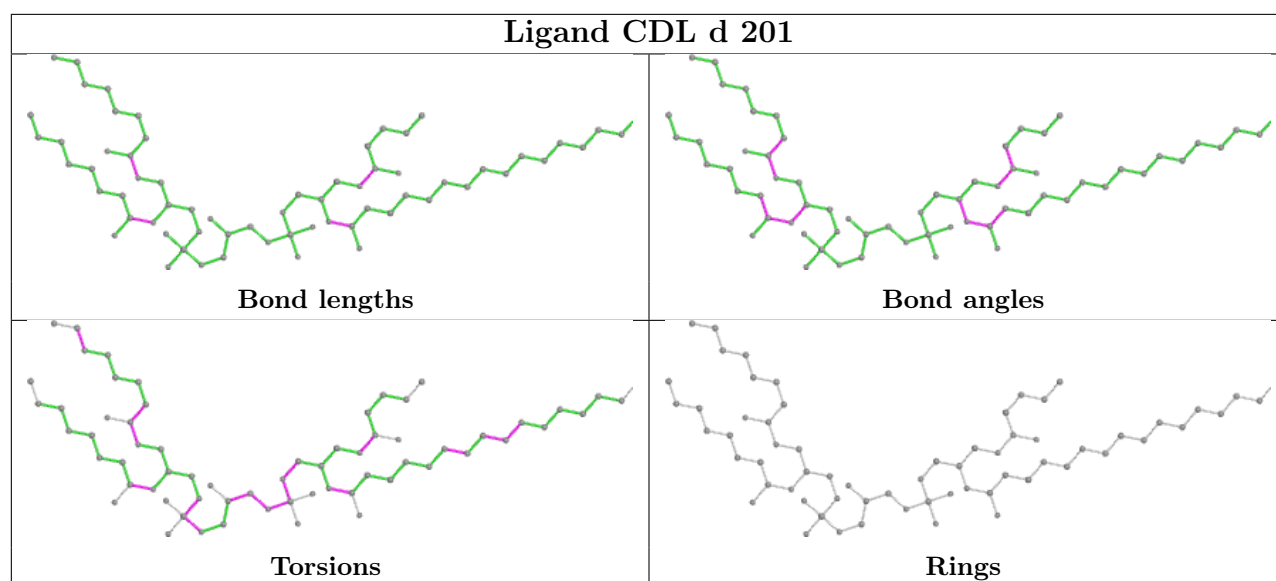
No monomer is involved in short contacts.

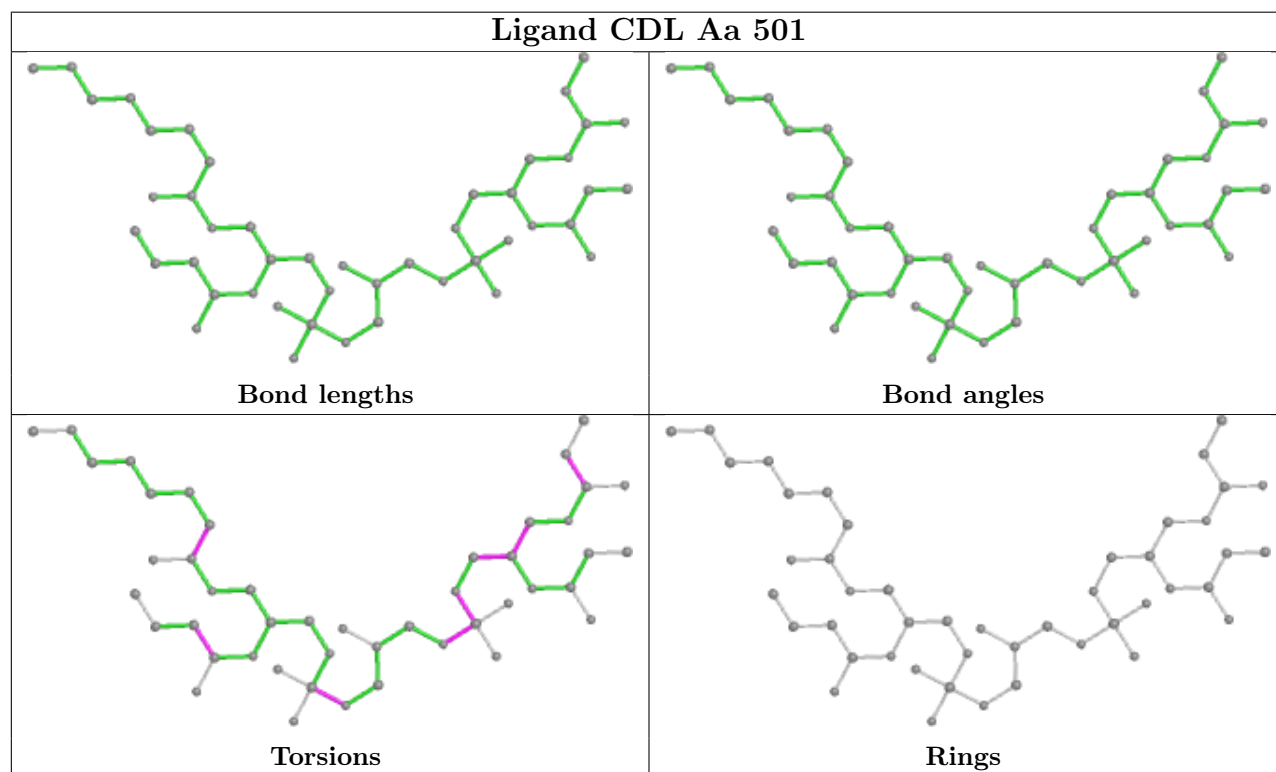
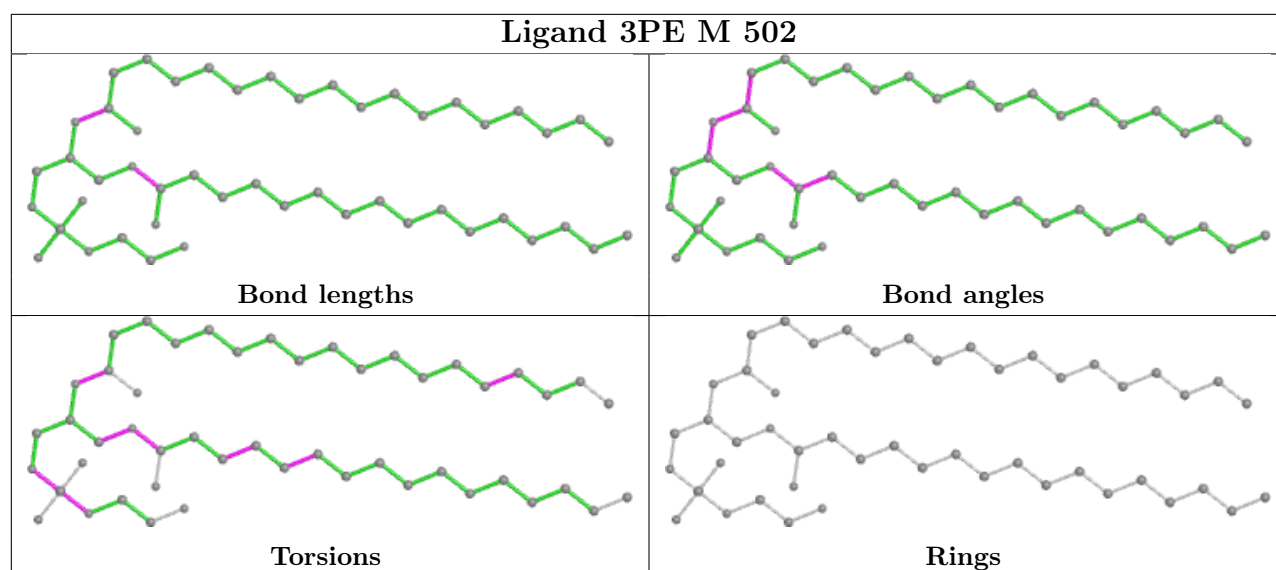
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand HEM AC 402

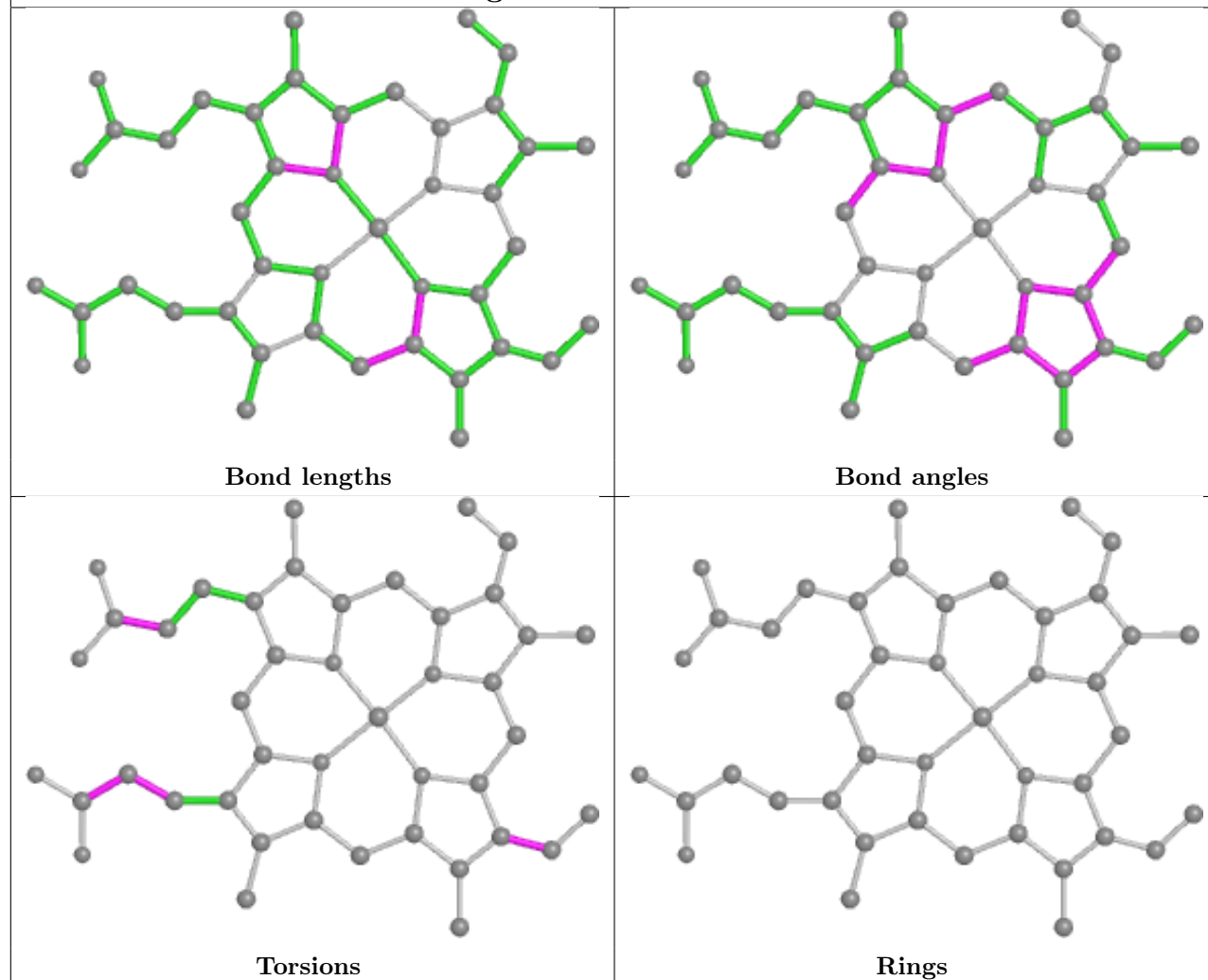




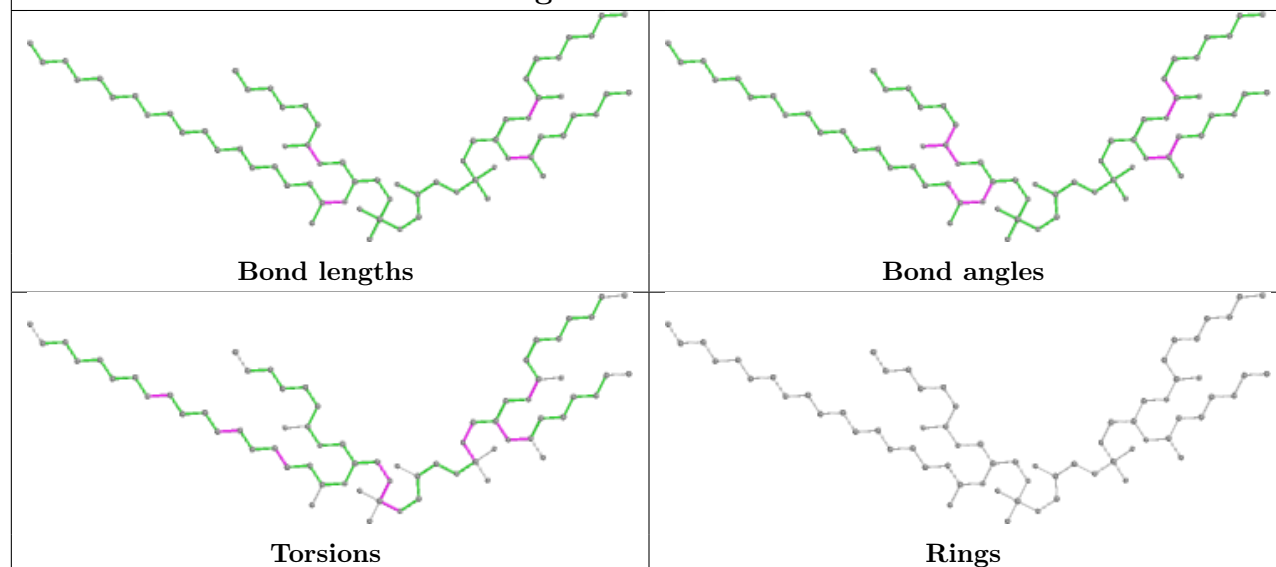


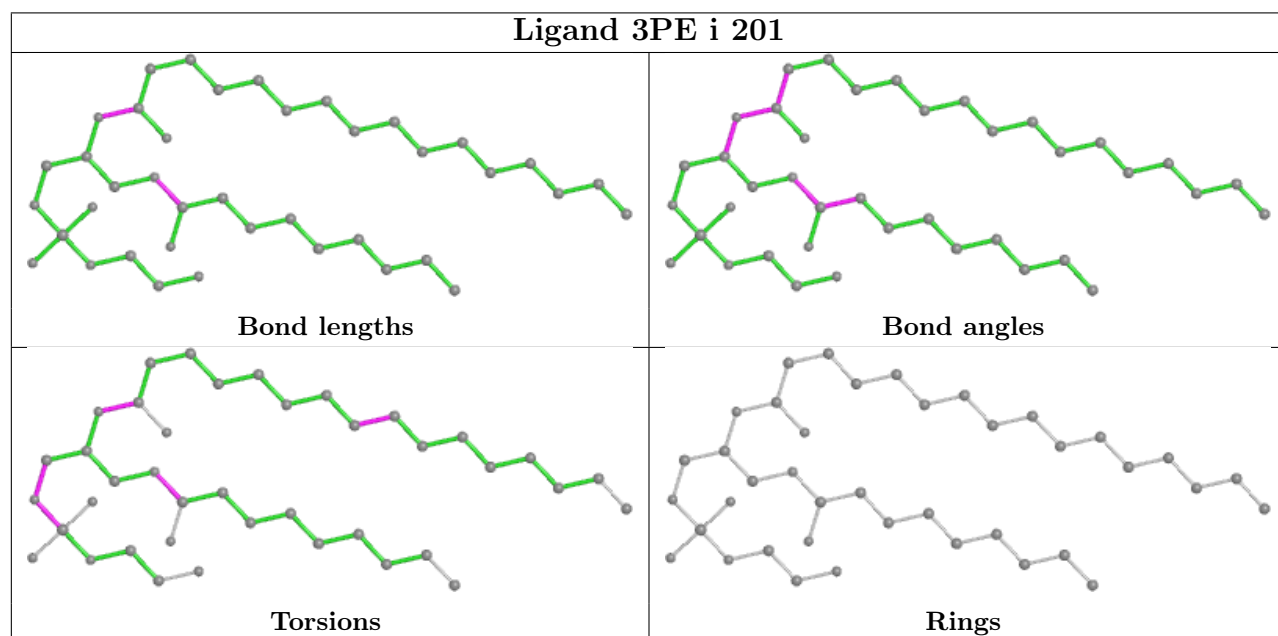
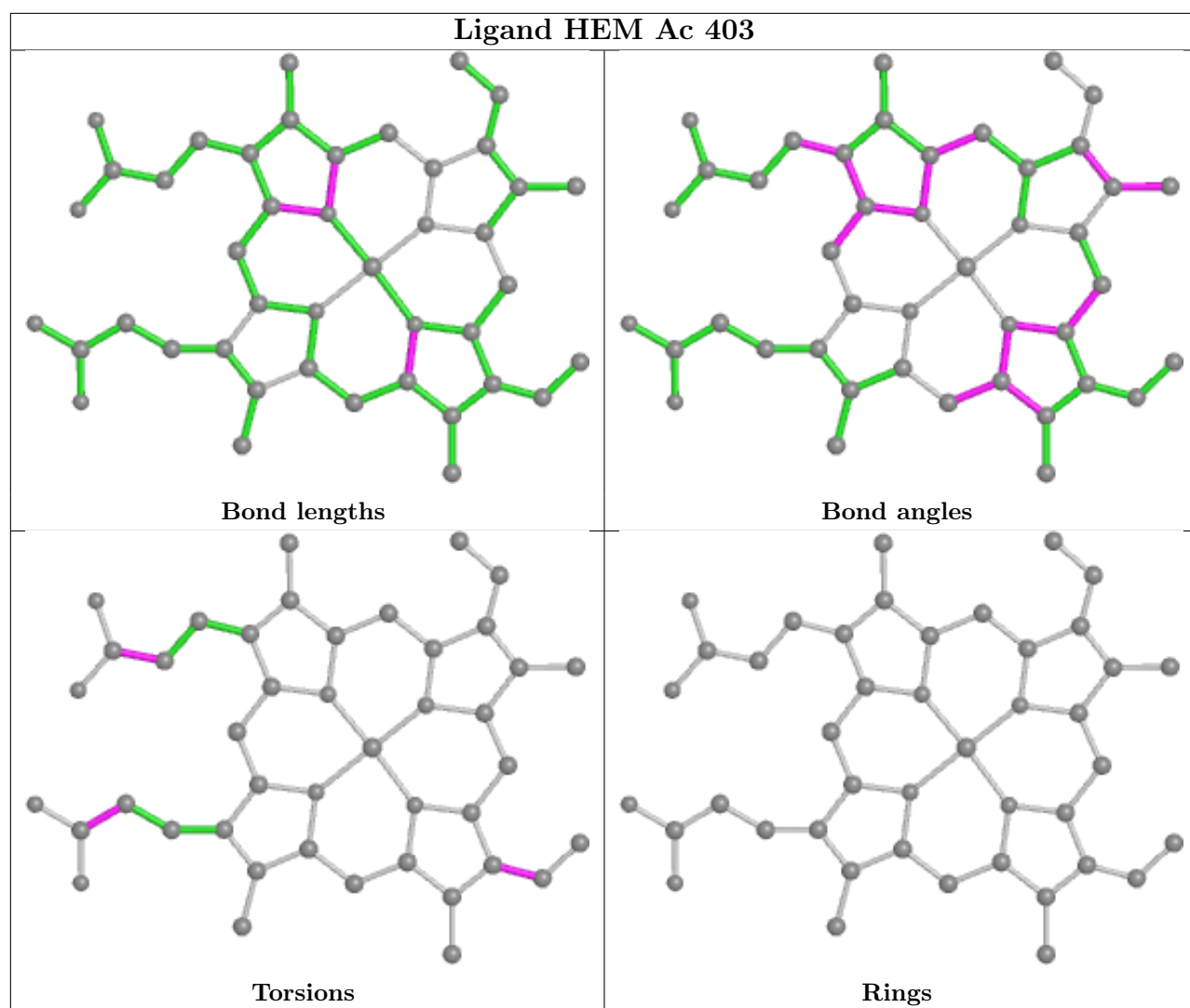


