



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 01:17 AM UTC

PDB ID : 9G9Y / pdb_00009g9y
EMDB ID : EMD-51161
Title : Respiratory supercomplex CI2-CIII2-CIV2 (megacomplex) from alphaproteobacterium
Authors : Yaikhomba, M.; Hirst, J.; Croll, T.I.; Spikes, T.E.; Agip, A.N.A.
Deposited on : 2024-07-25
Resolution : 4.91 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

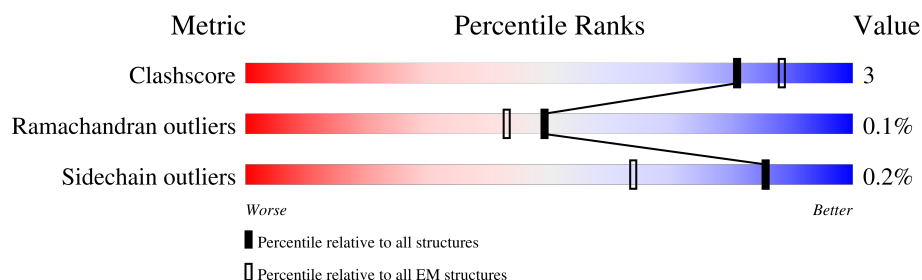
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.91 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.













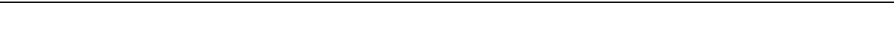

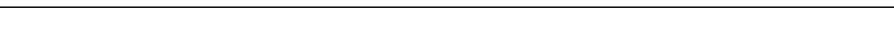
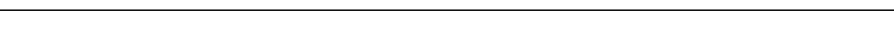






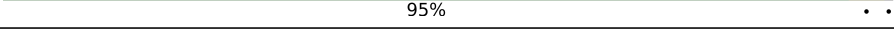
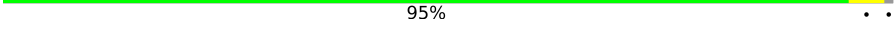
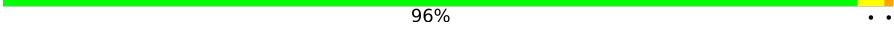
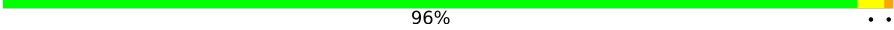

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	121	92% 8%
1	A1	121	95% 5%
2	B	175	82% 11% 7%
2	B1	175	84% 9% 7%
3	C	208	88% 5% 7%
3	C1	208	88% 5% 7%
4	D	412	92% 8%
4	D1	412	91% 9%
5	E	239	90% 9% .

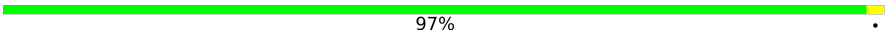
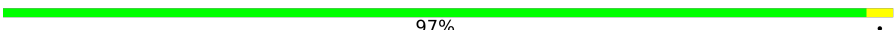


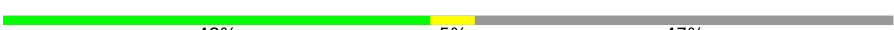





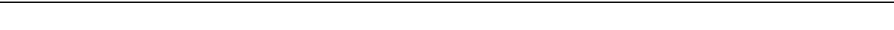

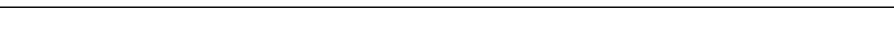
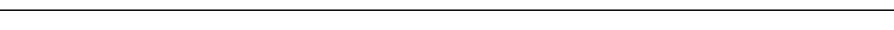
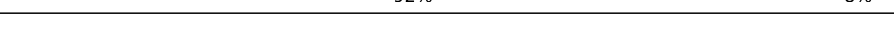




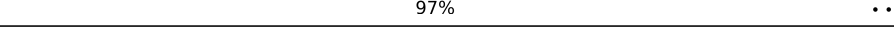
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Mol	Chain	Length	Quality of chain
5	E1	239	 92% 7% .
6	F	431	 88% 10% .
6	F1	431	 88% 10% .
7	G	674	 92% 6% .
7	G1	674	 92% 6% .
8	H	345	 91% 8% .
8	H1	345	 92% 7% .
9	I	163	 91% 8% .
9	I1	163	 93% 7% .
10	J	199	 96% .
10	J1	199	 97% .
11	K	101	 93% 6% .
11	K1	101	 92% 7% .
12	L	703	 88% 6% 6%
12	L1	703	 88% 6% 6%
13	M	513	 89% 8% .
13	M1	513	 89% 8% .
14	N	499	 91% 5% .
14	N1	499	 92% . .
15	P	330	 95% . .
15	P1	330	 95% . .
16	Q	103	 96% . .
16	Q1	103	 96% . .
17	R	62	 92% 6% .
17	R1	62	 92% 6% .

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Mol	Chain	Length	Quality of chain
18	Z	217	 97% .
18	Z1	217	 97% .
19	a	440	 92% 7% .
19	d	440	 91% 7% .
20	b	450	 48% 5% 47%
20	e	450	 48% 5% 47%
21	c	195	 86% 7% 7%
21	f	195	 86% 7% 7%
22	g	558	 88% 9% .
22	k	558	 90% 8% .
23	h	298	 77% 8% 15%
23	l	298	 76% 8% 15%
24	i	274	 91% 9%
24	m	274	 92% 8%
25	j	66	 64% . 35%
25	n	66	 64% . 35%
26	o	176	 23% . 75%
26	p	176	 23% . 75%
27	q	124	 97% ..
27	q1	124	 96% ..

2 Entry composition

There are 45 unique types of molecules in this entry. The entry contains 120030 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-quinone oxidoreductase subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	121	Total	C	N	O	S	0	0
			969	658	141	164	6		
1	A1	121	Total	C	N	O	S	0	0
			969	658	141	164	6		

- Molecule 2 is a protein called NADH-quinone oxidoreductase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	162	Total	C	N	O	S	0	0
			1270	799	227	231	13		
2	B1	162	Total	C	N	O	S	0	0
			1270	799	227	231	13		

- Molecule 3 is a protein called NADH-quinone oxidoreductase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	194	Total	C	N	O	S	0	0
			1586	1020	274	290	2		
3	C1	194	Total	C	N	O	S	0	0
			1586	1020	274	290	2		

- Molecule 4 is a protein called NADH-quinone oxidoreductase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	411	Total	C	N	O	S	0	0
			3277	2072	582	601	22		
4	D1	411	Total	C	N	O	S	0	0
			3277	2072	582	601	22		

- Molecule 5 is a protein called NADH dehydrogenase subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	237	Total	C	N	O	S	0	0
			1822	1155	314	340	13		
5	E1	237	Total	C	N	O	S	0	0
			1822	1155	314	340	13		

- Molecule 6 is a protein called NADH-quinone oxidoreductase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	422	Total	C	N	O	S	0	0
			3241	2027	583	600	31		
6	F1	422	Total	C	N	O	S	0	0
			3241	2027	583	600	31		

- Molecule 7 is a protein called NADH-quinone oxidoreductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	665	Total	C	N	O	S	0	0
			5068	3149	917	969	33		
7	G1	665	Total	C	N	O	S	0	0
			5068	3149	917	969	33		

- Molecule 8 is a protein called NADH-quinone oxidoreductase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	341	Total	C	N	O	S	0	0
			2722	1848	413	439	22		
8	H1	341	Total	C	N	O	S	0	0
			2722	1848	413	439	22		

- Molecule 9 is a protein called NADH-quinone oxidoreductase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	162	Total	C	N	O	S	0	0
			1319	836	230	242	11		
9	I1	162	Total	C	N	O	S	0	0
			1319	836	230	242	11		

- Molecule 10 is a protein called NADH-quinone oxidoreductase subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	199	Total	C	N	O	S	0	0
			1528	1014	246	257	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	J1	199	Total	C	N	O	S	0	0
			1528	1014	246	257	11		

- Molecule 11 is a protein called NADH-quinone oxidoreductase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			764	508	123	128	5		
11	K1	101	Total	C	N	O	S	0	0
			764	508	123	128	5		

- Molecule 12 is a protein called NADH dehydrogenase subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	661	Total	C	N	O	S	0	0
			5215	3472	853	857	33		
12	L1	661	Total	C	N	O	S	0	0
			5215	3472	853	857	33		

- Molecule 13 is a protein called NADH dehydrogenase subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	503	Total	C	N	O	S	0	0
			3915	2615	610	658	32		
13	M1	503	Total	C	N	O	S	0	0
			3915	2615	610	658	32		

- Molecule 14 is a protein called NADH-quinone oxidoreductase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	480	Total	C	N	O	S	0	0
			3556	2342	565	617	32		
14	N1	480	Total	C	N	O	S	0	0
			3556	2342	565	617	32		

- Molecule 15 is a protein called NAD-dependent epimerase/dehydratase.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	328	Total	C	N	O	S	0	0
			2468	1541	463	452	12		
15	P1	328	Total	C	N	O	S	0	0
			2468	1541	463	452	12		

- Molecule 16 is a protein called ETC complex I subunit conserved region.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	103	Total	C	N	O	S	0	0
			849	523	167	156	3		
16	Q1	103	Total	C	N	O	S	0	0
			849	523	167	156	3		

- Molecule 17 is a protein called Zinc finger CHCC-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	61	Total	C	N	O	S	0	0
			488	304	90	91	3		
17	R1	61	Total	C	N	O	S	0	0
			488	304	90	91	3		

- Molecule 18 is a protein called Protein-L-isoaspartate O-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	216	Total	C	N	O	S	0	0
			1642	1033	294	306	9		
18	Z1	216	Total	C	N	O	S	0	0
			1642	1033	294	306	9		

- Molecule 19 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	434	Total	C	N	O	S	0	0
			3513	2378	553	564	18		
19	d	434	Total	C	N	O	S	0	0
			3513	2378	553	564	18		

- Molecule 20 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	b	239	Total	C	N	O	S	0	0
			1855	1181	311	354	9		
20	e	239	Total	C	N	O	S	0	0
			1855	1181	311	354	9		

- Molecule 21 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	c	181	Total	C	N	O	S	0	0
			1361	842	246	266	7		
21	f	181	Total	C	N	O	S	0	0
			1361	842	246	266	7		

- Molecule 22 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	g	544	Total	C	N	O	S	0	0
			4322	2890	684	715	33		
22	k	544	Total	C	N	O	S	0	0
			4322	2890	684	715	33		

- Molecule 23 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	h	252	Total	C	N	O	S	0	0
			1976	1295	319	354	8		
23	l	252	Total	C	N	O	S	0	0
			1976	1295	319	354	8		

- Molecule 24 is a protein called cytochrome-c oxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	i	273	Total	C	N	O	S	0	0
			2183	1483	341	348	11		
24	m	273	Total	C	N	O	S	0	0
			2183	1483	341	348	11		

- Molecule 25 is a protein called Aa3 type cytochrome c oxidase subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	j	43	Total	C	N	O	S	0	0
			332	214	58	59	1		
25	n	43	Total	C	N	O	S	0	0
			332	214	58	59	1		

- Molecule 26 is a protein called Cytochrome c, class I.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	o	44	Total	C	N	O	S	0	0
			324	215	49	58	2		

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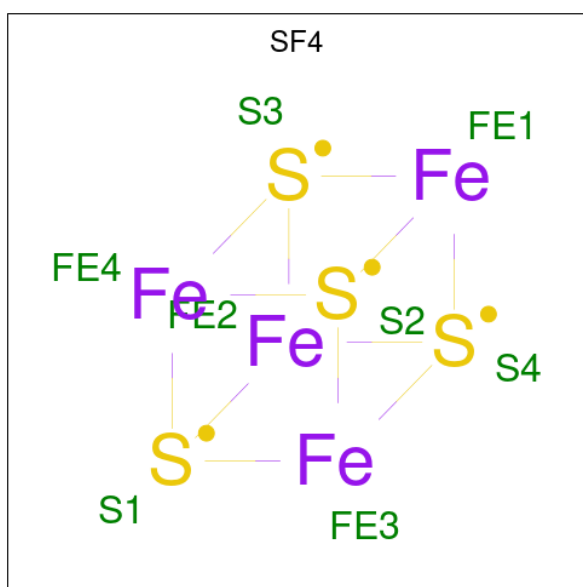
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Mol	Chain	Residues	Atoms					AltConf	Trace
26	p	44	Total	C	N	O	S	0	0
			324	215	49	58	2		

- Molecule 27 is a protein called NADH:ubiquinone oxidoreductase 17.2 kD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	q	123	Total	C	N	O	S	0	0
			1018	651	181	185	1		
27	q1	123	Total	C	N	O	S	0	0
			1018	651	181	185	1		

- Molecule 28 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



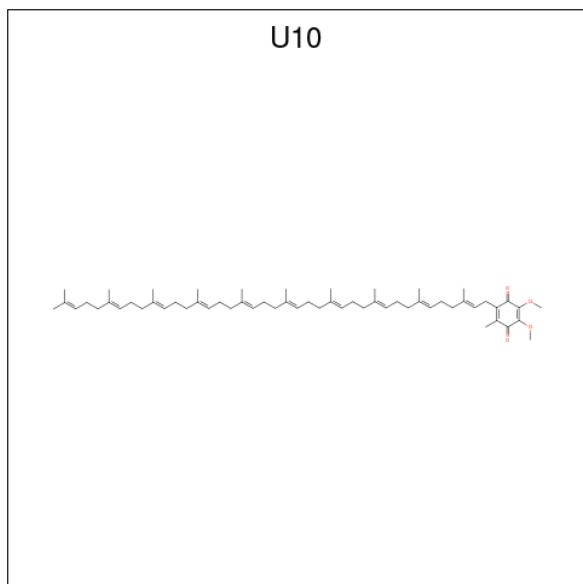
Mol	Chain	Residues	Atoms			AltConf
28	B	1	Total	Fe	S	0
			8	4	4	
28	B1	1	Total	Fe	S	0
			8	4	4	
28	F	1	Total	Fe	S	0
			8	4	4	
28	F1	1	Total	Fe	S	0
			8	4	4	
28	G	1	Total	Fe	S	0
			8	4	4	
28	G	1	Total	Fe	S	0
			8	4	4	

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Mol	Chain	Residues	Atoms			AltConf
28	G1	1	Total	Fe	S	0
			8	4	4	
28	G1	1	Total	Fe	S	0
			8	4	4	
28	I	1	Total	Fe	S	0
			8	4	4	
28	I	1	Total	Fe	S	0
			8	4	4	
28	I1	1	Total	Fe	S	0
			8	4	4	
28	I1	1	Total	Fe	S	0
			8	4	4	

- Molecule 29 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			AltConf
29	B	1	Total	C	O	0
			63	59	4	
29	B1	1	Total	C	O	0
			63	59	4	
29	a	1	Total	C	O	0
			63	59	4	
29	a	1	Total	C	O	0
			63	59	4	
29	d	1	Total	C	O	0
			63	59	4	

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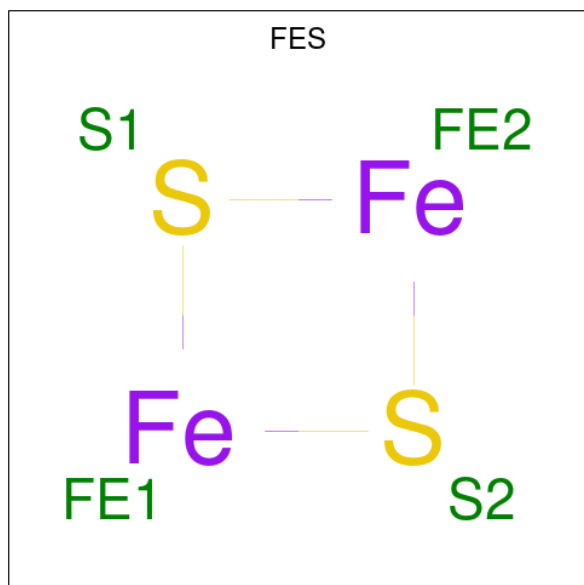
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Mol	Chain	Residues	Atoms			AltConf
29	d	1	Total	C	O	0
			63	59	4	

- Molecule 30 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
30	D	1	Total	Ca	0
			1	1	
30	D1	1	Total	Ca	0
			1	1	
30	b	1	Total	Ca	0
			1	1	
30	e	1	Total	Ca	0
			1	1	
30	g	1	Total	Ca	0
			1	1	
30	k	1	Total	Ca	0
			1	1	

- Molecule 31 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



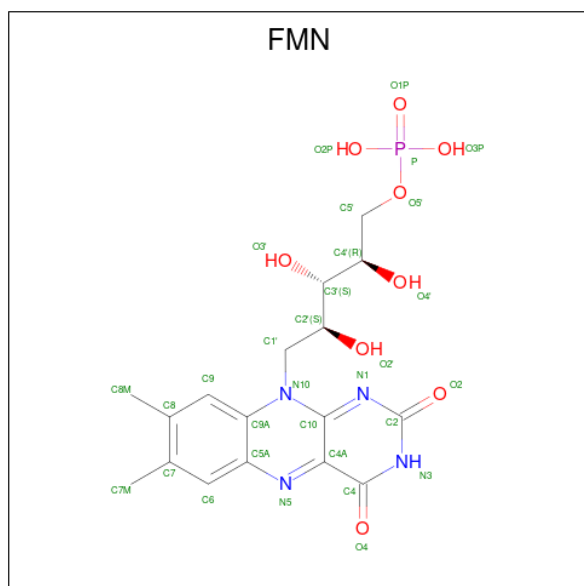
Mol	Chain	Residues	Atoms			AltConf
31	E	1	Total	Fe	S	0
			4	2	2	
31	E1	1	Total	Fe	S	0
			4	2	2	

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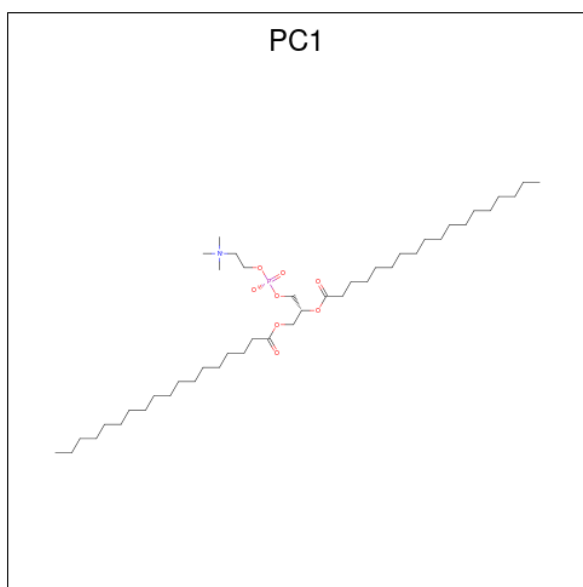
Mol	Chain	Residues	Atoms			AltConf
31	G	1	Total	Fe	S	0
			4	2	2	
31	G1	1	Total	Fe	S	0
			4	2	2	
31	c	1	Total	Fe	S	0
			4	2	2	
31	f	1	Total	Fe	S	0
			4	2	2	

- Molecule 32 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



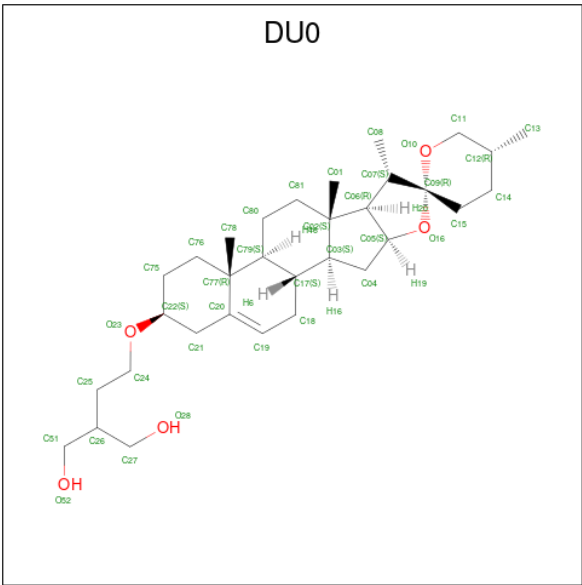
Mol	Chain	Residues	Atoms					AltConf
32	F	1	Total	C	N	O	P	0
			31	17	4	9	1	
32	F1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 33 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



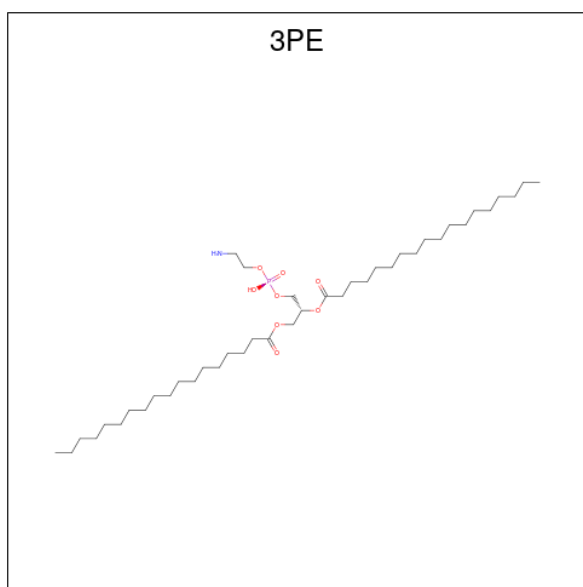
Mol	Chain	Residues	Atoms					AltConf
33	H	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	H1	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	H1	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	L1	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	M	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	M1	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	i	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	i	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	j	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	m	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	m	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	n	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 34 is 2-[2-[(1 {S},2 {S},4 {S},5' {R},6 {R},7 {S},8 {R},9 {S},12 {S},13 {R},16 {S})-5',7,9,13-tetramethylspiro[5-oxapentacyclo[10.8.0.0^{2,9}.0^{4,8}.0^{13,18}]]icos-18-ene-6,2'-oxane]-16-yl]oxyethyl]propane-1,3-diol (CCD ID: DU0) (formula: C₃₂H₅₂O₅).



