



Full wwPDB EM Validation Report ⓘ

Aug 26, 2026 – 04:46 pm BST

PDB ID : 9GAE / pdb_00009gae
EMDB ID : EMD-51181
Title : Respiratory supercomplex CI1-CIII2-CIV2 from alphaproteobacterium
Authors : Yaikhomba, M.; Hirst, J.; Croll, T.I.; Spikes, T.E.; Agip, A.N.A.
Deposited on : 2024-07-26
Resolution : 3.00 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:

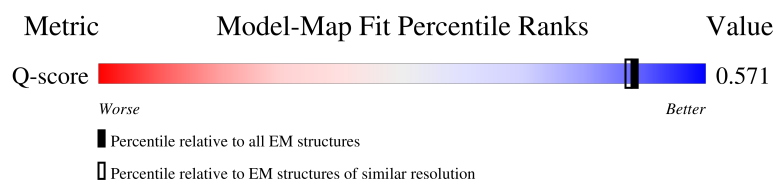
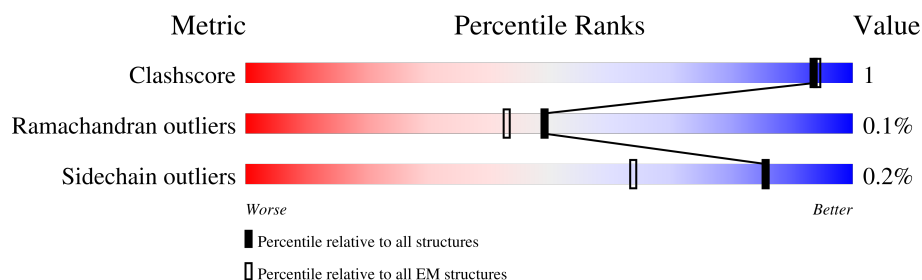
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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.



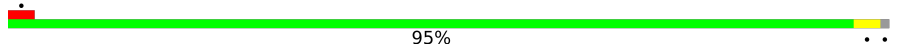
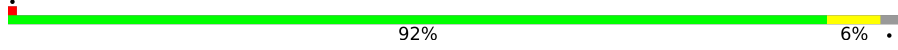
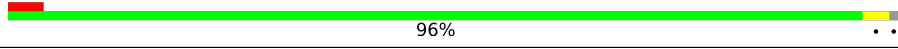
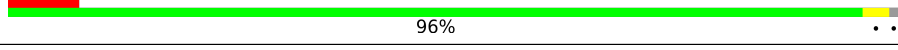
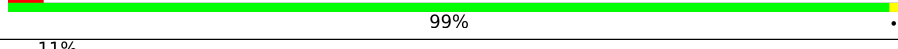
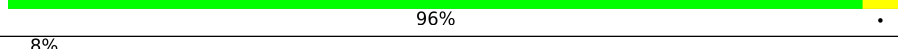
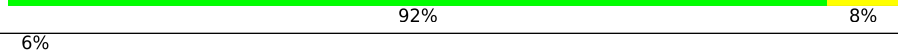
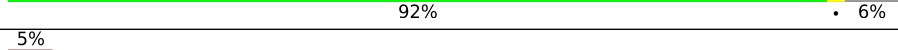
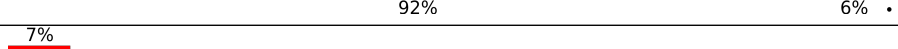
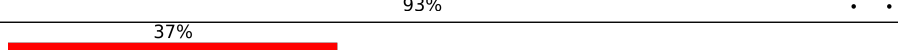
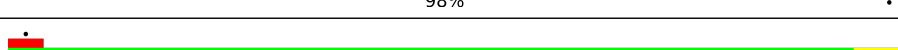
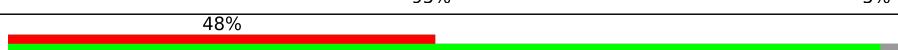
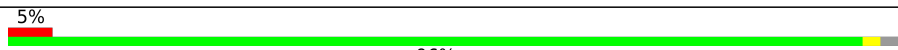
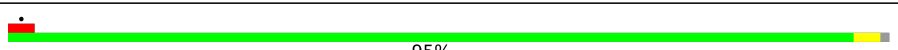
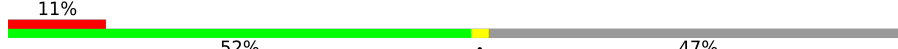
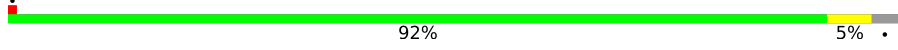
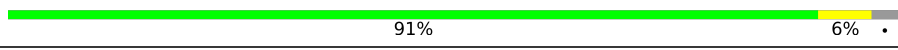
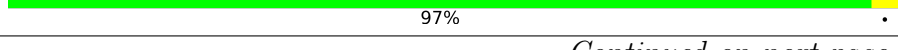
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	121	14% 95% 5%
2	B	175	10% 86% 7% 7%
3	C	208	10% 91% 7%
4	D	412	11% 96% .

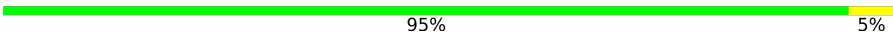
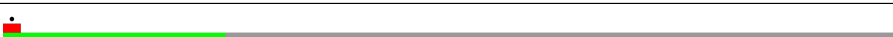
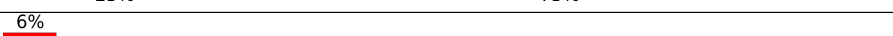
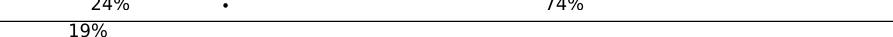
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	239	
6	F	431	
7	G	674	
8	H	345	
9	I	163	
10	J	199	
11	K	101	
12	L	703	
13	M	513	
14	N	499	
15	P	330	
16	Q	103	
17	R	62	
18	Z	217	
19	a	440	
19	d	440	
20	b	450	
20	e	450	
21	c	195	
21	f	195	
22	g	558	
22	k	558	
23	h	298	
23	l	298	
24	i	274	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
24	m	274	 95% 5%
25	j	66	 64% 35%
25	n	66	 65% 35%
26	o	176	 25% 75%
26	p	176	 24% 74%
27	q	124	 98% ..

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
42	HEC	b	502	X	-	-	-

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 82894 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- 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		

- Molecule 19 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	433	Total	C	N	O	S	0	0
			3504	2373	552	561	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	180	Total	C	N	O	S	0	0
			1353	838	245	263	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		

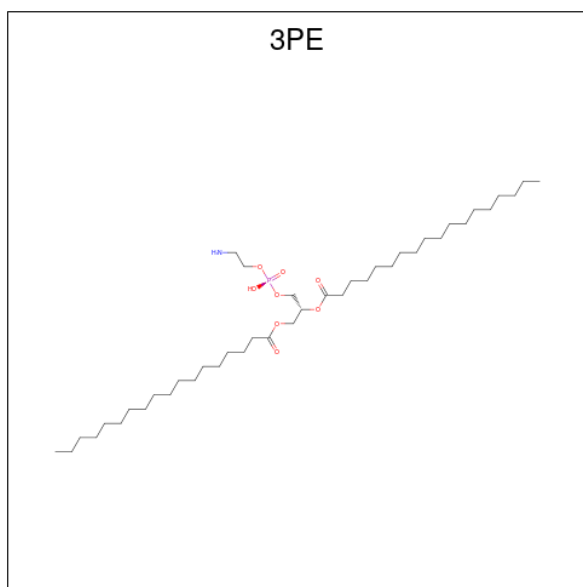
- Molecule 26 is a protein called Cytochrome c, class I.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	o	44	Total	C	N	O	S	0	0
			324	215	49	58	2		
26	p	45	Total	C	N	O	S	0	0
			330	218	50	60	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		

- Molecule 28 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
28	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
28	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
28	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
28	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
28	H	1	Total	C	N	O	P	0
			51	41	1	8	1	
28	L	1	Total	C	N	O	P	0
			51	41	1	8	1	

Continued on next page...

Continued from previous page...