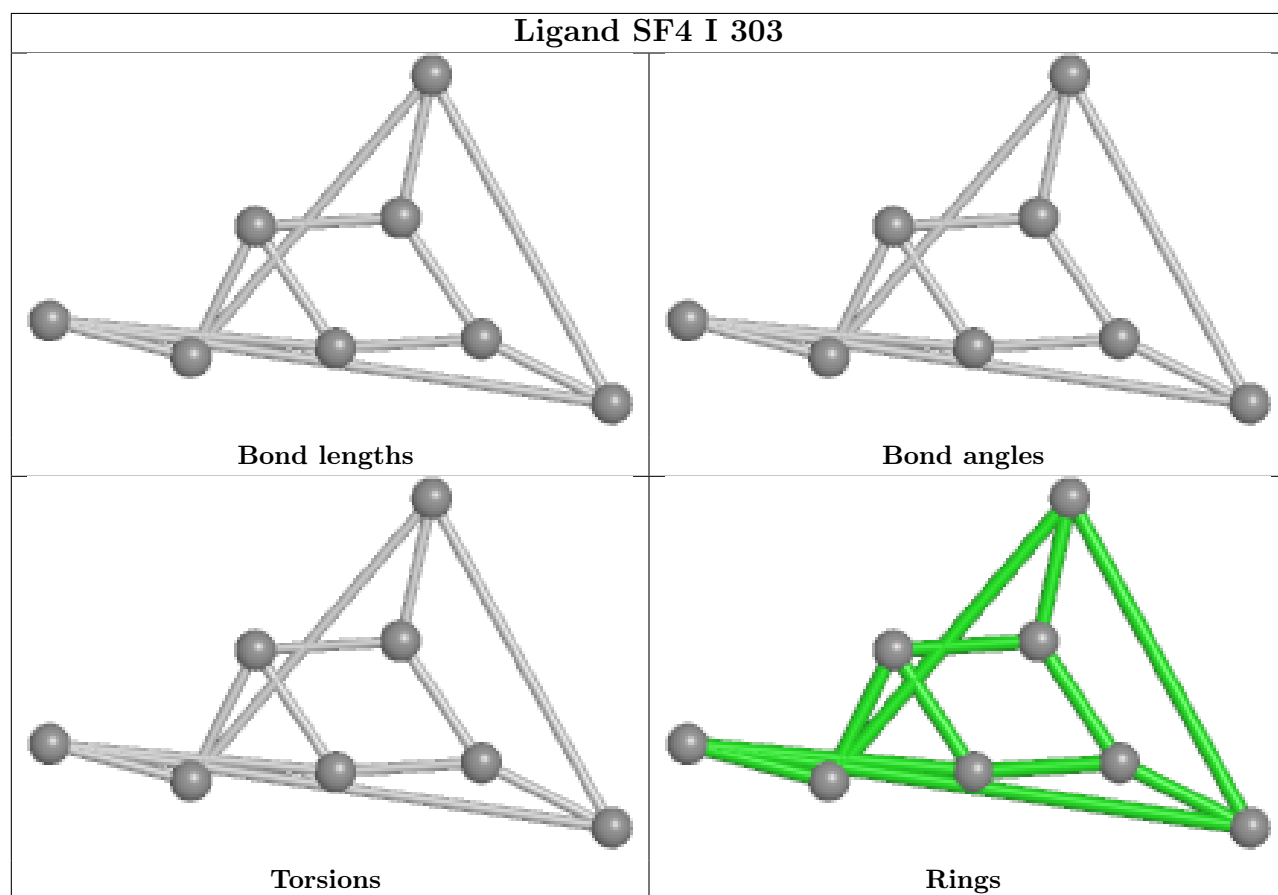
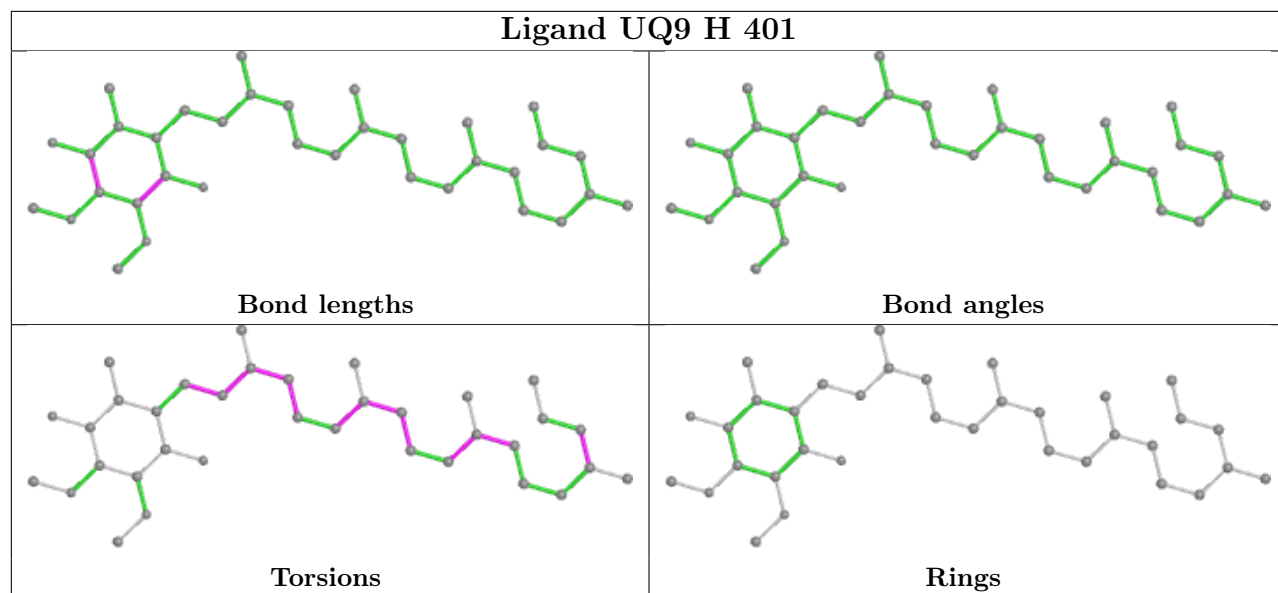
Ligand HEM AC 401

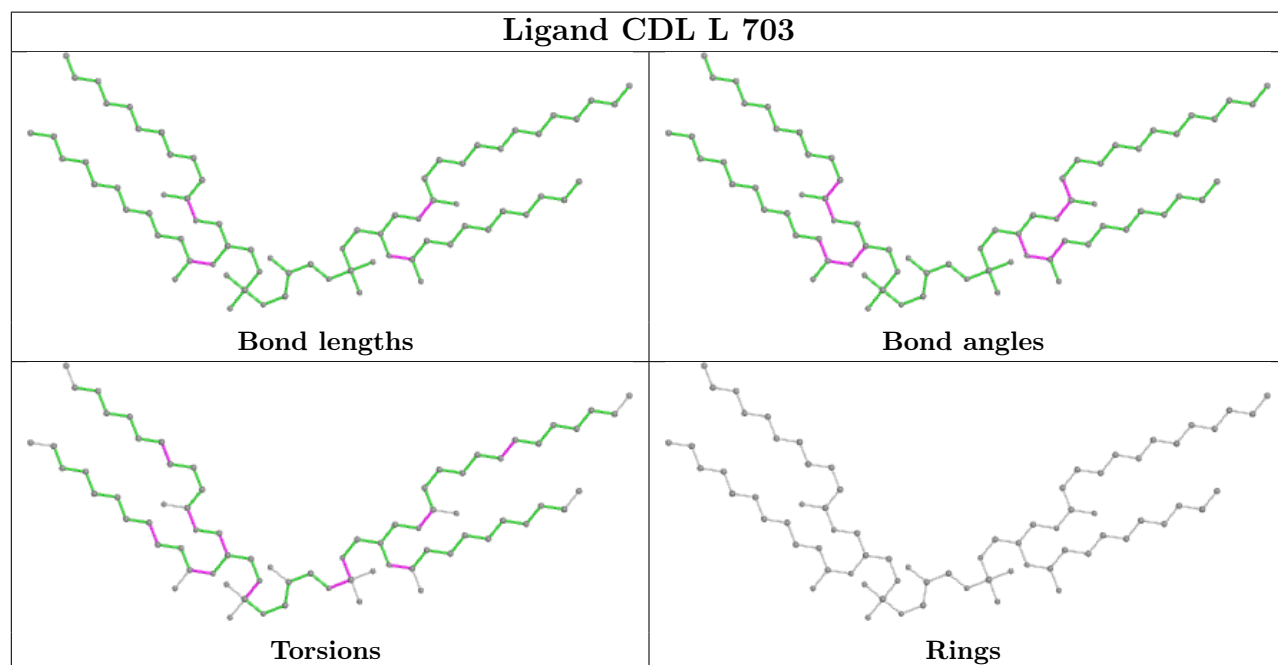
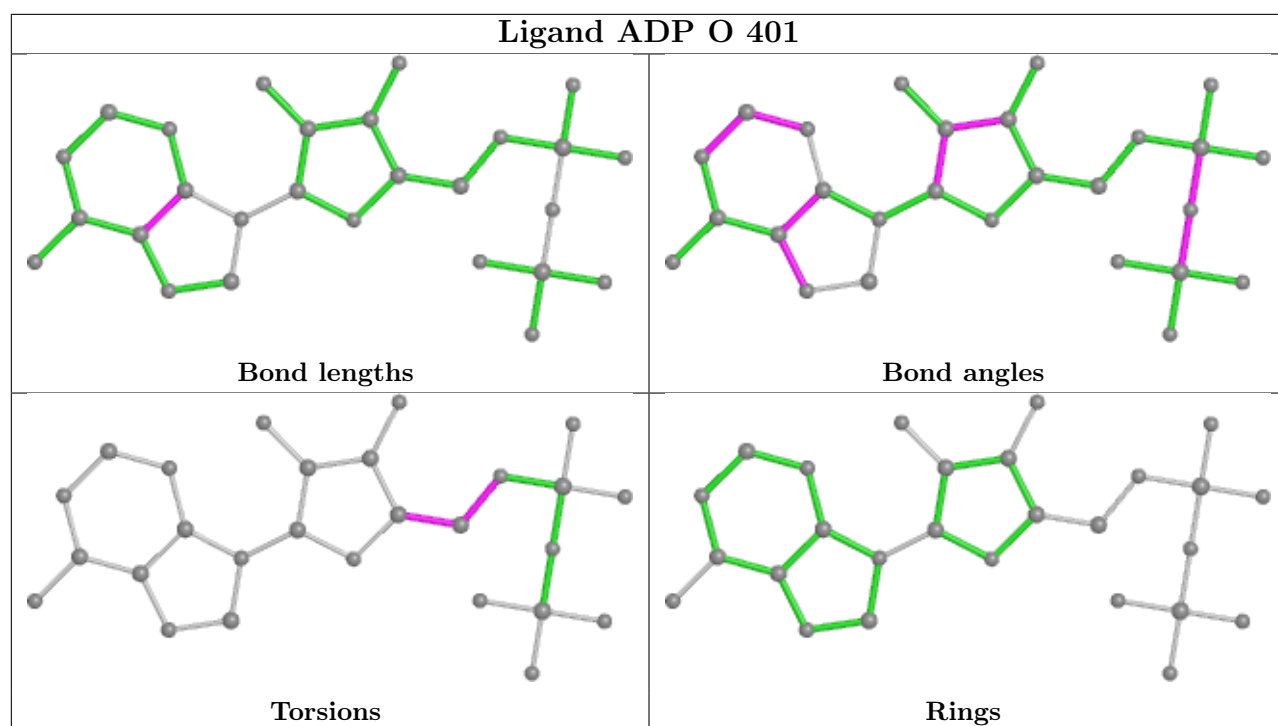


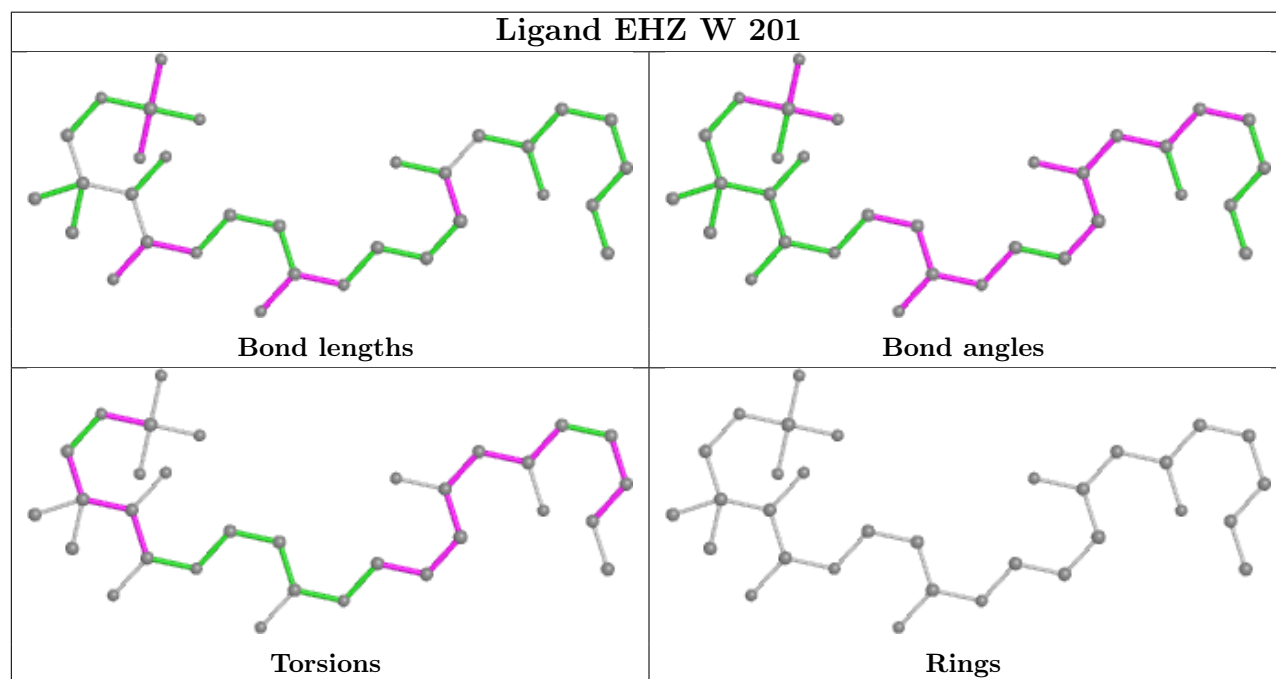
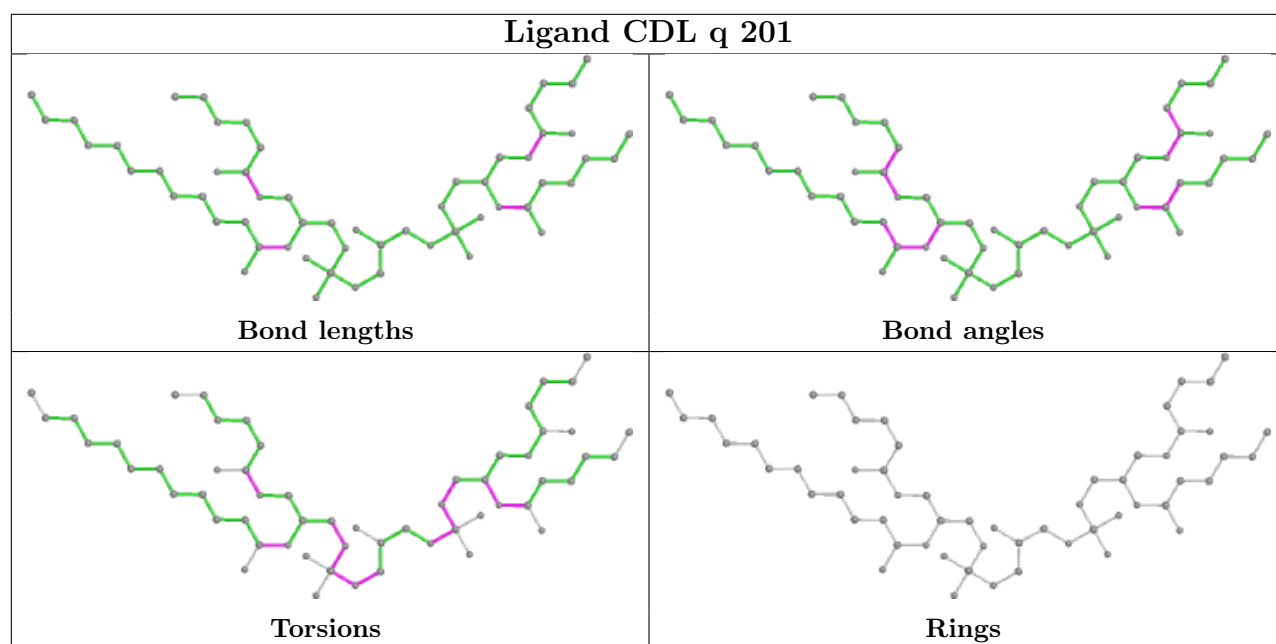
Ligand CDL h 201