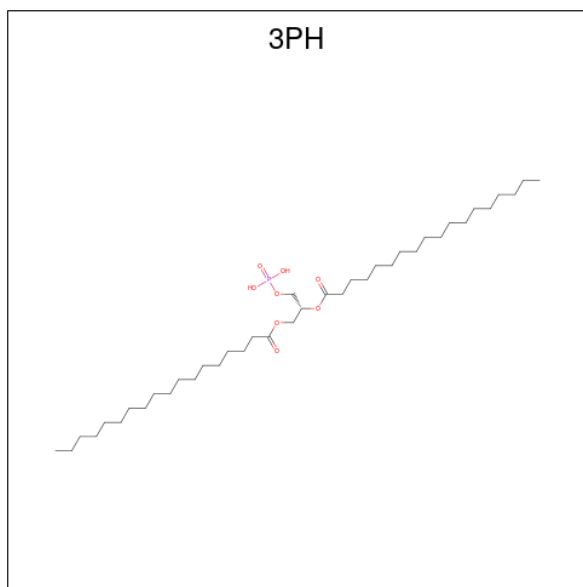
Mol	Chain	Residues	Atoms			AltConf
34	K	1	Total	C	O	0
			37	32	5	
34	M	1	Total	C	O	0
			37	32	5	
34	M1	1	Total	C	O	0
			37	32	5	
34	a	1	Total	C	O	0
			37	32	5	
34	d	1	Total	C	O	0
			37	32	5	

- Molecule 35 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



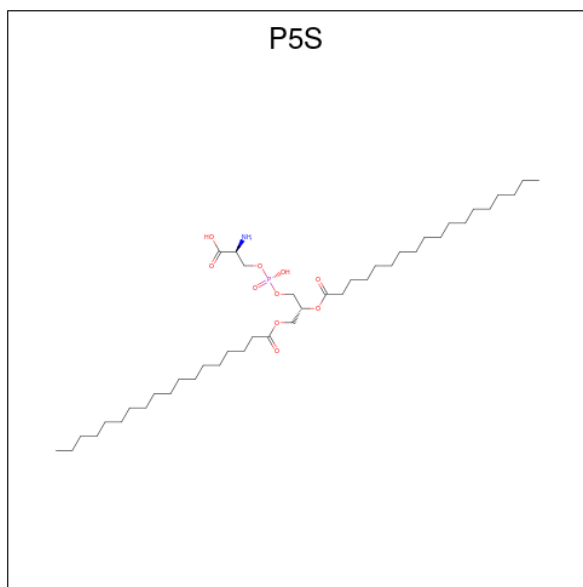
Mol	Chain	Residues	Atoms					AltConf
35	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
35	L1	1	Total	C	N	O	P	0
			51	41	1	8	1	
35	b	1	Total	C	N	O	P	0
			51	41	1	8	1	
35	e	1	Total	C	N	O	P	0
			51	41	1	8	1	
35	g	1	Total	C	N	O	P	0
			51	41	1	8	1	
35	i	1	Total	C	N	O	P	0
			51	41	1	8	1	
35	k	1	Total	C	N	O	P	0
			51	41	1	8	1	
35	m	1	Total	C	N	O	P	0
			51	41	1	8	1	
35	m	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 36 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
36	L	1	Total	C	O	P	0
			48	39	8	1	
36	L1	1	Total	C	O	P	0
			48	39	8	1	
36	f	1	Total	C	O	P	0
			48	39	8	1	
36	g	1	Total	C	O	P	0
			48	39	8	1	
36	k	1	Total	C	O	P	0
			48	39	8	1	
36	p	1	Total	C	O	P	0
			48	39	8	1	

- Molecule 37 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: C₄₂H₈₂NO₁₀P).

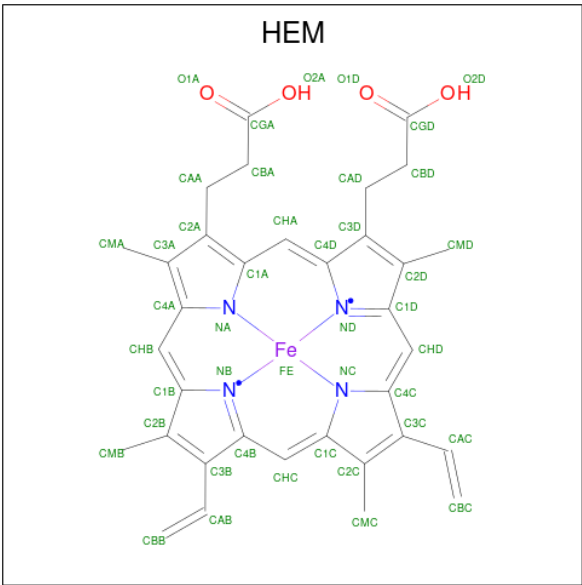


Mol	Chain	Residues	Atoms					AltConf
37	L	1	Total	C	N	O	P	0
			54	42	1	10	1	
37	L1	1	Total	C	N	O	P	0
			54	42	1	10	1	

- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

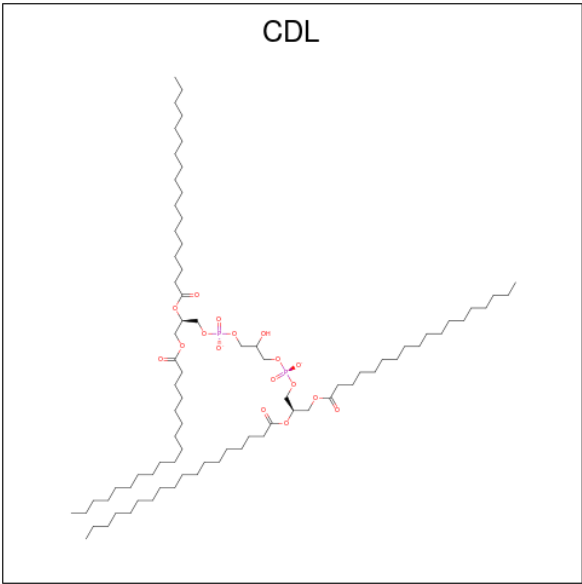
Mol	Chain	Residues	Atoms		AltConf
38	R	1	Total	Zn	0
			1	1	
38	R1	1	Total	Zn	0
			1	1	
38	i	1	Total	Zn	0
			1	1	
38	m	1	Total	Zn	0
			1	1	

- Molecule 39 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



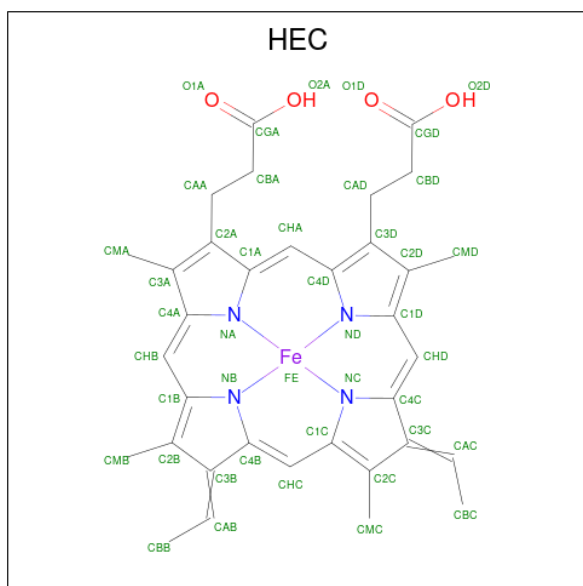
Mol	Chain	Residues	Atoms					AltConf
39	a	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
39	a	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
39	d	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
39	d	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 40 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



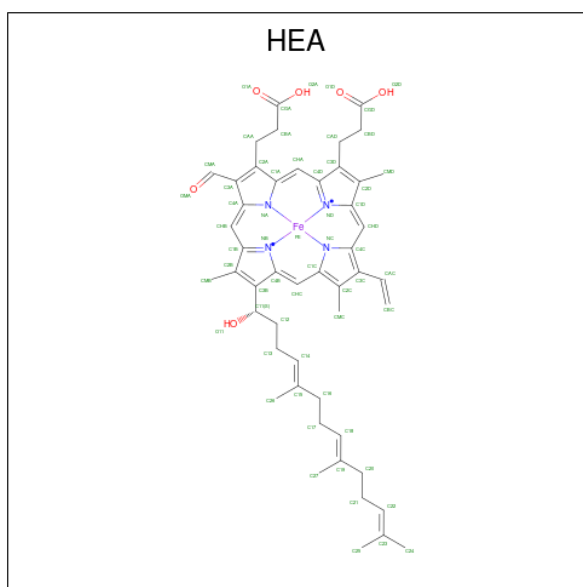
Mol	Chain	Residues	Atoms				AltConf
40	a	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 41 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
41	b	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
41	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 42 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
42	g	1	Total 60	C 49	Fe 1	N 4	O 6	0
42	g	1	Total 60	C 49	Fe 1	N 4	O 6	0
42	k	1	Total 60	C 49	Fe 1	N 4	O 6	0
42	k	1	Total 60	C 49	Fe 1	N 4	O 6	0

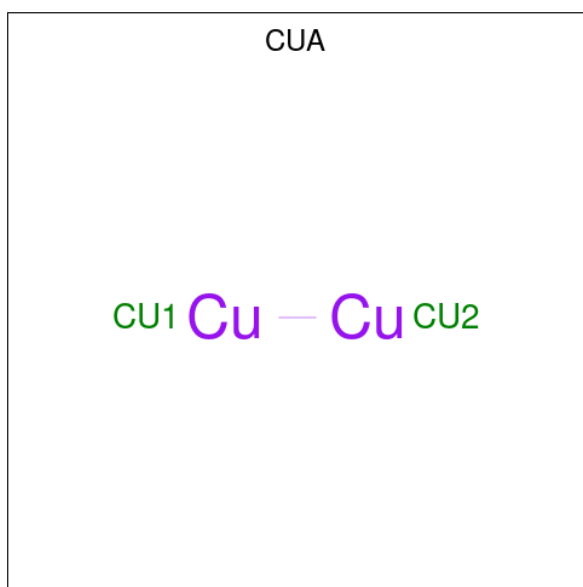
- Molecule 43 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
43	g	1	Total	Cu	0
			1	1	
43	k	1	Total	Cu	0
			1	1	

- Molecule 44 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
44	g	1	Total	Mn	0
			1	1	
44	k	1	Total	Mn	0
			1	1	

- Molecule 45 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



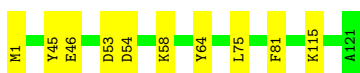
Mol	Chain	Residues	Atoms		AltConf
45	h	1	Total 2	Cu 2	0
45	l	1	Total 2	Cu 2	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

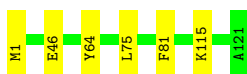
- Molecule 1: NADH-quinone oxidoreductase subunit A

Chain A: 




- Molecule 1: NADH-quinone oxidoreductase subunit A

Chain A1: 




- Molecule 2: NADH-quinone oxidoreductase subunit B

Chain B: 




- Molecule 2: NADH-quinone oxidoreductase subunit B

Chain B1: 




- Molecule 3: NADH-quinone oxidoreductase subunit C

Chain C: 



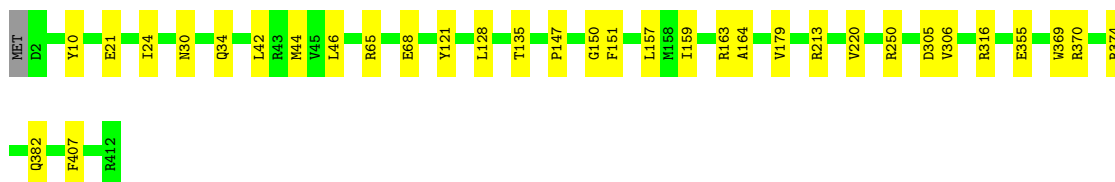
- Molecule 3: NADH-quinone oxidoreductase subunit C

Chain C1: 



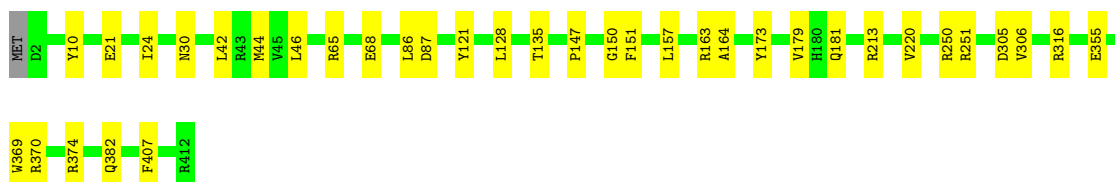
- Molecule 4: NADH-quinone oxidoreductase subunit D

Chain D: 92% 8%



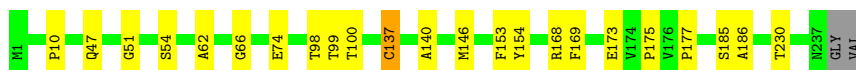
- Molecule 4: NADH-quinone oxidoreductase subunit D

Chain D1: 91% 9%



- Molecule 5: NADH dehydrogenase subunit E

Chain E: 90% 9%



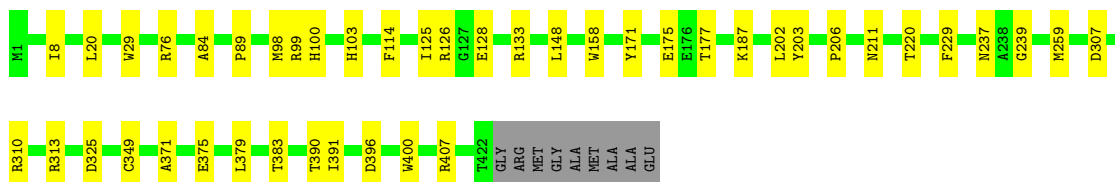
- Molecule 5: NADH dehydrogenase subunit E

Chain E1: 92% 7%




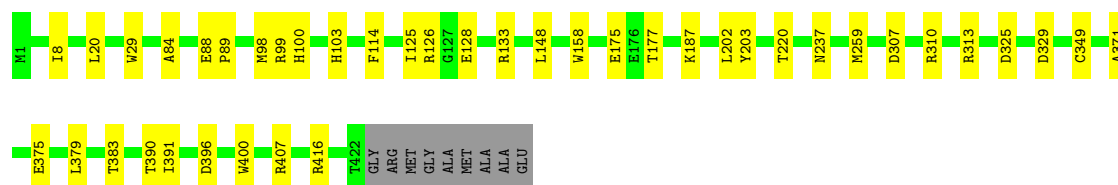
- Molecule 6: NADH-quinone oxidoreductase subunit F

Chain F: 88% 10%



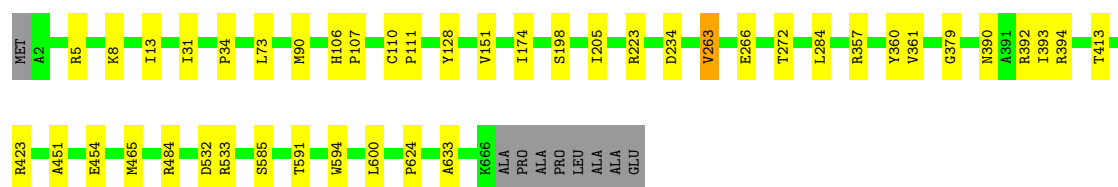
- Molecule 6: NADH-quinone oxidoreductase subunit F

Chain F1:  88% 10% .



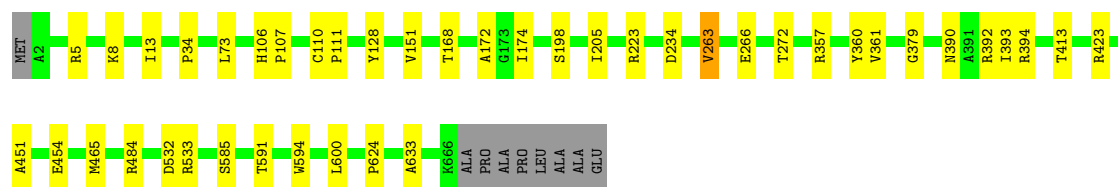
• Molecule 7: NADH-quinone oxidoreductase

Chain G:  92% 6% .



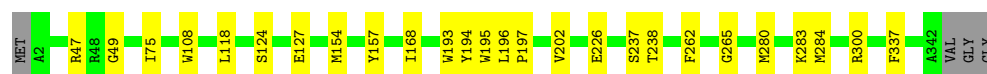
• Molecule 7: NADH-quinone oxidoreductase

Chain G1:  92% 6% .



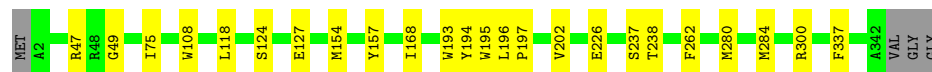
• Molecule 8: NADH-quinone oxidoreductase subunit H

Chain H:  91% 8% .




• Molecule 8: NADH-quinone oxidoreductase subunit H

Chain H1:  92% 7% .



• Molecule 9: NADH-quinone oxidoreductase subunit I

Chain I:  91% 8% .



- Molecule 9: NADH-quinone oxidoreductase subunit I

Chain I1:  93% 7%



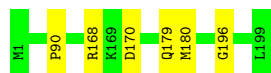
- Molecule 10: NADH-quinone oxidoreductase subunit J

Chain J:  96%



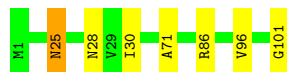
- Molecule 10: NADH-quinone oxidoreductase subunit J

Chain J1:  97%



- Molecule 11: NADH-quinone oxidoreductase subunit K

Chain K:  93% 6%




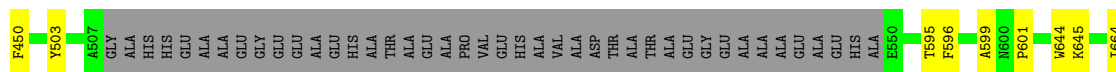
- Molecule 11: NADH-quinone oxidoreductase subunit K

Chain K1:  92% 7%




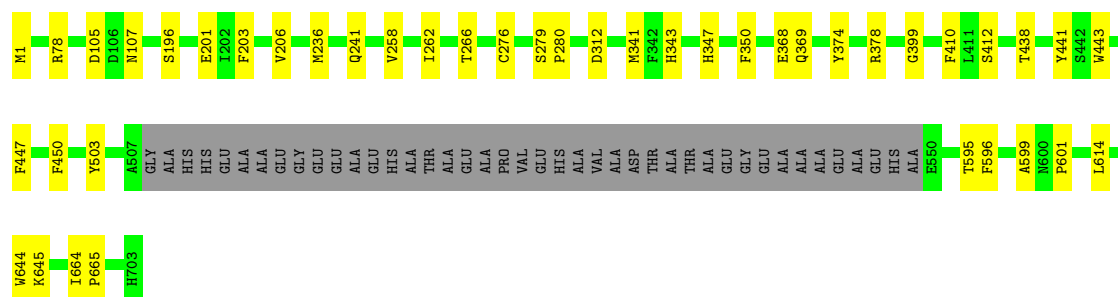
- Molecule 12: NADH dehydrogenase subunit L

Chain L:  88% 6% 6%



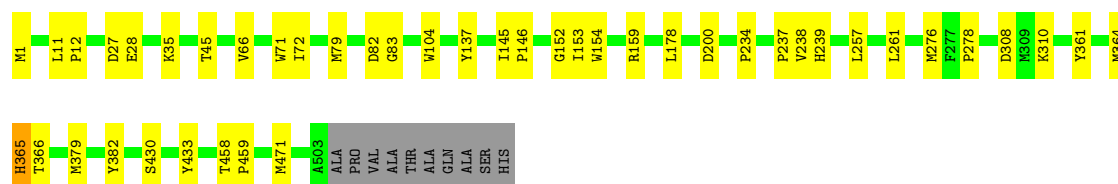
- Molecule 12: NADH dehydrogenase subunit L

Chain L1:  88% 6% 6%



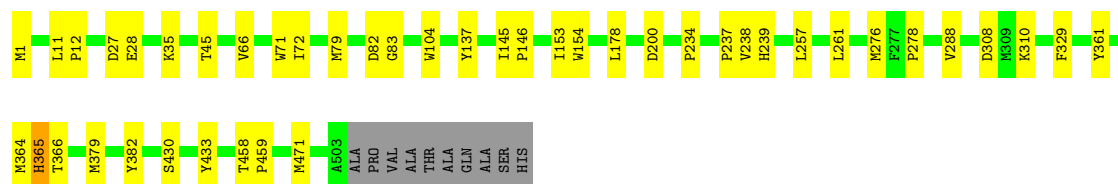
• Molecule 13: NADH dehydrogenase subunit M

Chain M:  89% 8% .




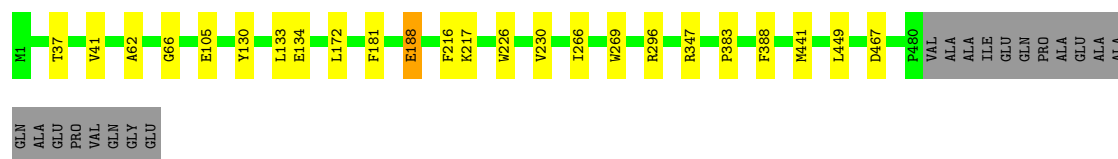
• Molecule 13: NADH dehydrogenase subunit M

Chain M1:  89% 8% .



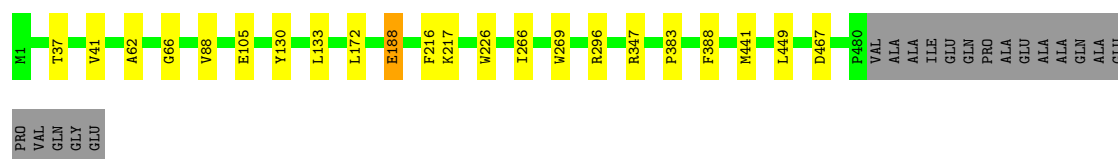
• Molecule 14: NADH-quinone oxidoreductase subunit N

Chain N:  91% 5% .



• Molecule 14: NADH-quinone oxidoreductase subunit N

Chain N1:  92% . .



- Molecule 15: NAD-dependent epimerase/dehydratase

Chain P:  95% ..



- Molecule 15: NAD-dependent epimerase/dehydratase

Chain P1:  95% ..



- Molecule 16: ETC complex I subunit conserved region

Chain Q:  96% ..



- Molecule 16: ETC complex I subunit conserved region

Chain Q1:  96% ..



- Molecule 17: Zinc finger CHCC-type domain-containing protein

Chain R:  92% 6% .



- Molecule 17: Zinc finger CHCC-type domain-containing protein

Chain R1:  92% 6% .




- Molecule 18: Protein-L-isoaspartate O-methyltransferase

Chain Z:  97% .