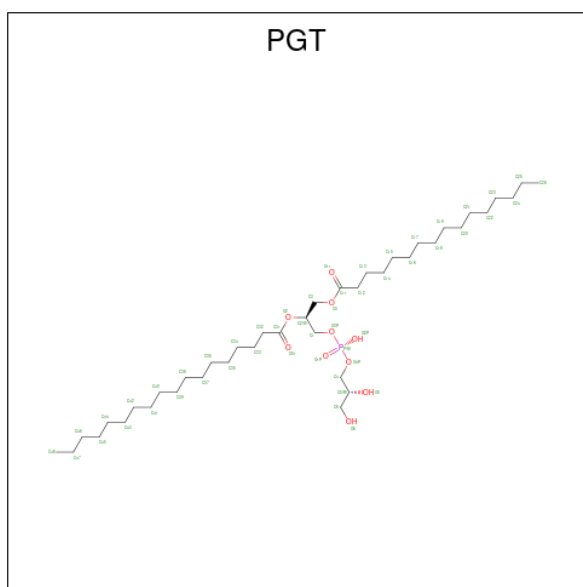
Mol	Chain	Residues	Atoms					AltConf
28	L	1	Total 51	C 41	N 1	O 8	P 1	0
28	L	1	Total 51	C 41	N 1	O 8	P 1	0
28	L	1	Total 51	C 41	N 1	O 8	P 1	0
28	P	1	Total 51	C 41	N 1	O 8	P 1	0
28	a	1	Total 51	C 41	N 1	O 8	P 1	0
28	a	1	Total 51	C 41	N 1	O 8	P 1	0
28	a	1	Total 51	C 41	N 1	O 8	P 1	0
28	a	1	Total 51	C 41	N 1	O 8	P 1	0
28	c	1	Total 51	C 41	N 1	O 8	P 1	0
28	d	1	Total 51	C 41	N 1	O 8	P 1	0
28	d	1	Total 51	C 41	N 1	O 8	P 1	0
28	d	1	Total 51	C 41	N 1	O 8	P 1	0
28	e	1	Total 51	C 41	N 1	O 8	P 1	0
28	e	1	Total 51	C 41	N 1	O 8	P 1	0
28	g	1	Total 51	C 41	N 1	O 8	P 1	0
28	g	1	Total 51	C 41	N 1	O 8	P 1	0
28	g	1	Total 51	C 41	N 1	O 8	P 1	0
28	h	1	Total 51	C 41	N 1	O 8	P 1	0
28	h	1	Total 51	C 41	N 1	O 8	P 1	0
28	i	1	Total 51	C 41	N 1	O 8	P 1	0
28	i	1	Total 51	C 41	N 1	O 8	P 1	0

Continued on next page...

Continued from previous page...

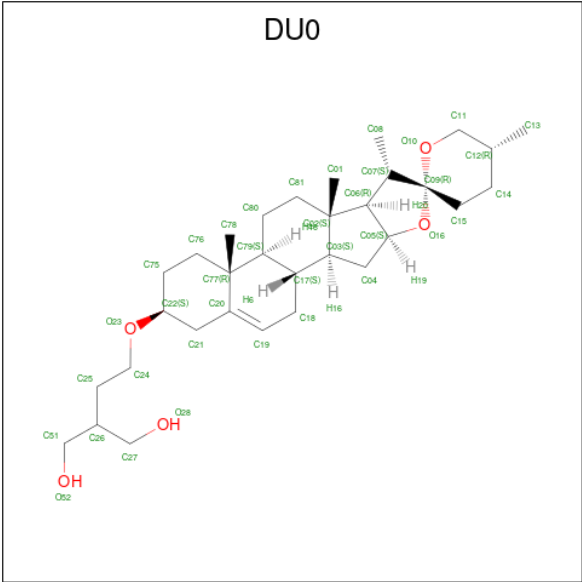
Mol	Chain	Residues	Atoms					AltConf
28	i	1	Total	C	N	O	P	0
			51	41	1	8	1	
28	i	1	Total	C	N	O	P	0
			51	41	1	8	1	
28	i	1	Total	C	N	O	P	0
			51	41	1	8	1	
28	k	1	Total	C	N	O	P	0
			51	41	1	8	1	
28	m	1	Total	C	N	O	P	0
			51	41	1	8	1	
28	m	1	Total	C	N	O	P	0
			51	41	1	8	1	
28	m	1	Total	C	N	O	P	0
			51	41	1	8	1	
28	m	1	Total	C	N	O	P	0
			51	41	1	8	1	
28	m	1	Total	C	N	O	P	0
			51	41	1	8	1	
28	n	1	Total	C	N	O	P	0
			51	41	1	8	1	
28	p	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 29 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	C	O	P	0
			51	40	10	1	
29	H	1	Total	C	O	P	0
			51	40	10	1	
29	J	1	Total	C	O	P	0
			51	40	10	1	
29	J	1	Total	C	O	P	0
			51	40	10	1	
29	K	1	Total	C	O	P	0
			51	40	10	1	
29	L	1	Total	C	O	P	0
			51	40	10	1	
29	M	1	Total	C	O	P	0
			51	40	10	1	
29	N	1	Total	C	O	P	0
			51	40	10	1	
29	P	1	Total	C	O	P	0
			51	40	10	1	
29	a	1	Total	C	O	P	0
			51	40	10	1	
29	g	1	Total	C	O	P	0
			51	40	10	1	
29	q	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 30 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).



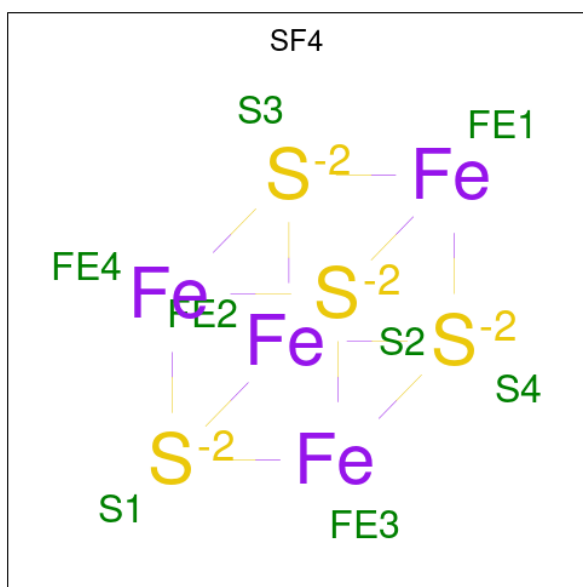
Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	C	O	0
			37	32	5	
30	H	1	Total	C	O	0
			37	32	5	
30	J	1	Total	C	O	0
			37	32	5	
30	J	1	Total	C	O	0
			37	32	5	
30	M	1	Total	C	O	0
			37	32	5	
30	M	1	Total	C	O	0
			37	32	5	
30	a	1	Total	C	O	0
			37	32	5	
30	c	1	Total	C	O	0
			37	32	5	
30	c	1	Total	C	O	0
			37	32	5	
30	d	1	Total	C	O	0
			37	32	5	
30	d	1	Total	C	O	0
			37	32	5	
30	d	1	Total	C	O	0
			37	32	5	
30	e	1	Total	C	O	0
			37	32	5	
30	f	1	Total	C	O	0
			37	32	5	

Continued on next page...

Continued from previous page...