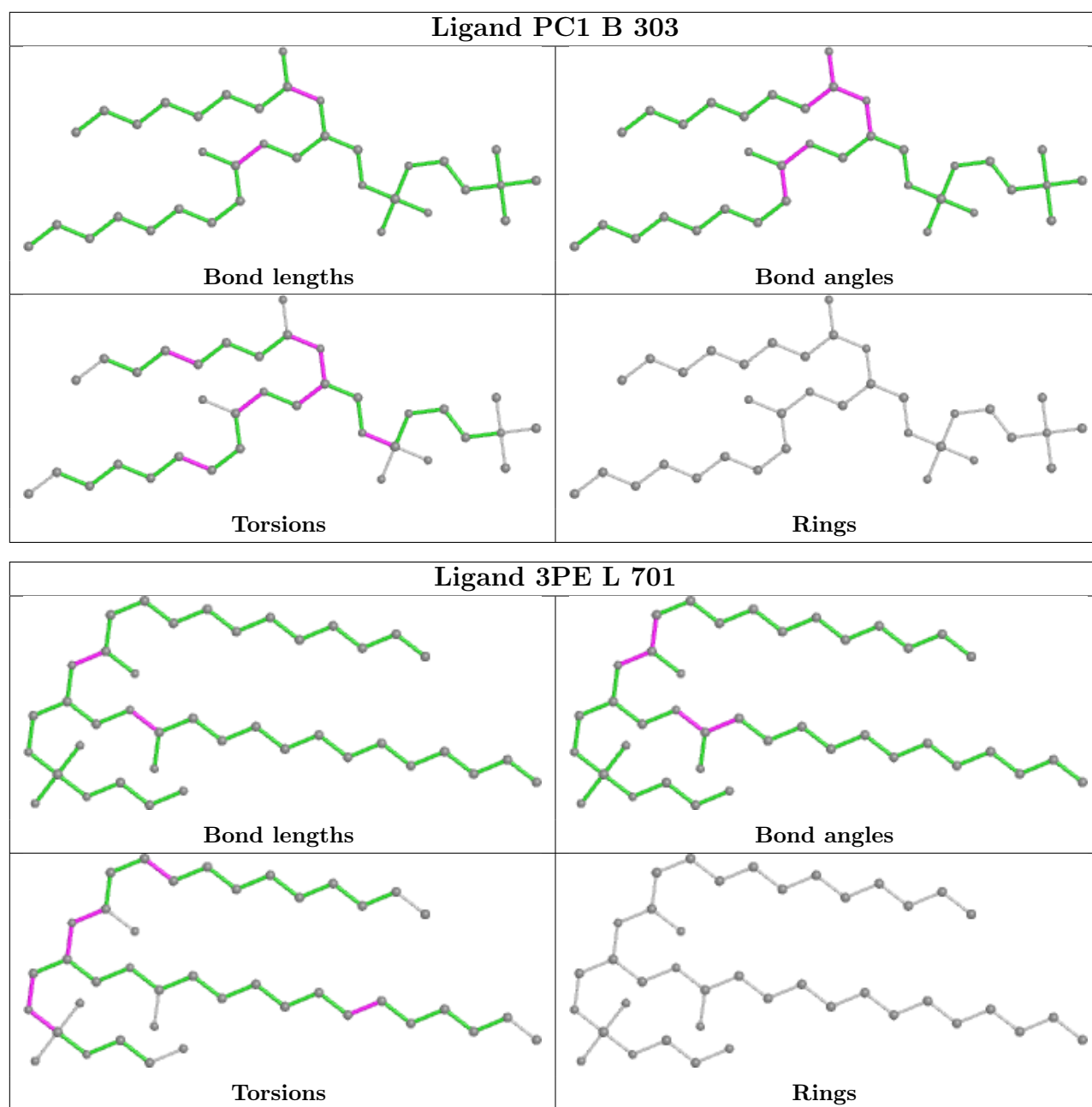


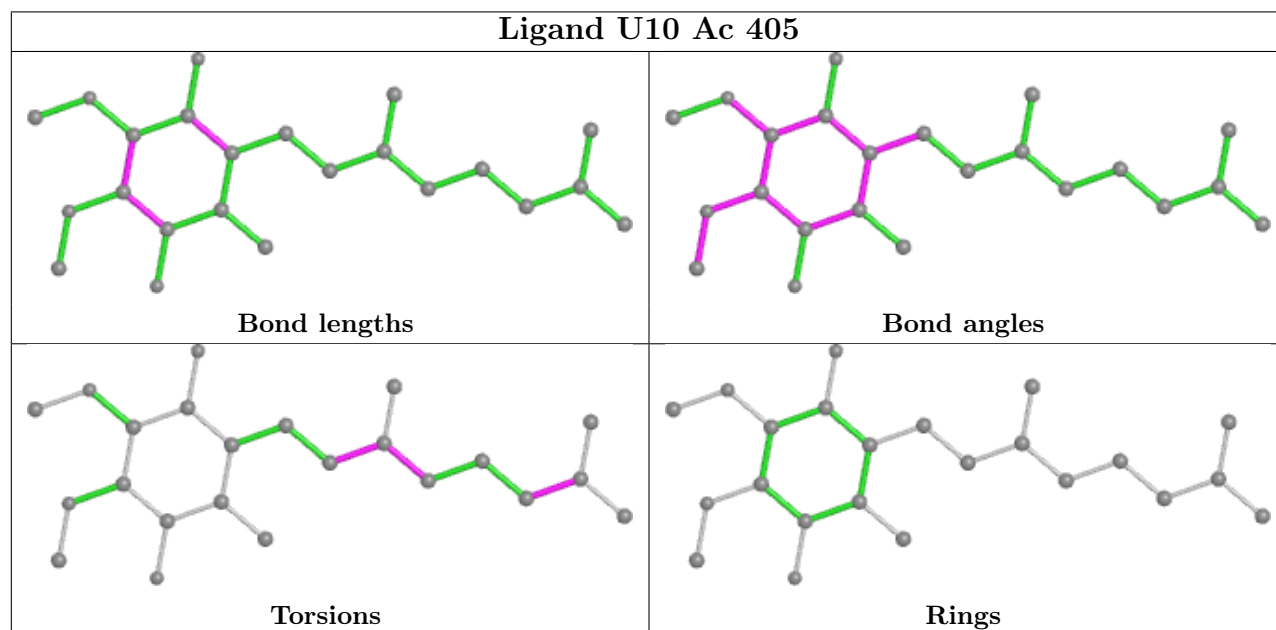
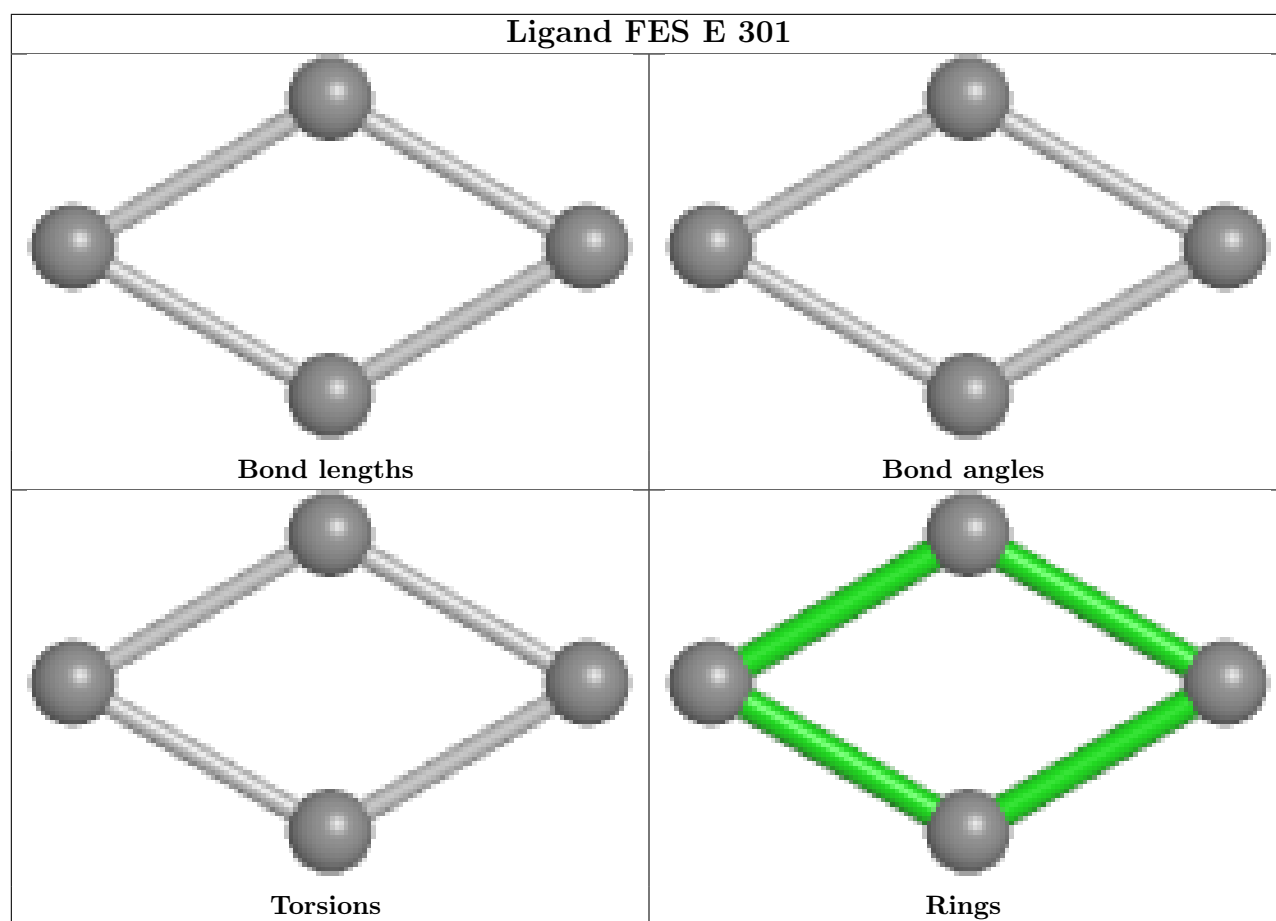




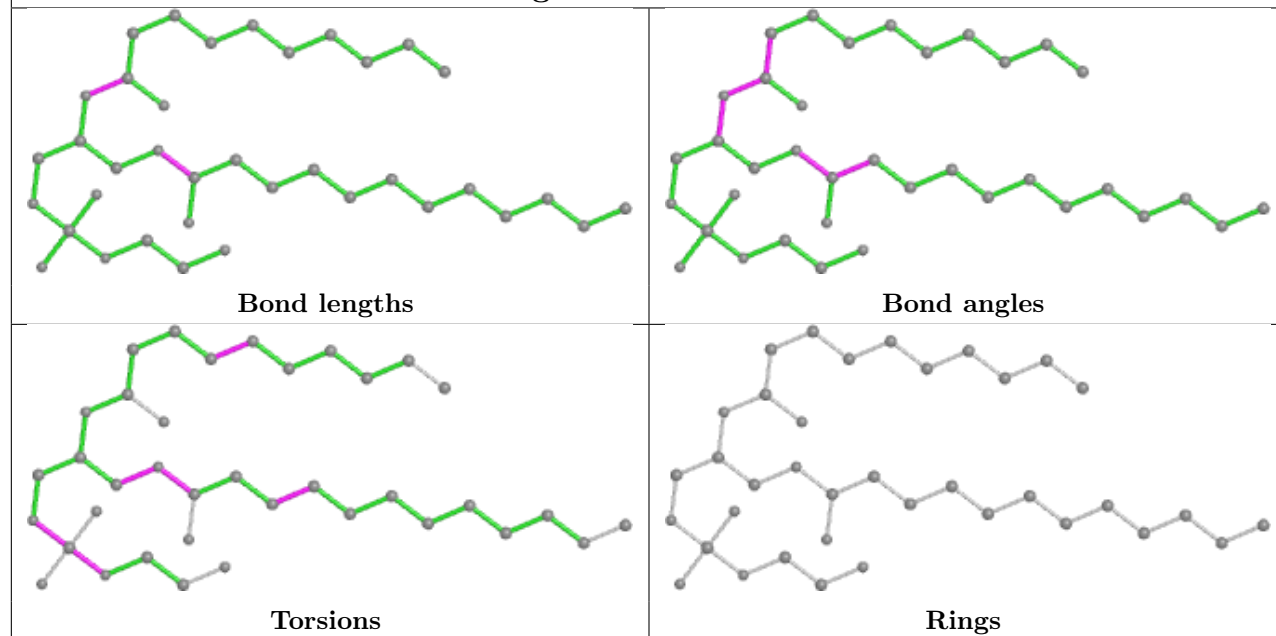




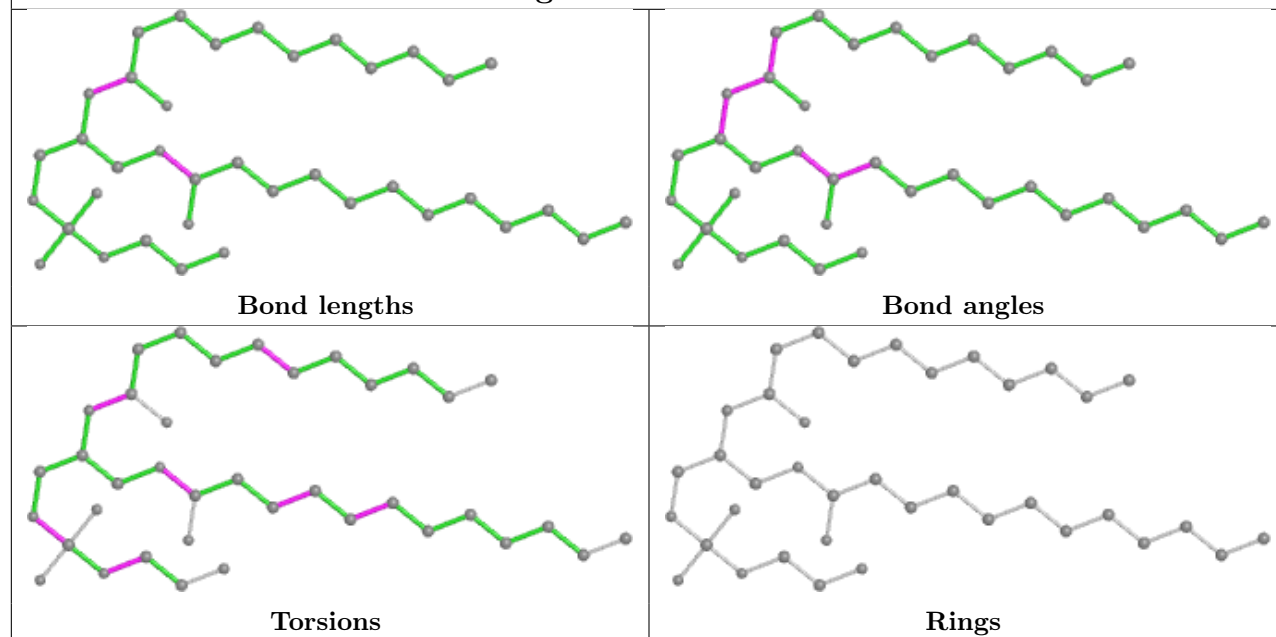


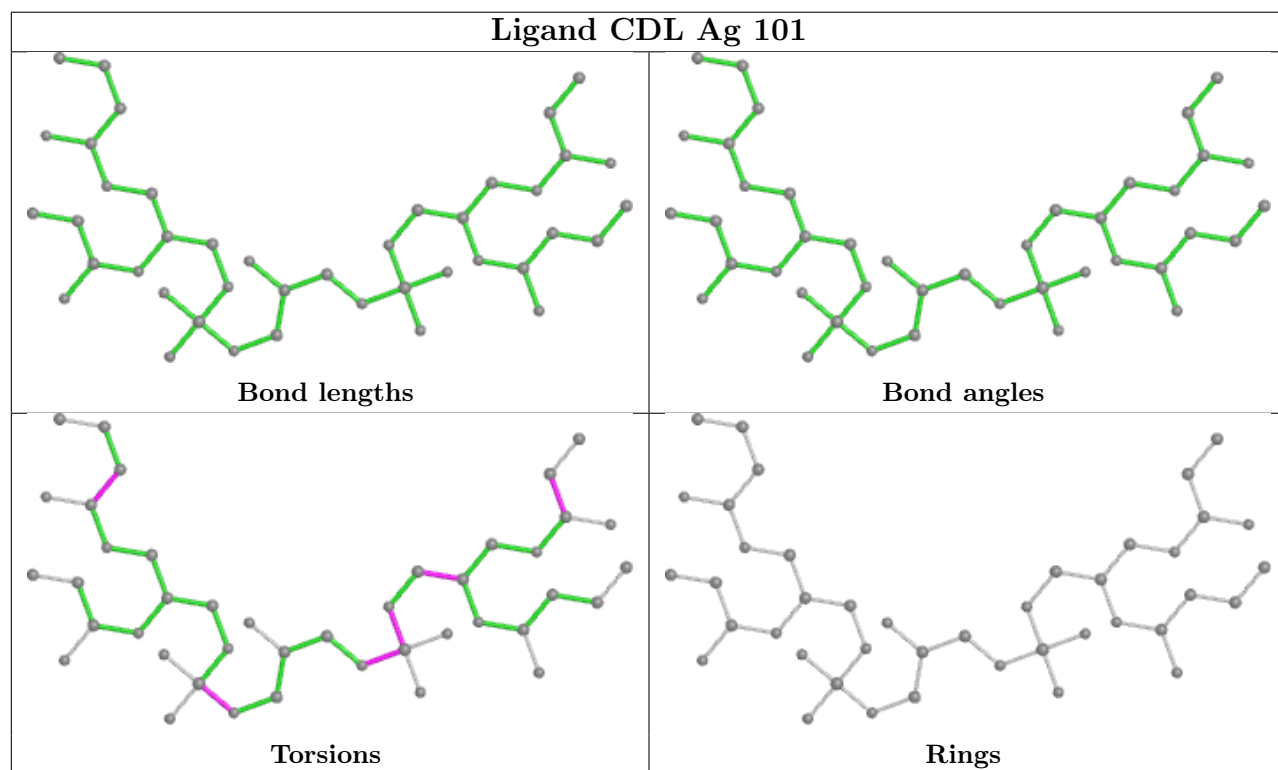
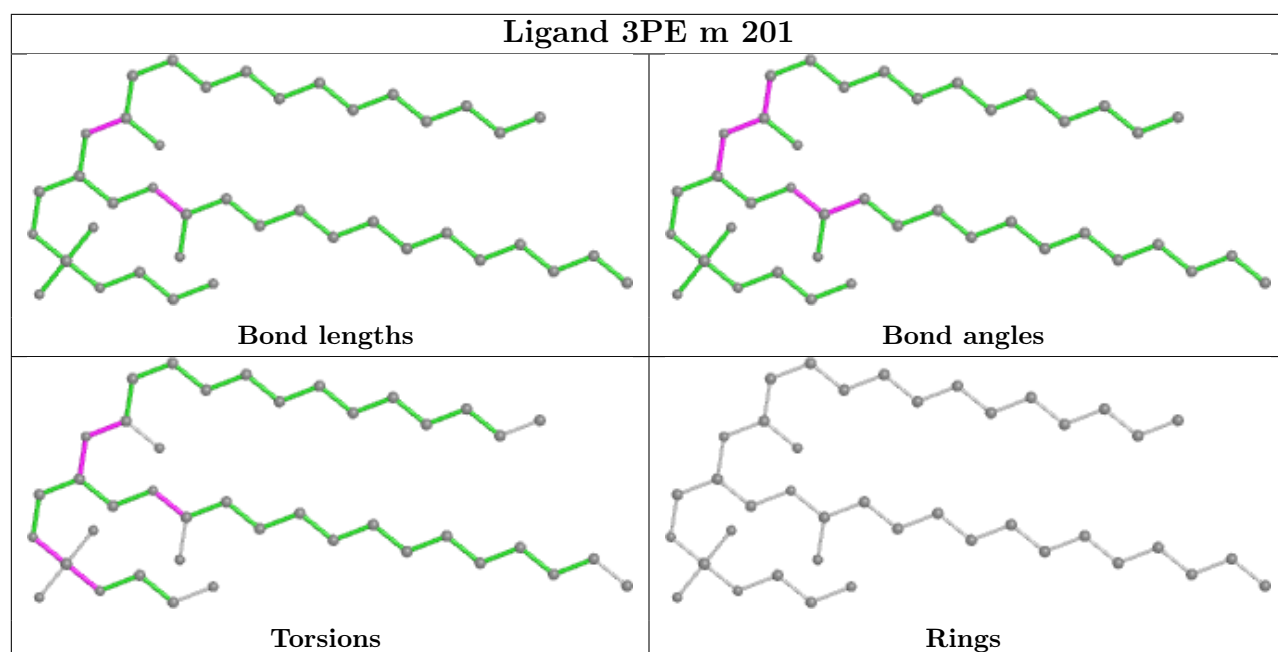


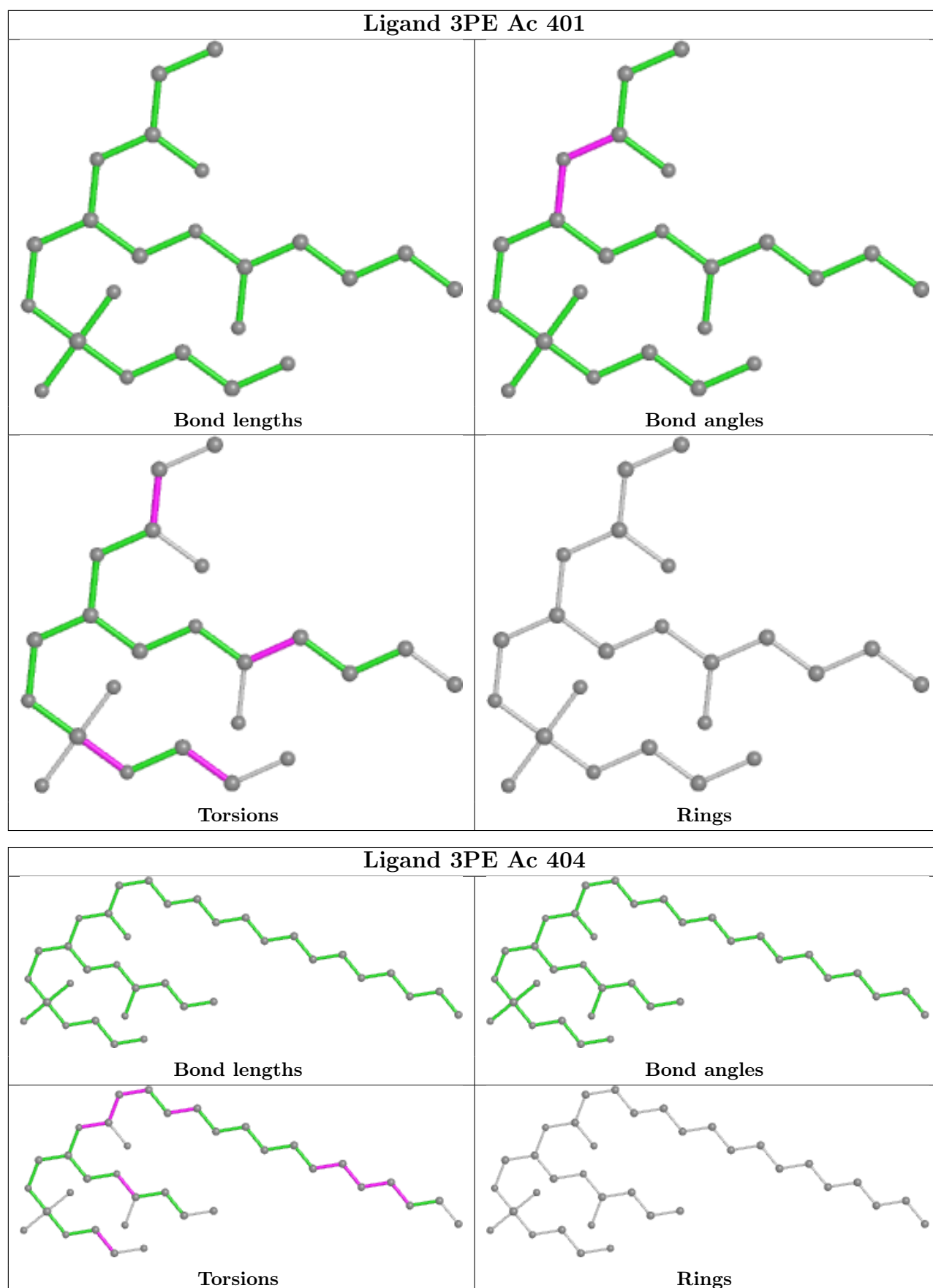
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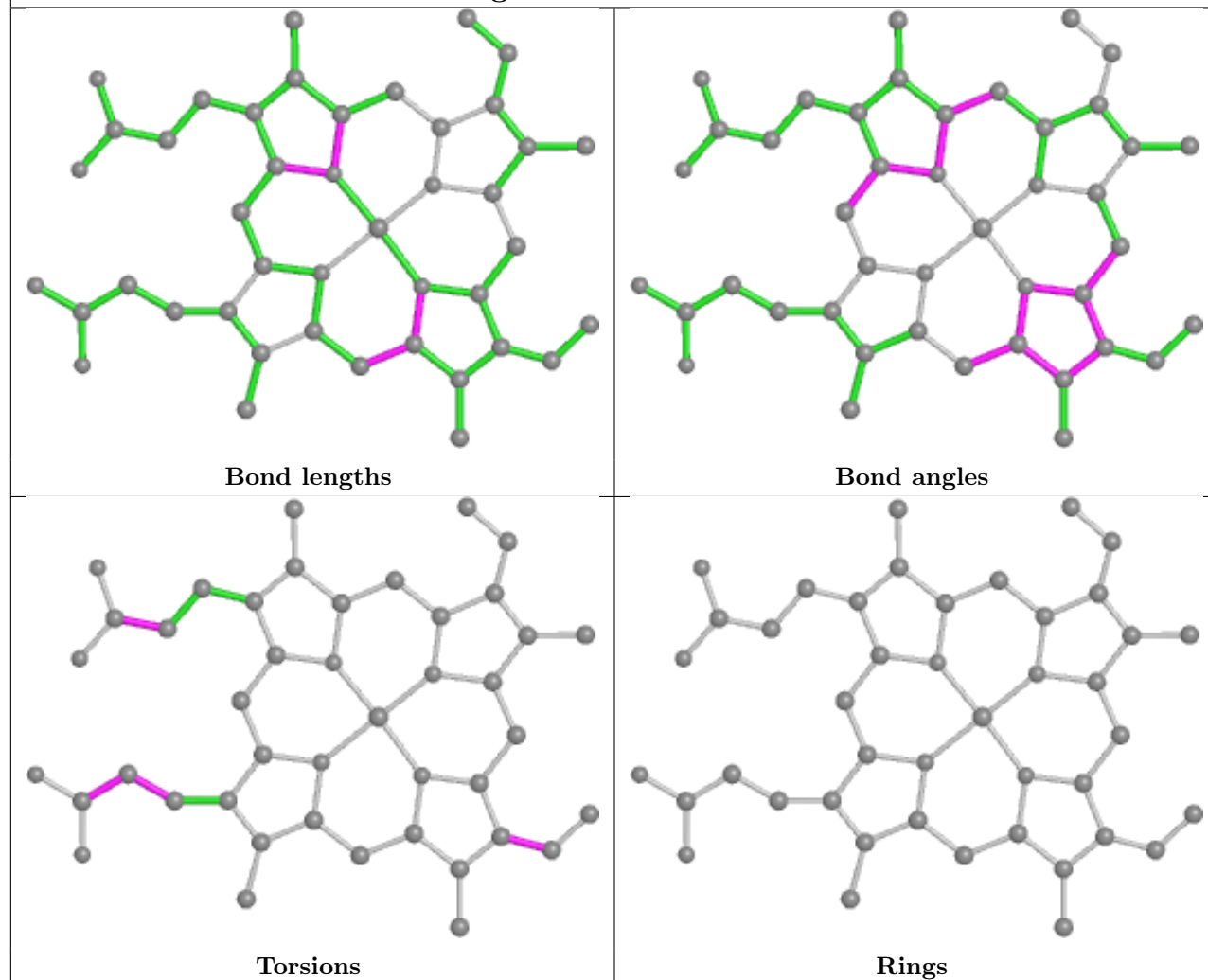
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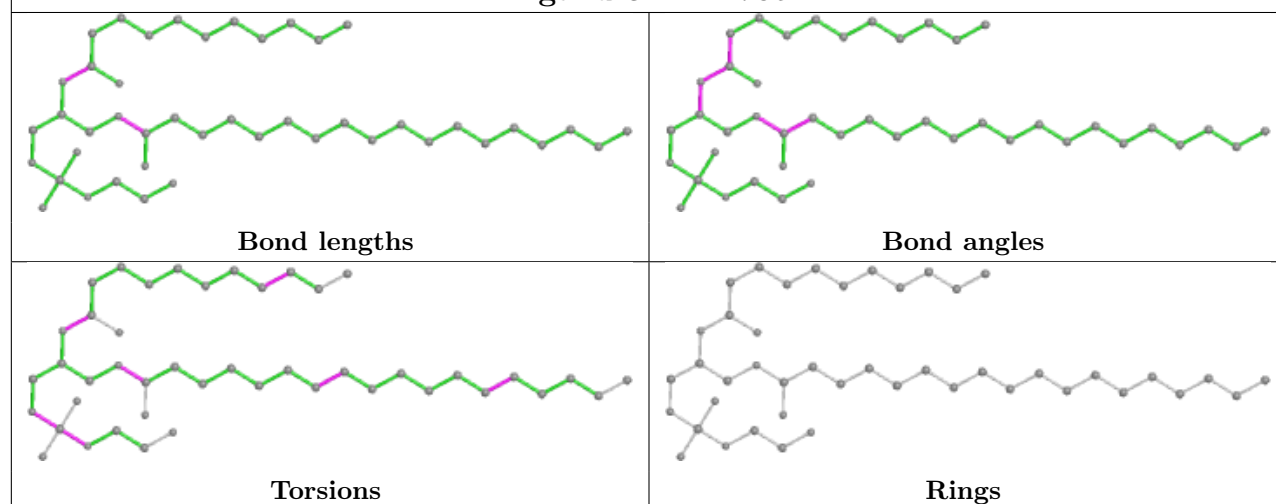