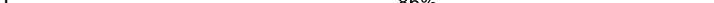
- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | LEU | LEU | ARG | ASN | ALA | SER | LEU | LEU | ALA | VAL | VAL | ALA | ALA | LEU | THR | THR | VAL | VAL | ALA | LEU | GLY | GLY | GLY | GLN | ASP | ALA | SER | THR | THR | ALA | ALA | PRO | GLY | GLY | SER | SER | TYR | HIS | THR | ASN | ALA | ALA | ALA | ALA | ASP | THR | ALA | ALA | PRO | PRO | ALA | ALA | ALA | GLY | ALA | ALA |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- Molecule 21: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain c:  86% 7% 7%



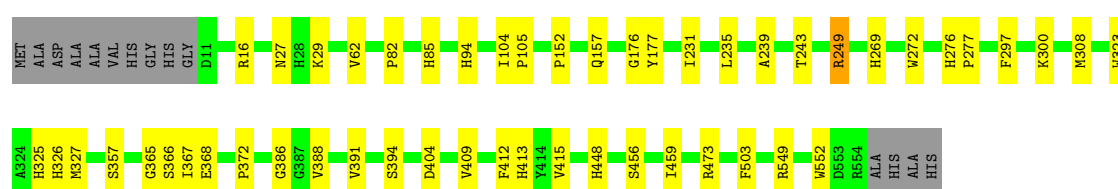
- Molecule 21: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain f:  86% 7% 7%

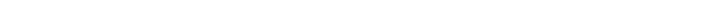


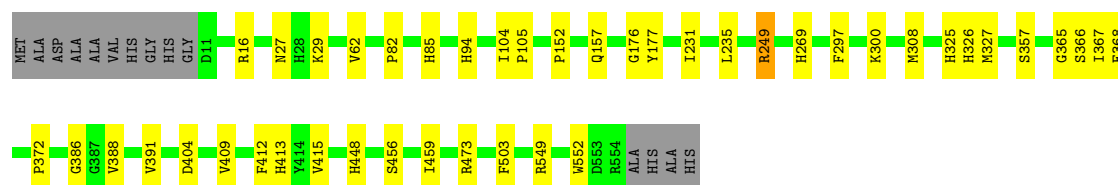
- Molecule 22: Cytochrome c oxidase subunit 1

Chain g: 88% 9%



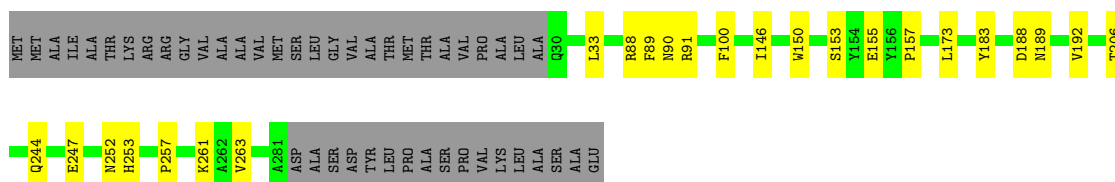
- Molecule 22: Cytochrome c oxidase subunit 1

Chain k:  90% 8%



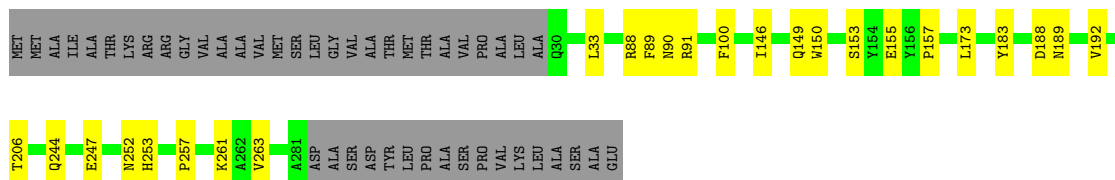
- Molecule 23: Cytochrome c oxidase subunit 2

Chain h: 77% 8% 15%



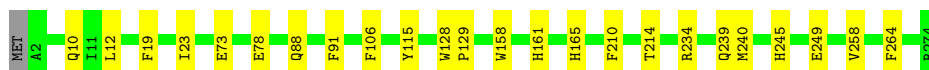
• Molecule 23: Cytochrome c oxidase subunit 2

Chain l: 76% 8% 15%



• Molecule 24: cytochrome-c oxidase

Chain i: 91% 9%



• Molecule 24: cytochrome-c oxidase

Chain m: 92% 8%



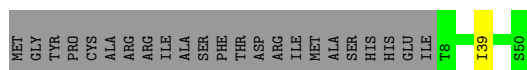
• Molecule 25: Aa3 type cytochrome c oxidase subunit IV

Chain j: 64% 35%



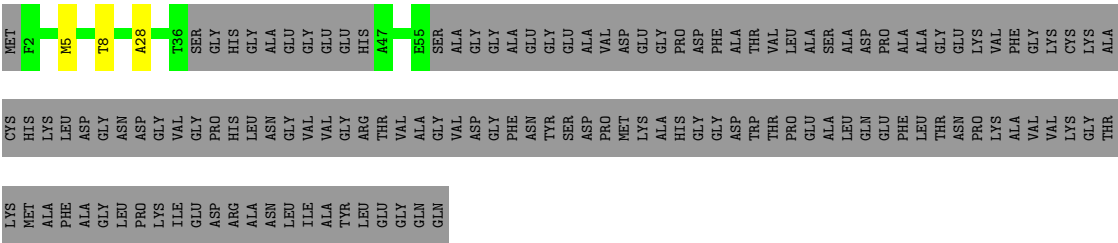
• Molecule 25: Aa3 type cytochrome c oxidase subunit IV

Chain n: 64% 35%

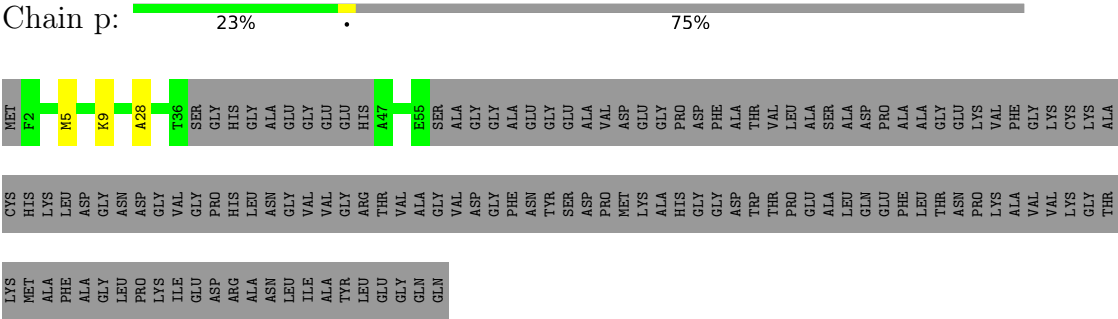


• Molecule 26: Cytochrome c, class I

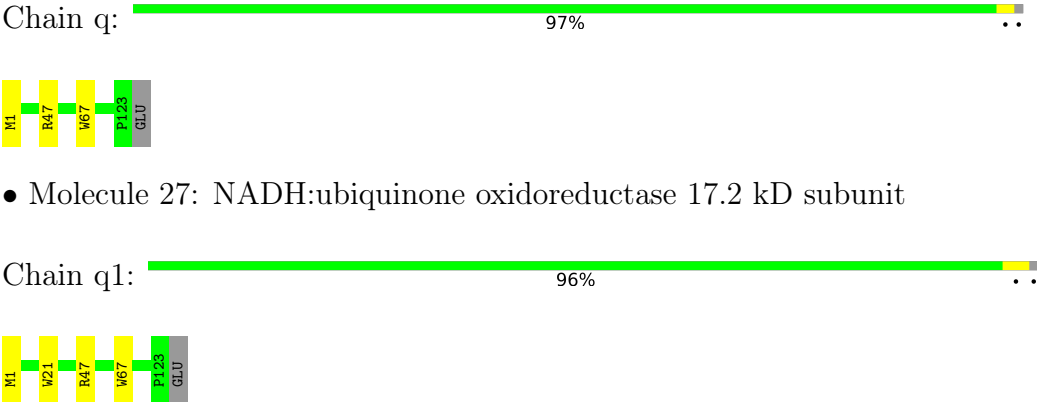
Chain o: 23% 75%



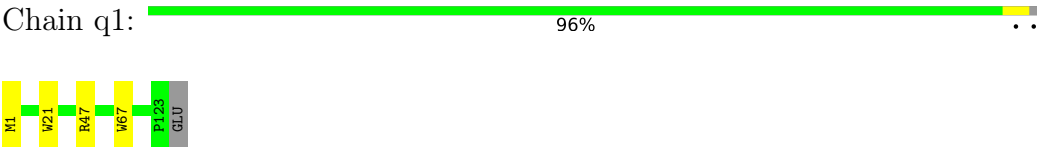
• Molecule 26: Cytochrome c, class I



• Molecule 27: NADH:ubiquinone oxidoreductase 17.2 kD subunit



• Molecule 27: NADH:ubiquinone oxidoreductase 17.2 kD subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	3002	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 ($e^-/\text{\AA}^2$)	55.2	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PE, CDL, HEM, 2MR, HEC, FES, ZN, U10, CU, MN, CA, PC1, P5S, FME, 3PH, DU0, CUA, SF4, HEA, FMN

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	0.27	0/988	0.54	0/1345
1	A1	0.27	0/988	0.54	0/1345
2	B	0.33	0/1297	0.66	0/1758
2	B1	0.33	0/1297	0.66	0/1758
3	C	0.29	0/1624	0.68	0/2208
3	C1	0.29	0/1624	0.68	0/2208
4	D	0.28	0/3339	0.60	0/4520
4	D1	0.28	0/3339	0.60	0/4520
5	E	0.23	0/1865	0.61	0/2537
5	E1	0.23	0/1865	0.61	0/2537
6	F	0.23	0/3308	0.62	0/4456
6	F1	0.23	0/3308	0.62	0/4456
7	G	0.24	0/5156	0.64	0/6982
7	G1	0.24	0/5156	0.64	0/6982
8	H	0.30	0/2815	0.61	0/3837
8	H1	0.30	0/2815	0.60	0/3837
9	I	0.29	0/1354	0.59	0/1828
9	I1	0.29	0/1354	0.59	0/1828
10	J	0.29	0/1548	0.59	0/2104
10	J1	0.29	0/1548	0.60	0/2104
11	K	0.33	0/775	0.58	1/1050 (0.1%)
11	K1	0.33	0/775	0.58	1/1050 (0.1%)
12	L	0.27	0/5379	0.56	1/7323 (0.0%)
12	L1	0.27	0/5379	0.56	1/7323 (0.0%)
13	M	0.30	0/4010	0.59	0/5460
13	M1	0.30	0/4010	0.59	0/5460
14	N	0.30	0/3634	0.55	0/4935
14	N1	0.30	0/3634	0.55	0/4935
15	P	0.27	0/2511	0.62	0/3409
15	P1	0.27	0/2511	0.62	0/3409
16	Q	0.26	0/872	0.63	0/1181

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	Q1	0.26	0/872	0.63	0/1181
17	R	0.23	0/503	0.63	0/685
17	R1	0.22	0/503	0.64	0/685
18	Z	0.27	0/1669	0.62	0/2266
18	Z1	0.27	0/1669	0.62	0/2266
19	a	0.40	0/3650	0.59	0/5005
19	d	0.40	0/3650	0.59	0/5005
20	b	0.33	0/1906	0.62	0/2592
20	e	0.33	0/1906	0.62	0/2592
21	c	0.27	0/1390	0.56	0/1891
21	f	0.27	0/1390	0.56	0/1891
22	g	0.30	0/4483	0.63	0/6118
22	k	0.29	0/4483	0.61	0/6118
23	h	0.25	0/2033	0.60	0/2787
23	l	0.25	0/2033	0.60	0/2787
24	i	0.32	0/2270	0.55	0/3107
24	m	0.32	0/2270	0.55	0/3107
25	j	0.27	0/339	0.55	0/457
25	n	0.27	0/339	0.56	0/457
26	o	0.32	0/330	0.51	0/448
26	p	0.32	0/330	0.52	0/448
27	q	0.25	0/1049	0.62	0/1434
27	q1	0.25	0/1049	0.62	0/1434
All	All	0.29	0/120194	0.60	4/163446 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	B1	0	1
4	D	0	1
4	D1	0	1
7	G	0	2
7	G1	0	2
9	I	0	2
9	I1	0	1
14	N	0	1
14	N1	0	1
16	Q	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	Q1	0	2
22	g	0	1
22	k	0	1
All	All	0	19

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K1	25	ASN	N-CA-C	5.82	119.56	112.23
11	K	25	ASN	N-CA-C	5.80	119.54	112.23
12	L	266	THR	N-CA-C	5.47	119.52	111.04
12	L1	266	THR	N-CA-C	5.45	119.49	111.04

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	134	ARG	Sidechain
2	B1	134	ARG	Sidechain
4	D	250	ARG	Sidechain
4	D1	250	ARG	Sidechain
7	G	223	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	969	0	970	9	0
1	A1	969	0	970	7	0
2	B	1270	0	1268	10	0
2	B1	1270	0	1268	8	0
3	C	1586	0	1562	9	0
3	C1	1586	0	1562	9	0
4	D	3277	0	3217	23	0
4	D1	3277	0	3217	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1822	0	1796	14	0
5	E1	1822	0	1796	11	0
6	F	3241	0	3188	26	0
6	F1	3241	0	3188	24	0
7	G	5068	0	5037	21	0
7	G1	5068	0	5037	21	0
8	H	2722	0	2744	17	0
8	H1	2722	0	2744	16	0
9	I	1319	0	1259	7	0
9	I1	1319	0	1259	7	0
10	J	1528	0	1612	7	0
10	J1	1528	0	1612	6	0
11	K	764	0	817	4	0
11	K1	764	0	817	5	0
12	L	5215	0	5174	22	0
12	L1	5215	0	5174	24	0
13	M	3915	0	4024	25	0
13	M1	3915	0	4024	23	0
14	N	3556	0	3656	16	0
14	N1	3556	0	3656	12	0
15	P	2468	0	2498	9	0
15	P1	2468	0	2498	9	0
16	Q	849	0	812	1	0
16	Q1	849	0	812	1	0
17	R	488	0	450	2	0
17	R1	488	0	450	2	0
18	Z	1642	0	1643	3	0
18	Z1	1642	0	1643	4	0
19	a	3513	0	3489	24	0
19	d	3513	0	3489	25	0
20	b	1855	0	1773	14	0
20	e	1855	0	1773	15	0
21	c	1361	0	1301	8	0
21	f	1361	0	1301	8	0
22	g	4322	0	4225	31	0
22	k	4322	0	4225	27	0
23	h	1976	0	1960	16	0
23	l	1976	0	1960	17	0
24	i	2183	0	2144	19	0
24	m	2183	0	2144	15	0
25	j	332	0	331	2	0
25	n	332	0	331	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	o	324	0	330	3	0
26	p	324	0	330	4	0
27	q	1018	0	942	1	0
27	q1	1018	0	942	2	0
28	B	8	0	0	0	0
28	B1	8	0	0	0	0
28	F	8	0	0	1	0
28	F1	8	0	0	1	0
28	G	16	0	0	0	0
28	G1	16	0	0	0	0
28	I	16	0	0	0	0
28	I1	16	0	0	0	0
29	B	63	0	90	1	0
29	B1	63	0	90	0	0
29	a	126	0	180	15	0
29	d	126	0	180	12	0
30	D	1	0	0	0	0
30	D1	1	0	0	0	0
30	b	1	0	0	0	0
30	e	1	0	0	0	0
30	g	1	0	0	0	0
30	k	1	0	0	0	0
31	E	4	0	0	1	0
31	E1	4	0	0	1	0
31	G	4	0	0	0	0
31	G1	4	0	0	0	0
31	c	4	0	0	0	0
31	f	4	0	0	0	0
32	F	31	0	19	2	0
32	F1	31	0	19	1	0
33	H	54	0	88	1	0
33	H1	108	0	176	2	0
33	L1	54	0	88	0	0
33	M	54	0	88	0	0
33	M1	54	0	88	0	0
33	i	108	0	176	8	0
33	j	54	0	88	5	0
33	m	108	0	176	3	0
33	n	54	0	88	0	0
34	K	37	0	0	0	0
34	M	37	0	0	0	0
34	M1	37	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	a	37	0	0	0	0
34	d	37	0	0	0	0
35	L	51	0	82	0	0
35	L1	51	0	82	0	0
35	b	51	0	82	0	0
35	e	51	0	82	1	0
35	g	51	0	82	2	0
35	i	51	0	82	0	0
35	k	51	0	82	2	0
35	m	102	0	164	0	0
36	L	48	0	75	0	0
36	L1	48	0	75	0	0
36	f	48	0	75	0	0
36	g	48	0	75	0	0
36	k	48	0	75	0	0
36	p	48	0	75	0	0
37	L	54	0	80	0	0
37	L1	54	0	80	0	0
38	R	1	0	0	0	0
38	R1	1	0	0	0	0
38	i	1	0	0	0	0
38	m	1	0	0	0	0
39	a	86	0	60	4	0
39	d	86	0	60	4	0
40	a	100	0	156	1	0
41	b	43	0	30	1	0
41	e	43	0	30	1	0
42	g	120	0	108	2	0
42	k	120	0	108	3	0
43	g	1	0	0	0	0
43	k	1	0	0	0	0
44	g	1	0	0	0	0
44	k	1	0	0	0	0
45	h	2	0	0	0	0
45	l	2	0	0	0	0
All	All	120030	0	119978	622	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 622 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LEU:HD11	11:K:71:ALA:HB3	1.67	0.76
1:A1:75:LEU:HD11	11:K1:71:ALA:HB3	1.67	0.76
29:a:1002:U10:H301	29:d:504:U10:H351	1.71	0.72
22:k:365:GLY:HA2	23:l:89:PHE:HB3	1.77	0.67
22:g:365:GLY:HA2	23:h:89:PHE:HB3	1.77	0.66

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
1	A1	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
2	B	160/175 (91%)	153 (96%)	6 (4%)	1 (1%)	21	58
2	B1	160/175 (91%)	154 (96%)	5 (3%)	1 (1%)	21	58
3	C	192/208 (92%)	187 (97%)	5 (3%)	0	100	100
3	C1	192/208 (92%)	187 (97%)	5 (3%)	0	100	100
4	D	408/412 (99%)	398 (98%)	10 (2%)	0	100	100
4	D1	408/412 (99%)	398 (98%)	10 (2%)	0	100	100
5	E	235/239 (98%)	225 (96%)	9 (4%)	1 (0%)	30	67
5	E1	235/239 (98%)	225 (96%)	9 (4%)	1 (0%)	30	67
6	F	420/431 (97%)	404 (96%)	16 (4%)	0	100	100
6	F1	420/431 (97%)	403 (96%)	17 (4%)	0	100	100
7	G	663/674 (98%)	637 (96%)	24 (4%)	2 (0%)	36	71
7	G1	663/674 (98%)	637 (96%)	24 (4%)	2 (0%)	36	71
8	H	339/345 (98%)	329 (97%)	10 (3%)	0	100	100
8	H1	339/345 (98%)	329 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
9	I1	160/163 (98%)	156 (98%)	4 (2%)	0	100	100
10	J	197/199 (99%)	193 (98%)	4 (2%)	0	100	100
10	J1	197/199 (99%)	193 (98%)	4 (2%)	0	100	100
11	K	99/101 (98%)	98 (99%)	0	1 (1%)	12	47
11	K1	99/101 (98%)	98 (99%)	0	1 (1%)	12	47
12	L	657/703 (94%)	628 (96%)	29 (4%)	0	100	100
12	L1	657/703 (94%)	628 (96%)	29 (4%)	0	100	100
13	M	501/513 (98%)	494 (99%)	6 (1%)	1 (0%)	43	77
13	M1	501/513 (98%)	494 (99%)	6 (1%)	1 (0%)	43	77
14	N	478/499 (96%)	470 (98%)	8 (2%)	0	100	100
14	N1	478/499 (96%)	470 (98%)	8 (2%)	0	100	100
15	P	326/330 (99%)	317 (97%)	9 (3%)	0	100	100
15	P1	326/330 (99%)	315 (97%)	11 (3%)	0	100	100
16	Q	101/103 (98%)	101 (100%)	0	0	100	100
16	Q1	101/103 (98%)	101 (100%)	0	0	100	100
17	R	59/62 (95%)	54 (92%)	4 (7%)	1 (2%)	7	35
17	R1	59/62 (95%)	54 (92%)	4 (7%)	1 (2%)	7	35
18	Z	214/217 (99%)	209 (98%)	5 (2%)	0	100	100
18	Z1	214/217 (99%)	209 (98%)	5 (2%)	0	100	100
19	a	432/440 (98%)	424 (98%)	8 (2%)	0	100	100
19	d	432/440 (98%)	423 (98%)	9 (2%)	0	100	100
20	b	237/450 (53%)	234 (99%)	2 (1%)	1 (0%)	30	67
20	e	237/450 (53%)	233 (98%)	3 (1%)	1 (0%)	30	67
21	c	179/195 (92%)	174 (97%)	4 (2%)	1 (1%)	21	58
21	f	179/195 (92%)	174 (97%)	5 (3%)	0	100	100
22	g	542/558 (97%)	528 (97%)	14 (3%)	0	100	100
22	k	542/558 (97%)	528 (97%)	14 (3%)	0	100	100
23	h	250/298 (84%)	240 (96%)	10 (4%)	0	100	100
23	l	250/298 (84%)	240 (96%)	10 (4%)	0	100	100
24	i	271/274 (99%)	260 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	m	271/274 (99%)	261 (96%)	10 (4%)	0	100	100
25	j	41/66 (62%)	39 (95%)	2 (5%)	0	100	100
25	n	41/66 (62%)	39 (95%)	2 (5%)	0	100	100
26	o	40/176 (23%)	39 (98%)	1 (2%)	0	100	100
26	p	40/176 (23%)	39 (98%)	1 (2%)	0	100	100
27	q	121/124 (98%)	115 (95%)	6 (5%)	0	100	100
27	q1	121/124 (98%)	115 (95%)	6 (5%)	0	100	100
All	All	14882/16152 (92%)	14441 (97%)	424 (3%)	17 (0%)	49	83

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	137	CYS
5	E1	137	CYS
13	M	238	VAL
13	M1	238	VAL
20	b	369	ASN

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	97/97 (100%)	97 (100%)	0	100	100
1	A1	97/97 (100%)	97 (100%)	0	100	100
2	B	136/145 (94%)	134 (98%)	2 (2%)	57	71
2	B1	136/145 (94%)	135 (99%)	1 (1%)	76	79
3	C	172/183 (94%)	172 (100%)	0	100	100
3	C1	172/183 (94%)	172 (100%)	0	100	100
4	D	341/342 (100%)	341 (100%)	0	100	100
4	D1	341/342 (100%)	341 (100%)	0	100	100
5	E	189/190 (100%)	189 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E1	189/190 (100%)	189 (100%)	0	100	100
6	F	331/335 (99%)	331 (100%)	0	100	100
6	F1	331/335 (99%)	330 (100%)	1 (0%)	86	84
7	G	530/535 (99%)	528 (100%)	2 (0%)	84	83
7	G1	530/535 (99%)	530 (100%)	0	100	100
8	H	277/279 (99%)	277 (100%)	0	100	100
8	H1	277/279 (99%)	277 (100%)	0	100	100
9	I	136/137 (99%)	136 (100%)	0	100	100
9	I1	136/137 (99%)	136 (100%)	0	100	100
10	J	158/158 (100%)	158 (100%)	0	100	100
10	J1	158/158 (100%)	158 (100%)	0	100	100
11	K	81/81 (100%)	80 (99%)	1 (1%)	63	74
11	K1	81/81 (100%)	80 (99%)	1 (1%)	63	74
12	L	520/543 (96%)	520 (100%)	0	100	100
12	L1	520/543 (96%)	520 (100%)	0	100	100
13	M	410/416 (99%)	408 (100%)	2 (0%)	81	82
13	M1	410/416 (99%)	408 (100%)	2 (0%)	81	82
14	N	357/369 (97%)	356 (100%)	1 (0%)	86	84
14	N1	357/369 (97%)	355 (99%)	2 (1%)	78	81
15	P	248/250 (99%)	248 (100%)	0	100	100
15	P1	248/250 (99%)	248 (100%)	0	100	100
16	Q	87/87 (100%)	86 (99%)	1 (1%)	65	74
16	Q1	87/87 (100%)	86 (99%)	1 (1%)	65	74
17	R	51/52 (98%)	51 (100%)	0	100	100
17	R1	51/52 (98%)	51 (100%)	0	100	100
18	Z	167/168 (99%)	167 (100%)	0	100	100
18	Z1	167/168 (99%)	167 (100%)	0	100	100
19	a	361/366 (99%)	361 (100%)	0	100	100
19	d	361/366 (99%)	361 (100%)	0	100	100
20	b	192/319 (60%)	192 (100%)	0	100	100
20	e	192/319 (60%)	192 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	c	140/151 (93%)	140 (100%)	0	100	100
21	f	140/151 (93%)	140 (100%)	0	100	100
22	g	447/454 (98%)	447 (100%)	0	100	100
22	k	447/454 (98%)	447 (100%)	0	100	100
23	h	211/243 (87%)	210 (100%)	1 (0%)	81	82
23	l	211/243 (87%)	210 (100%)	1 (0%)	81	82
24	i	220/221 (100%)	219 (100%)	1 (0%)	81	82
24	m	220/221 (100%)	219 (100%)	1 (0%)	81	82
25	j	34/53 (64%)	34 (100%)	0	100	100
25	n	34/53 (64%)	34 (100%)	0	100	100
26	o	33/126 (26%)	33 (100%)	0	100	100
26	p	33/126 (26%)	33 (100%)	0	100	100
27	q	103/104 (99%)	103 (100%)	0	100	100
27	q1	103/104 (99%)	103 (100%)	0	100	100
All	All	12058/12808 (94%)	12037 (100%)	21 (0%)	85	86

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	N1	188	GLU
23	h	88	ARG
24	m	258	VAL
24	i	258	VAL
16	Q1	73	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