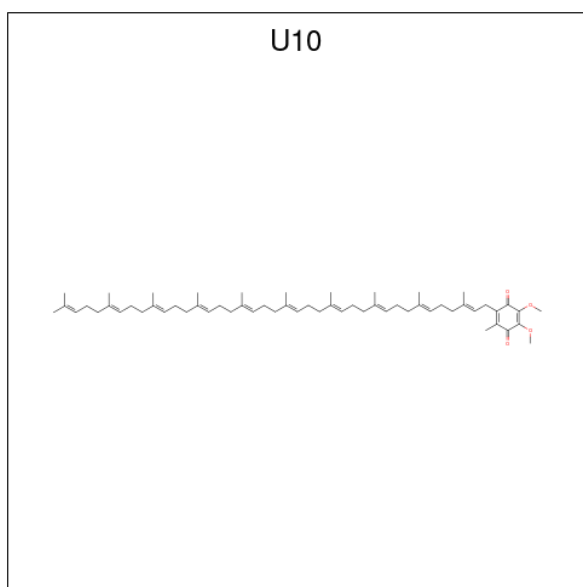
Mol	Chain	Residues	Atoms			AltConf
30	g	1	Total	C	O	0
			37	32	5	
30	g	1	Total	C	O	0
			37	32	5	
30	g	1	Total	C	O	0
			37	32	5	
30	g	1	Total	C	O	0
			37	32	5	
30	h	1	Total	C	O	0
			37	32	5	
30	h	1	Total	C	O	0
			37	32	5	
30	h	1	Total	C	O	0
			37	32	5	
30	i	1	Total	C	O	0
			37	32	5	
30	i	1	Total	C	O	0
			37	32	5	
30	i	1	Total	C	O	0
			37	32	5	
30	i	1	Total	C	O	0
			37	32	5	
30	j	1	Total	C	O	0
			37	32	5	
30	k	1	Total	C	O	0
			37	32	5	
30	m	1	Total	C	O	0
			37	32	5	
30	m	1	Total	C	O	0
			37	32	5	

- Molecule 31 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



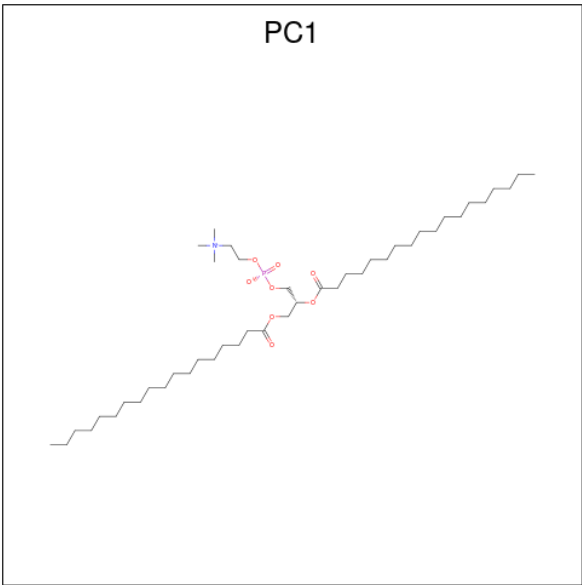
Mol	Chain	Residues	Atoms			AltConf
31	B	1	Total	Fe	S	0
			8	4	4	
31	F	1	Total	Fe	S	
			8	4	4	
31	G	1	Total	Fe	S	
			8	4	4	
31	G	1	Total	Fe	S	0
			8	4	4	
31	I	1	Total	Fe	S	
			8	4	4	
31	I	1	Total	Fe	S	
			8	4	4	

- Molecule 32 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄).



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

- 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	D	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	H	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	H	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	L	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	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	
33	N	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	
33	a	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	a	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	a	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	b	1	Total	C	N	O	P	0
			54	44	1	8	1	

Continued on next page...

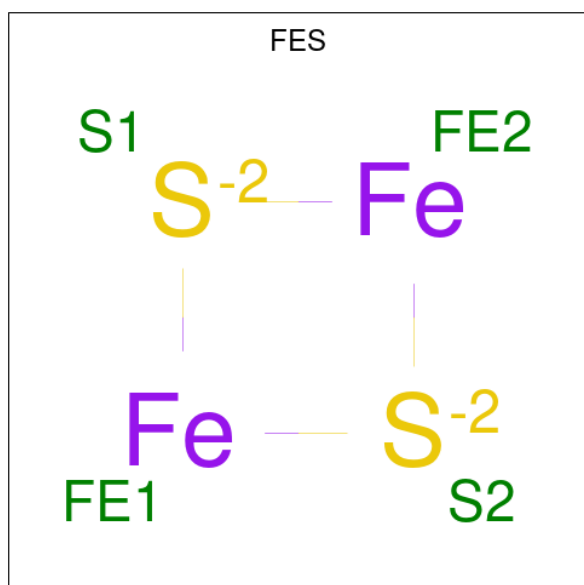
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
33	b	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	c	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	d	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	d	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	f	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	g	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	h	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	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	k	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	k	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	l	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	l	1	Total	C	N	O	P	0
			54	44	1	8	1	
33	l	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	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 CALCIUM ION (CCD ID: CA) (formula: Ca).

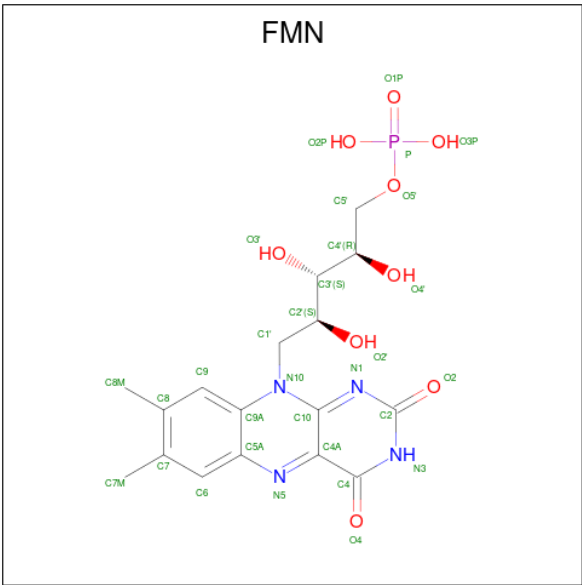
Mol	Chain	Residues	Atoms		AltConf
34	D	1	Total	Ca	0
			1	1	
34	b	1	Total	Ca	0
			1	1	
34	e	1	Total	Ca	0
			1	1	
34	g	1	Total	Ca	0
			1	1	
34	k	1	Total	Ca	0
			1	1	

- Molecule 35 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
35	E	1	Total	Fe	S	0
			4	2	2	
35	G	1	Total	Fe	S	0
			4	2	2	
35	c	1	Total	Fe	S	0
			4	2	2	
35	f	1	Total	Fe	S	0
			4	2	2	

- Molecule 36 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by depositor).



Continued from previous page...

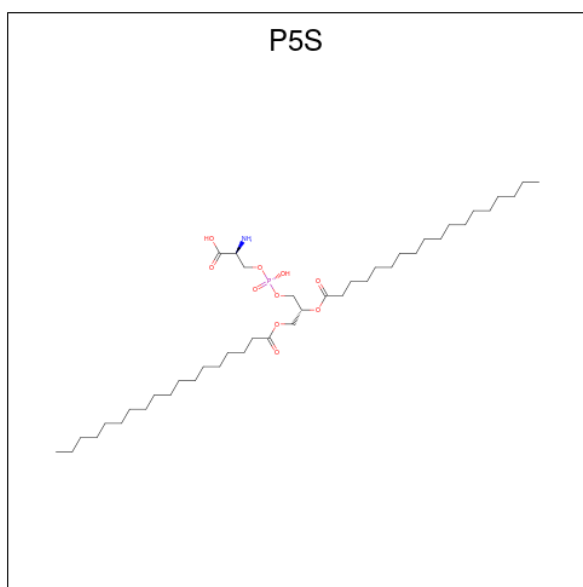
Mol	Chain	Residues	Atoms				AltConf
37	L	1	Total 48	C 39	O 8	P 1	0
37	L	1	Total 48	C 39	O 8	P 1	0
37	L	1	Total 48	C 39	O 8	P 1	0
37	M	1	Total 48	C 39	O 8	P 1	0
37	M	1	Total 48	C 39	O 8	P 1	0
37	M	1	Total 48	C 39	O 8	P 1	0
37	M	1	Total 48	C 39	O 8	P 1	0
37	N	1	Total 48	C 39	O 8	P 1	0
37	P	1	Total 48	C 39	O 8	P 1	0
37	a	1	Total 48	C 39	O 8	P 1	0
37	a	1	Total 48	C 39	O 8	P 1	0
37	a	1	Total 48	C 39	O 8	P 1	0
37	c	1	Total 48	C 39	O 8	P 1	0
37	d	1	Total 48	C 39	O 8	P 1	0
37	d	1	Total 48	C 39	O 8	P 1	0
37	d	1	Total 48	C 39	O 8	P 1	0
37	f	1	Total 48	C 39	O 8	P 1	0
37	f	1	Total 48	C 39	O 8	P 1	0
37	g	1	Total 48	C 39	O 8	P 1	0
37	g	1	Total 48	C 39	O 8	P 1	0
37	i	1	Total 48	C 39	O 8	P 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
37	i	1	Total	C	O	P	0
			48	39	8	1	
37	i	1	Total	C	O	P	0
			48	39	8	1	
37	i	1	Total	C	O	P	0
			48	39	8	1	
37	i	1	Total	C	O	P	0
			48	39	8	1	
37	j	1	Total	C	O	P	0
			48	39	8	1	
37	k	1	Total	C	O	P	0
			48	39	8	1	
37	k	1	Total	C	O	P	0
			48	39	8	1	
37	m	1	Total	C	O	P	0
			48	39	8	1	
37	m	1	Total	C	O	P	0
			48	39	8	1	
37	o	1	Total	C	O	P	0
			48	39	8	1	

- Molecule 38 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: C₄₂H₈₂NO₁₀P).