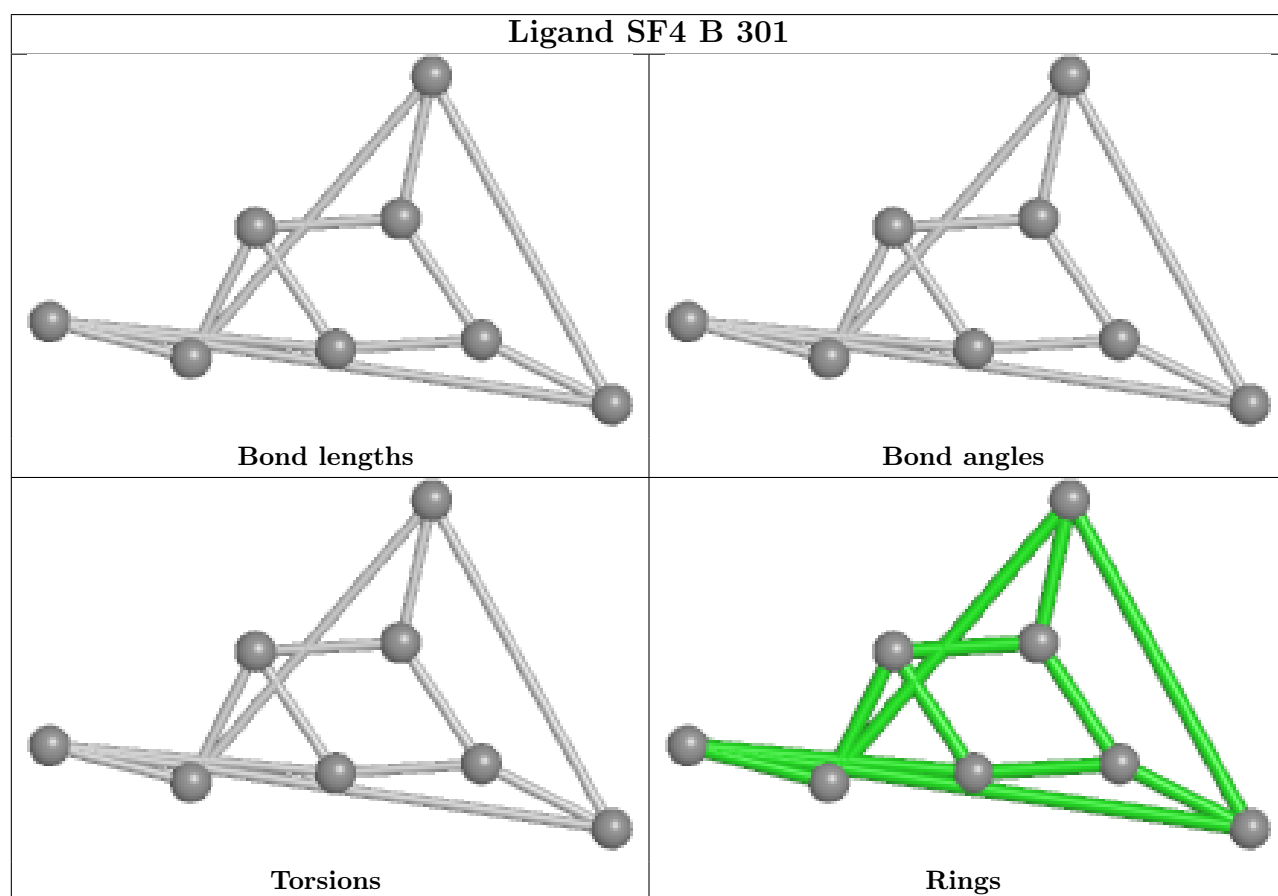
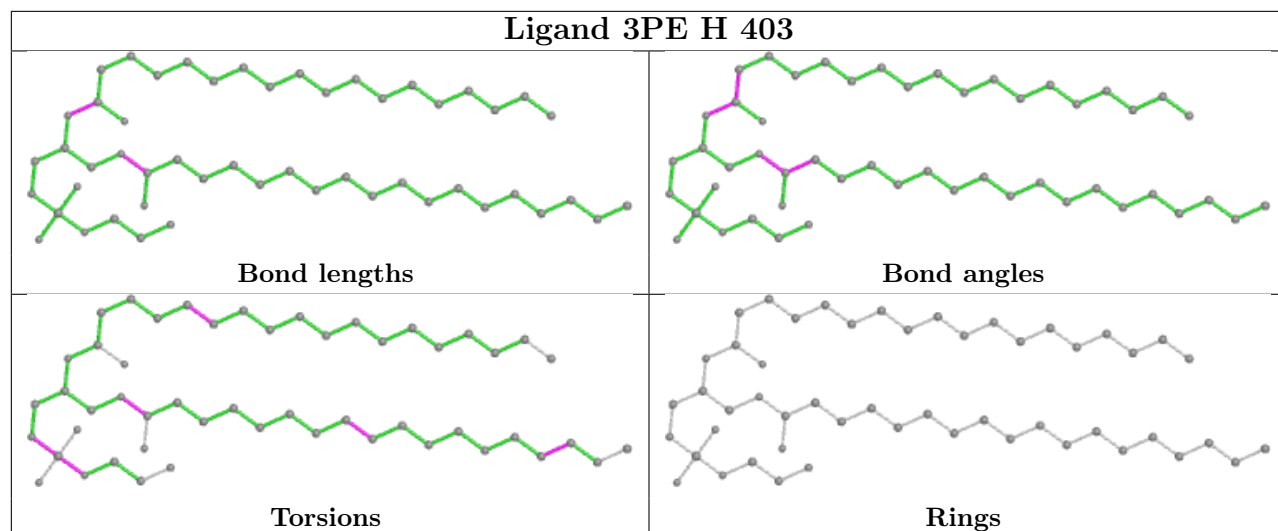


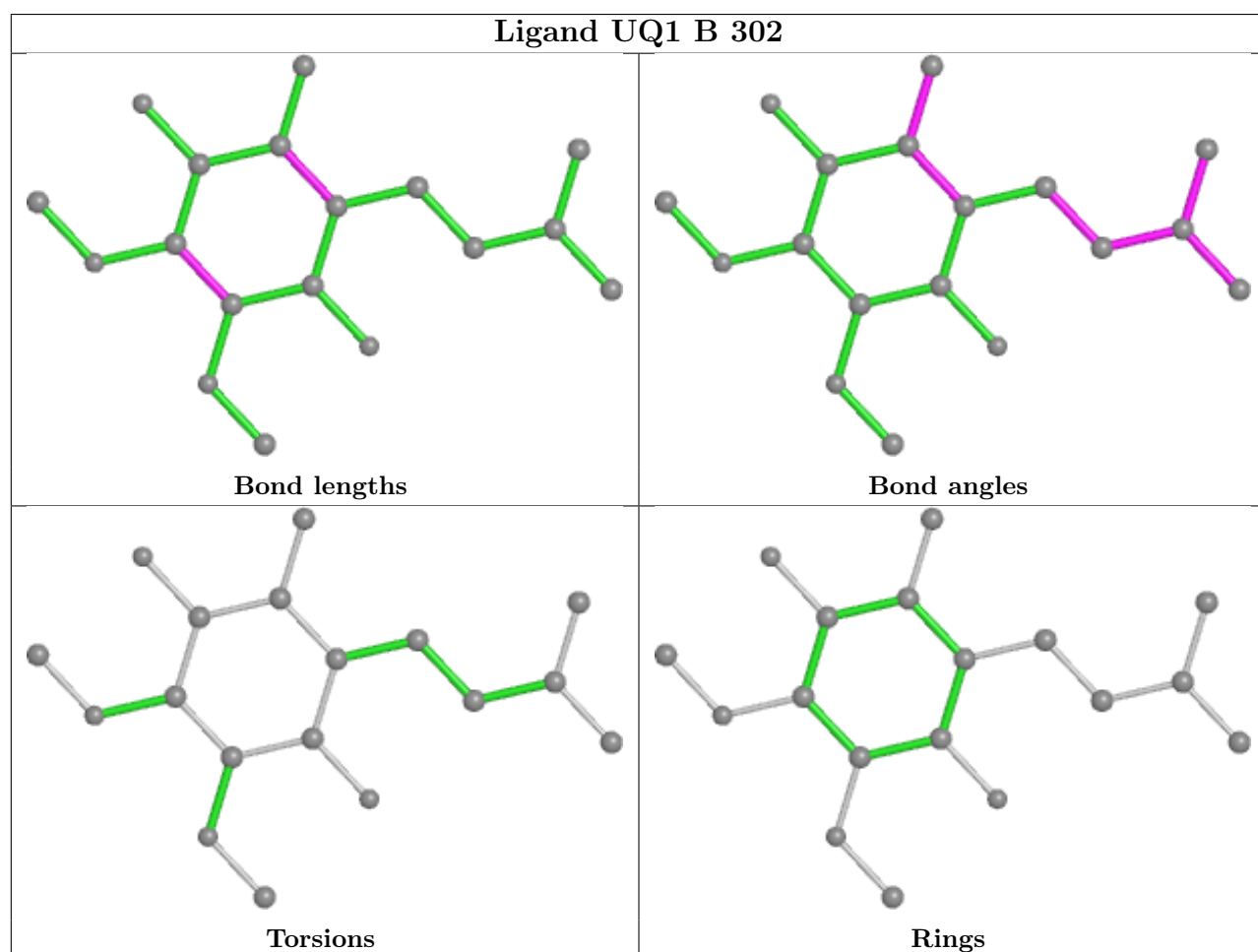
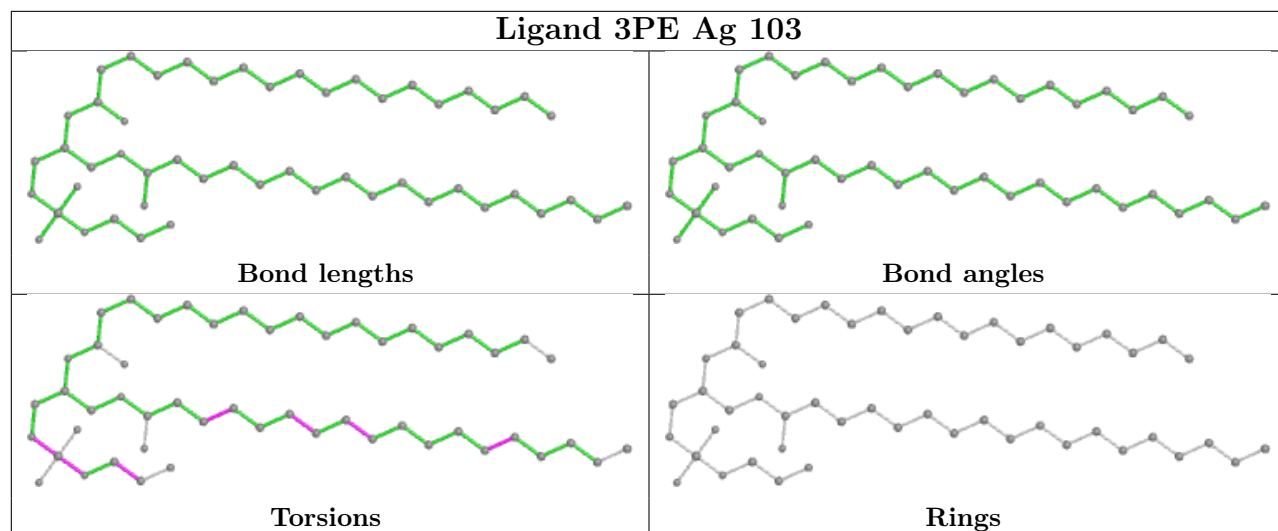
Ligand HEM Ac 402

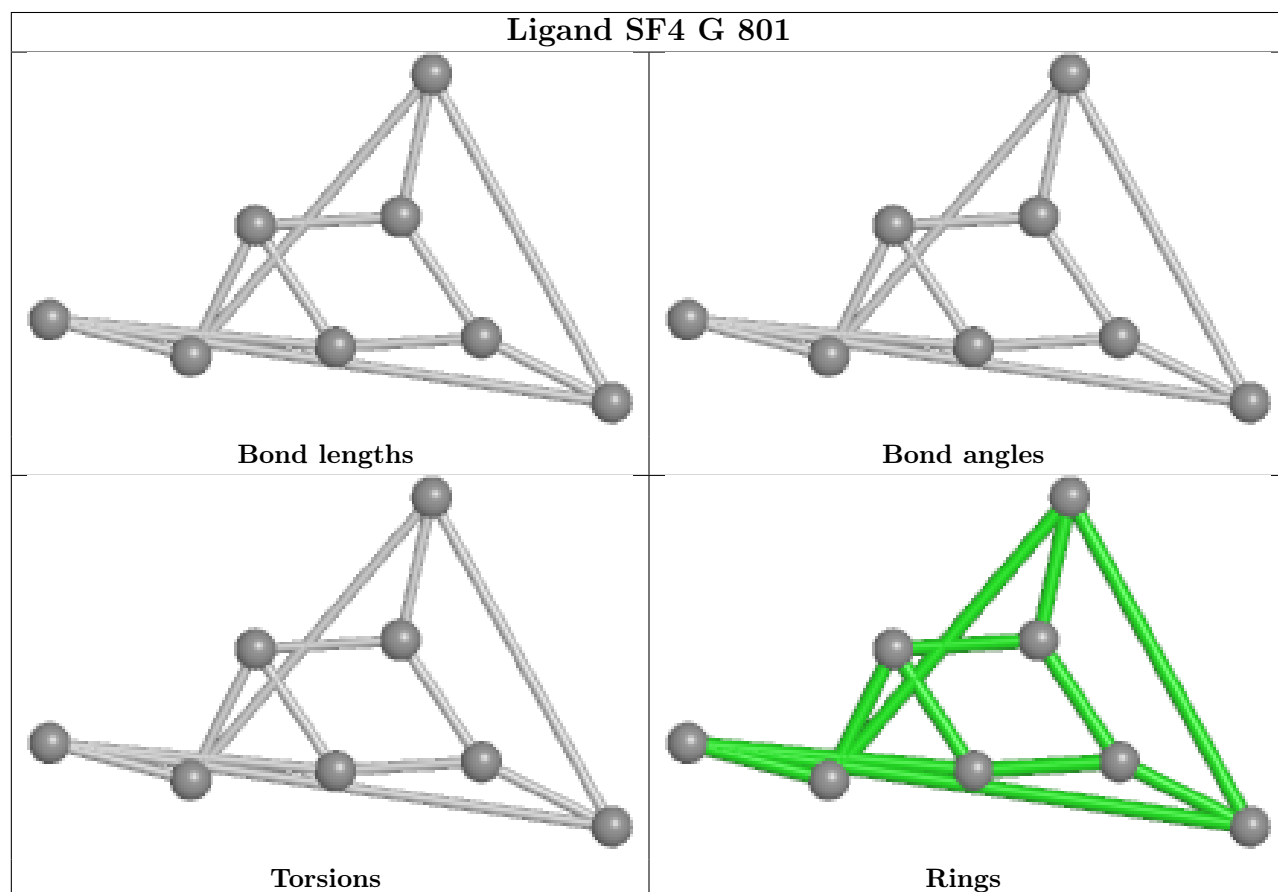
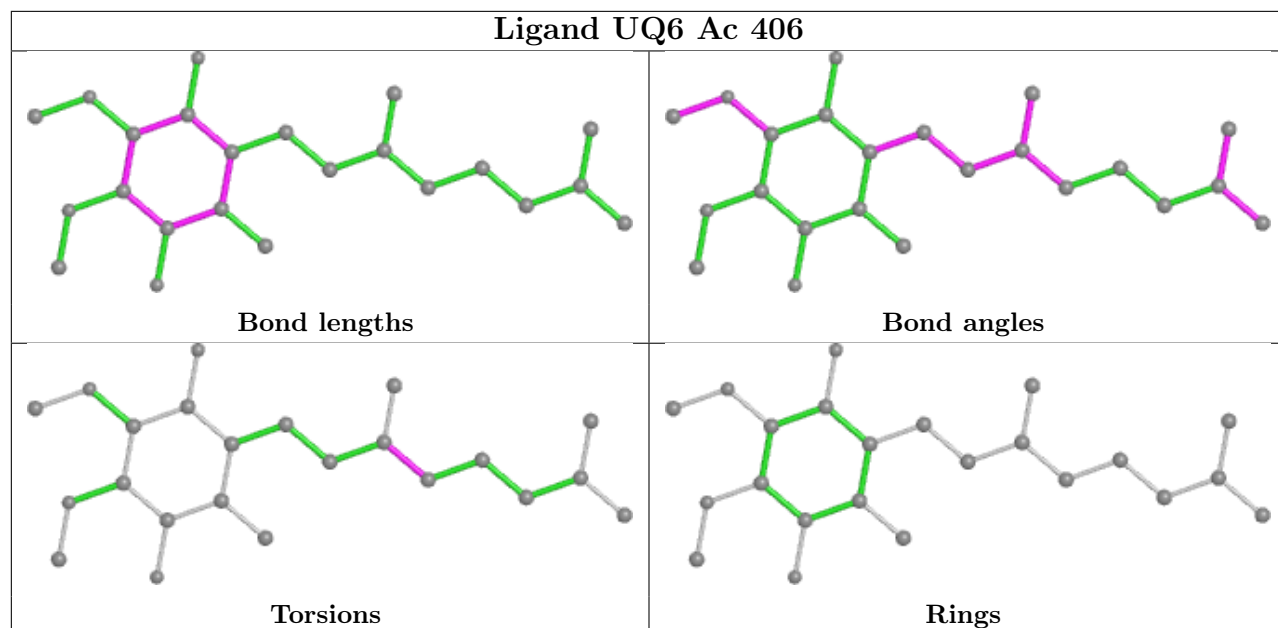