Mol	Chain	Res	Type
18	Z1	6	GLN
21	f	121	ASN
19	a	99	ASN
21	c	121	ASN
23	h	94	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
27	FME	q1	1	27	8,9,10	0.96	0	8,9,11	1.10	1 (12%)
13	FME	M1	1	13	8,9,10	0.97	0	8,9,11	1.13	1 (12%)
4	2MR	D	65	4	10,12,13	2.49	3 (30%)	5,13,15	1.12	0
1	FME	A1	1	1	8,9,10	0.94	0	8,9,11	1.07	1 (12%)
10	FME	J	1	10	8,9,10	0.99	0	8,9,11	0.71	0
12	FME	L1	1	12	8,9,10	0.93	0	8,9,11	1.26	1 (12%)
27	FME	q	1	27	8,9,10	0.96	0	8,9,11	1.10	1 (12%)
4	2MR	D1	65	4	10,12,13	2.49	3 (30%)	5,13,15	1.13	1 (20%)
10	FME	J1	1	10	8,9,10	1.03	0	8,9,11	0.71	0
13	FME	M	1	13	8,9,10	0.96	0	8,9,11	1.13	1 (12%)
1	FME	A	1	1	8,9,10	0.96	0	8,9,11	1.08	1 (12%)
12	FME	L	1	12	8,9,10	0.95	0	8,9,11	1.27	1 (12%)

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
27	FME	q1	1	27	-	0/7/9/11	-
13	FME	M1	1	13	-	3/7/9/11	-
4	2MR	D	65	4	-	0/10/13/15	-
1	FME	A1	1	1	-	1/7/9/11	-
10	FME	J	1	10	-	0/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	L1	1	12	-	1/7/9/11	-
27	FME	q	1	27	-	0/7/9/11	-
4	2MR	D1	65	4	-	0/10/13/15	-
10	FME	J1	1	10	-	1/7/9/11	-
13	FME	M	1	13	-	3/7/9/11	-
1	FME	A	1	1	-	1/7/9/11	-
12	FME	L	1	12	-	1/7/9/11	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D1	65	2MR	CZ-NH2	5.23	1.44	1.33
4	D	65	2MR	CZ-NH2	5.22	1.44	1.33
4	D	65	2MR	CZ-NE	5.05	1.45	1.34
4	D1	65	2MR	CZ-NE	5.05	1.45	1.34
4	D	65	2MR	CQ1-NH1	-2.08	1.42	1.46

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	1	FME	C-CA-N	2.78	114.86	109.50
12	L	1	FME	C-CA-N	2.76	114.83	109.50
12	L1	1	FME	C-CA-N	2.76	114.83	109.50
13	M1	1	FME	C-CA-N	2.76	114.82	109.50
27	q1	1	FME	C-CA-N	2.57	114.46	109.50

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	J1	1	FME	O-C-CA-CB
12	L	1	FME	O-C-CA-CB
12	L1	1	FME	O-C-CA-CB
13	M	1	FME	N-CA-CB-CG
13	M1	1	FME	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 87 ligands modelled in this entry, 14 are monoatomic - leaving 73 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
28	SF4	I1	201	9	0,12,12	-	-	-		
28	SF4	G	701	7	0,12,12	-	-	-		
35	3PE	m	304	-	50,50,50	0.97	4 (8%)	53,55,55	0.97	2 (3%)
29	U10	B	1002	-	63,63,63	0.69	0	78,79,79	1.27	6 (7%)
31	FES	E	401	5	0,4,4	-	-	-		
28	SF4	G	702	7	0,12,12	-	-	-		
32	FMN	F1	501	-	33,33,33	1.06	3 (9%)	48,50,50	1.27	6 (12%)
45	CUA	h	301	23	0,1,1	-	-	-		
28	SF4	F	501	6	0,12,12	-	-	-		
33	PC1	H1	1002	-	53,53,53	0.97	3 (5%)	59,61,61	0.86	2 (3%)
36	3PH	L	802	-	47,47,47	1.37	5 (10%)	50,52,52	1.04	4 (8%)
33	PC1	M	601	-	53,53,53	0.97	3 (5%)	59,61,61	0.87	2 (3%)
36	3PH	L1	804	-	47,47,47	1.37	5 (10%)	50,52,52	1.04	4 (8%)
36	3PH	p	201	-	47,47,47	1.37	5 (10%)	50,52,52	0.98	4 (8%)
37	P5S	L	803	-	52,53,53	0.94	3 (5%)	54,60,60	0.83	3 (5%)
32	FMN	F	502	-	33,33,33	1.05	3 (9%)	48,50,50	1.27	6 (12%)
33	PC1	L1	801	-	53,53,53	0.98	3 (5%)	59,61,61	0.93	2 (3%)
35	3PE	e	501	-	50,50,50	0.95	4 (8%)	53,55,55	1.00	3 (5%)
33	PC1	H	1001	-	53,53,53	0.97	3 (5%)	59,61,61	0.83	1 (1%)
31	FES	G	703	7	0,4,4	-	-	-		
31	FES	c	1000	21	0,4,4	-	-	-		
33	PC1	i	304	-	53,53,53	0.96	3 (5%)	59,61,61	0.87	2 (3%)
34	DU0	M	602	-	42,42,42	0.70	0	64,66,66	0.91	2 (3%)
39	HEM	a	1001	19	50,50,50	1.52	8 (16%)	67,82,82	1.06	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	SF4	G1	703	7	0,12,12	-	-	-		
28	SF4	I	201	9	0,12,12	-	-	-		
34	DU0	a	1005	-	42,42,42	0.73	0	64,66,66	0.82	1 (1%)
35	3PE	L1	802	-	50,50,50	0.96	4 (8%)	53,55,55	0.99	4 (7%)
34	DU0	M1	602	-	42,42,42	0.68	0	64,66,66	0.94	4 (6%)
42	HEA	g	605	22	67,67,67	1.39	8 (11%)	81,103,103	2.28	33 (40%)
29	U10	d	501	-	63,63,63	0.68	0	78,79,79	1.07	4 (5%)
33	PC1	m	302	-	53,53,53	0.97	3 (5%)	59,61,61	0.84	2 (3%)
34	DU0	d	503	-	42,42,42	0.73	0	64,66,66	0.82	1 (1%)
35	3PE	i	303	-	50,50,50	0.97	4 (8%)	53,55,55	1.03	2 (3%)
37	P5S	L1	803	-	52,53,53	0.94	3 (5%)	54,60,60	0.83	3 (5%)
35	3PE	m	301	-	50,50,50	0.97	4 (8%)	53,55,55	0.99	4 (7%)
33	PC1	i	301	-	53,53,53	0.97	3 (5%)	59,61,61	0.84	1 (1%)
39	HEM	a	1003	19	50,50,50	1.46	6 (12%)	67,82,82	0.99	3 (4%)
29	U10	d	504	-	63,63,63	0.73	0	78,79,79	1.05	4 (5%)
36	3PH	f	201	-	47,47,47	1.39	5 (10%)	50,52,52	1.02	4 (8%)
35	3PE	L	801	-	50,50,50	0.95	4 (8%)	53,55,55	0.99	4 (7%)
28	SF4	B	1001	2	0,12,12	-	-	-		
28	SF4	G1	702	7	0,12,12	-	-	-		
33	PC1	j	1001	-	53,53,53	0.97	3 (5%)	59,61,61	0.88	3 (5%)
40	CDL	a	1006	-	99,99,99	0.92	6 (6%)	105,111,111	0.89	4 (3%)
36	3PH	k	602	-	47,47,47	1.40	6 (12%)	50,52,52	1.02	4 (8%)
31	FES	G1	701	7	0,4,4	-	-	-		
33	PC1	n	1001	-	53,53,53	0.96	3 (5%)	59,61,61	0.89	3 (5%)
28	SF4	I1	202	9	0,12,12	-	-	-		
45	CUA	l	301	23	0,1,1	-	-	-		
28	SF4	B1	1001	2	0,12,12	-	-	-		
31	FES	f	202	21	0,4,4	-	-	-		
33	PC1	m	303	-	53,53,53	0.95	3 (5%)	59,61,61	0.91	3 (5%)
34	DU0	K	1000	-	42,42,42	0.73	0	64,66,66	0.84	1 (1%)
33	PC1	M1	601	-	53,53,53	0.97	3 (5%)	59,61,61	0.87	2 (3%)
35	3PE	b	502	-	50,50,50	0.95	4 (8%)	53,55,55	1.00	4 (7%)
29	U10	B1	1002	-	63,63,63	0.69	0	78,79,79	1.23	6 (7%)
29	U10	a	1004	-	63,63,63	0.69	0	78,79,79	1.09	5 (6%)
35	3PE	g	607	-	50,50,50	0.95	4 (8%)	53,55,55	1.01	3 (5%)
33	PC1	H1	1001	-	53,53,53	0.97	3 (5%)	59,61,61	0.83	1 (1%)
31	FES	E1	401	5	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	HEM	d	505	19	50,50,50	1.52	8 (16%)	67,82,82	1.07	2 (2%)
41	HEC	e	503	20	46,50,50	2.01	10 (21%)	58,82,82	1.83	9 (15%)
28	SF4	I	202	9	0,12,12	-	-	-	-	-
42	HEA	k	603	22	67,67,67	1.40	8 (11%)	81,103,103	2.29	31 (38%)
35	3PE	k	607	-	50,50,50	0.94	4 (8%)	53,55,55	1.01	3 (5%)
36	3PH	g	602	-	47,47,47	1.39	5 (10%)	50,52,52	1.04	5 (10%)
42	HEA	k	605	22	67,67,67	1.39	9 (13%)	81,103,103	2.28	32 (39%)
29	U10	a	1002	-	63,63,63	0.68	0	78,79,79	1.06	2 (2%)
39	HEM	d	502	19	50,50,50	1.47	7 (14%)	67,82,82	0.99	3 (4%)
28	SF4	F1	502	6	0,12,12	-	-	-	-	-
42	HEA	g	601	22	67,67,67	1.40	7 (10%)	81,103,103	2.28	30 (37%)
41	HEC	b	503	20	46,50,50	2.00	10 (21%)	58,82,82	1.82	10 (17%)

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
28	SF4	I1	201	9	-	-	0/6/5/5
28	SF4	G	701	7	-	-	0/6/5/5
35	3PE	m	304	-	-	7/54/54/54	-
29	U10	B	1002	-	-	13/63/87/87	0/1/1/1
31	FES	E	401	5	-	-	0/1/1/1
32	FMN	F1	501	-	-	9/18/18/18	0/3/3/3
28	SF4	G	702	7	-	-	0/6/5/5
28	SF4	F	501	6	-	-	0/6/5/5
33	PC1	H1	1002	-	-	5/57/57/57	-
36	3PH	L	802	-	-	5/49/49/49	-
33	PC1	M	601	-	-	11/57/57/57	-
36	3PH	L1	804	-	-	6/49/49/49	-
36	3PH	p	201	-	-	9/49/49/49	-
37	P5S	L	803	-	-	3/59/59/59	-
32	FMN	F	502	-	-	1/18/18/18	0/3/3/3
33	PC1	L1	801	-	-	18/57/57/57	-
35	3PE	e	501	-	-	11/54/54/54	-
33	PC1	H	1001	-	-	11/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	DU0	M	602	-	-	0/10/98/98	0/6/6/6
39	HEM	a	1001	19	-	8/14/54/54	-
33	PC1	i	304	-	-	10/57/57/57	-
42	HEA	g	605	22	-	5/36/76/76	-
42	HEA	k	603	22	-	7/36/76/76	-
28	SF4	G1	703	7	-	-	0/6/5/5
28	SF4	I	201	9	-	-	0/6/5/5
31	FES	G	703	7	-	-	0/1/1/1
35	3PE	L1	802	-	-	7/54/54/54	-
34	DU0	M1	602	-	-	0/10/98/98	0/6/6/6
31	FES	c	1000	21	-	-	0/1/1/1
29	U10	d	501	-	-	9/63/87/87	0/1/1/1
33	PC1	m	302	-	-	6/57/57/57	-
34	DU0	d	503	-	-	0/10/98/98	0/6/6/6
35	3PE	i	303	-	-	12/54/54/54	-
37	P5S	L1	803	-	-	4/59/59/59	-
35	3PE	m	301	-	-	10/54/54/54	-
28	SF4	F1	502	6	-	-	0/6/5/5
33	PC1	i	301	-	-	6/57/57/57	-
39	HEM	a	1003	19	-	9/14/54/54	-
29	U10	d	504	-	-	15/63/87/87	0/1/1/1
36	3PH	f	201	-	-	8/49/49/49	-
35	3PE	L	801	-	-	7/54/54/54	-
33	PC1	j	1001	-	-	13/57/57/57	-
28	SF4	B	1001	2	-	-	0/6/5/5
28	SF4	G1	702	7	-	-	0/6/5/5
40	CDL	a	1006	-	-	21/110/110/110	-
36	3PH	k	602	-	-	7/49/49/49	-
31	FES	G1	701	7	-	-	0/1/1/1
33	PC1	n	1001	-	-	18/57/57/57	-
28	SF4	I1	202	9	-	-	0/6/5/5
33	PC1	m	303	-	-	12/57/57/57	-
28	SF4	B1	1001	2	-	-	0/6/5/5
31	FES	f	202	21	-	-	0/1/1/1
34	DU0	K	1000	-	-	0/10/98/98	0/6/6/6
33	PC1	M1	601	-	-	10/57/57/57	-
35	3PE	b	502	-	-	13/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	U10	a	1004	-	-	13/63/87/87	0/1/1/1
29	U10	B1	1002	-	-	8/63/87/87	0/1/1/1
35	3PE	g	607	-	-	10/54/54/54	-
33	PC1	H1	1001	-	-	11/57/57/57	-
39	HEM	d	505	19	-	8/14/54/54	-
41	HEC	e	503	20	-	7/14/54/54	-
31	FES	E1	401	5	-	-	0/1/1/1
28	SF4	I	202	9	-	-	0/6/5/5
35	3PE	k	607	-	-	11/54/54/54	-
36	3PH	g	602	-	-	5/49/49/49	-
42	HEA	k	605	22	-	5/36/76/76	-
29	U10	a	1002	-	-	8/63/87/87	0/1/1/1
39	HEM	d	502	19	-	9/14/54/54	-
34	DU0	a	1005	-	-	0/10/98/98	0/6/6/6
42	HEA	g	601	22	-	7/36/76/76	-
41	HEC	b	503	20	-	7/14/54/54	-

The worst 5 of 202 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	f	201	3PH	P-O11	7.45	1.83	1.60
36	k	602	3PH	P-O11	7.41	1.83	1.60
36	g	602	3PH	P-O11	7.34	1.83	1.60
36	p	201	3PH	P-O11	7.29	1.83	1.60
36	L1	804	3PH	P-O11	7.28	1.83	1.60

The worst 5 of 291 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	k	603	HEA	C3A-C2A-C1A	-6.83	100.59	107.05
42	g	601	HEA	C3A-C2A-C1A	-6.77	100.64	107.05
42	k	605	HEA	C3A-C2A-C1A	-6.63	100.77	107.05
42	g	605	HEA	C3A-C2A-C1A	-6.58	100.82	107.05
41	e	503	HEC	CBB-CAB-C3B	-6.41	114.62	127.43

There are no chirality outliers.

5 of 435 torsion outliers are listed below:

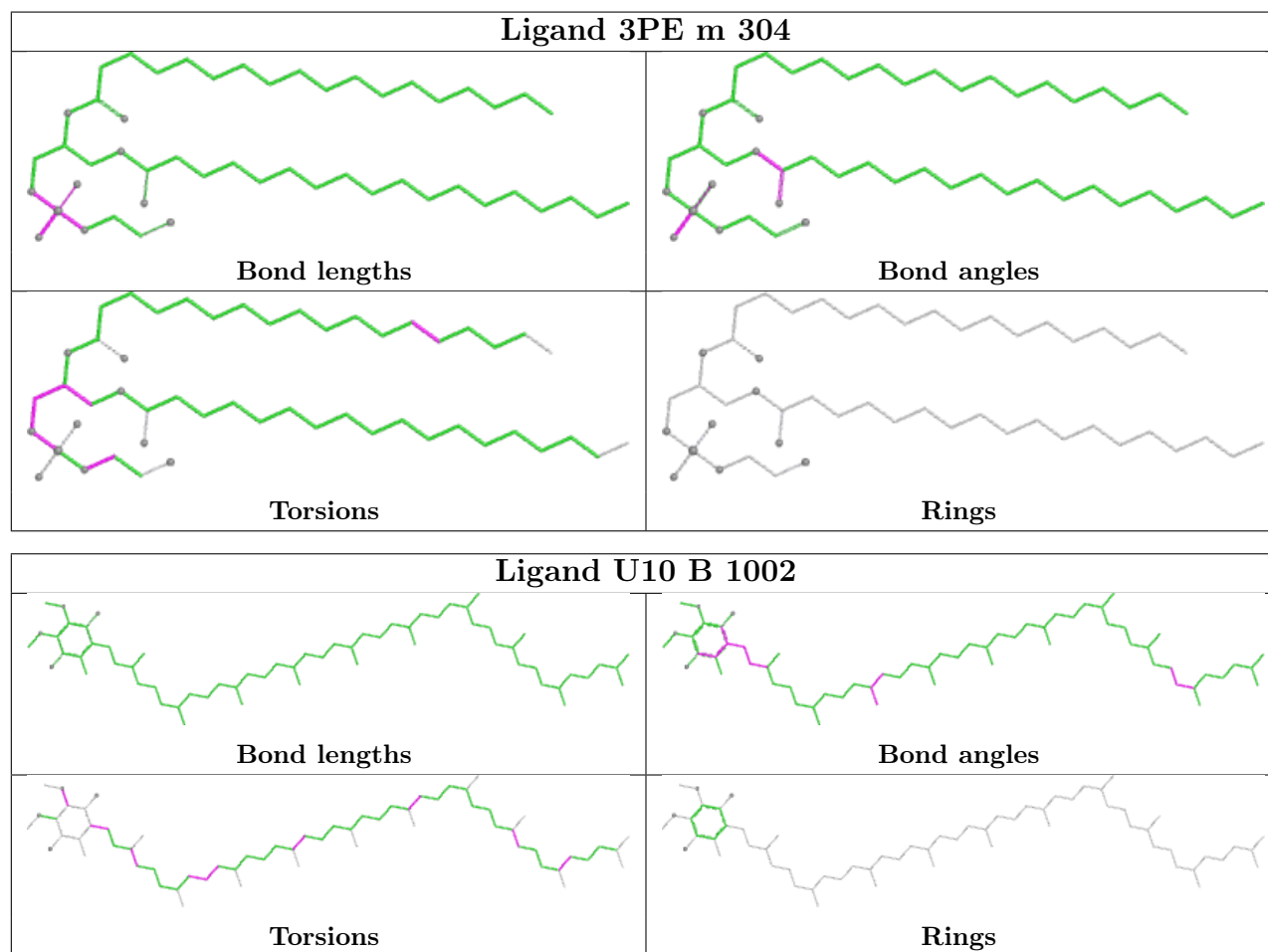
Mol	Chain	Res	Type	Atoms
29	B	1002	U10	C1-C6-C7-C8
29	B	1002	U10	C5-C6-C7-C8
29	B	1002	U10	C16-C17-C18-C19
29	B1	1002	U10	C1-C6-C7-C8
29	B1	1002	U10	C5-C6-C7-C8

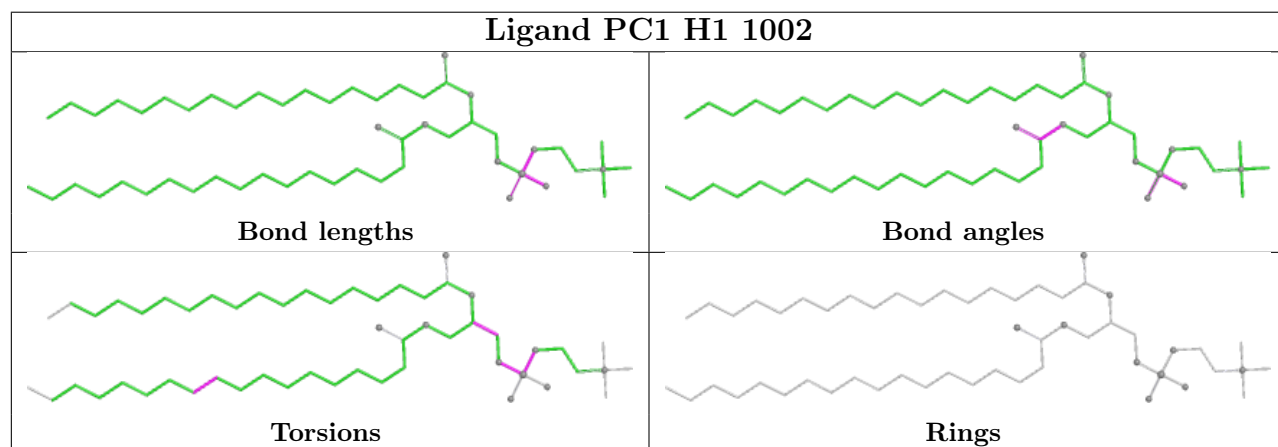
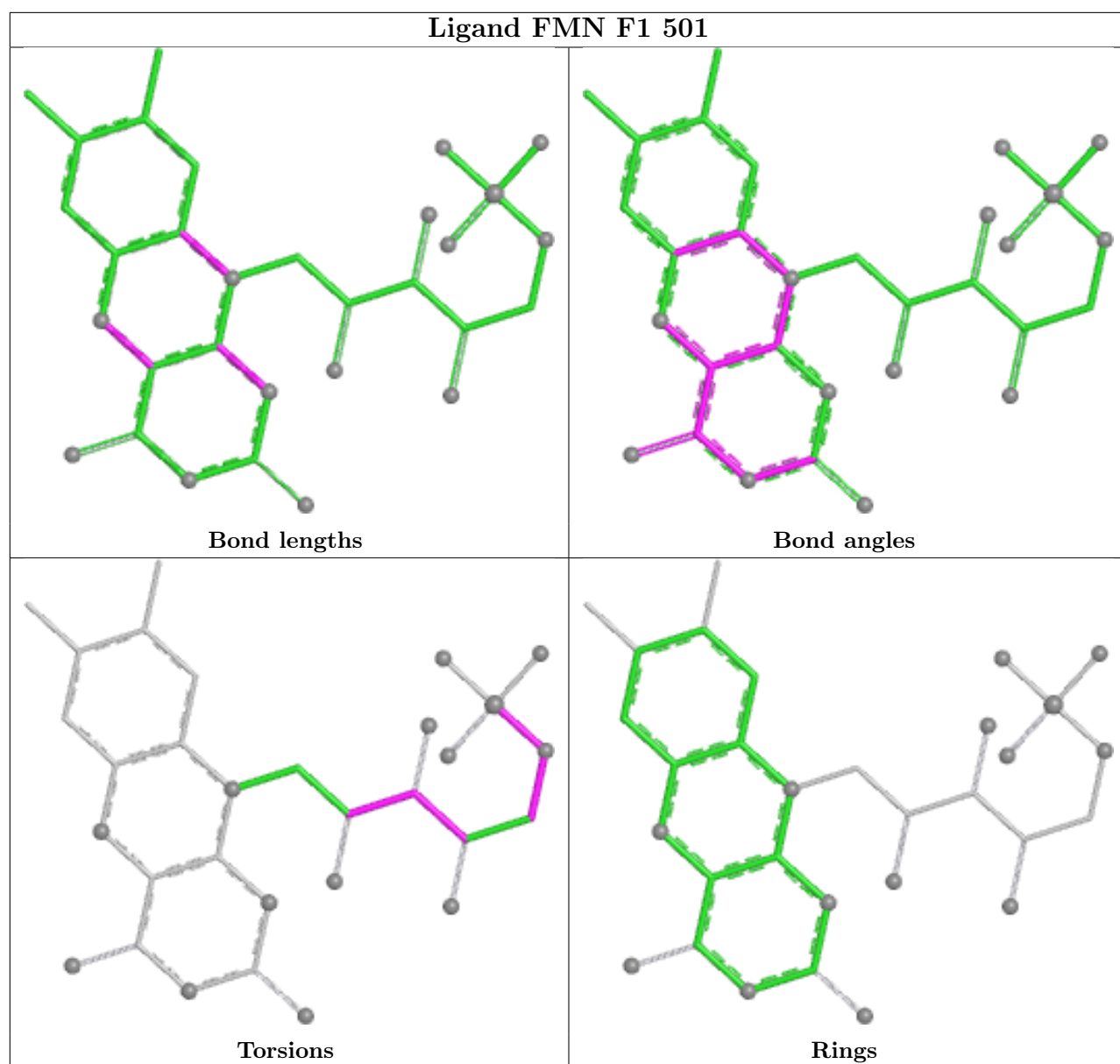
There are no ring outliers.