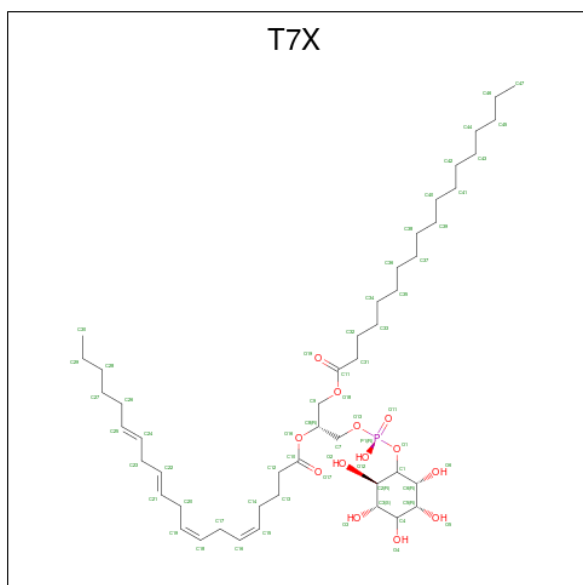
Mol	Chain	Residues	Atoms					AltConf
38	I	1	Total	C	N	O	P	0
			54	42	1	10	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
38	L	1	Total	C	N	O	P
			54	42	1	10	1
38	a	1	Total	C	N	O	P
			54	42	1	10	1

- Molecule 39 is Phosphatidylinositol (CCD ID: T7X) (formula: $C_{47}H_{83}O_{13}P$).

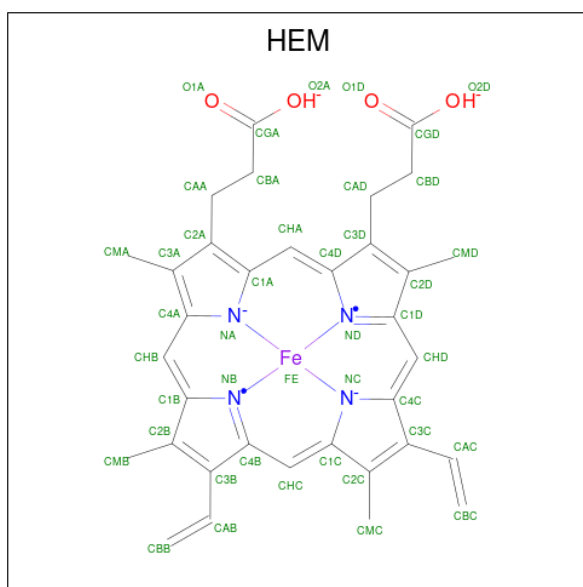


Mol	Chain	Residues	Atoms				AltConf
39	J	1	Total	C	O	P	0
			61	47	13	1	
39	g	1	Total	C	O	P	0
			61	47	13	1	

- Molecule 40 is ZINC ION (CCD ID: ZN) (formula: Zn).

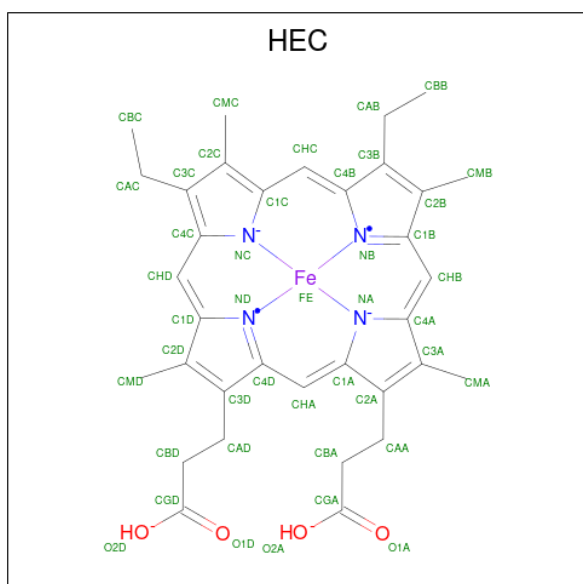
Mol	Chain	Residues	Atoms		AltConf
40	R	1	Total	Zn	0
			1	1	
40	i	1	Total	Zn	0
			1	1	
40	m	1	Total	Zn	0
			1	1	

- Molecule 41 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



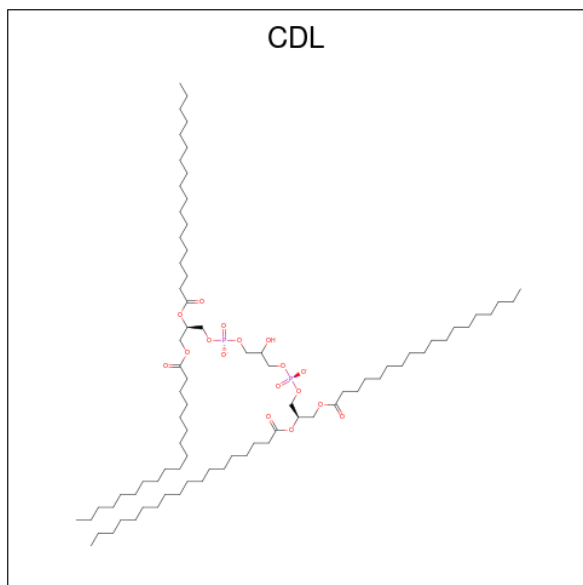
Mol	Chain	Residues	Atoms					AltConf
41	a	1	Total 43	C 34	Fe 1	N 4	O 4	0
41	a	1	Total 43	C 34	Fe 1	N 4	O 4	0
41	d	1	Total 43	C 34	Fe 1	N 4	O 4	0
41	d	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 42 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$) (labeled as "Ligand of Interest" by depositor).



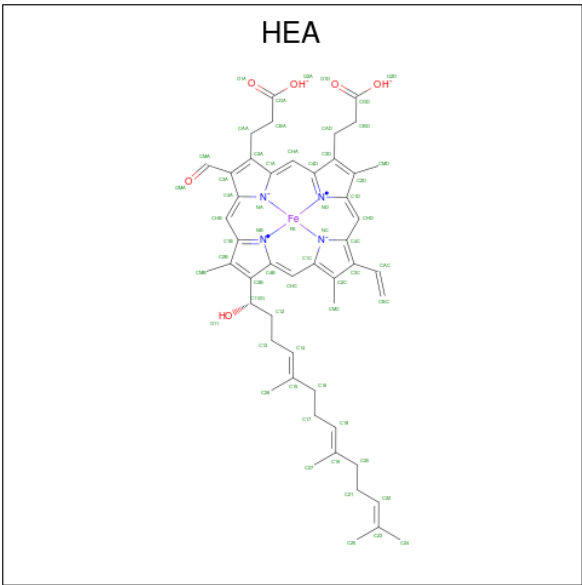
Mol	Chain	Residues	Atoms					AltConf
42	b	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
42	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 43 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
43	d	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 44 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
44	g	1	Total 60	C 49	Fe 1	N 4	O 6	0
44	g	1	Total 60	C 49	Fe 1	N 4	O 6	0
44	k	1	Total 60	C 49	Fe 1	N 4	O 6	0
44	k	1	Total 60	C 49	Fe 1	N 4	O 6	0