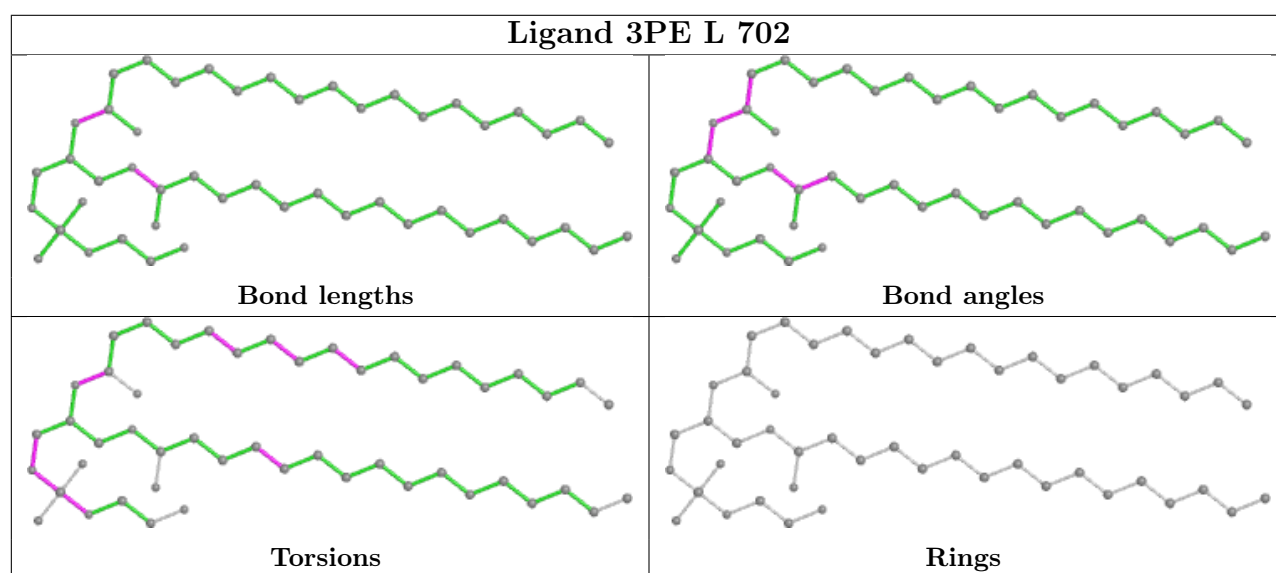
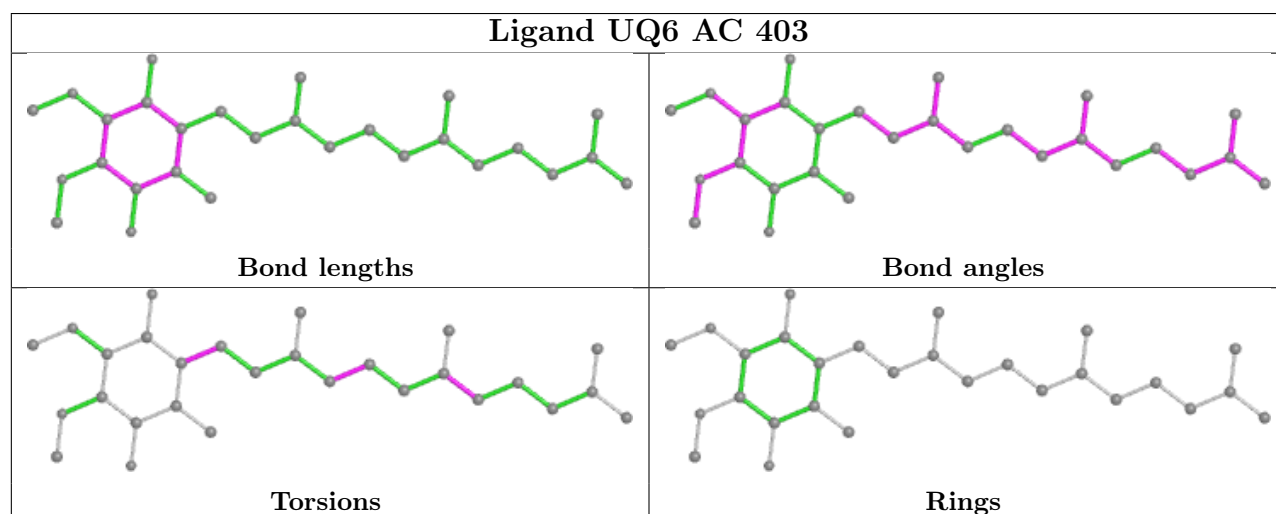
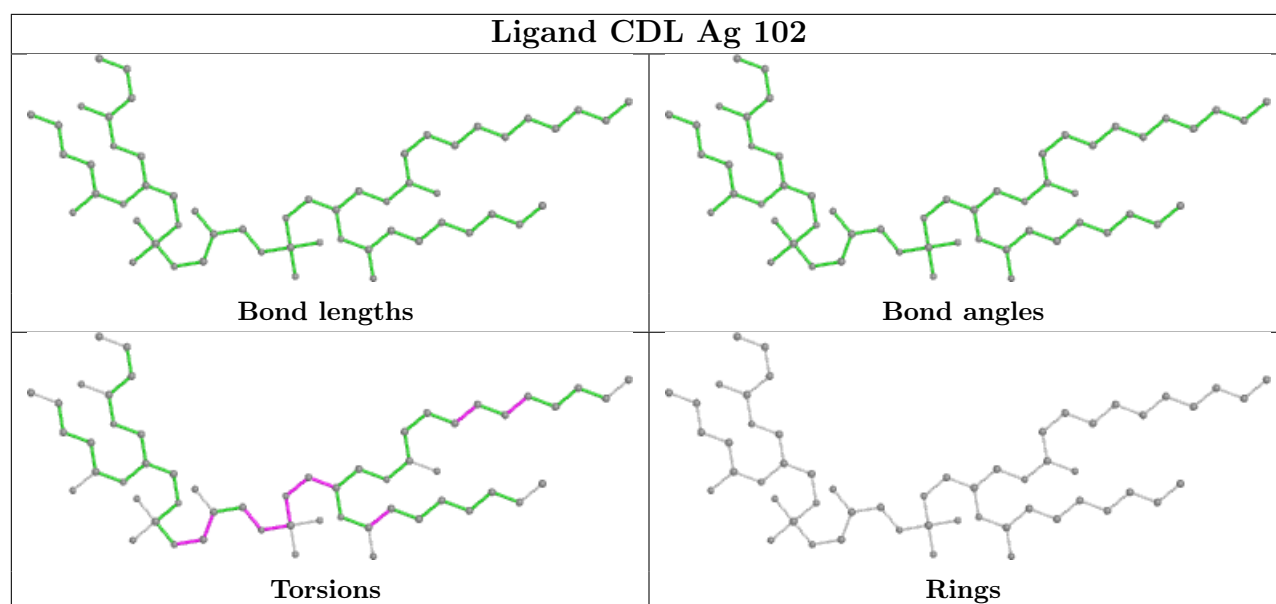
Ligand 3PE L 705

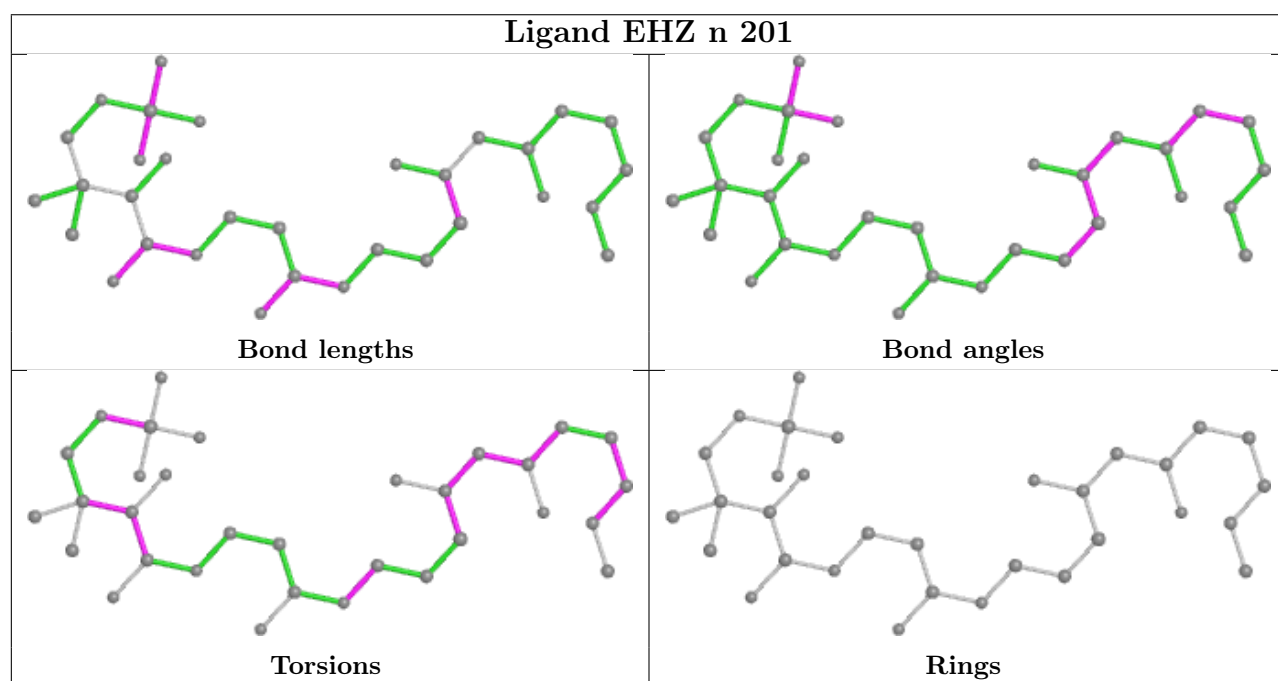
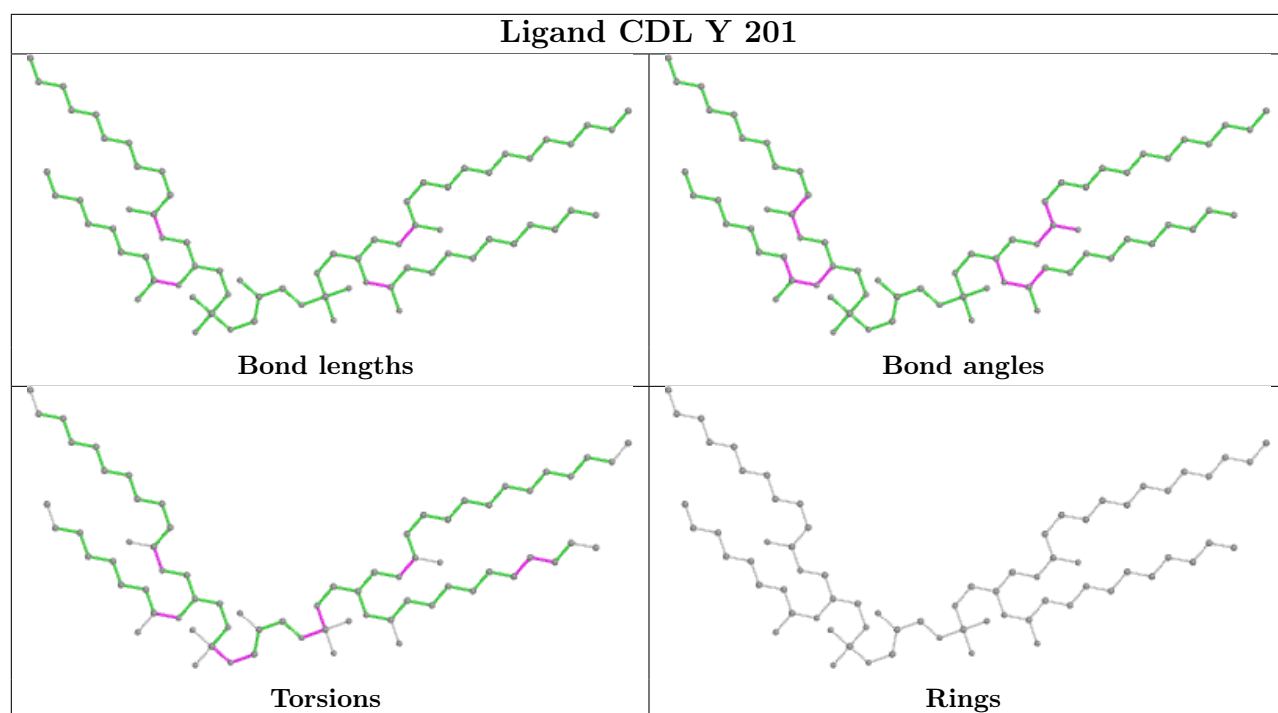


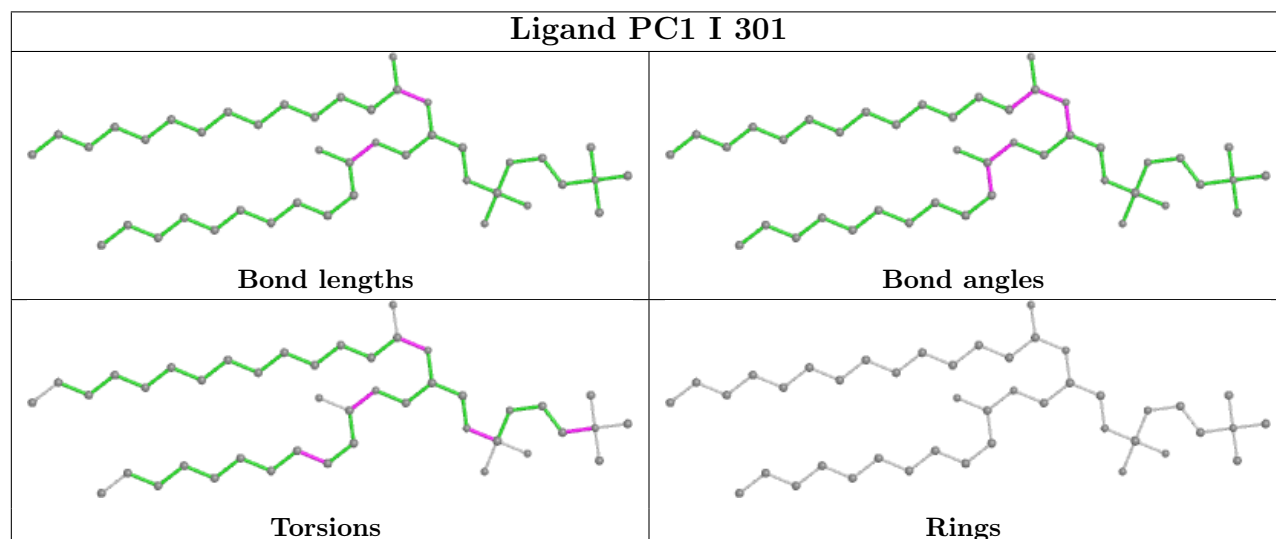
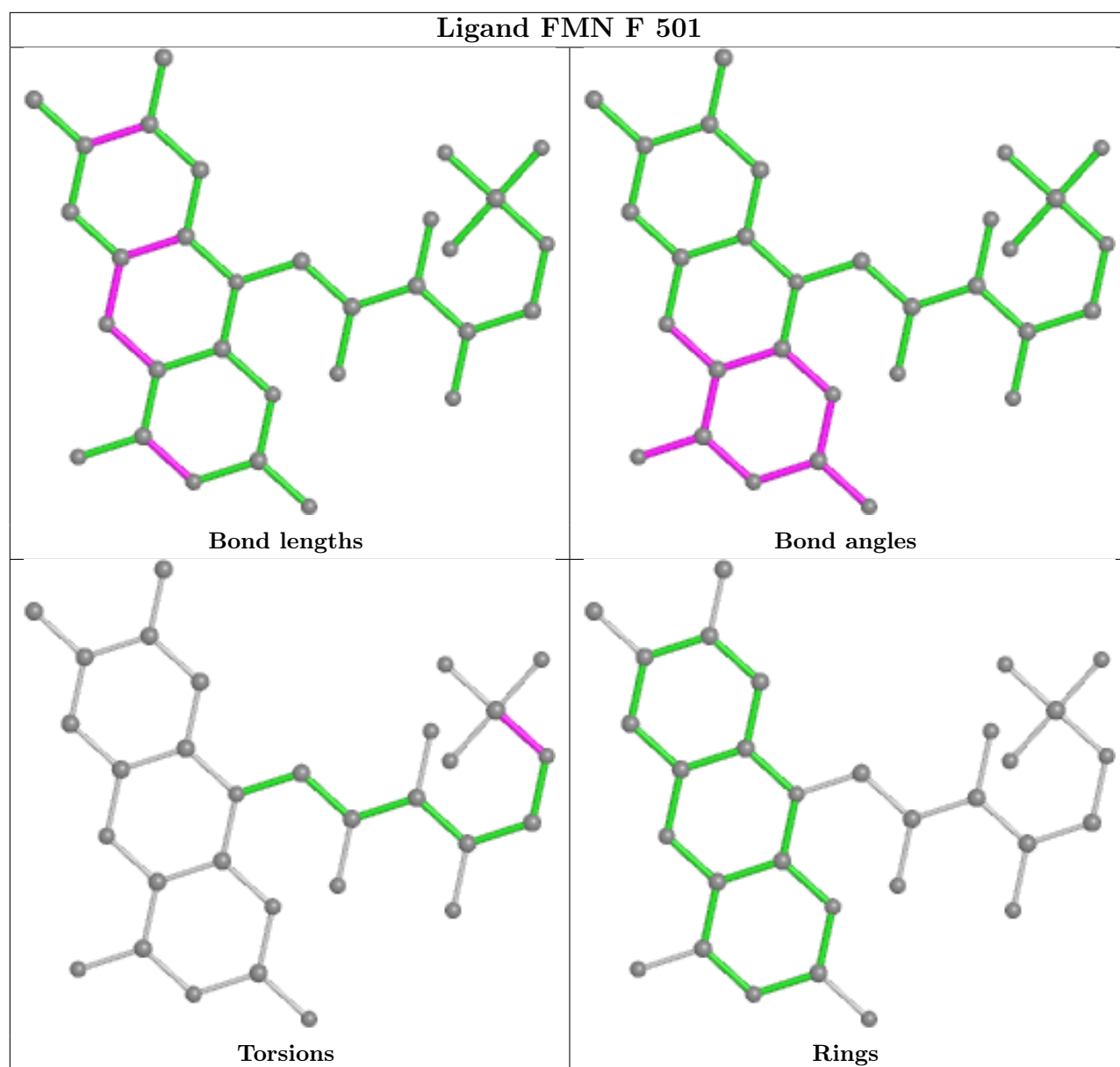