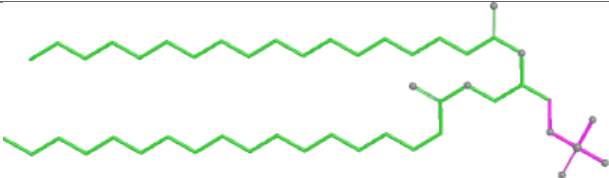

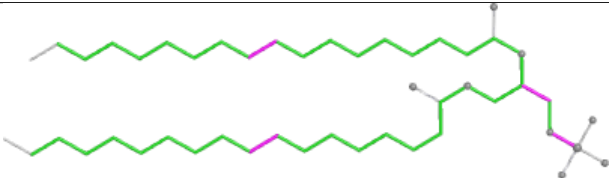
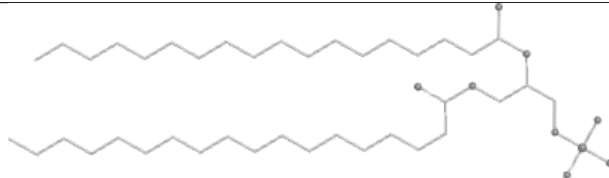
33 monomers are involved in 68 short contacts:

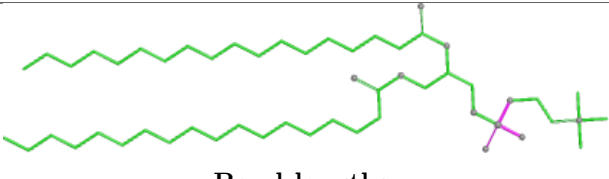
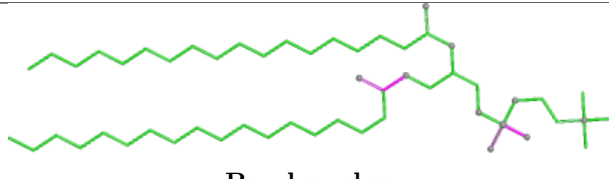
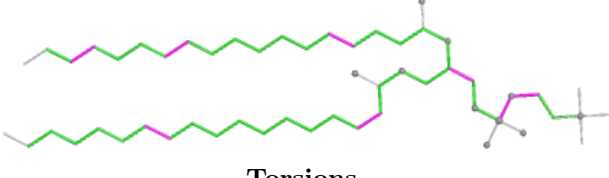
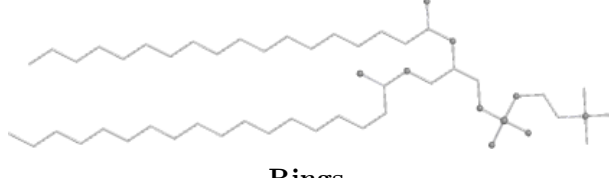
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	B	1002	U10	1	0
31	E	401	FES	1	0
32	F1	501	FMN	1	0
28	F	501	SF4	1	0
33	H1	1002	PC1	1	0
32	F	502	FMN	2	0
35	e	501	3PE	1	0
33	H	1001	PC1	1	0
33	i	304	PC1	7	0
39	a	1001	HEM	2	0
42	g	605	HEA	1	0
29	d	501	U10	7	0
33	m	302	PC1	2	0
33	i	301	PC1	1	0
39	a	1003	HEM	2	0
29	d	504	U10	5	0
33	j	1001	PC1	5	0
40	a	1006	CDL	1	0
33	m	303	PC1	1	0
29	a	1004	U10	1	0
35	g	607	3PE	2	0
33	H1	1001	PC1	1	0
31	E1	401	FES	1	0
39	d	505	HEM	2	0
41	e	503	HEC	1	0
42	k	603	HEA	2	0
35	k	607	3PE	2	0
42	k	605	HEA	1	0
29	a	1002	U10	14	0
39	d	502	HEM	2	0
28	F1	502	SF4	1	0
42	g	601	HEA	1	0
41	b	503	HEC	1	0

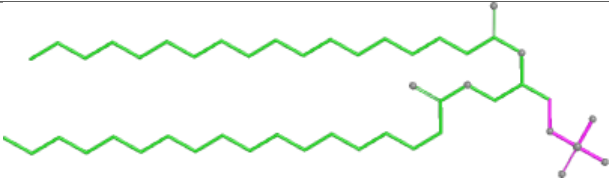

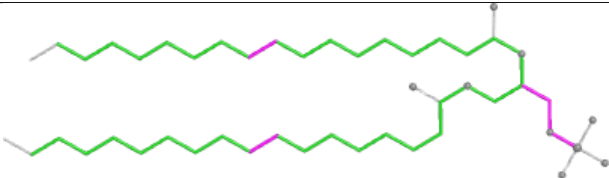
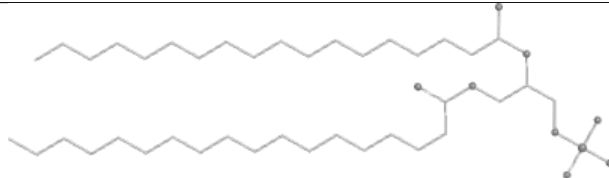
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

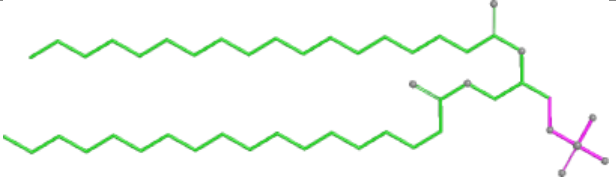
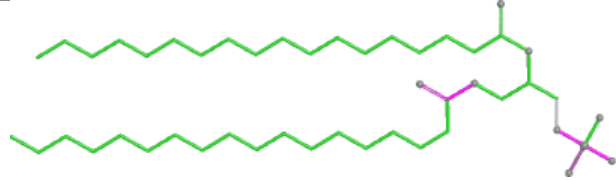
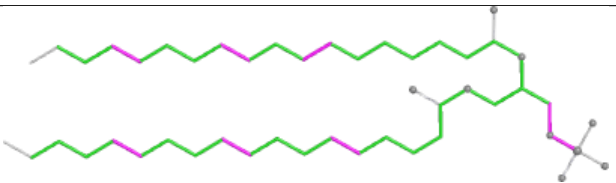
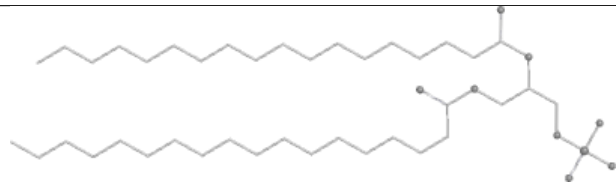
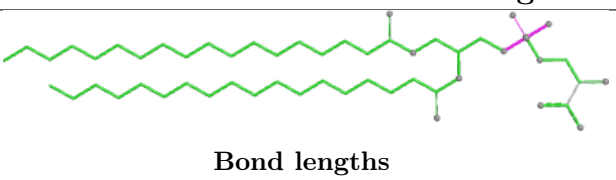
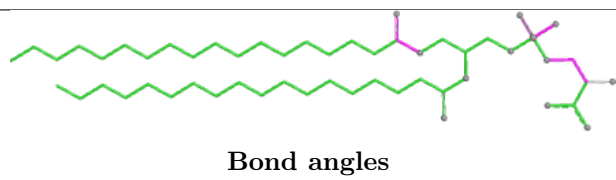
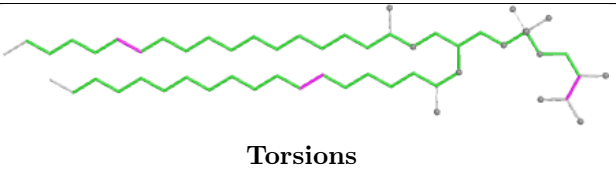
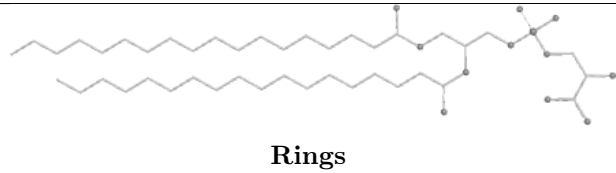


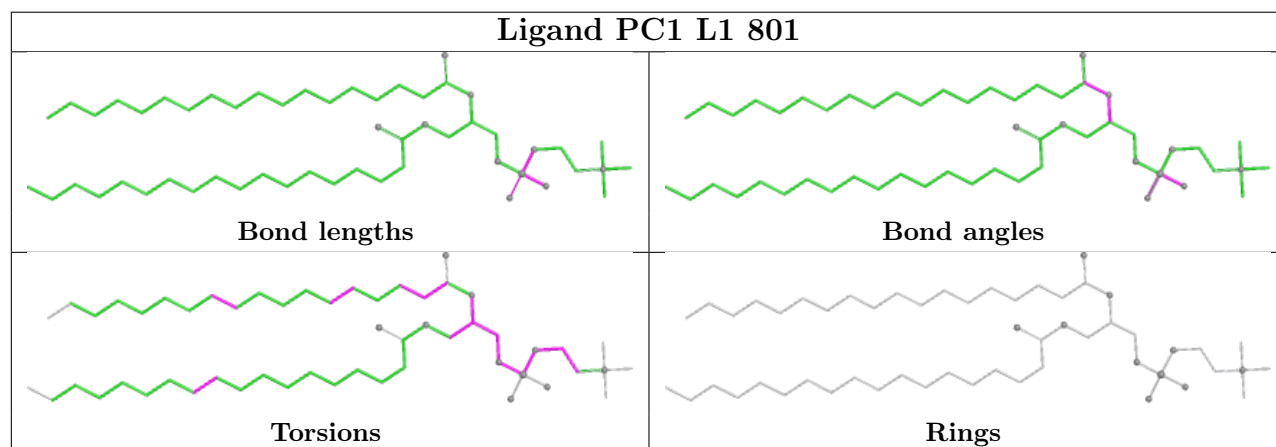
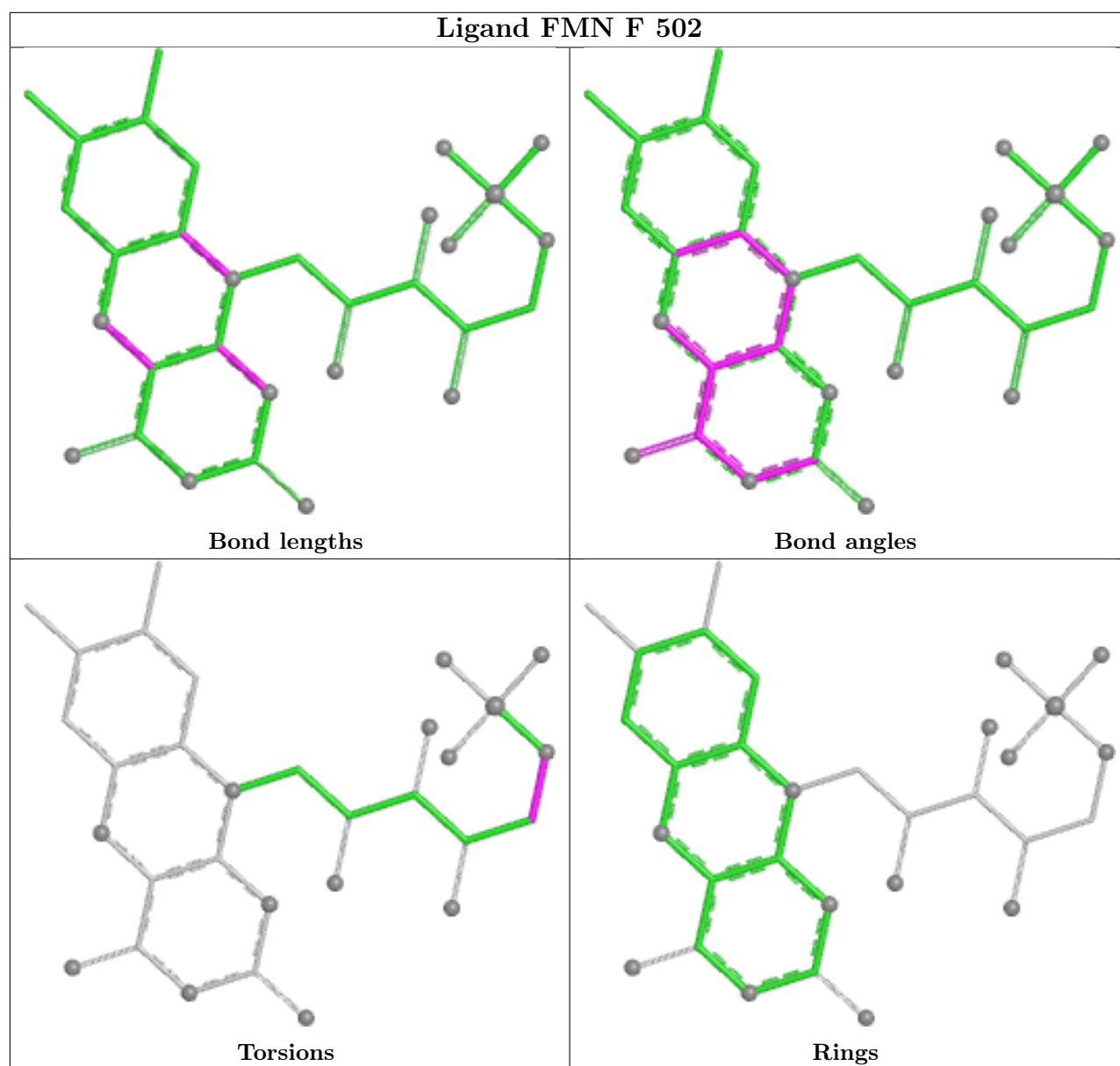


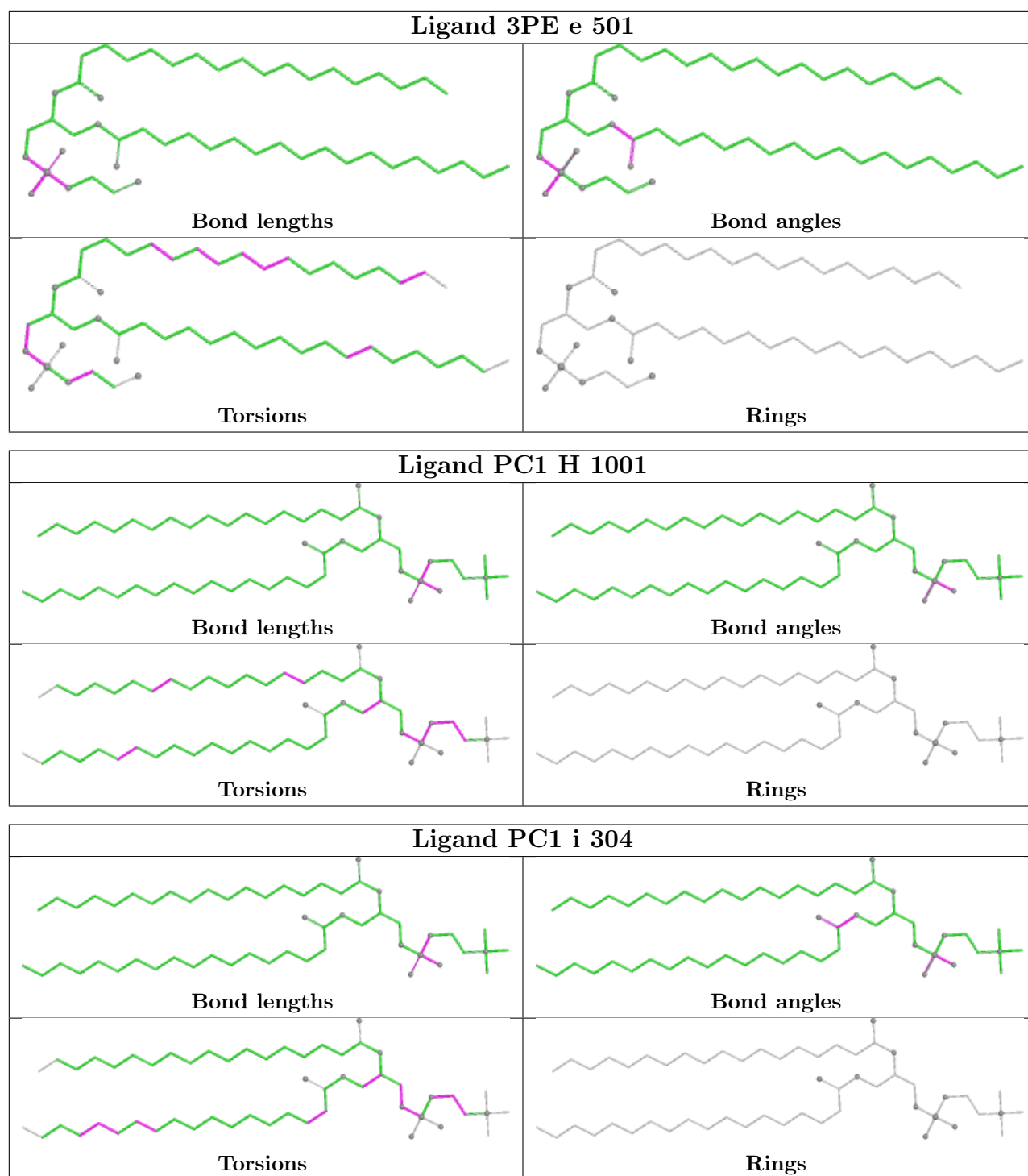
Ligand 3PH L 802			
 <p>Bond lengths</p>		 <p>Bond angles</p>	
 <p>Torsions</p>		 <p>Rings</p>	

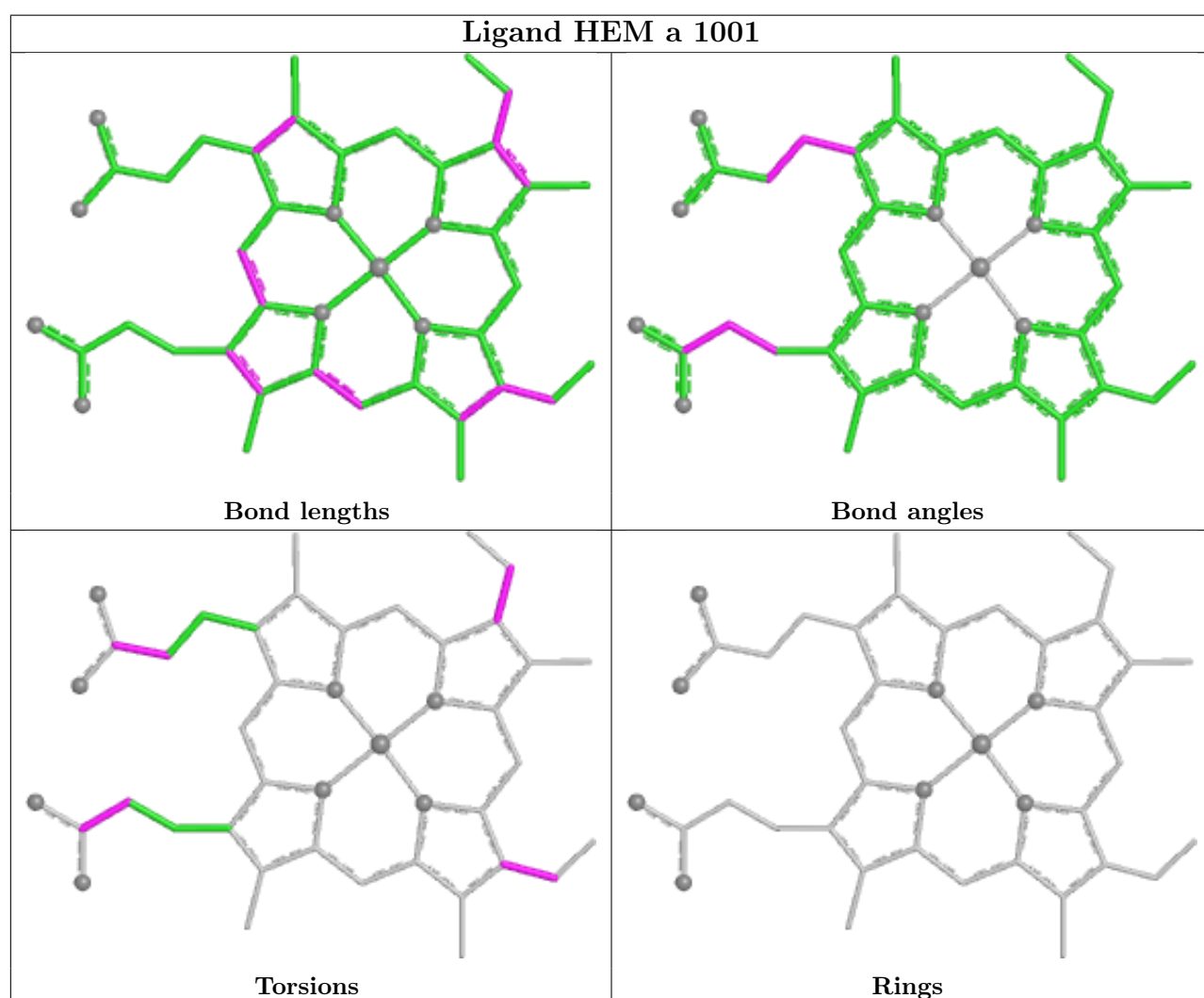
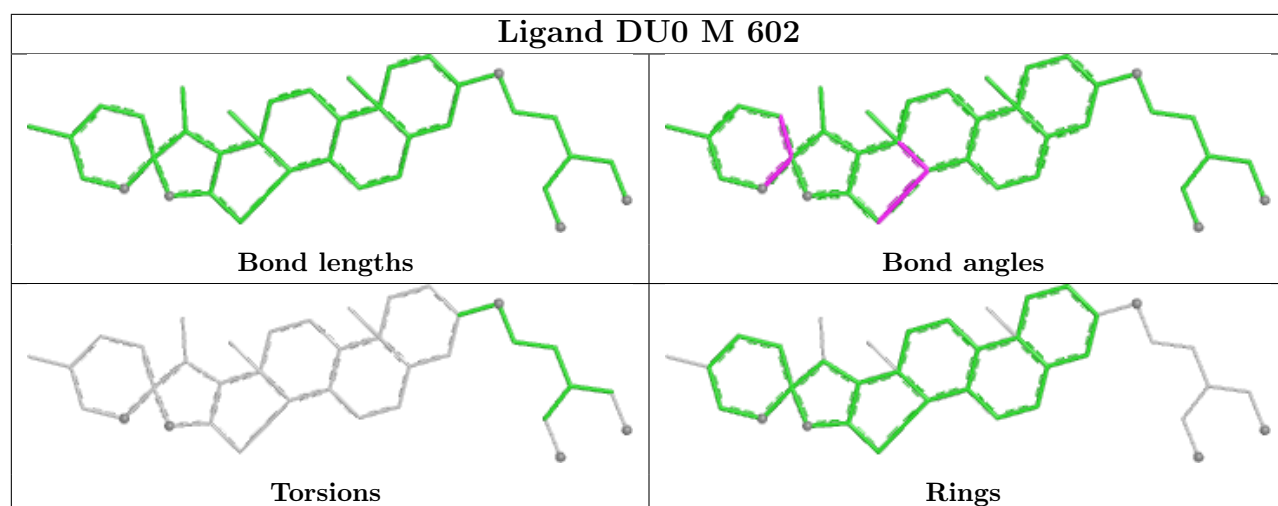
Ligand PC1 M 601			
 <p>Bond lengths</p>		 <p>Bond angles</p>	
 <p>Torsions</p>		 <p>Rings</p>	