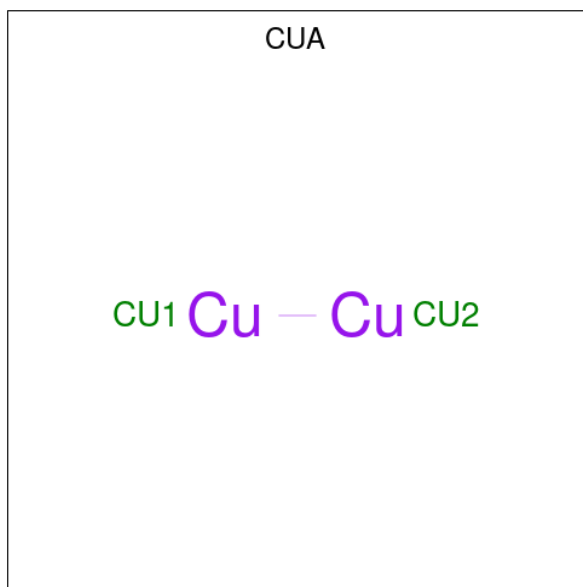
- Molecule 45 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- Molecule 46 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 47 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).

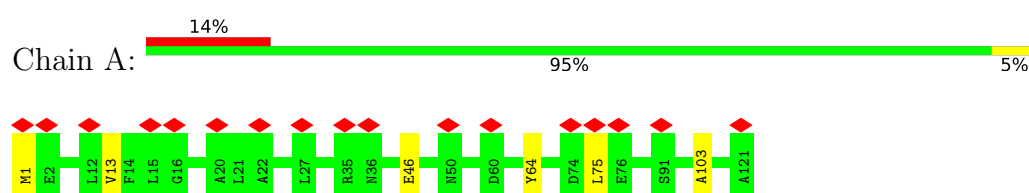


Mol	Chain	Residues	Atoms		AltConf
47	h	1	Total	Cu	0
			2	2	
47	l	1	Total	Cu	0
			2	2	

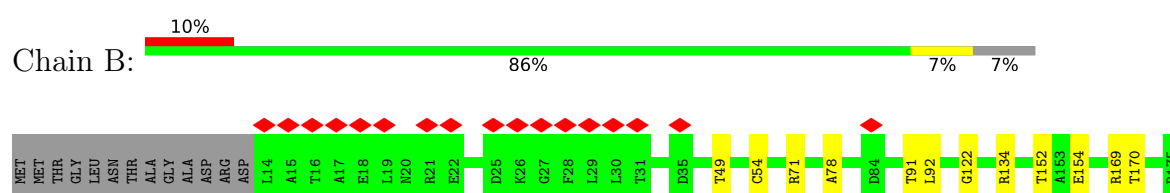
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

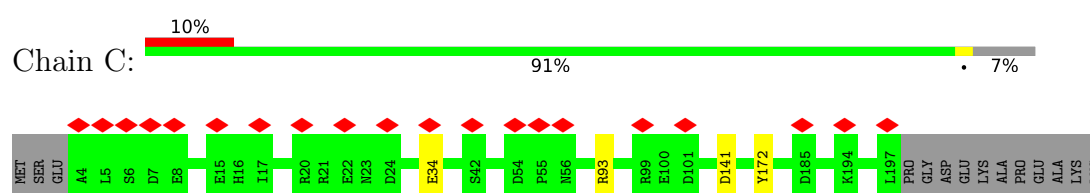
- Molecule 1: NADH-quinone oxidoreductase subunit A



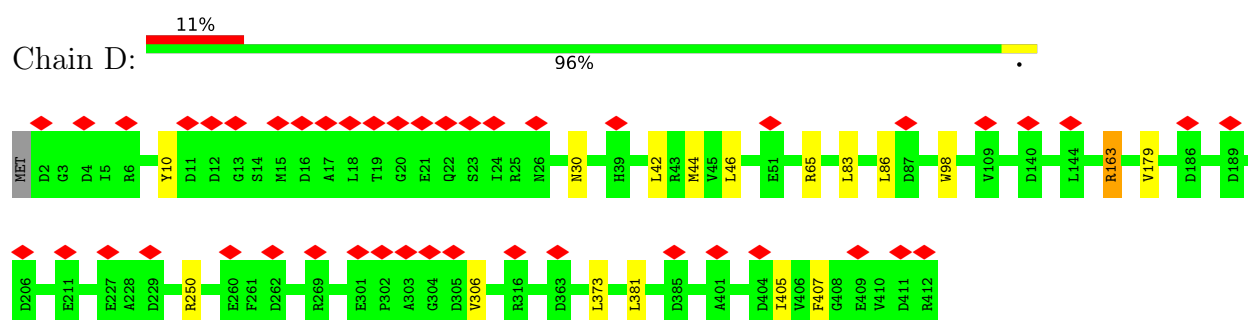
- Molecule 2: NADH-quinone oxidoreductase subunit B



- Molecule 3: NADH-quinone oxidoreductase subunit C

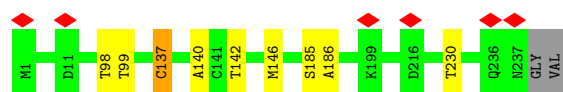


- Molecule 4: NADH-quinone oxidoreductase subunit D



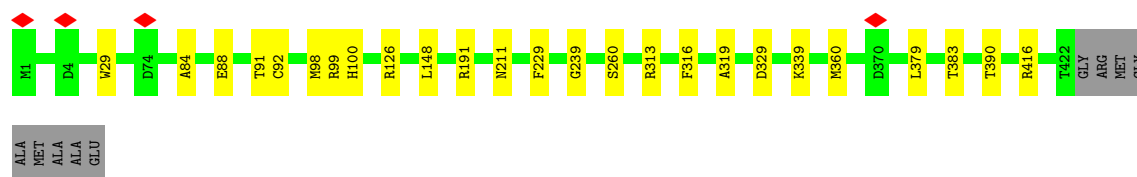
- Molecule 5: NADH dehydrogenase subunit E





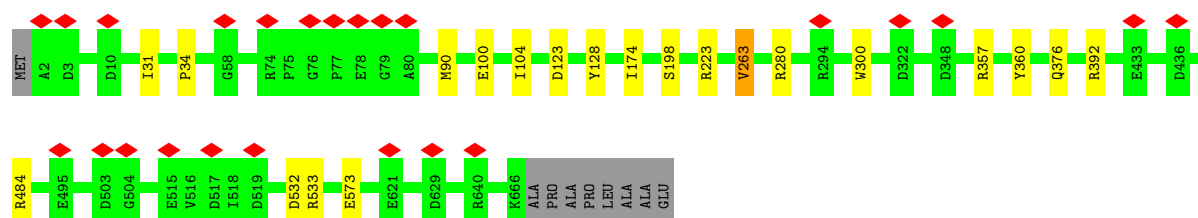
- Molecule 6: NADH-quinone oxidoreductase subunit F

Chain F: 92% 6%



- Molecule 7: NADH-quinone oxidoreductase

Chain G: 96%



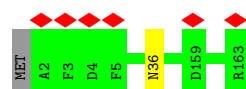
- Molecule 8: NADH-quinone oxidoreductase subunit H

Chain H: 8% 96%



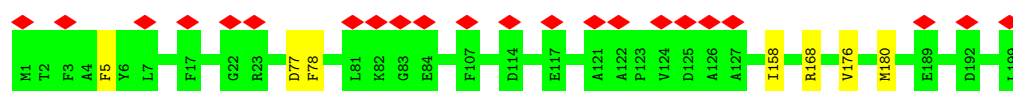
- Molecule 9: NADH-quinone oxidoreductase subunit I