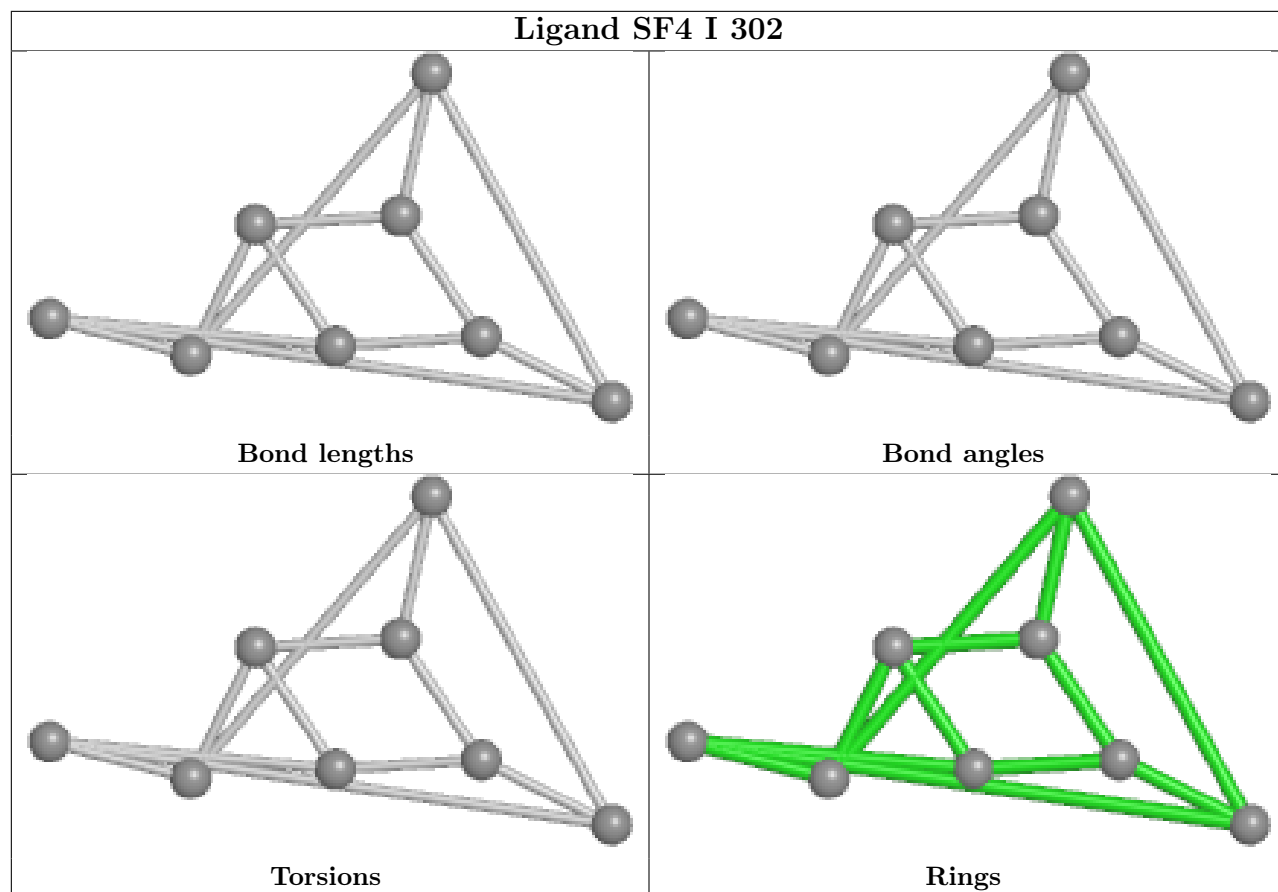




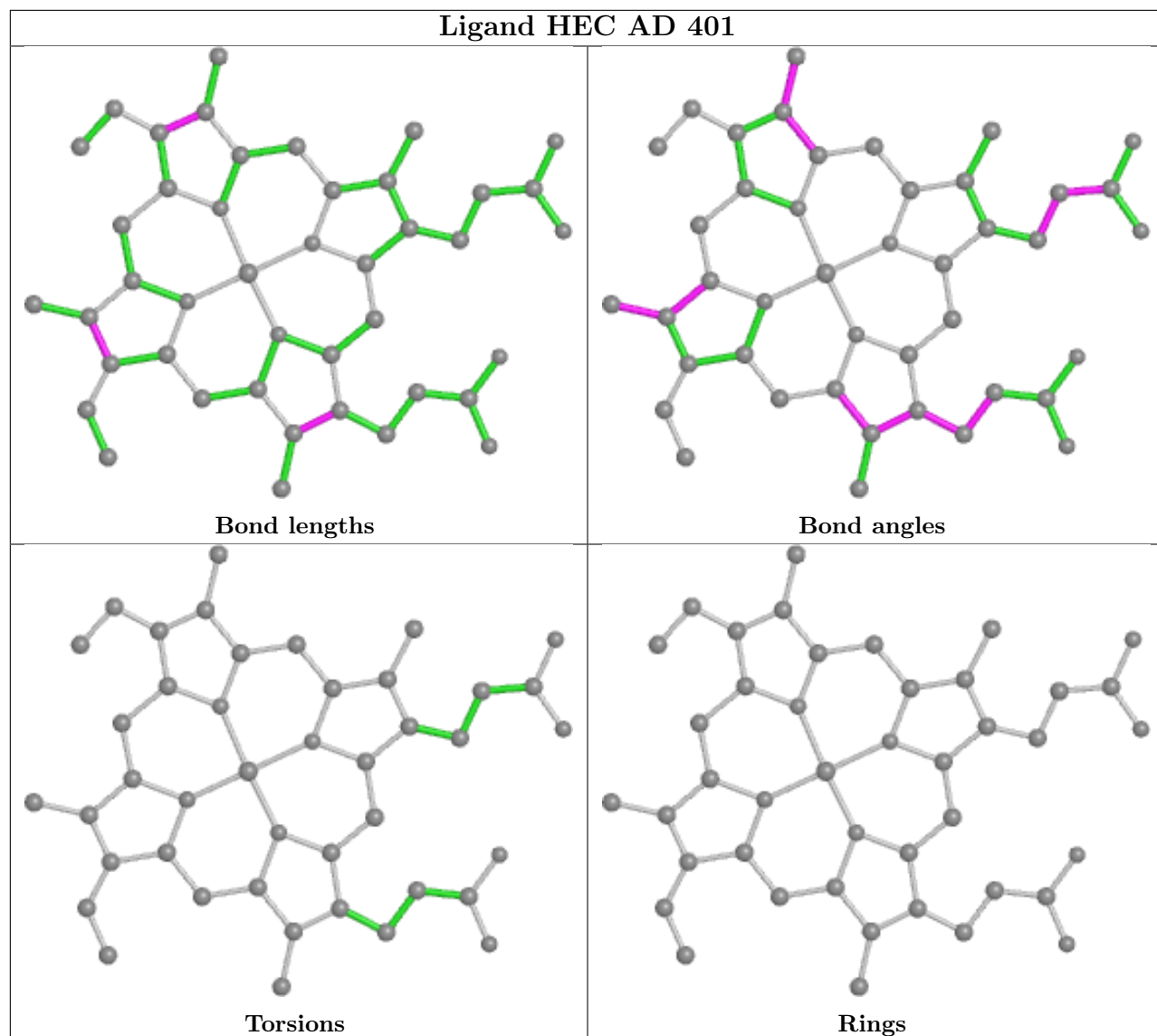


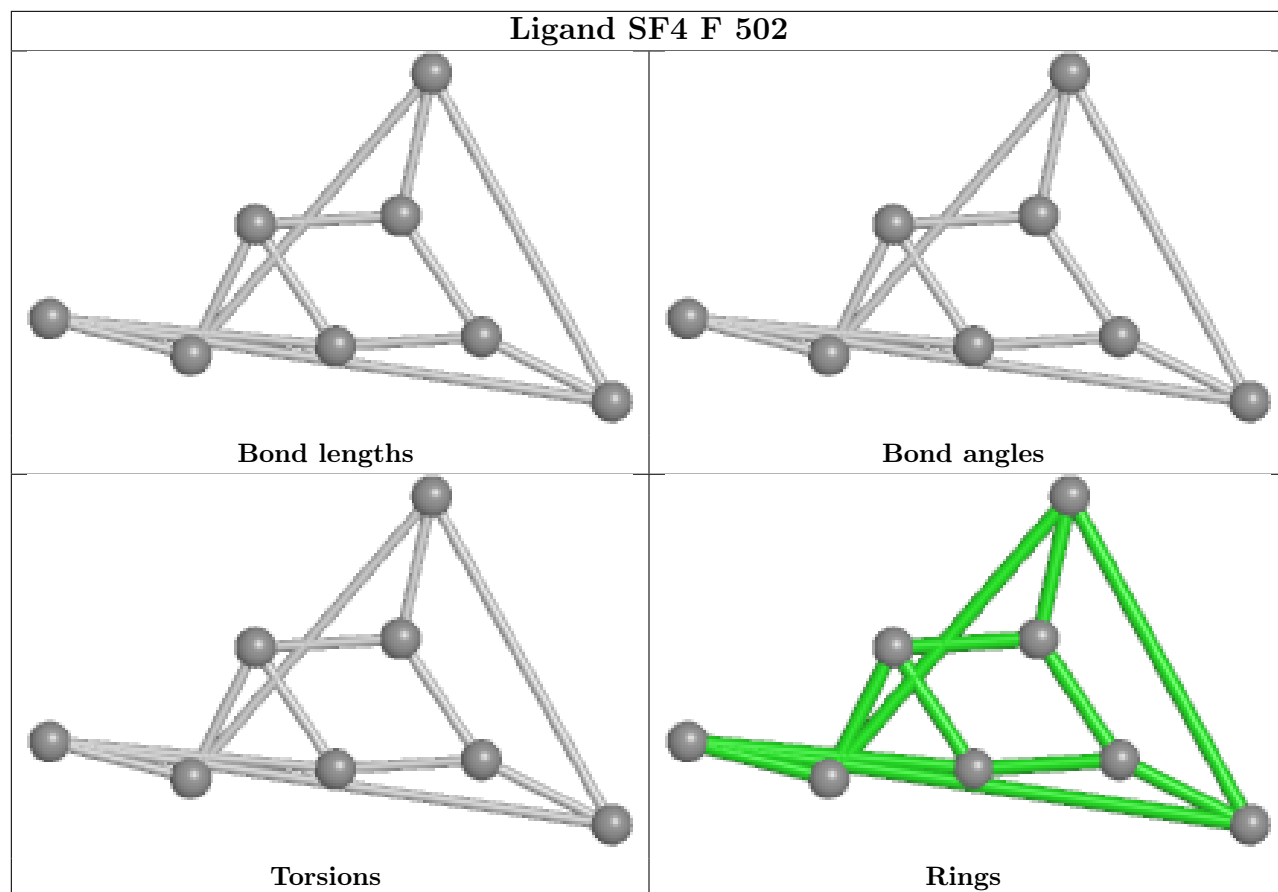


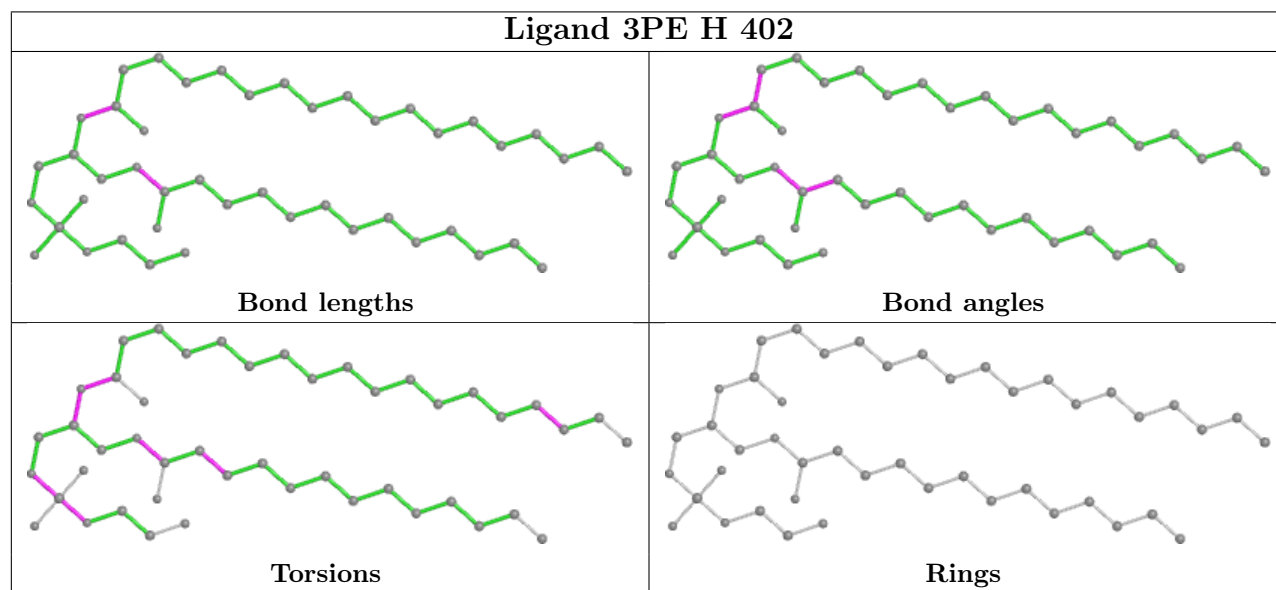
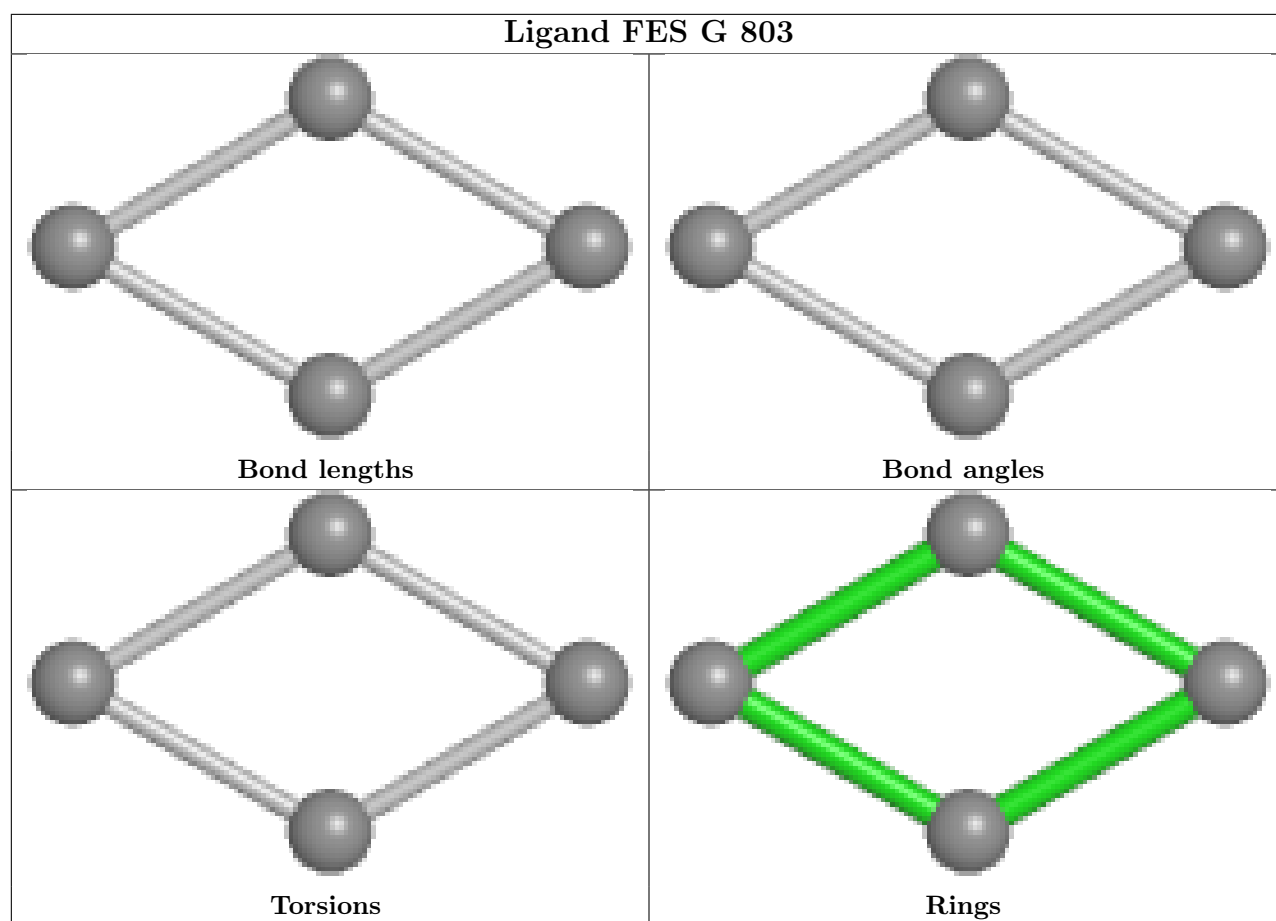


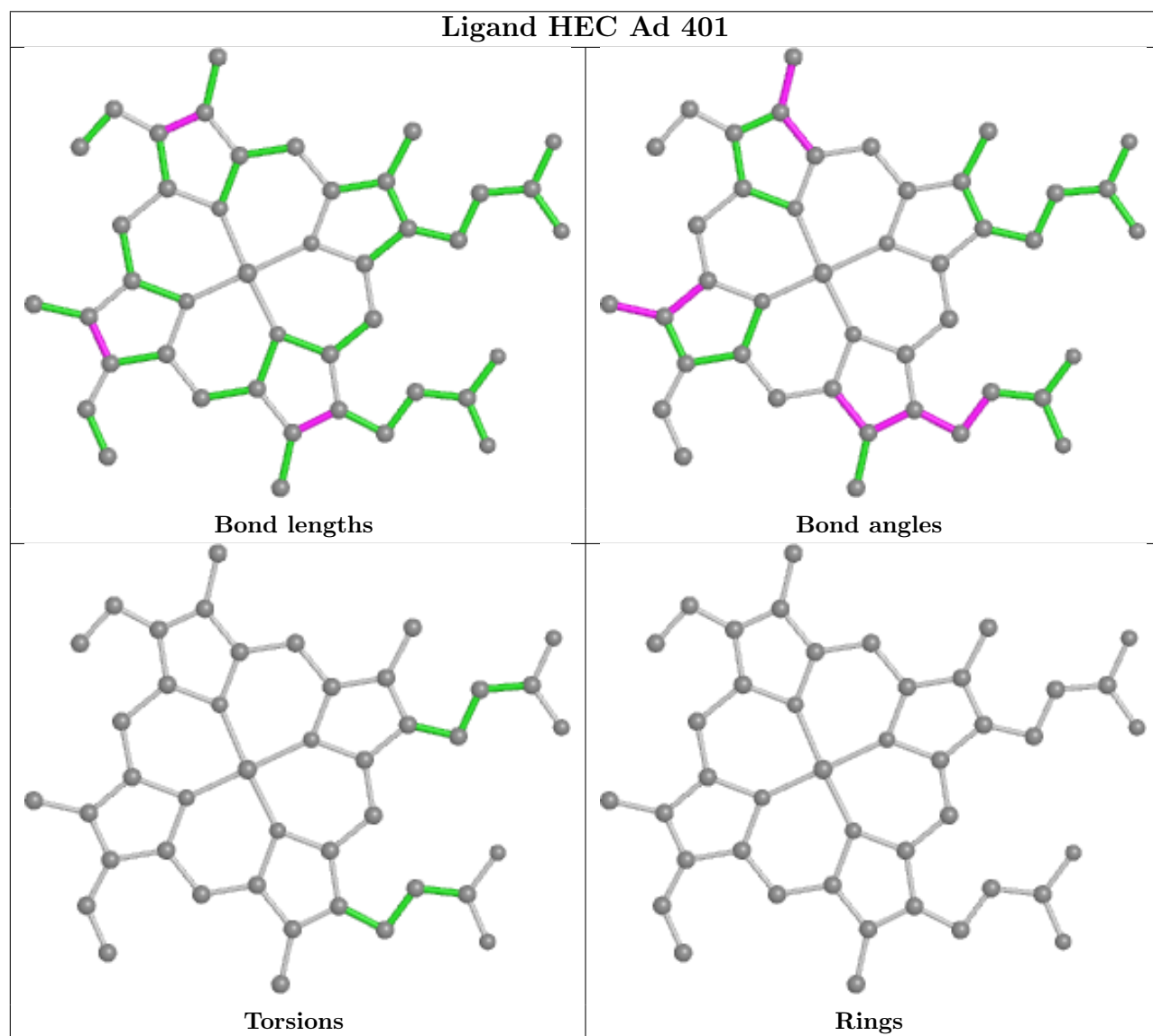
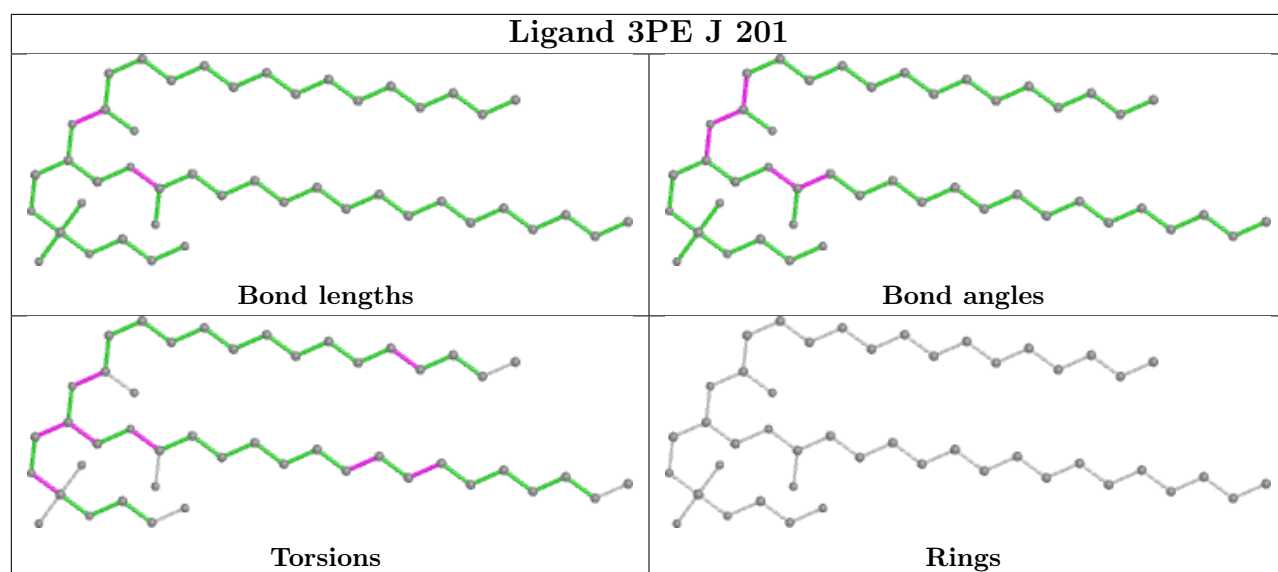


Ligand HEC AD 401









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.

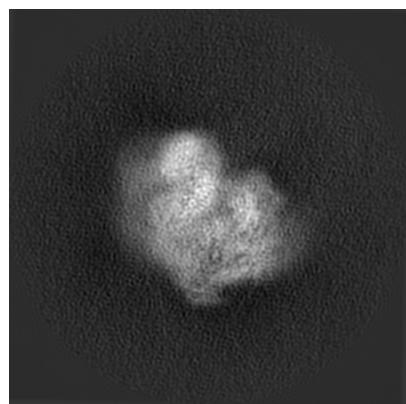
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35352. These allow visual inspection of the internal detail of the map and identification of artifacts.