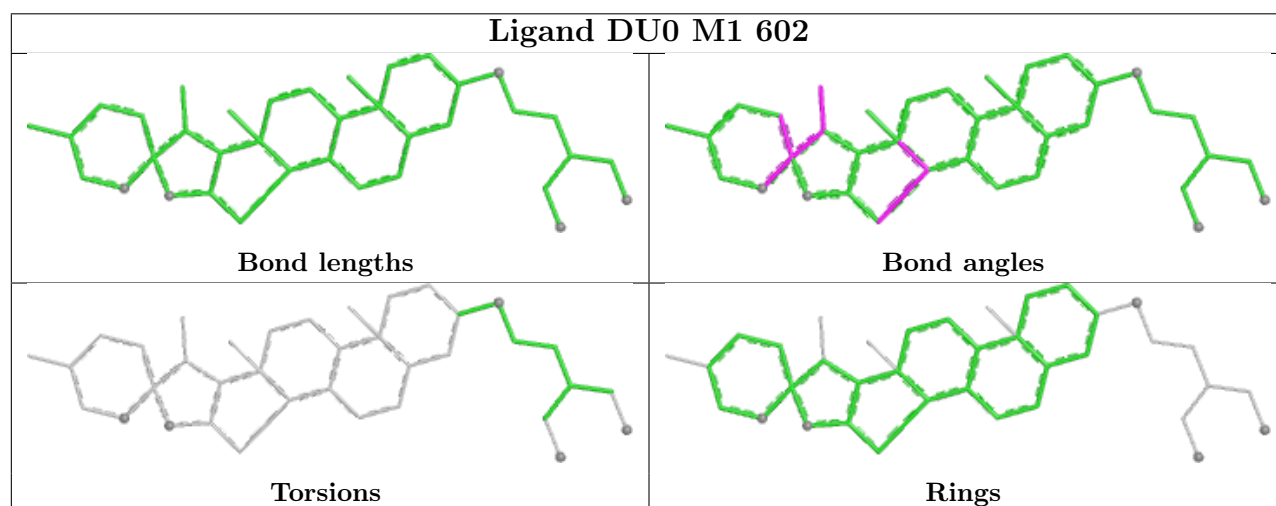
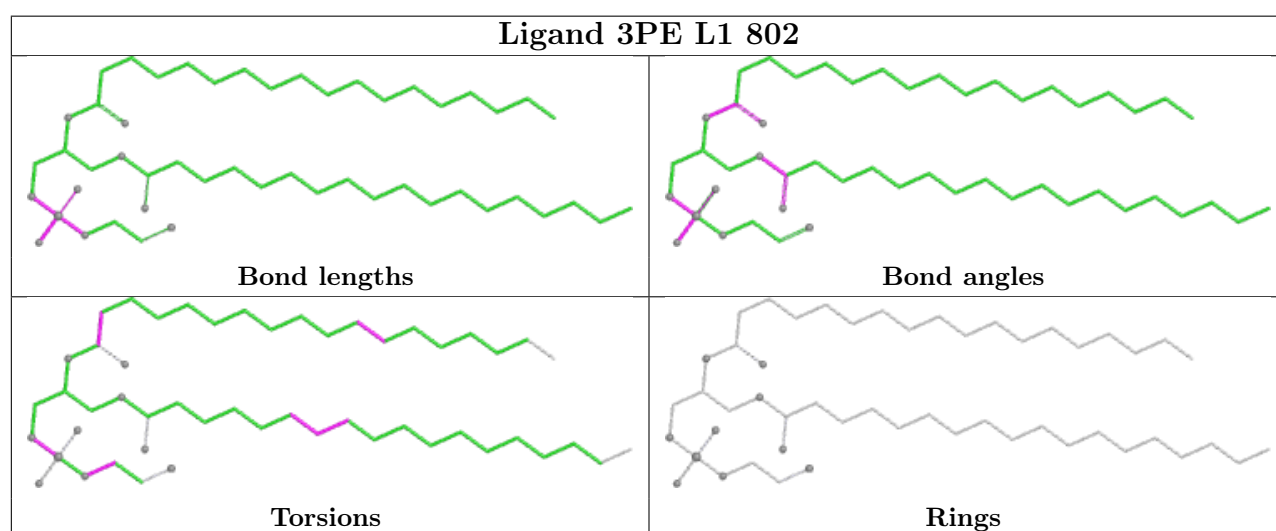
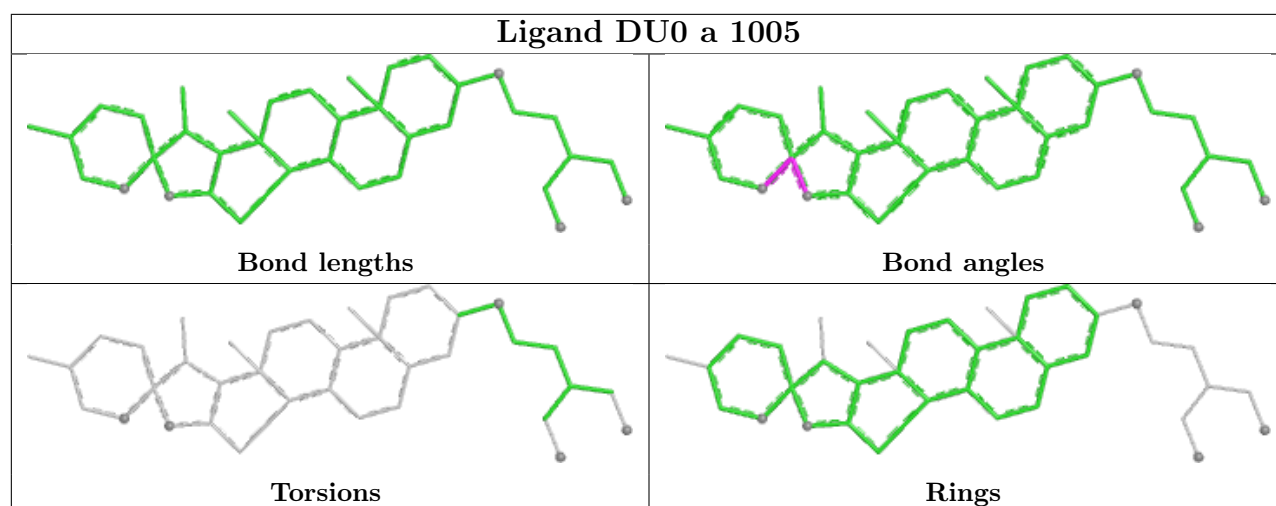
Ligand 3PH L1 804			
 <p>Bond lengths</p>		 <p>Bond angles</p>	
 <p>Torsions</p>		 <p>Rings</p>	

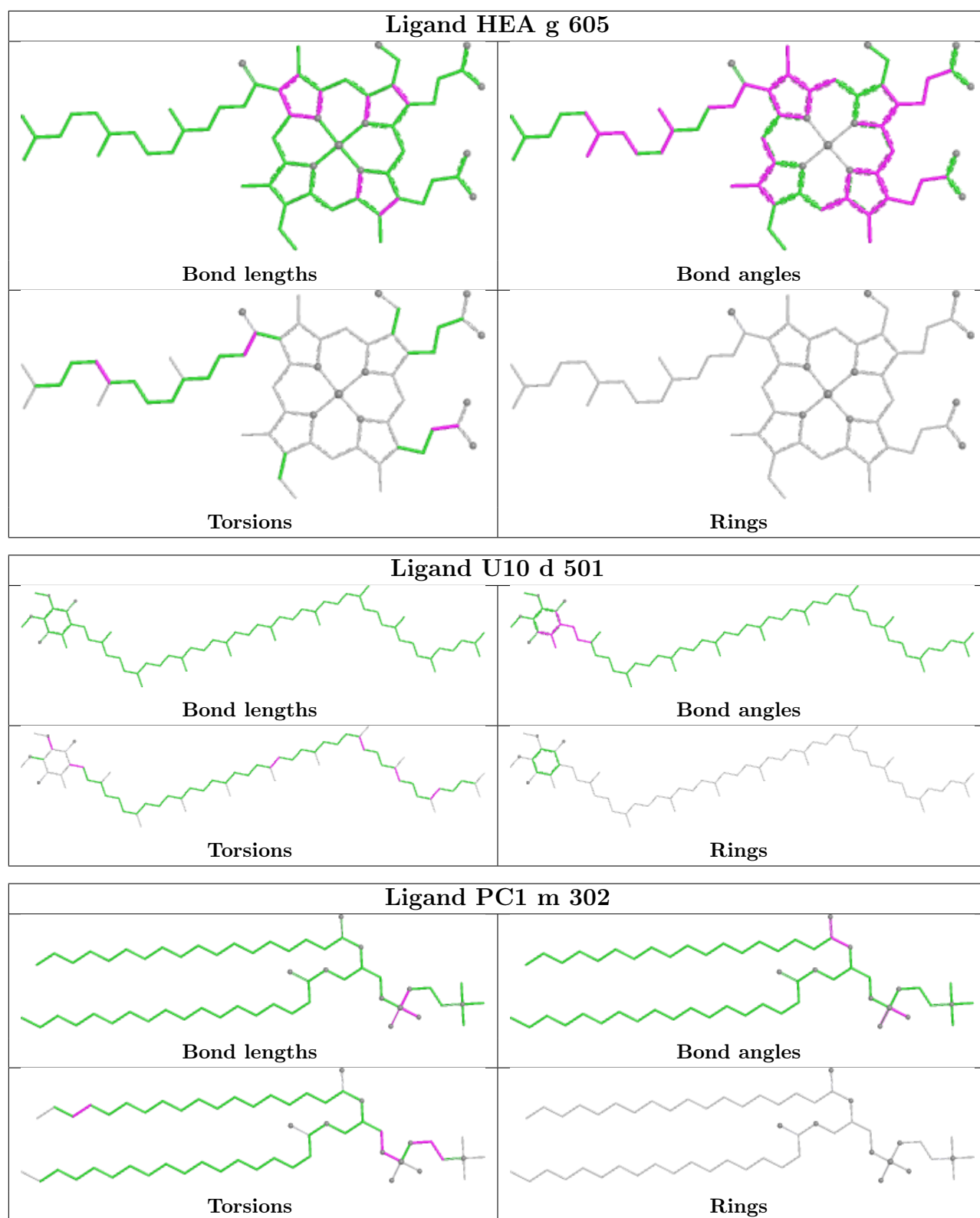
Ligand 3PH p 201	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand P5S L 803	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

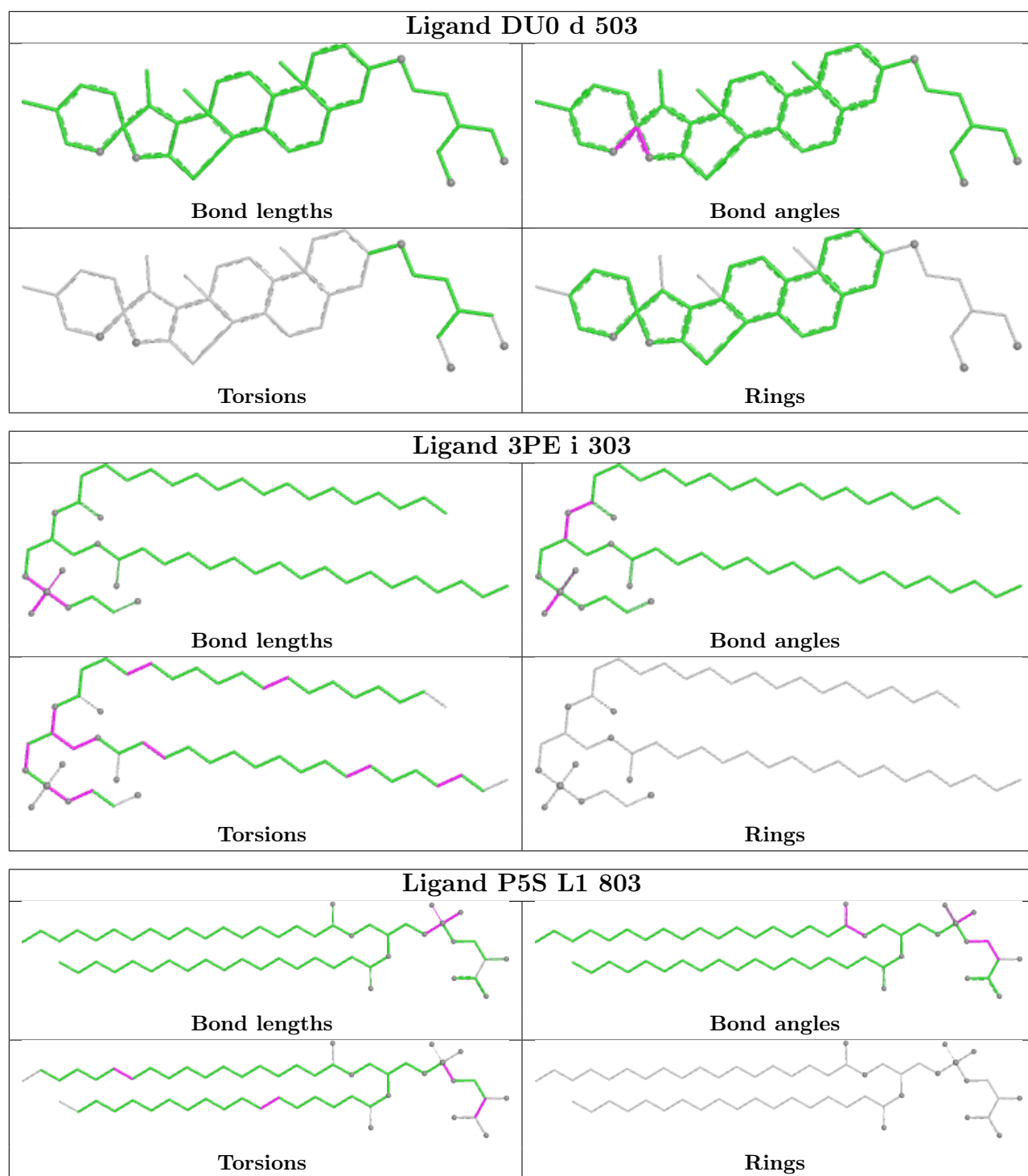


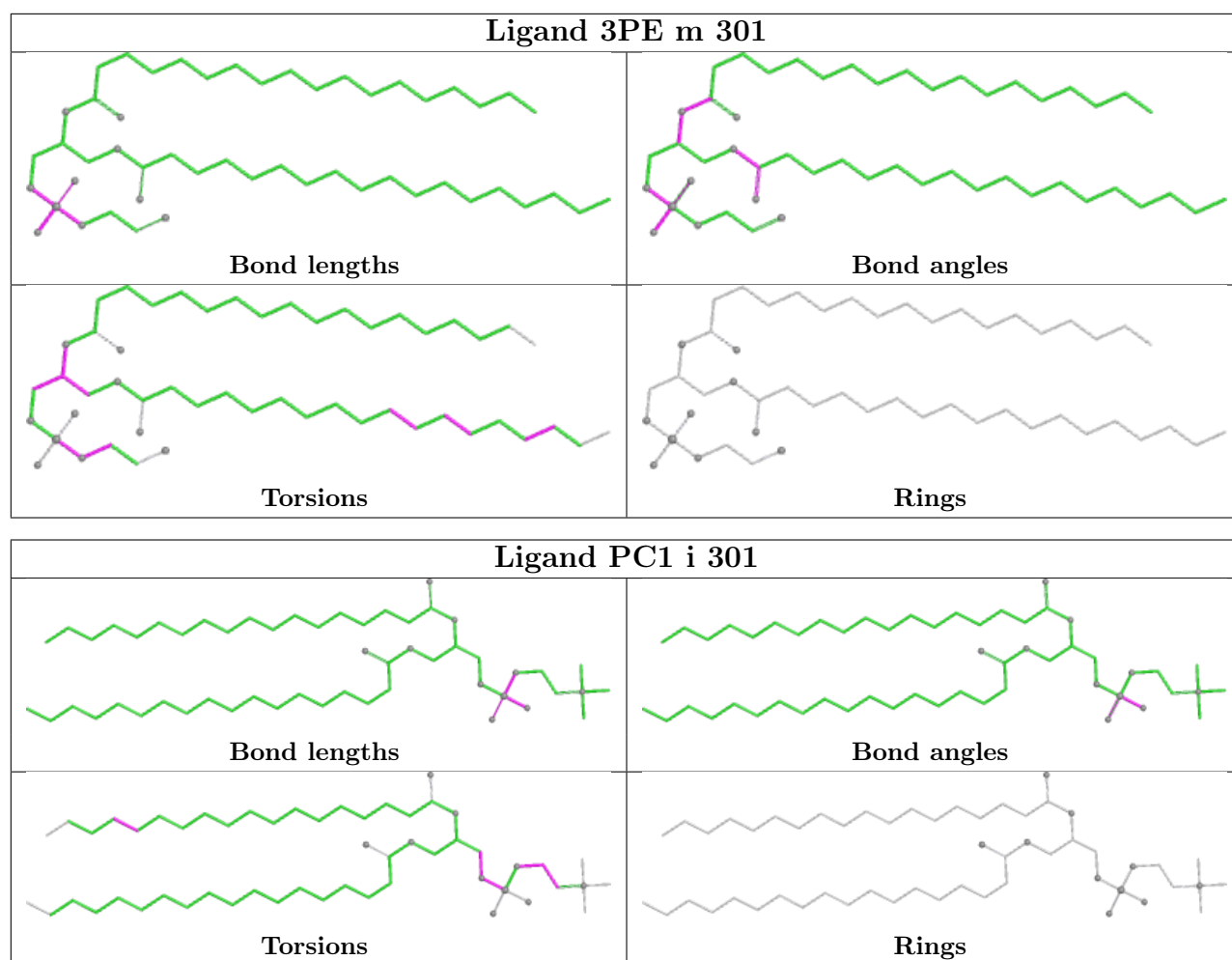


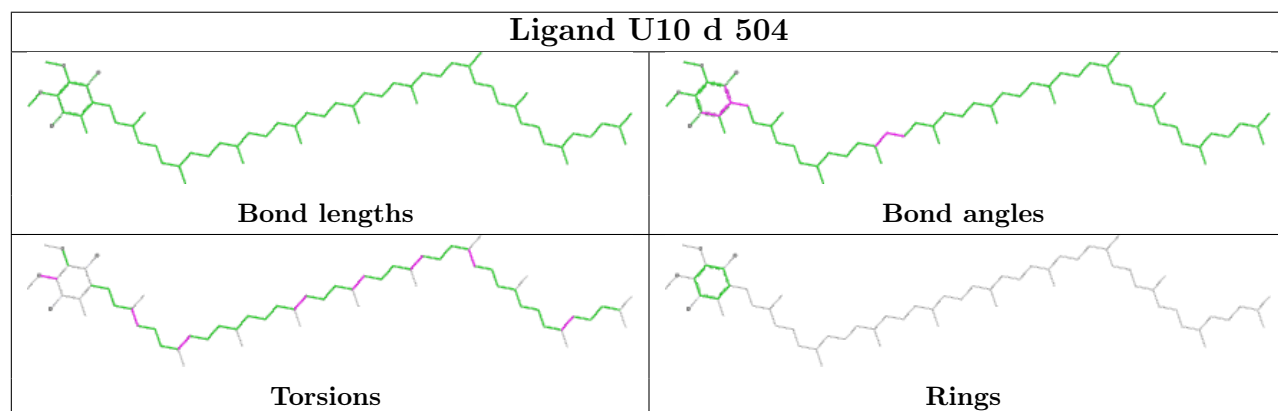
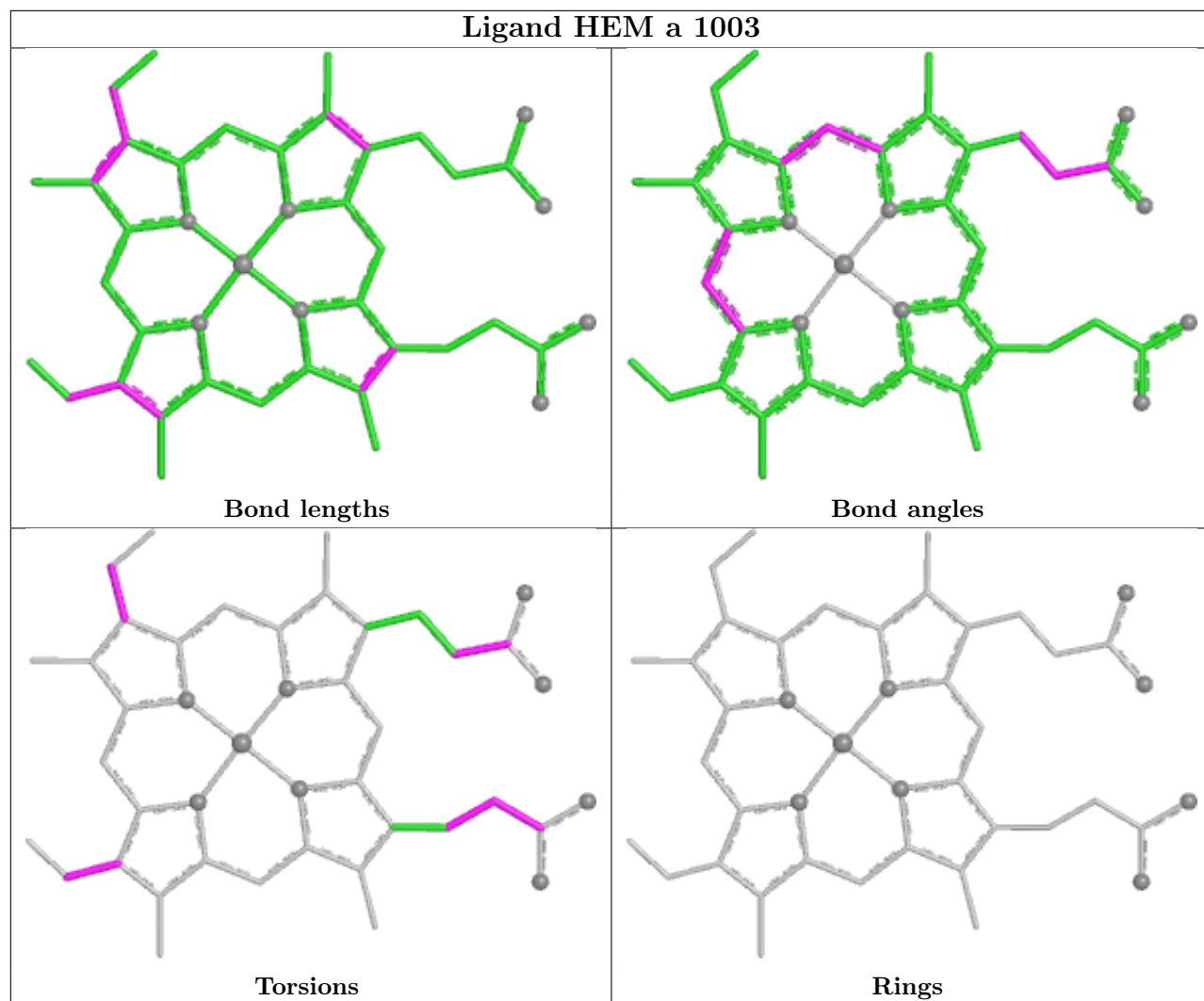