Chain I: 99%

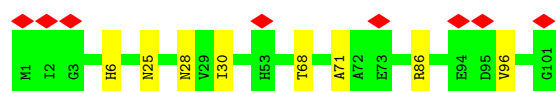


- Molecule 10: NADH-quinone oxidoreductase subunit J

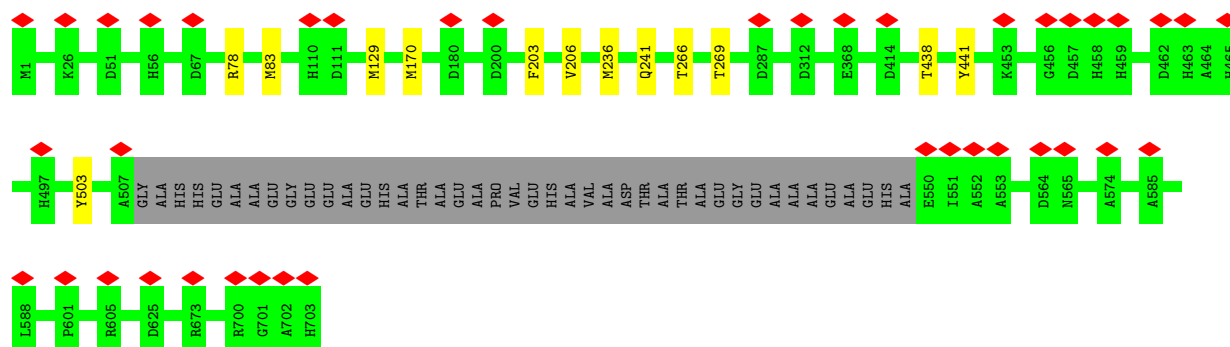
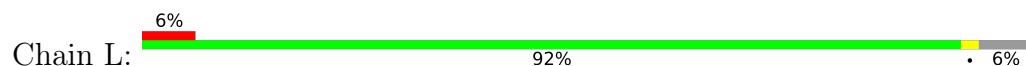
Chain J: 11% 96%



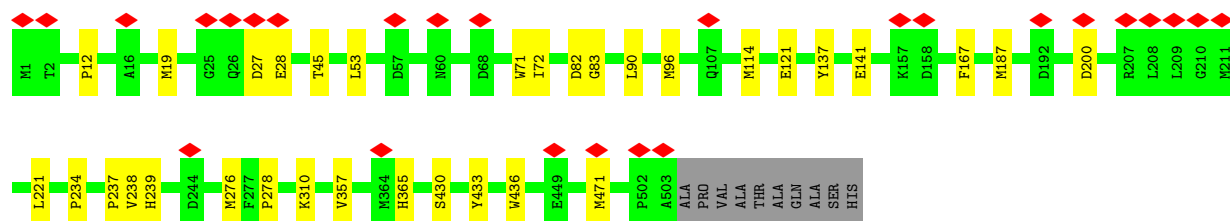
- Molecule 11: NADH-quinone oxidoreductase subunit K



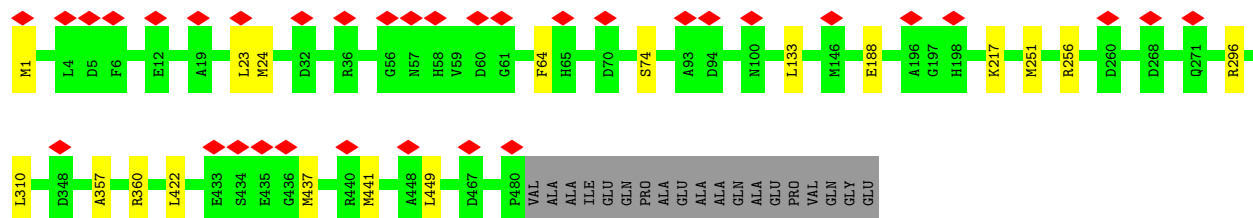
• Molecule 12: NADH dehydrogenase subunit L



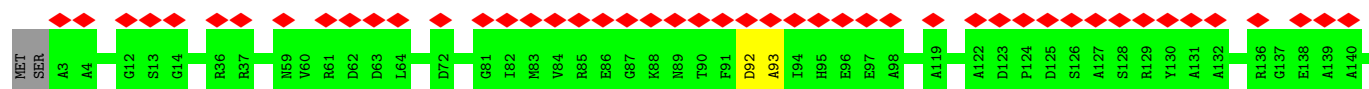
• Molecule 13: NADH dehydrogenase subunit M

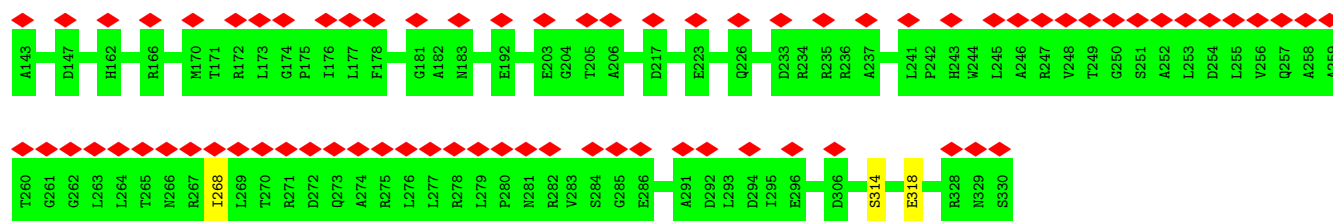


• Molecule 14: NADH-quinone oxidoreductase subunit N

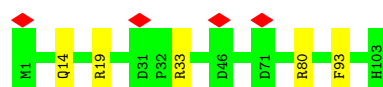


• Molecule 15: NAD-dependent epimerase/dehydratase

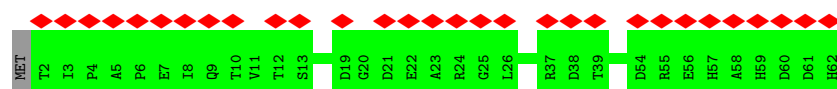




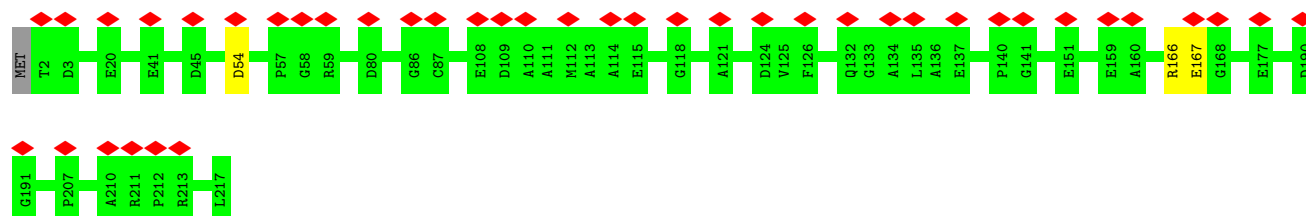
- Molecule 16: ETC complex I subunit conserved region



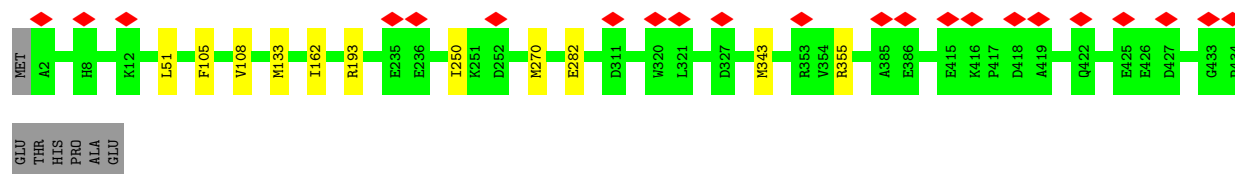
- Molecule 17: Zinc finger CHCC-type domain-containing protein