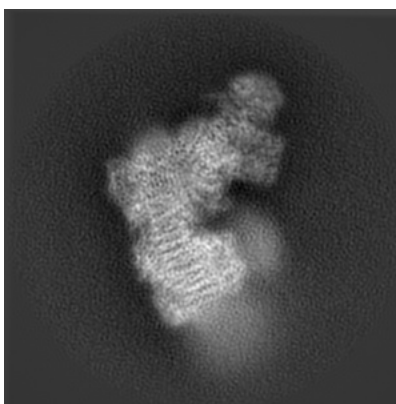
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

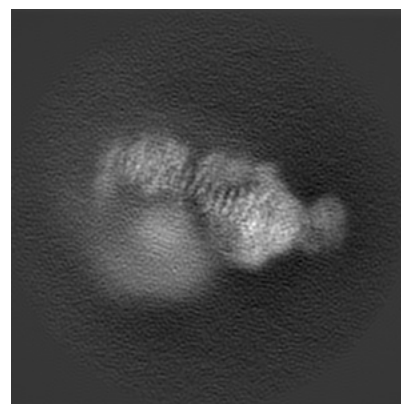
6.1.1 Primary map



X

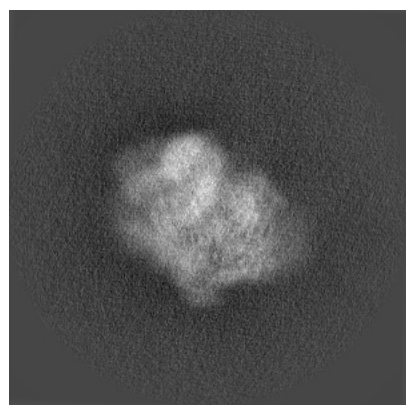


Y

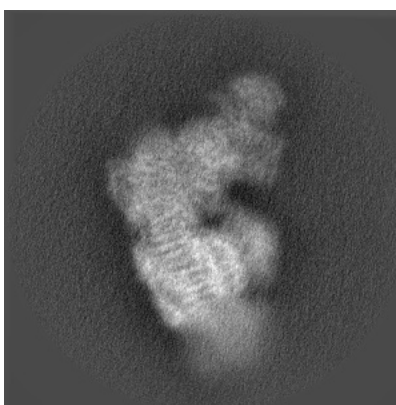


Z

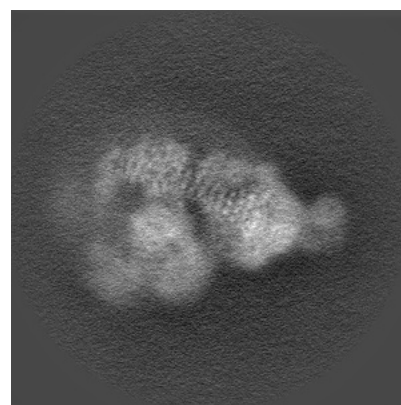
6.1.2 Raw map



X



Y

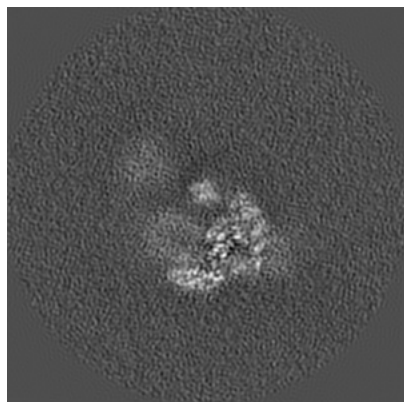


Z

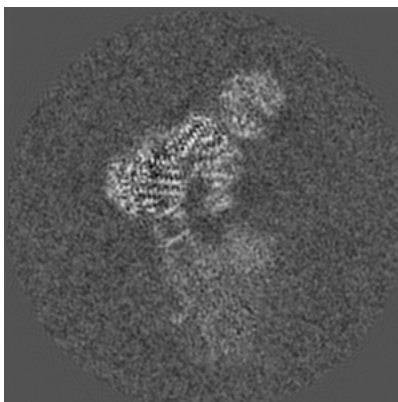
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

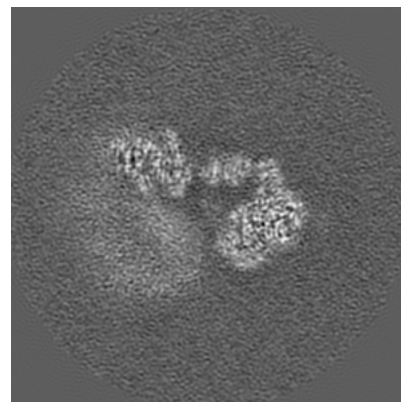
6.2.1 Primary map



X Index: 256

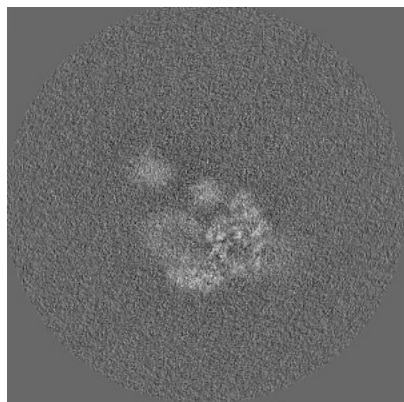


Y Index: 256

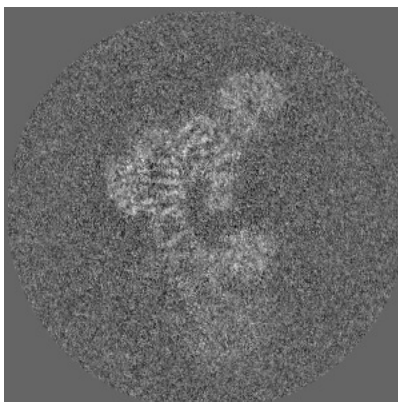


Z Index: 256

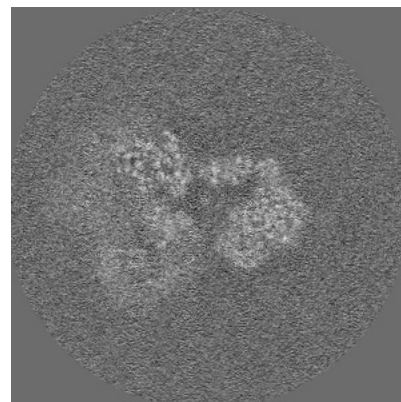
6.2.2 Raw map



X Index: 256



Y Index: 256

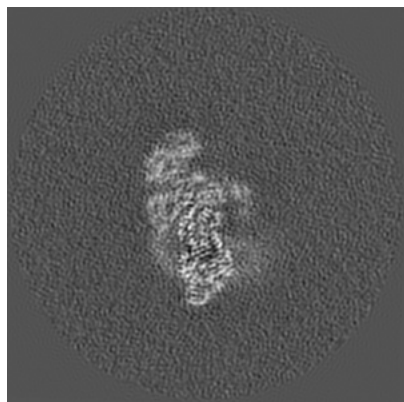


Z Index: 256

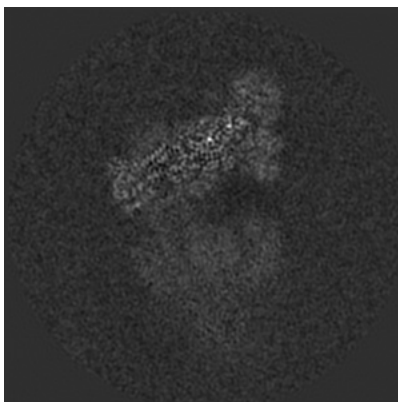
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

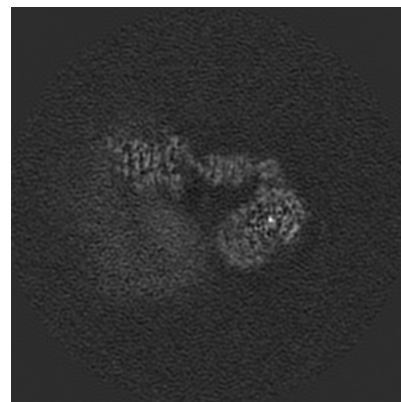
6.3.1 Primary map



X Index: 310

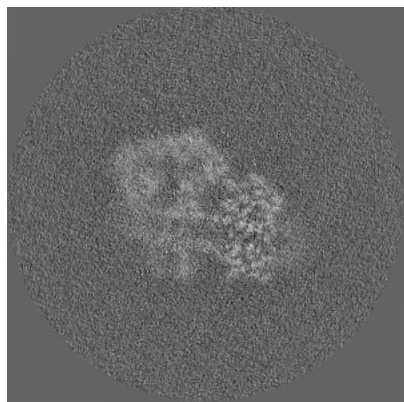


Y Index: 232

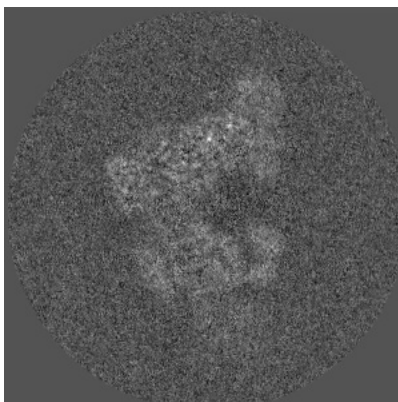


Z Index: 252

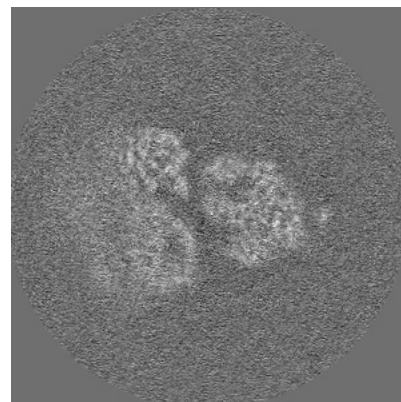
6.3.2 Raw map



X Index: 205



Y Index: 234

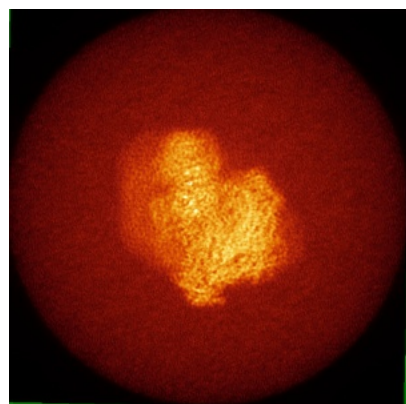


Z Index: 268

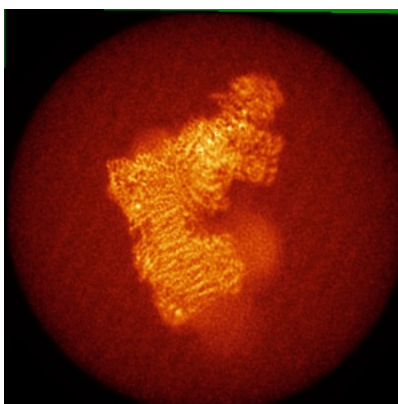
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

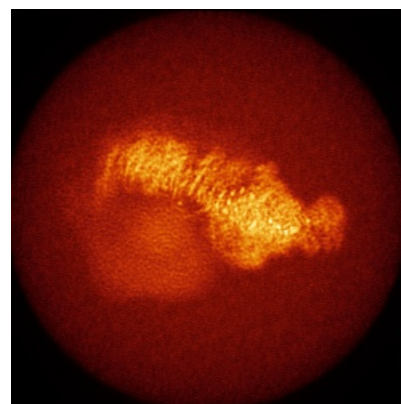
6.4.1 Primary map



X

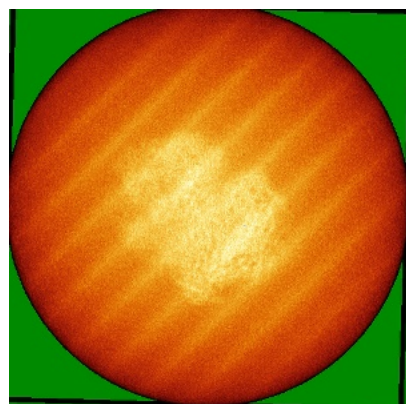


Y

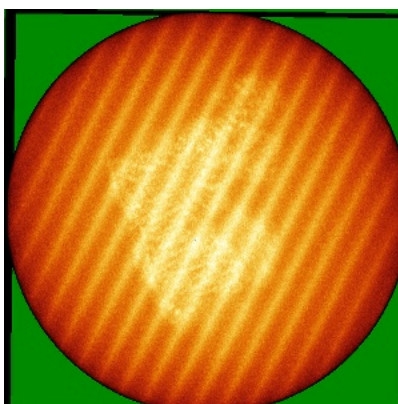


Z

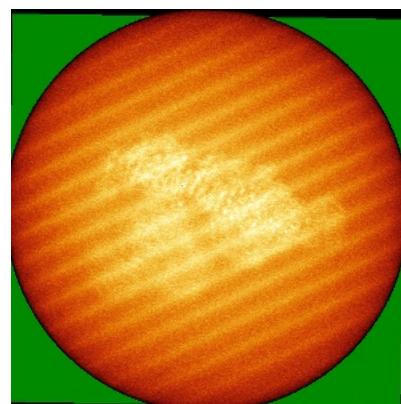
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



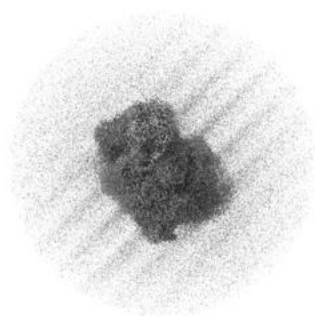
Y



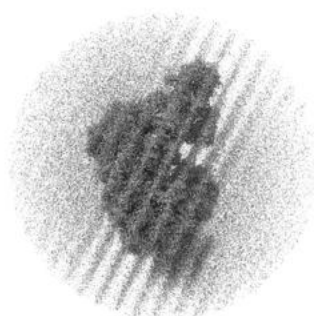
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0082. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

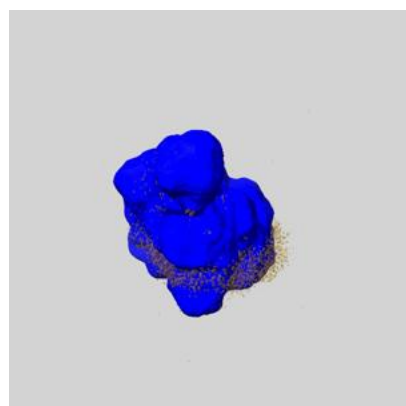
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

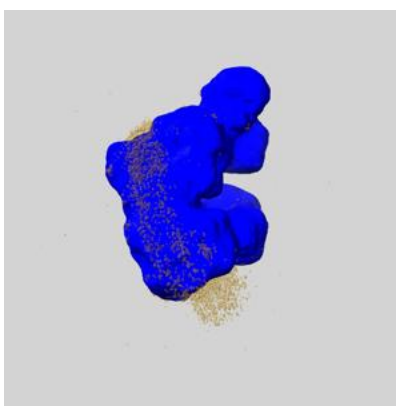
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

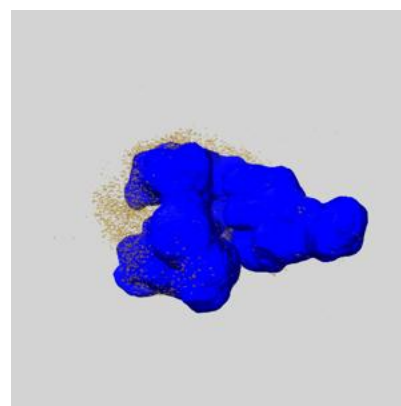
6.6.1 emd_35352_msk_1.map [i](#)



X



Y

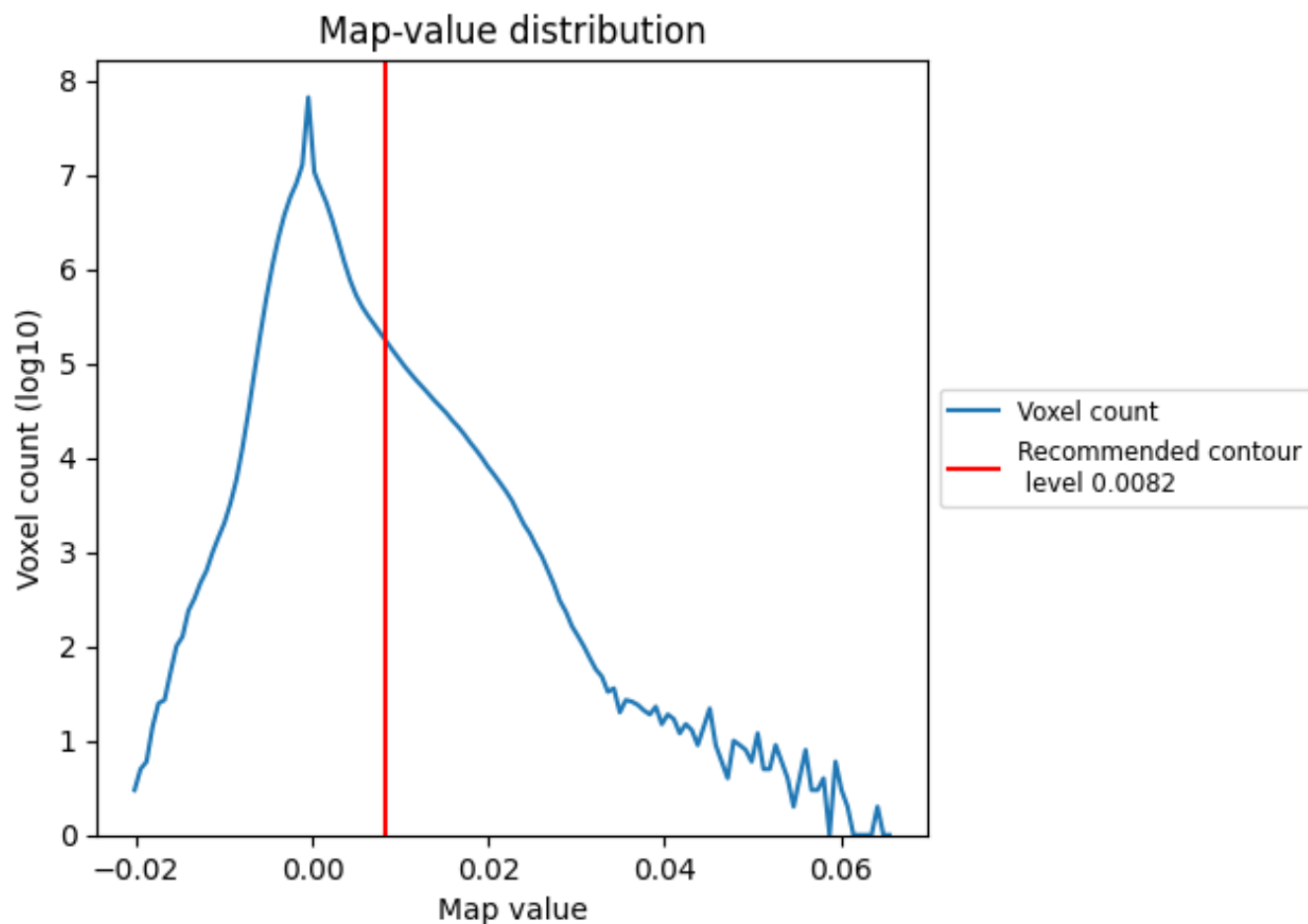


Z

7 Map analysis [i](#)

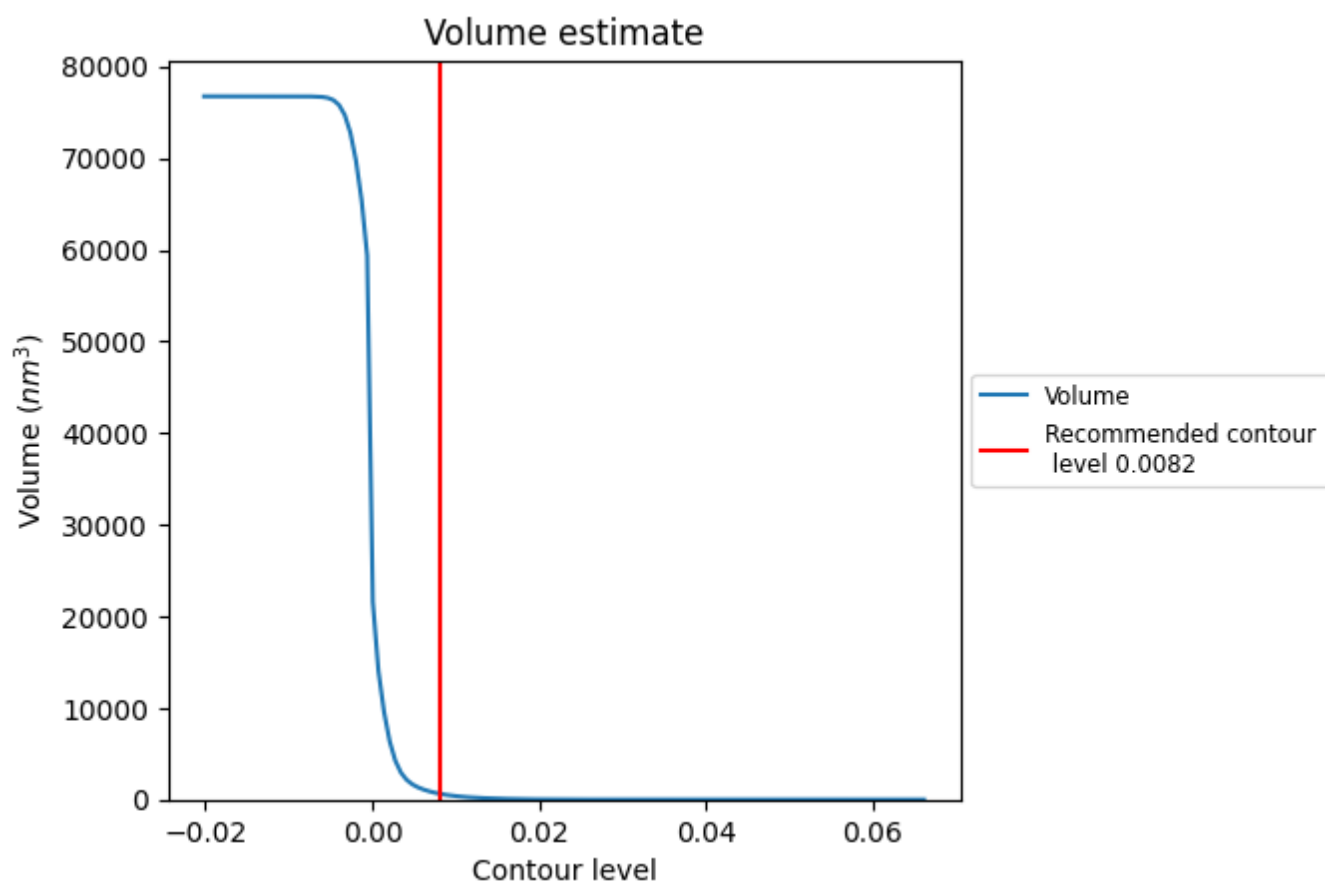
This section contains the results of statistical analysis of the map.