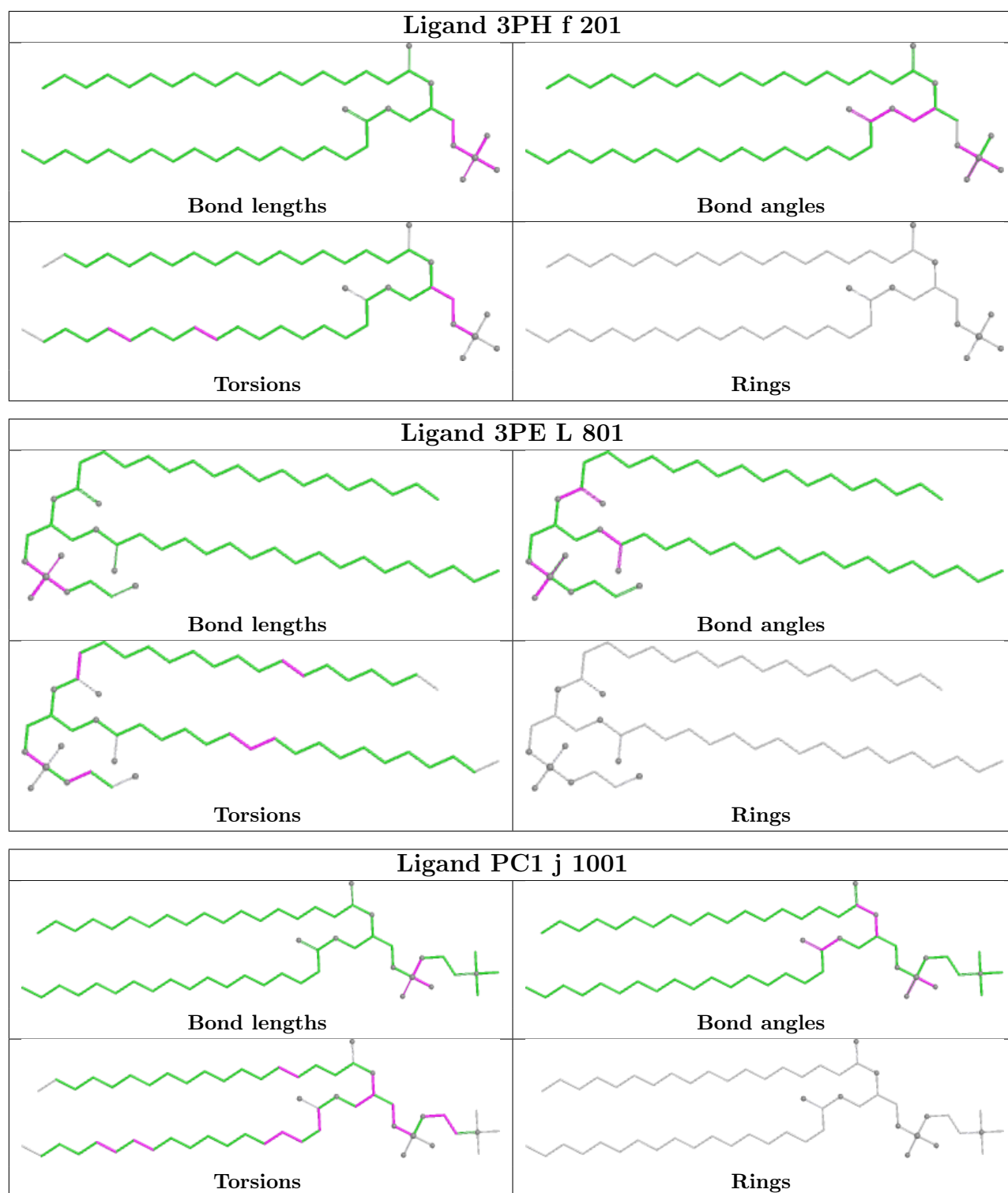


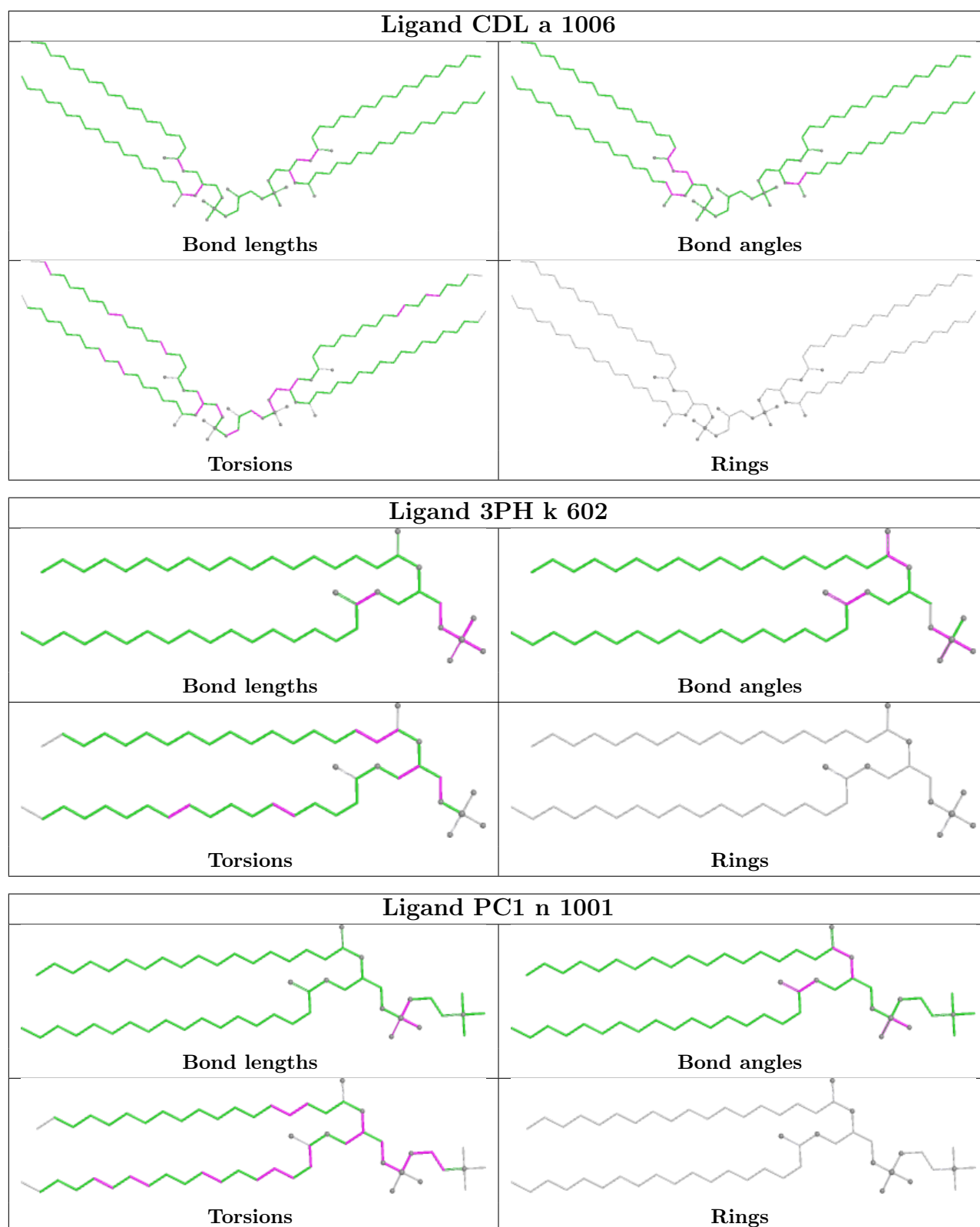


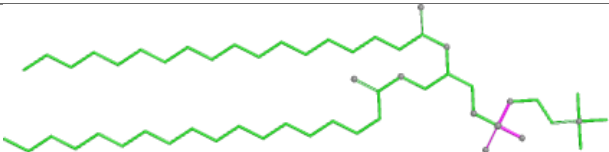
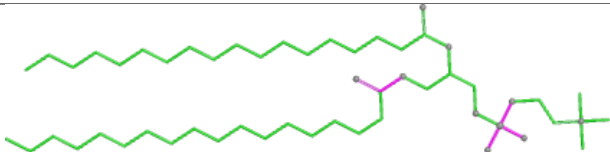
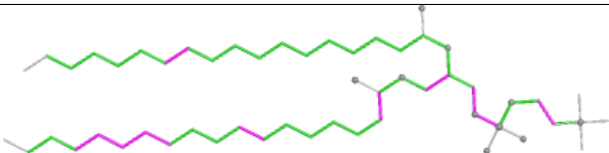
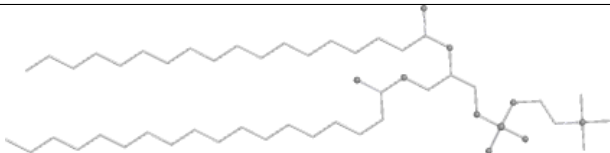
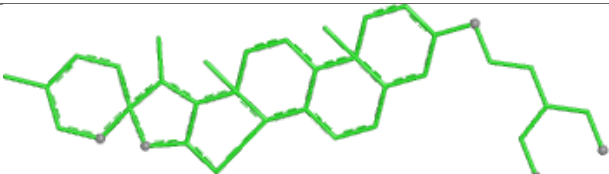
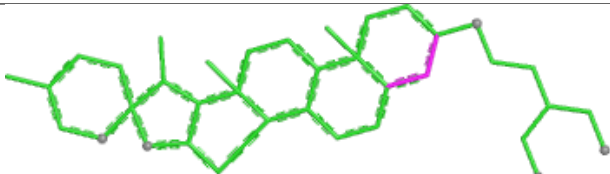
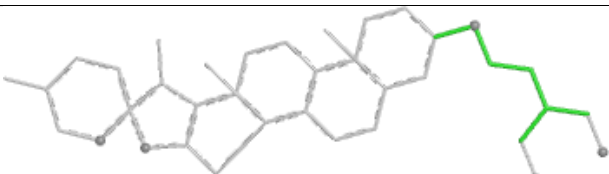
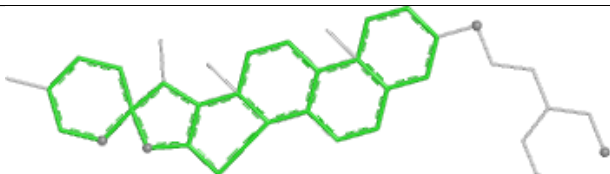
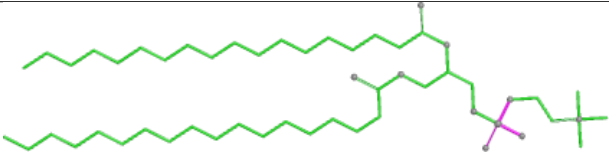
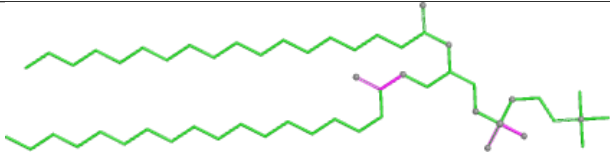
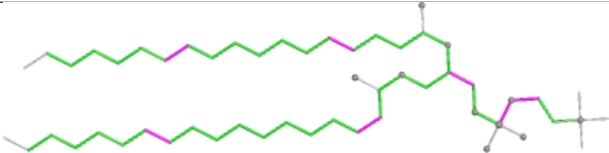
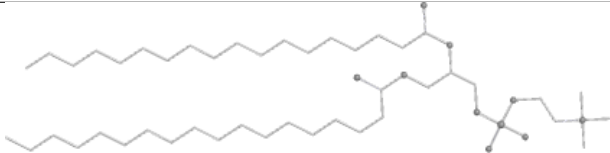


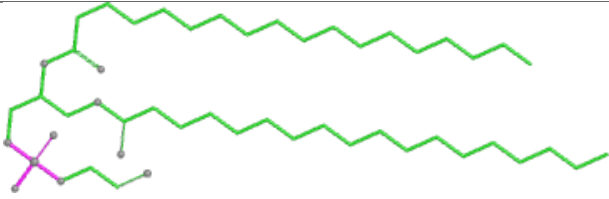
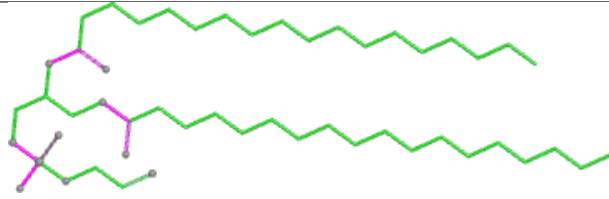
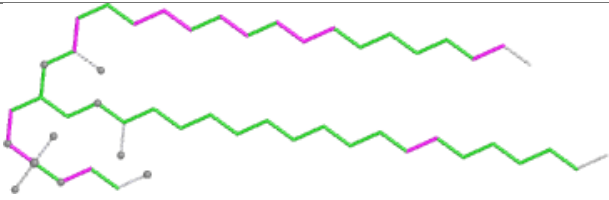
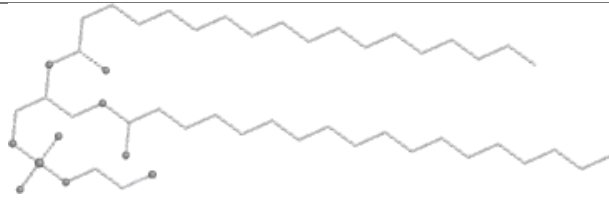




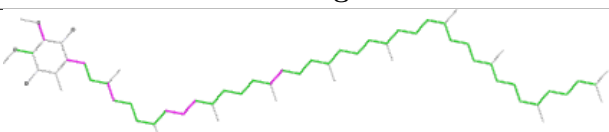



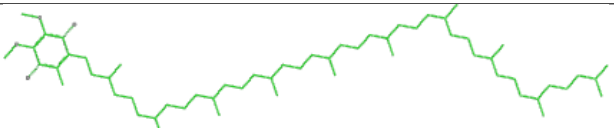
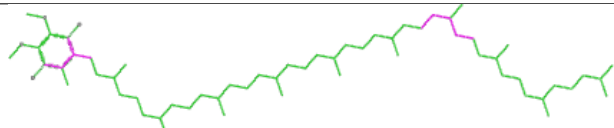
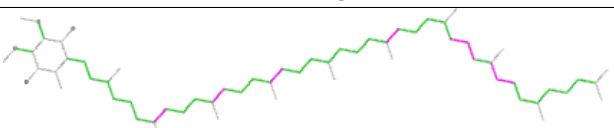



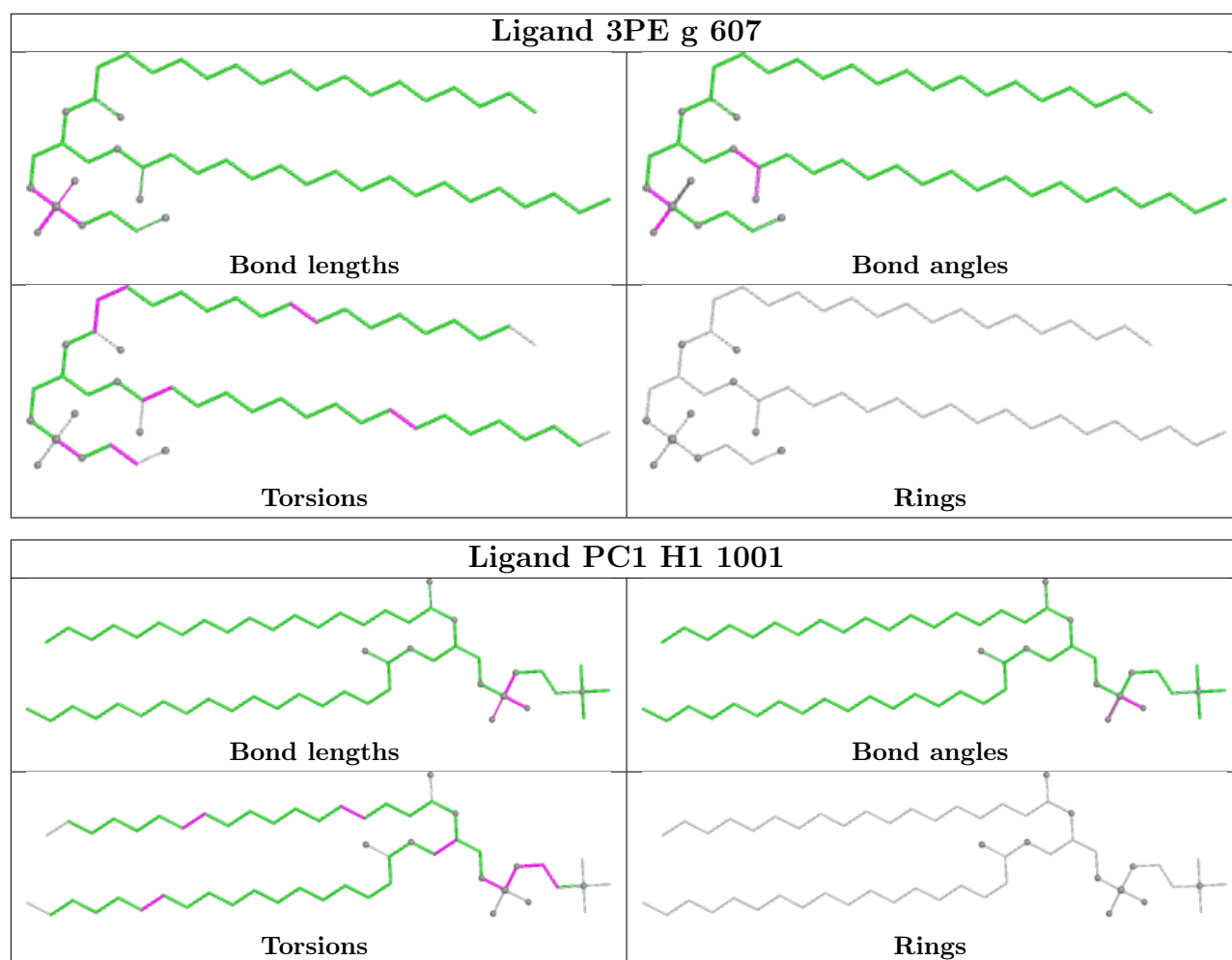


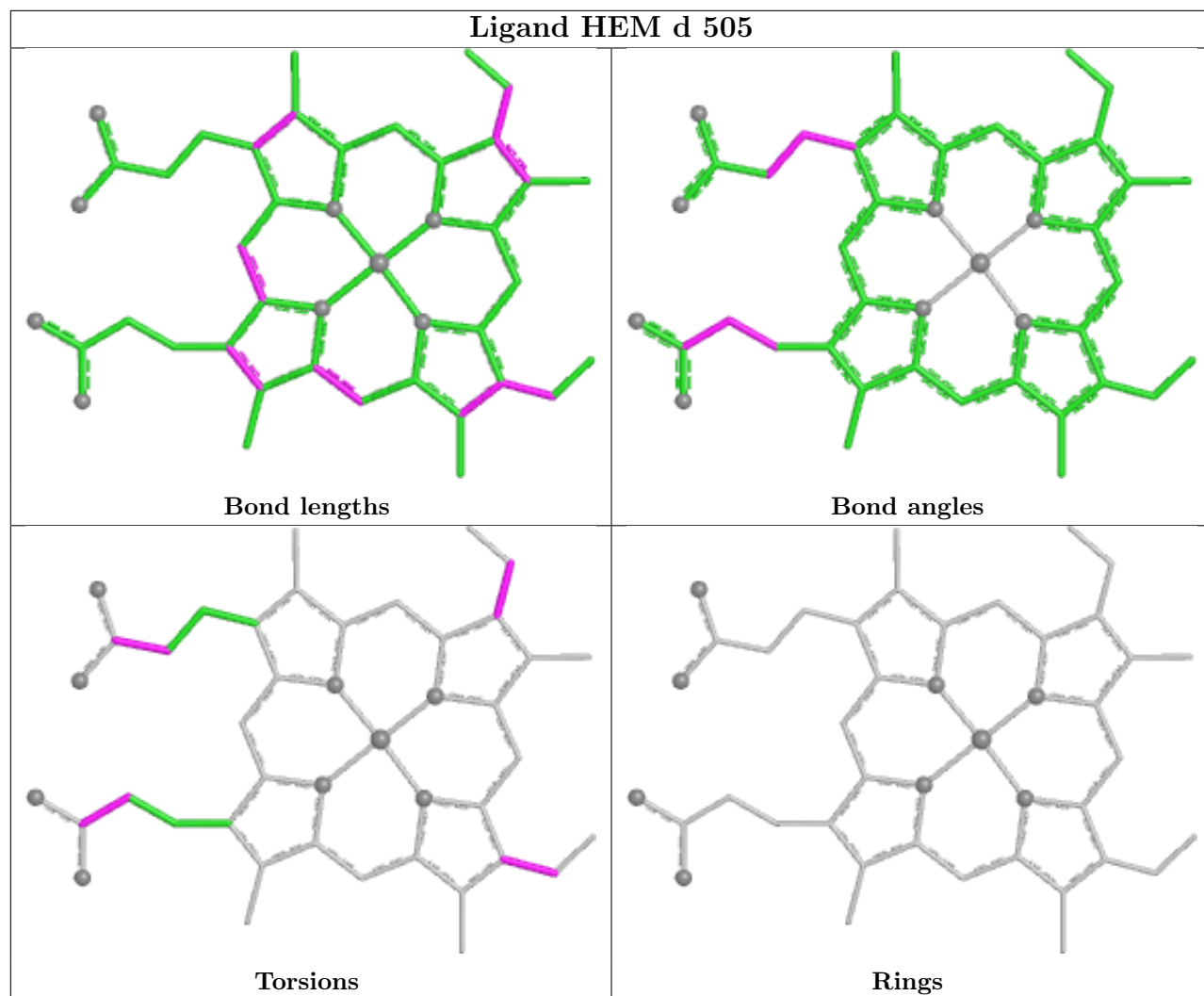
Ligand PC1 m 303	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand DU0 K 1000	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PC1 M1 601	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

Ligand 3PE b 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

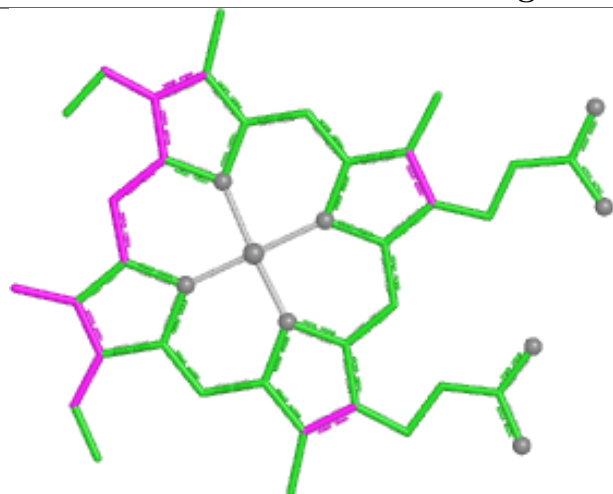
Ligand U10 B1 1002	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand U10 a 1004	
	