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

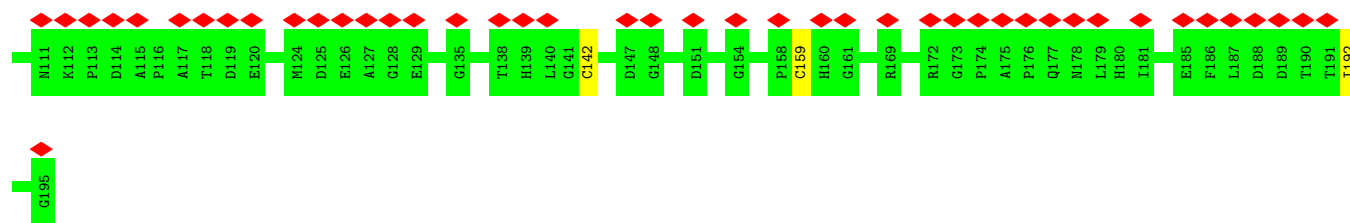


- Molecule 19: Cytochrome b



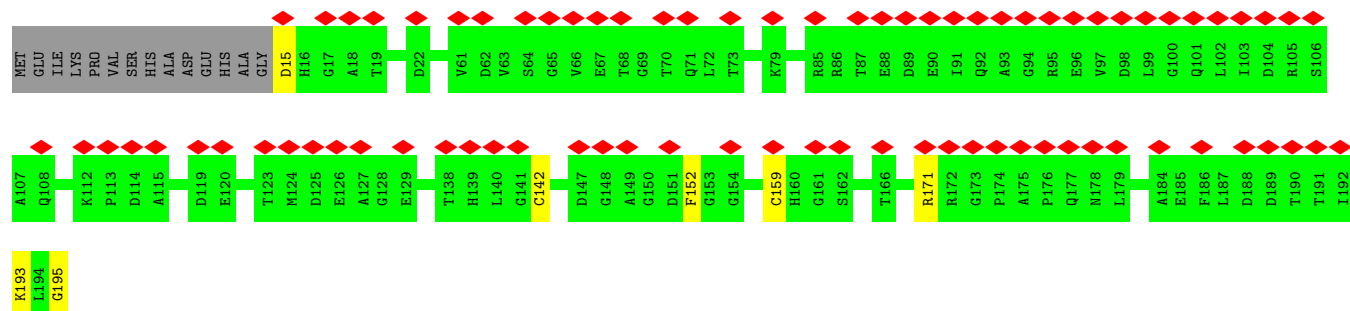
- Molecule 19: Cytochrome b





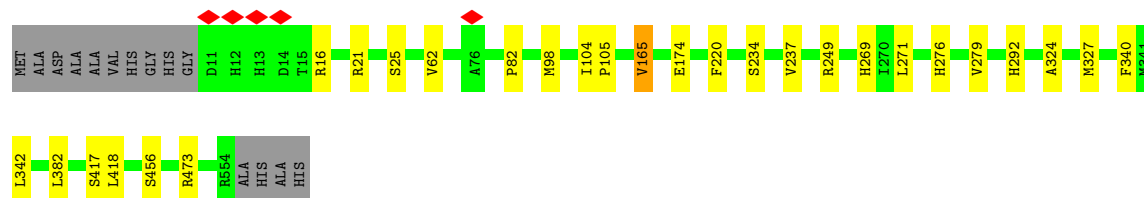
- Molecule 21: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain f: 41% 89% 7%



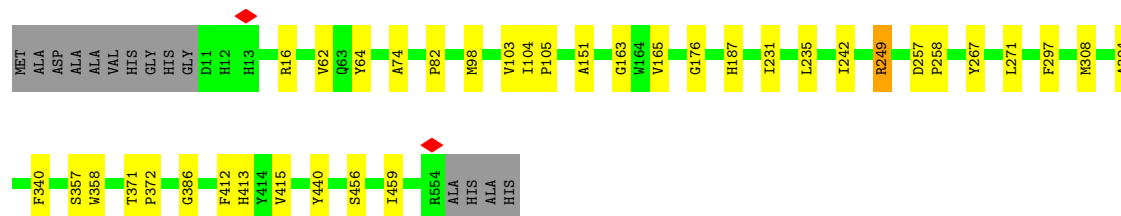
- Molecule 22: Cytochrome c oxidase subunit 1

Chain g: 92% 5%



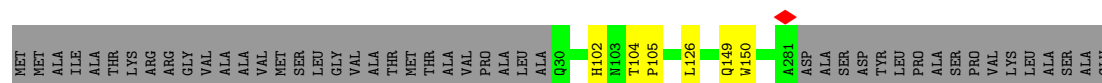
- Molecule 22: Cytochrome c oxidase subunit 1

Chain k: 91% 6%



- Molecule 23: Cytochrome c oxidase subunit 2

Chain h: 83% 15%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99946	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
Maximum map value	52.125	Depositor
Minimum map value	-28.966	Depositor
Average map value	0.036	Depositor
Map value standard deviation	1.388	Depositor
Recommended contour level	5.34	Depositor
Map size ($\text{\AA}$)	393.0, 393.0, 393.0	wwPDB
Map dimensions	375, 375, 375	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.048, 1.048, 1.048	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEA, CUA, P5S, DU0, FME, MN, CA, 3PE, ZN, HEM, CU, 2MR, FES, PC1, U10, HEC, CDL, PGT, SF4, 3PH, FMN, T7X

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	0.23	0/988	0.50	0/1345
2	B	0.31	0/1297	0.57	0/1758
3	C	0.26	0/1624	0.56	0/2208
4	D	0.28	0/3339	0.55	0/4520
5	E	0.21	0/1865	0.51	0/2537
6	F	0.21	0/3308	0.52	0/4456
7	G	0.24	0/5156	0.53	0/6982
8	H	0.25	0/2815	0.54	0/3837
9	I	0.30	0/1354	0.57	0/1828
10	J	0.24	0/1548	0.56	0/2104
11	K	0.25	0/775	0.50	0/1050
12	L	0.21	0/5379	0.51	0/7323
13	M	0.23	0/4010	0.53	0/5460
14	N	0.24	0/3634	0.54	0/4935
15	P	0.22	0/2511	0.55	0/3409
16	Q	0.23	0/872	0.51	0/1181
17	R	0.20	0/503	0.50	0/685
18	Z	0.22	0/1669	0.57	0/2266
19	a	0.26	0/3641	0.52	0/4993
19	d	0.24	0/3650	0.51	0/5005
20	b	0.21	0/1906	0.47	0/2592
20	e	0.20	0/1906	0.53	0/2592
21	c	0.17	0/1382	0.44	0/1880
21	f	0.18	0/1390	0.46	0/1891
22	g	0.23	0/4483	0.54	0/6118
22	k	0.20	0/4483	0.53	0/6118
23	h	0.19	0/2033	0.51	0/2787
23	l	0.18	0/2033	0.51	0/2787
24	i	0.22	0/2270	0.49	0/3107
24	m	0.19	0/2270	0.49	0/3107
25	j	0.16	0/339	0.43	0/457

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
25	n	0.20	0/339	0.49	0/457
26	o	0.17	0/330	0.45	0/448
26	p	0.22	0/336	0.52	0/456
27	q	0.22	0/1049	0.51	0/1434
All	All	0.23	0/76487	0.52	0/104113

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
4	D	0	2
7	G	0	3
14	N	0	2
16	Q	0	3
19	a	0	1
22	g	0	1
22	k	0	1
All	All	0	14