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.

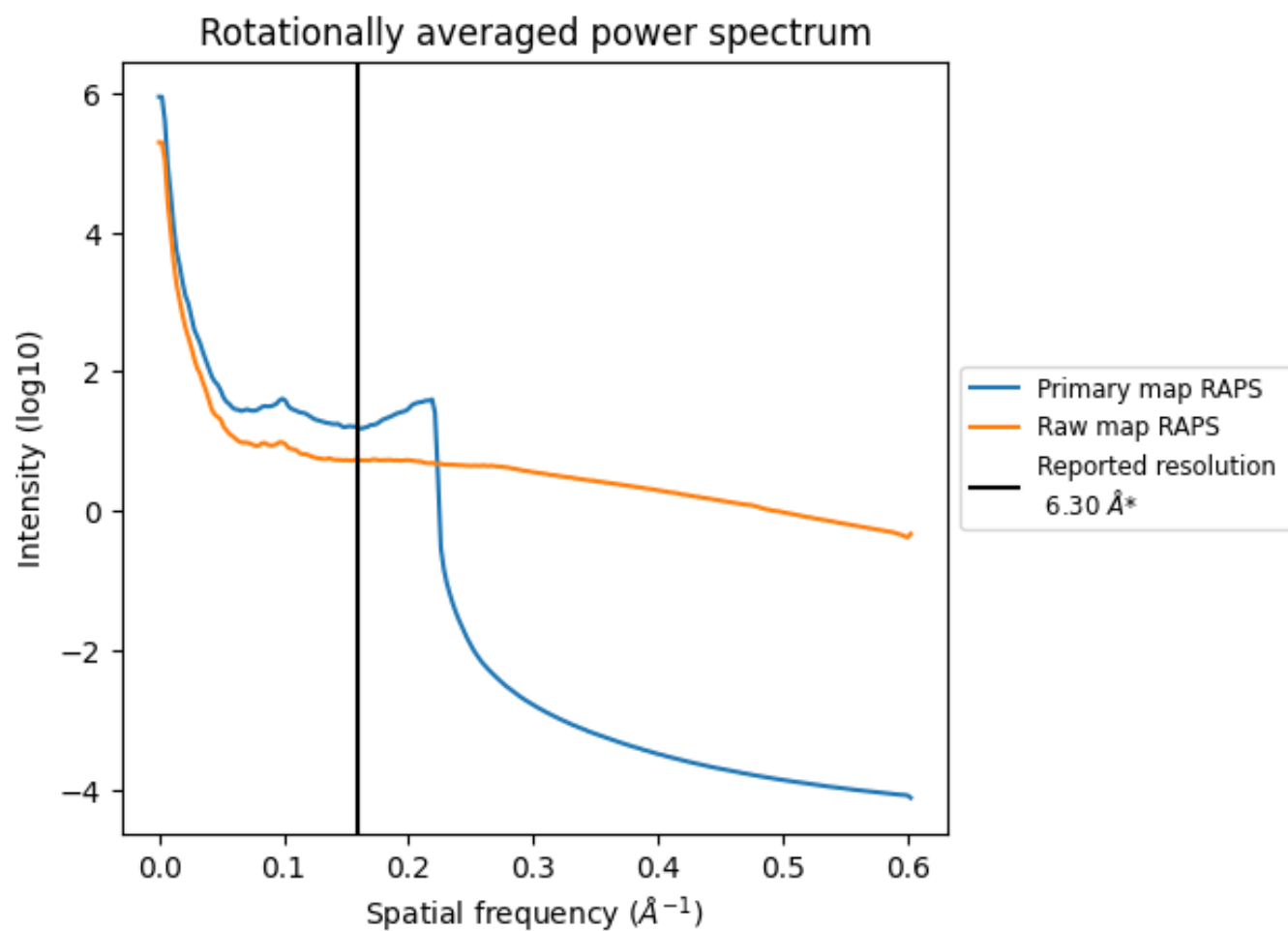
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 617 nm³; this corresponds to an approximate mass of 557 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 ⓘ

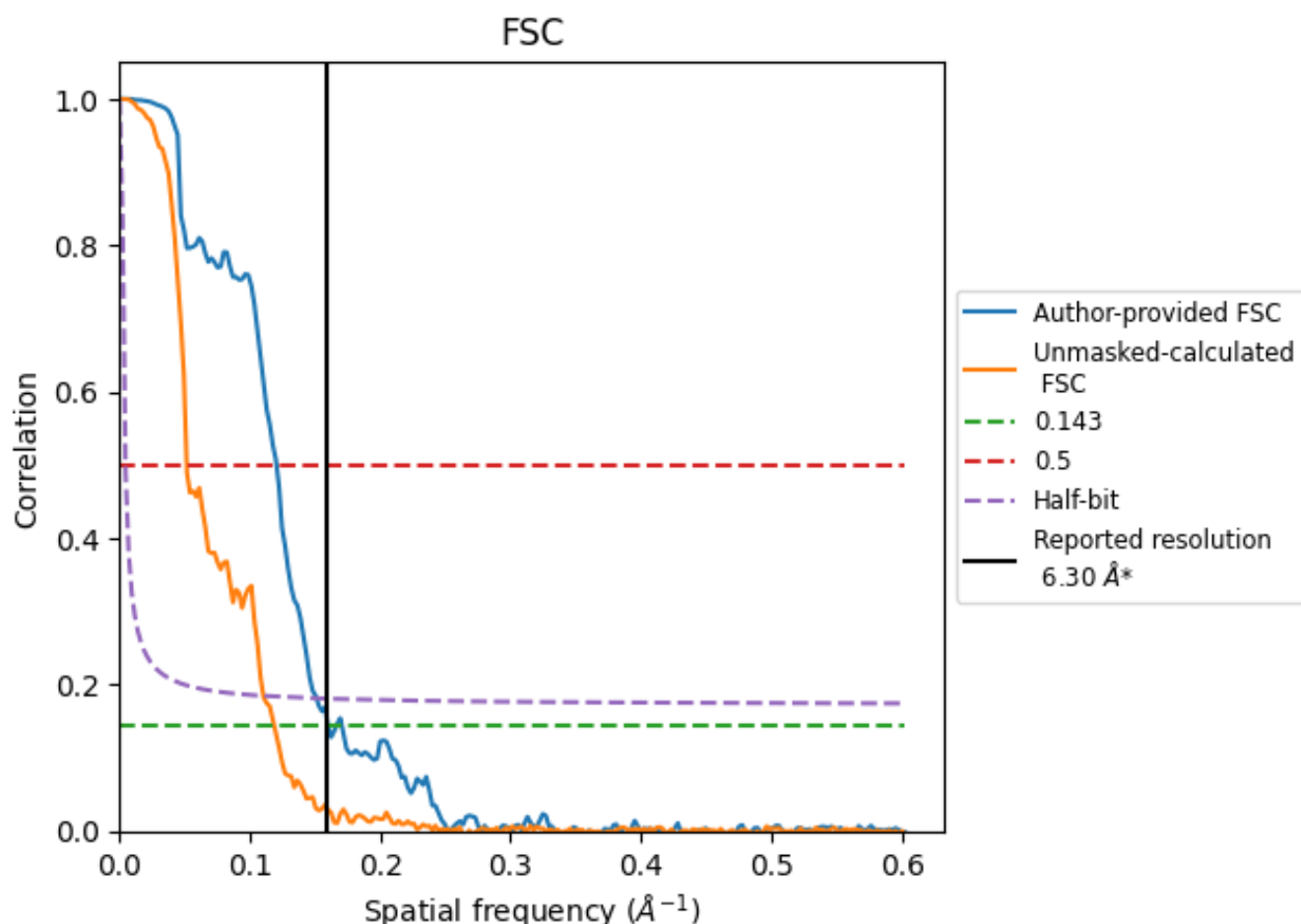


*Reported resolution corresponds to spatial frequency of 0.159 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.159 Å⁻¹

8.2 Resolution estimates [i](#)

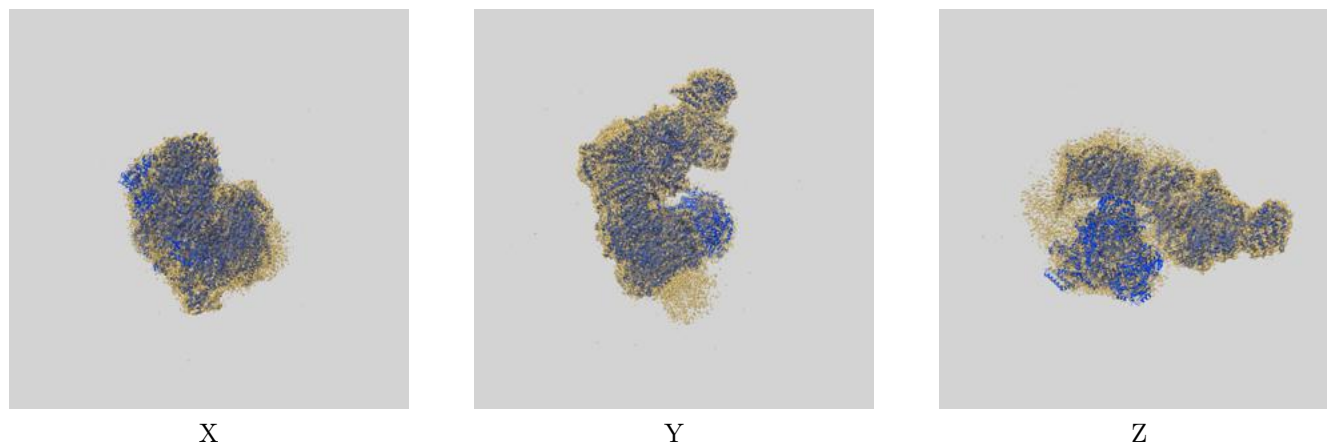
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.30	-	-
Author-provided FSC curve	6.25	8.30	6.61
Unmasked-calculated*	8.42	19.38	9.06

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.42 differs from the reported value 6.3 by more than 10 %

9 Map-model fit [i](#)

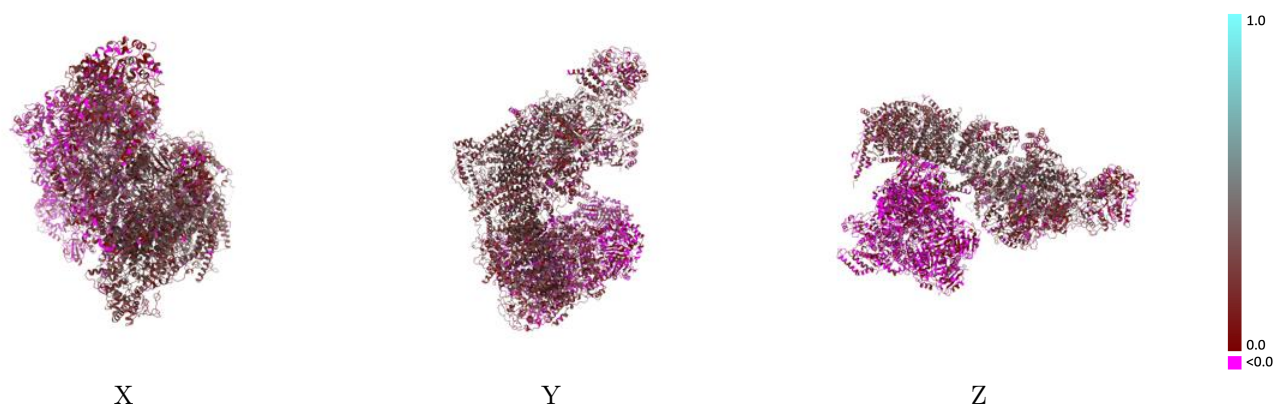
This section contains information regarding the fit between EMDB map EMD-35352 and PDB model 8IC2. Per-residue inclusion information can be found in section 3 on page 26.

9.1 Map-model overlay [i](#)



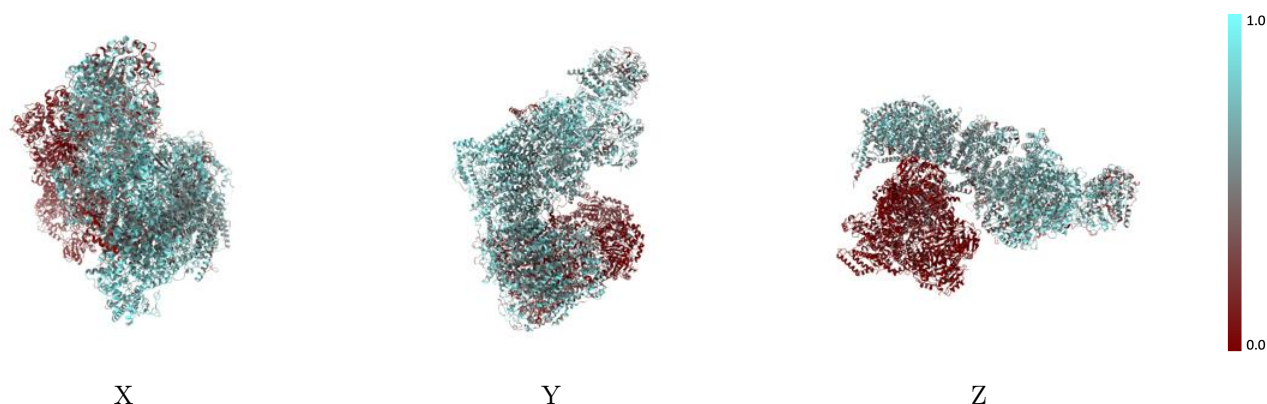
The images above show the 3D surface view of the map at the recommended contour level 0.0082 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



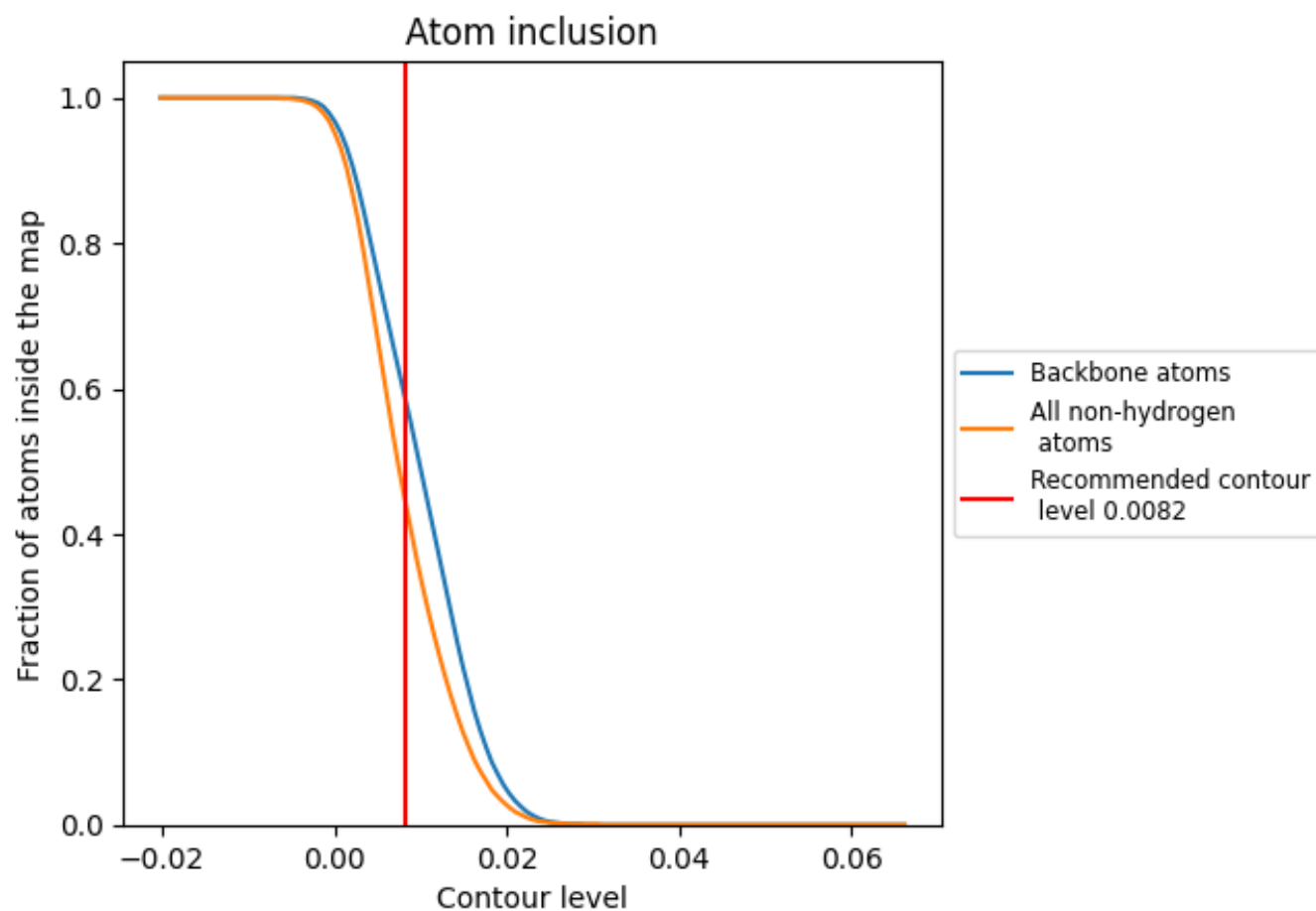
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0082).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 45% 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 (0.0082) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4470	 0.1620
A	 0.6300	 0.2860
AA	 0.0700	 0.0200
AB	 0.0460	 0.0120
AC	 0.0610	 -0.0060
AD	 0.0420	 -0.0050
AE	 0.0500	 -0.0000
AF	 0.0580	 0.0020
AG	 0.0440	 -0.0140
AH	 0.0140	 0.0180
AI	 0.0780	 -0.0240
AJ	 0.0650	 -0.0270
AK	 0.0500	 -0.0080
Aa	 0.0790	 0.0060
Ab	 0.0970	 0.0020
Ac	 0.1120	 0.0070
Ad	 0.0490	 -0.0020
Ae	 0.0270	 0.0020
Af	 0.0760	 0.0280
Ag	 0.1020	 0.0200
Ah	 0.0230	 0.0210
Aj	 0.0370	 -0.0150
Ak	 0.0460	 -0.0170
B	 0.7370	 0.2950
C	 0.7190	 0.2680
D	 0.7110	 0.3040
E	 0.5840	 0.1820
F	 0.5730	 0.1700
G	 0.6660	 0.2170
H	 0.6640	 0.2950
I	 0.7580	 0.3010
J	 0.5800	 0.2550
K	 0.6600	 0.2980
L	 0.6060	 0.2500
M	 0.6240	 0.2910



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
N	 0.6810	 0.3080
O	 0.6070	 0.2140
P	 0.6080	 0.1960
Q	 0.6230	 0.2630
R	 0.4540	 0.1950
S	 0.6130	 0.1520
T	 0.4760	 0.1260
U	 0.6600	 0.2200
V	 0.6430	 0.1750
W	 0.6640	 0.2260
X	 0.7620	 0.2650
Y	 0.4750	 0.2170
Z	 0.7340	 0.2500
a	 0.7750	 0.2800
b	 0.7270	 0.2540
c	 0.5820	 0.2290
d	 0.6170	 0.2230
e	 0.7340	 0.2790
f	 0.6200	 0.2590
g	 0.6070	 0.2300
h	 0.6340	 0.2510
i	 0.6070	 0.2300
j	 0.6300	 0.1610
k	 0.6270	 0.2090
l	 0.6080	 0.2260
m	 0.5370	 0.2100
n	 0.6180	 0.2200
o	 0.5820	 0.1390
p	 0.6770	 0.2430
q	 0.2250	 0.1500
r	 0.4090	 0.1190
s	 0.3530	 0.0670