Bond lengths	Bond angles
	
Torsions	Rings

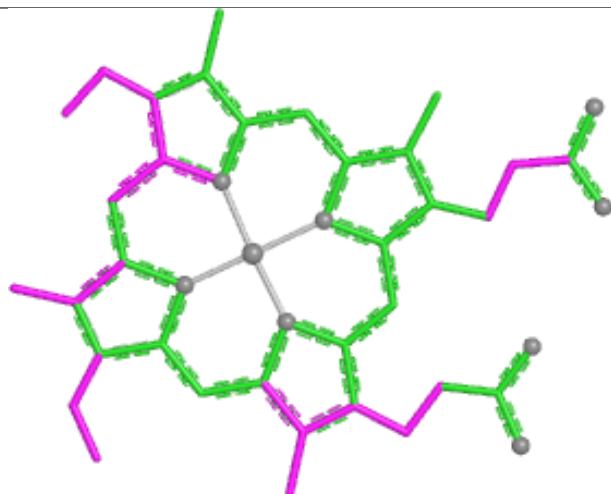




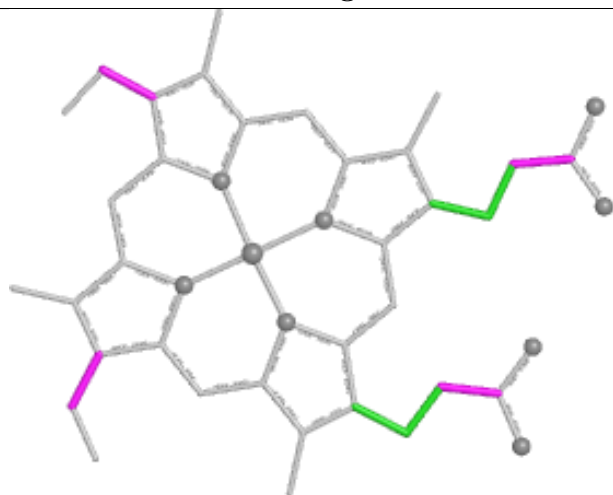
Ligand HEC e 503



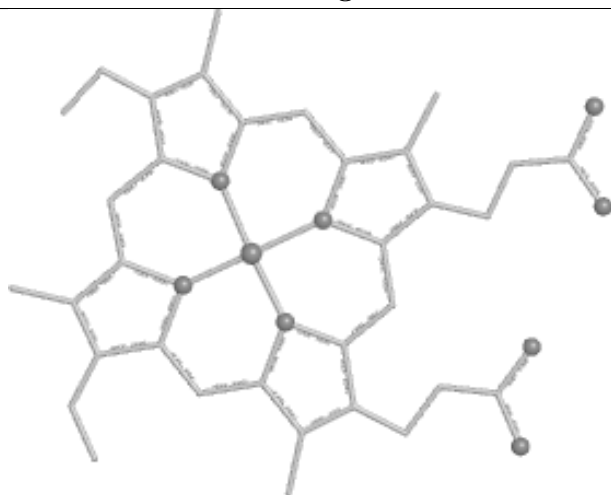
Bond lengths



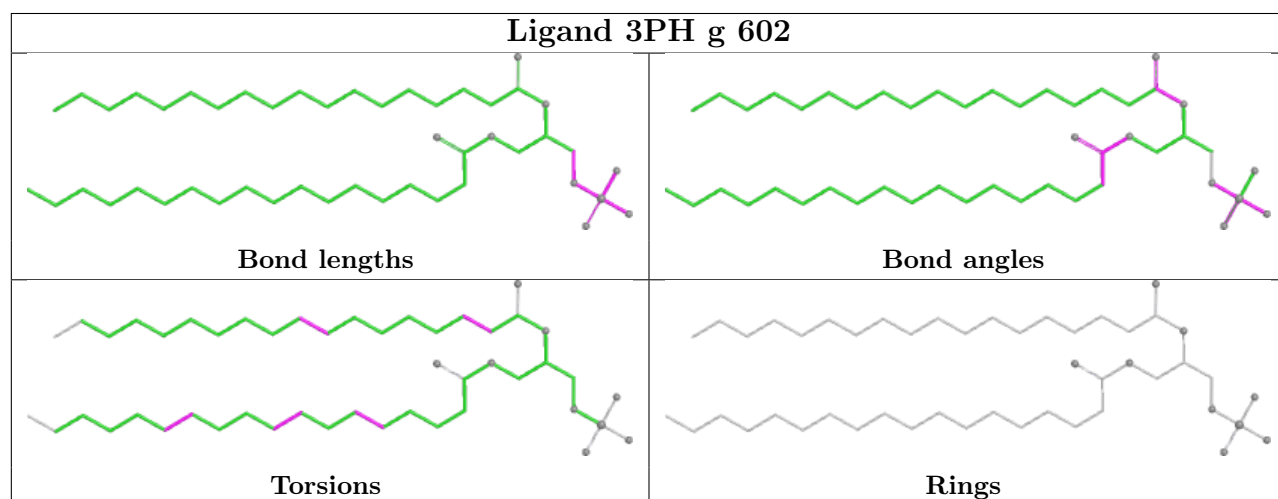
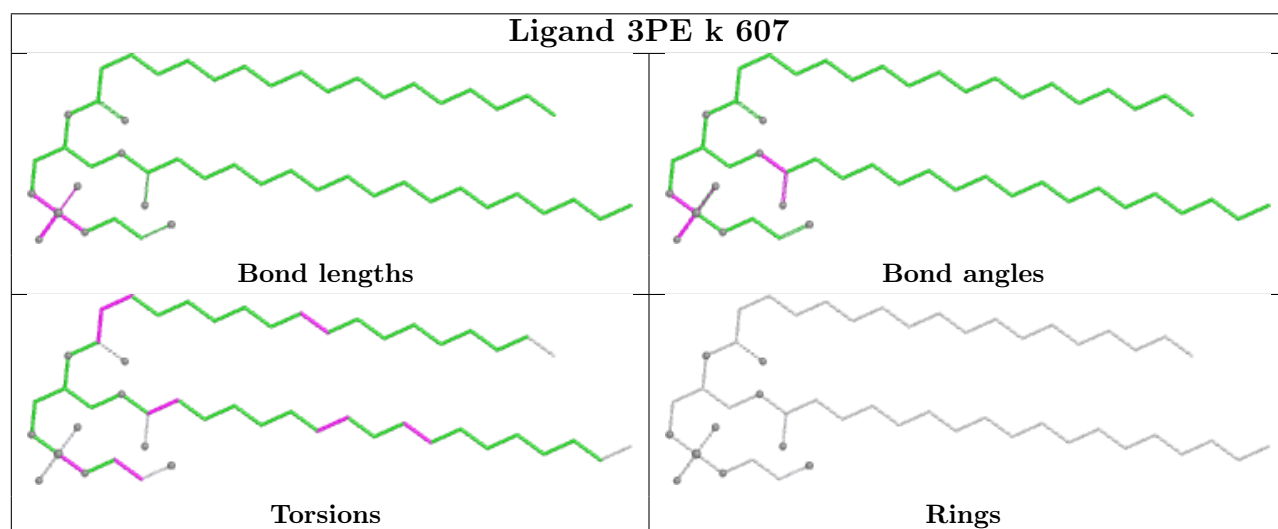
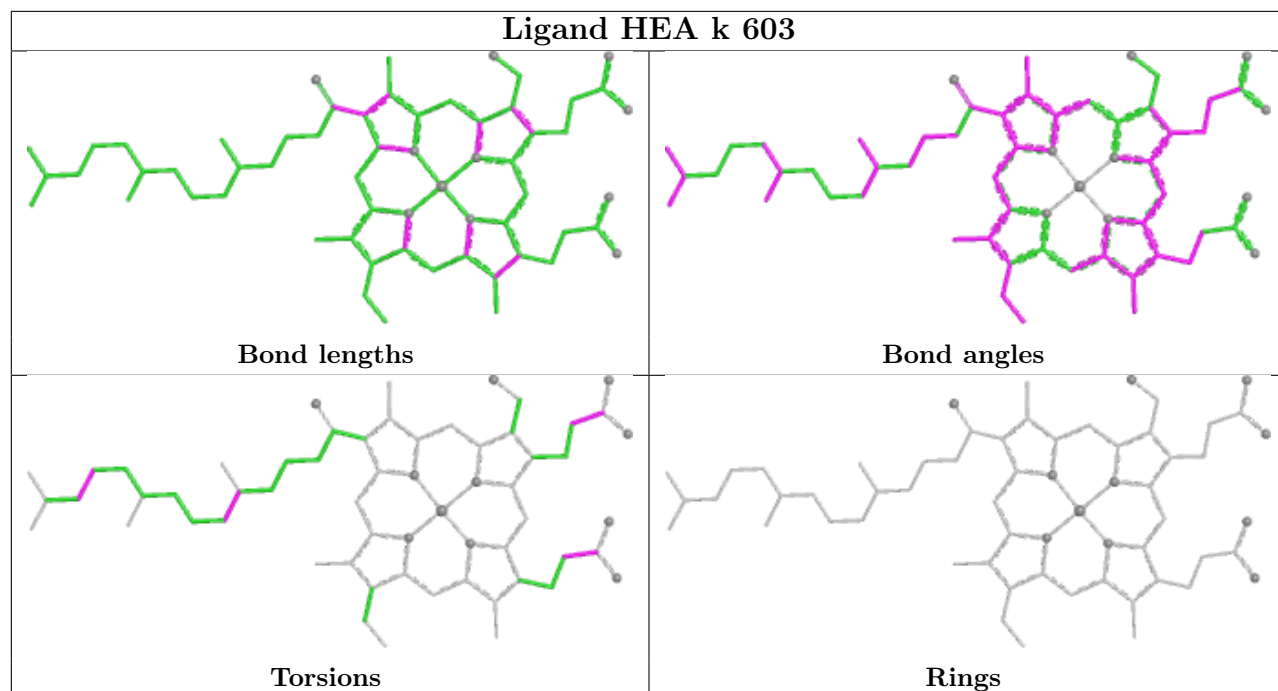
Bond angles

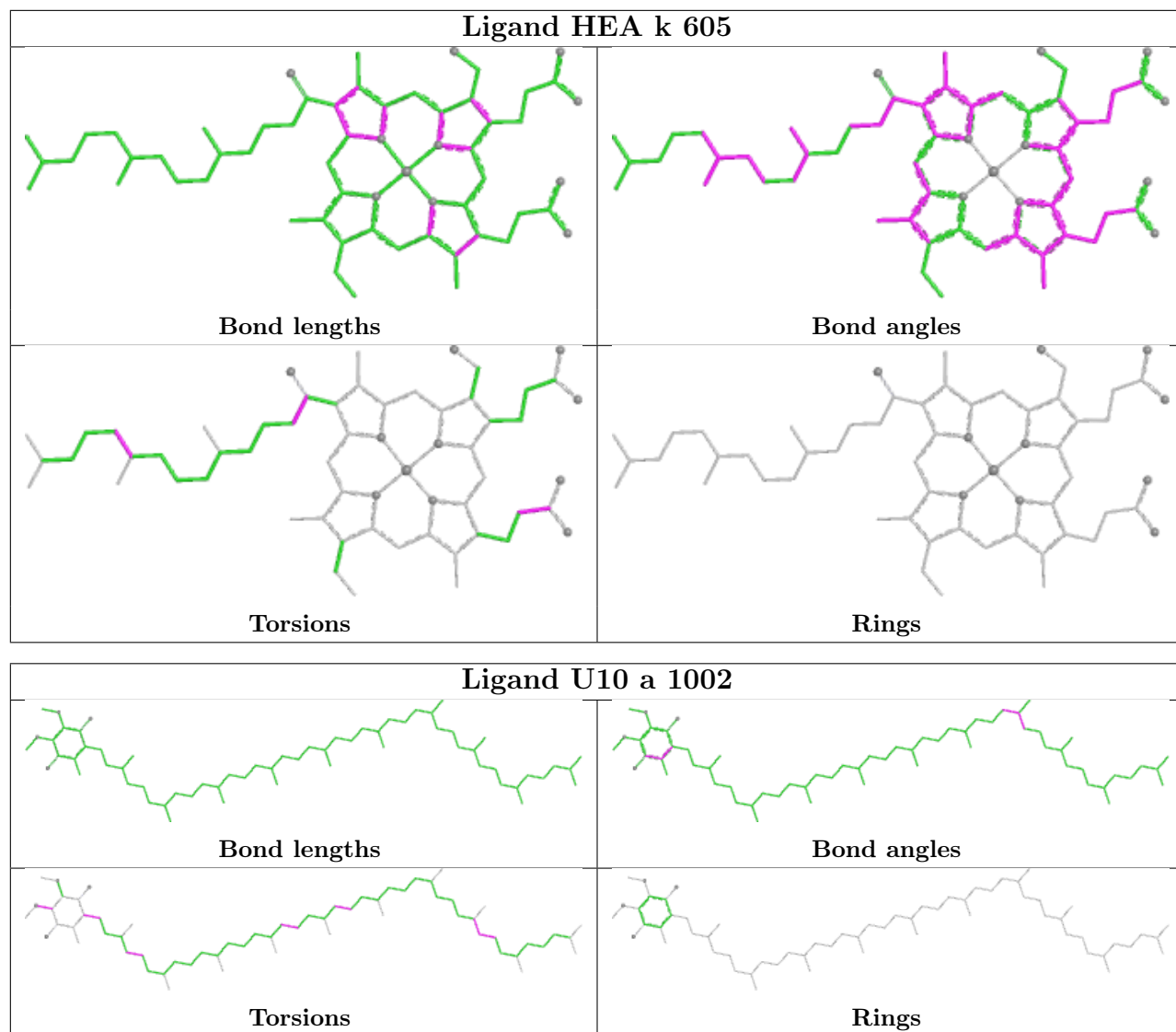


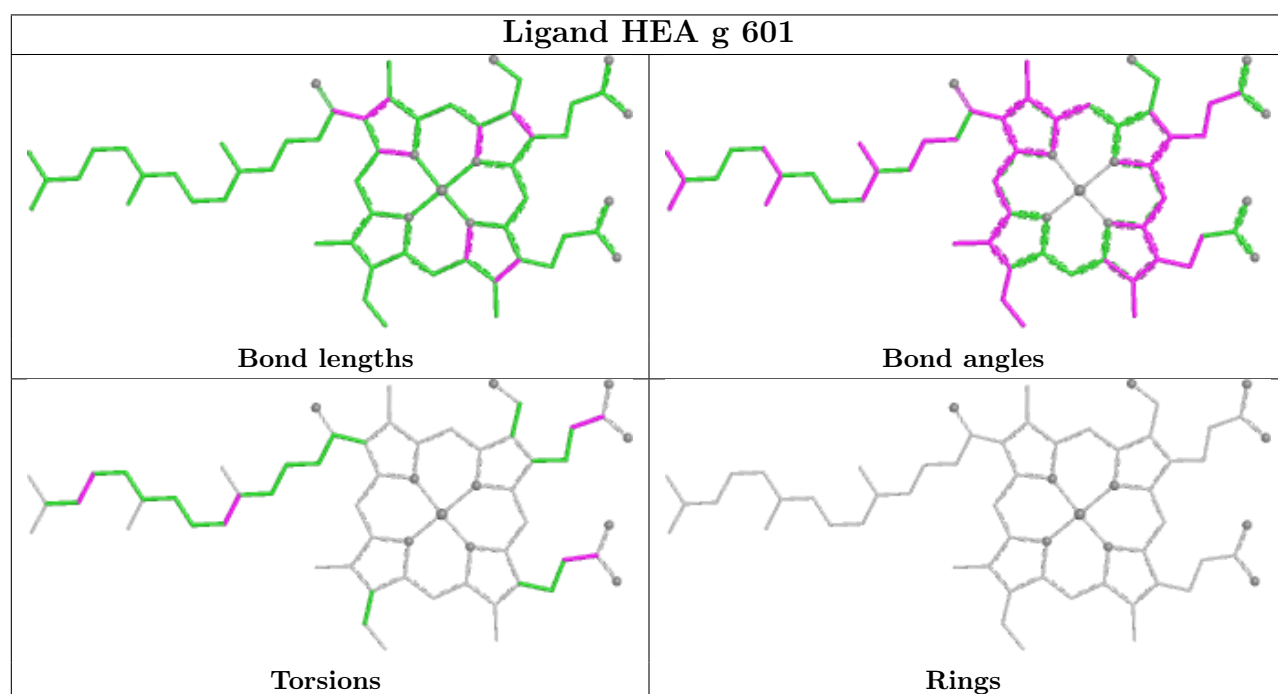
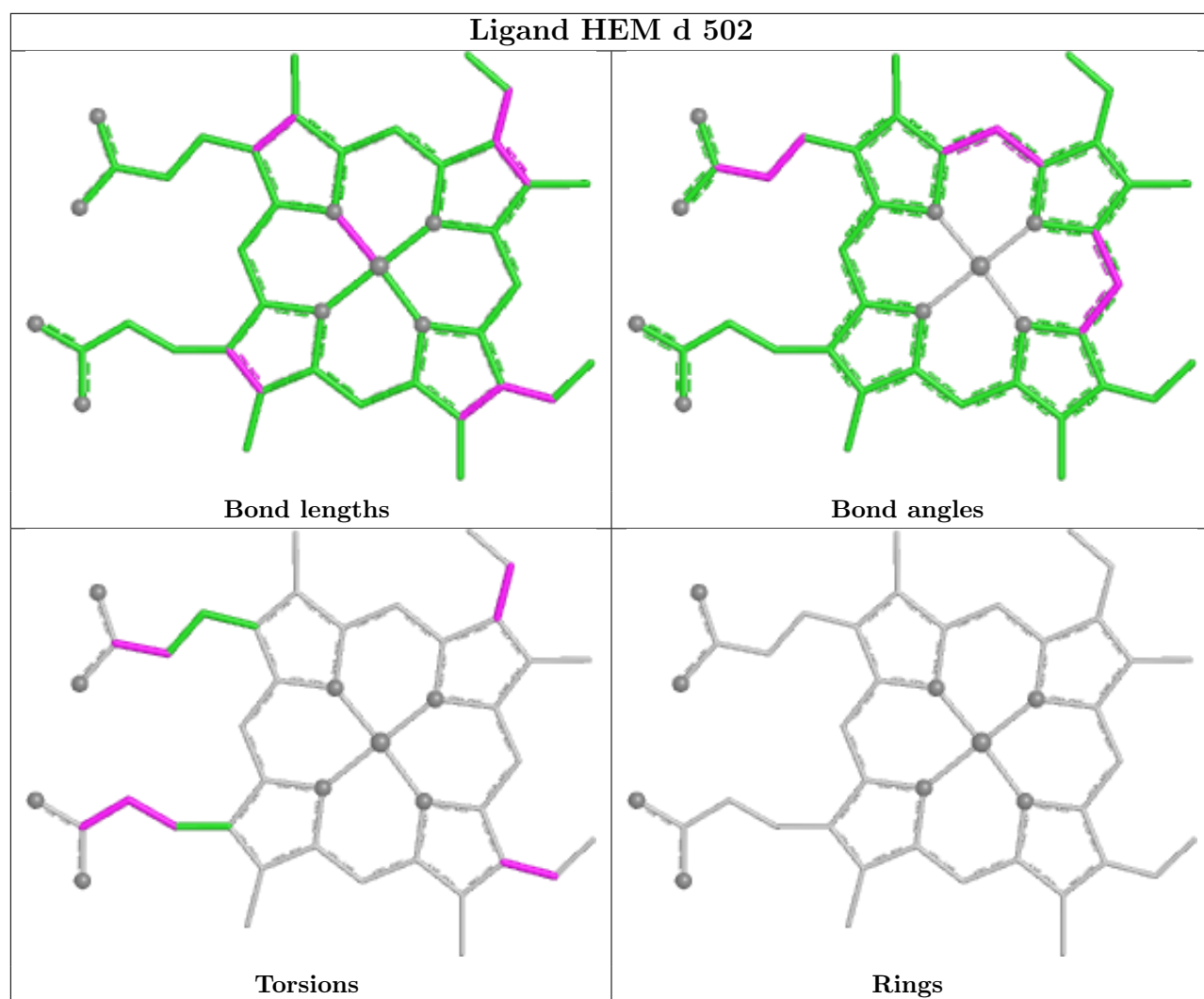
Torsions

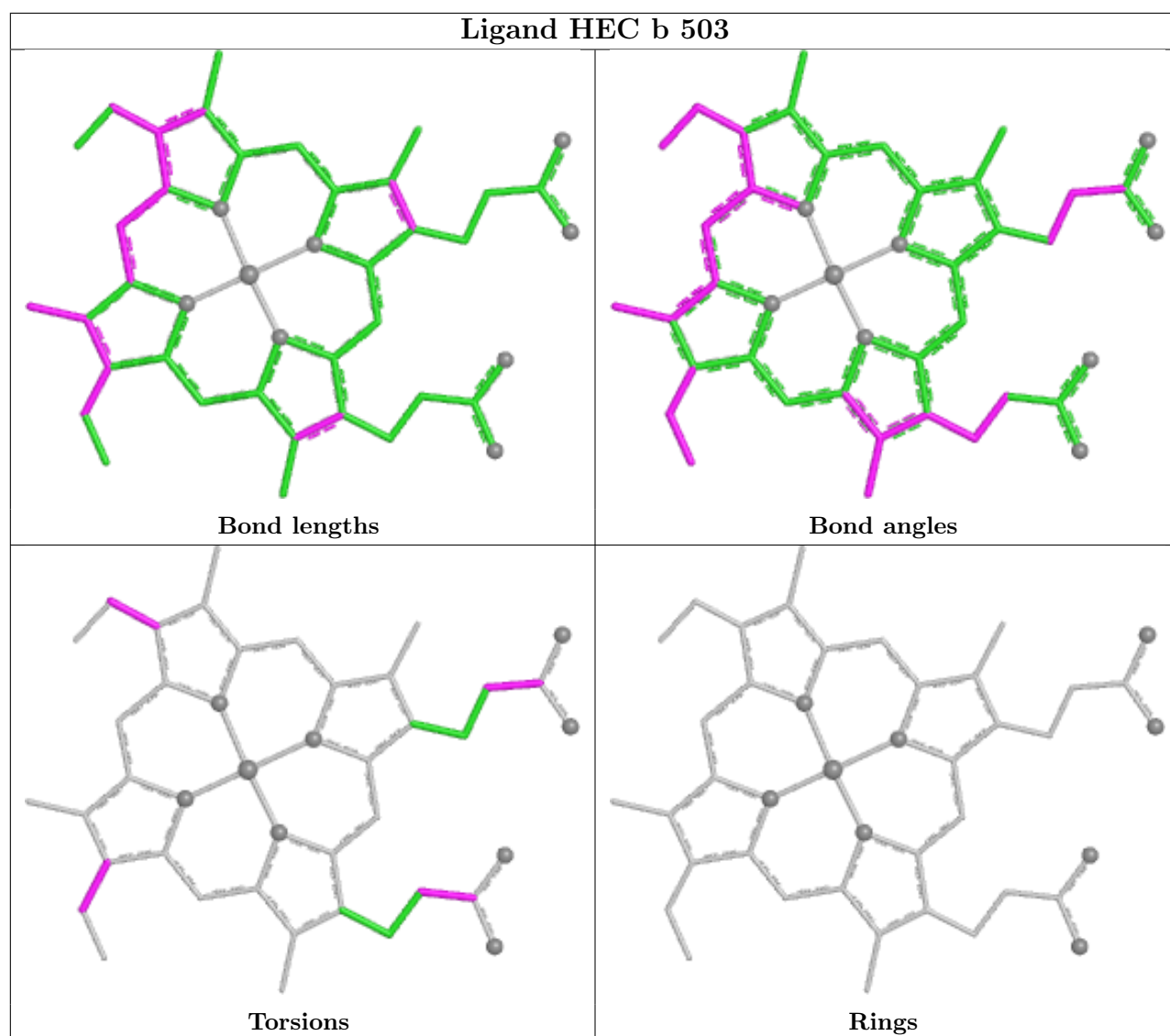


Rings









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51161. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

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

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.