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	134	ARG	Sidechain
4	D	163	ARG	Sidechain
4	D	250	ARG	Sidechain
7	G	223	ARG	Sidechain
7	G	280	ARG	Sidechain
7	G	484	ARG	Sidechain
14	N	296	ARG	Sidechain
14	N	360	ARG	Sidechain
16	Q	19	ARG	Sidechain
16	Q	33	ARG	Sidechain
16	Q	80	ARG	Sidechain
19	a	355	ARG	Sidechain
22	g	473	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
22	k	249	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	969	0	970	6	0
2	B	1270	0	1268	4	0
3	C	1586	0	1562	2	0
4	D	3277	0	3217	9	0
5	E	1822	0	1796	6	0
6	F	3241	0	3188	16	0
7	G	5068	0	5037	8	0
8	H	2722	0	2744	7	0
9	I	1319	0	1259	2	0
10	J	1528	0	1612	6	0
11	K	764	0	817	5	0
12	L	5215	0	5174	7	0
13	M	3915	0	4024	20	0
14	N	3556	0	3656	9	0
15	P	2468	0	2498	3	0
16	Q	849	0	812	2	0
17	R	488	0	450	0	0
18	Z	1642	0	1643	2	0
19	a	3504	0	3483	8	0
19	d	3513	0	3489	11	0
20	b	1855	0	1773	3	0
20	e	1855	0	1773	3	0
21	c	1353	0	1297	6	0
21	f	1361	0	1301	4	0
22	g	4322	0	4225	16	0
22	k	4322	0	4225	23	0
23	h	1976	0	1960	3	0
23	l	1976	0	1960	3	0
24	i	2183	0	2144	7	0
24	m	2183	0	2144	9	0
25	j	332	0	331	1	0
25	n	332	0	331	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	o	324	0	330	0	0
26	p	330	0	335	2	0
27	q	1018	0	942	0	0
28	A	51	0	82	1	0
28	H	204	0	328	0	0
28	L	204	0	328	0	0
28	P	51	0	82	1	0
28	a	204	0	328	0	0
28	c	51	0	82	0	0
28	d	153	0	246	0	0
28	e	102	0	164	0	0
28	g	153	0	246	0	0
28	h	102	0	164	0	0
28	i	255	0	410	0	0
28	k	51	0	82	0	0
28	m	306	0	492	2	0
28	n	51	0	82	0	0
28	p	51	0	82	0	0
29	A	51	0	78	0	0
29	H	51	0	78	1	0
29	J	102	0	156	1	0
29	K	51	0	78	0	0
29	L	51	0	78	0	0
29	M	51	0	78	0	0
29	N	51	0	78	0	0
29	P	51	0	78	0	0
29	a	51	0	78	0	0
29	g	51	0	78	0	0
29	q	51	0	78	0	0
30	A	37	0	0	0	0
30	H	37	0	0	0	0
30	J	74	0	0	0	0
30	M	74	0	0	0	0
30	a	37	0	0	0	0
30	c	74	0	0	2	0
30	d	111	0	0	0	0
30	e	37	0	0	0	0
30	f	37	0	0	0	0
30	g	148	0	0	0	0
30	h	111	0	0	0	0
30	i	148	0	0	0	0
30	j	37	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	k	37	0	0	0	0
30	m	74	0	0	0	0
31	B	8	0	0	0	0
31	F	8	0	0	1	0
31	G	16	0	0	0	0
31	I	16	0	0	0	0
32	B	63	0	90	3	0
32	a	126	0	180	4	0
32	d	126	0	180	10	0
33	D	54	0	88	2	0
33	H	108	0	176	2	0
33	L	54	0	88	0	0
33	M	162	0	264	0	0
33	N	162	0	264	0	0
33	a	162	0	264	0	0
33	b	108	0	176	1	0
33	c	54	0	88	0	0
33	d	108	0	176	0	0
33	f	54	0	88	0	0
33	g	54	0	88	0	0
33	h	54	0	88	0	0
33	i	162	0	264	1	0
33	j	54	0	88	0	0
33	k	108	0	176	1	0
33	l	162	0	264	1	0
33	m	216	0	352	4	0
33	n	54	0	88	0	0
34	D	1	0	0	0	0
34	b	1	0	0	0	0
34	e	1	0	0	0	0
34	g	1	0	0	0	0
34	k	1	0	0	0	0
35	E	4	0	0	0	0
35	G	4	0	0	0	0
35	c	4	0	0	0	0
35	f	4	0	0	0	0
36	F	31	0	19	1	0
37	H	48	0	75	0	0
37	L	192	0	300	2	0
37	M	192	0	300	2	0
37	N	48	0	75	0	0
37	P	48	0	75	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	a	144	0	225	0	0
37	c	48	0	75	0	0
37	d	144	0	225	0	0
37	f	96	0	150	1	0
37	g	96	0	150	0	0
37	i	240	0	375	1	0
37	j	48	0	75	0	0
37	k	96	0	150	0	0
37	m	96	0	150	0	0
37	o	48	0	75	0	0
38	I	54	0	80	0	0
38	L	54	0	80	0	0
38	a	54	0	80	0	0
39	J	61	0	0	0	0
39	g	61	0	0	0	0
40	R	1	0	0	0	0
40	i	1	0	0	0	0
40	m	1	0	0	0	0
41	a	86	0	60	0	0
41	d	86	0	60	0	0
42	b	43	0	30	1	0
42	e	43	0	30	2	0
43	d	100	0	156	0	0
44	g	120	0	108	3	0
44	k	120	0	108	6	0
45	g	1	0	0	0	0
45	k	1	0	0	0	0
46	g	1	0	0	0	0
46	k	1	0	0	0	0
47	h	2	0	0	0	0
47	l	2	0	0	0	0
All	All	82894	0	84720	214	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 1.

All (214) 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	1.58	0.84
19:d:144:PHE:HB2	32:d:506:U10:H1M3	1.70	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:k:308:MET:HE3	22:k:357:SER:HB2	1.73	0.70
5:E:98:THR:HG22	5:E:99:THR:H	1.56	0.69
4:D:42:LEU:HB2	4:D:407:PHE:CZ	2.33	0.64
22:g:98:MET:HB3	44:g:606:HEA:CAC	2.27	0.64
14:N:251:MET:HE1	14:N:310:LEU:HD23	1.79	0.64
22:k:98:MET:HB3	44:k:604:HEA:CAC	2.28	0.64
32:d:506:U10:H102	32:d:506:U10:H1M1	1.80	0.63
32:a:512:U10:H222	32:d:504:U10:H503	1.82	0.62
22:k:231:ILE:HG23	22:k:235:LEU:HD12	1.83	0.59
12:L:438:THR:HA	12:L:441:TYR:CE2	2.37	0.59
1:A:103:ALA:HB1	28:A:201:3PE:H2C1	1.84	0.59
8:H:168:ILE:HD11	8:H:262:PHE:CE1	2.38	0.58
19:d:162:ILE:HG13	32:d:506:U10:H3M3	1.86	0.58
4:D:86:LEU:HD11	4:D:373:LEU:HD13	1.85	0.57
13:M:53:LEU:HD21	37:M:604:3PH:H222	1.87	0.57
13:M:234:PRO:HB2	13:M:239:HIS:HA	1.86	0.57
23:h:149:GLN:HG2	23:h:150:TRP:CE2	2.40	0.57
22:k:16:ARG:HG3	22:k:16:ARG:HH11	1.69	0.56
1:A:75:LEU:HD13	11:K:68:THR:HA	1.87	0.56
21:c:16:HIS:CG	21:c:17:GLY:H	2.23	0.56
13:M:96:MET:HE3	13:M:121:GLU:HB2	1.87	0.56
4:D:163:ARG:HG2	4:D:163:ARG:HH11	1.70	0.56
22:g:16:ARG:HH11	22:g:16:ARG:HG3	1.71	0.55
24:m:210:PHE:O	24:m:214:THR:HG22	2.06	0.55
22:g:418:LEU:HD21	22:g:456:SER:HB3	1.89	0.54
19:a:105:PHE:HA	19:a:108:VAL:HG22	1.91	0.53
33:D:1001:PC1:H153	29:J:201:PGT:H322	1.91	0.53
32:d:506:U10:H101	32:d:506:U10:H153	1.90	0.53
19:d:108:VAL:HG21	19:d:139:MET:HE1	1.90	0.53
19:d:162:ILE:CG1	32:d:506:U10:H3M3	2.39	0.52
14:N:1:MET:HG2	14:N:64:PHE:CE2	2.45	0.52
37:L:811:3PH:H252	24:i:50:TRP:CE3	2.45	0.52
5:E:230:THR:O	5:E:230:THR:HG22	2.10	0.52
6:F:329:ASP:OD1	6:F:416:ARG:NH2	2.41	0.52
14:N:441:MET:HE1	14:N:449:LEU:HD22	1.92	0.51
29:H:406:PGT:H42	29:H:406:PGT:H31	1.92	0.51
22:g:62:VAL:HG21	22:g:82:PRO:HB3	1.93	0.51
20:b:218:ILE:HD11	20:b:220:PHE:CZ	2.46	0.51
22:k:62:VAL:HG21	22:k:82:PRO:HB3	1.92	0.51
22:k:64:TYR:CE1	22:k:74:ALA:HB2	2.46	0.51
24:m:244:GLN:CD	33:m:311:PC1:H132	2.36	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:211:ASN:ND2	36:F:502:FMN:O2	2.38	0.51
7:G:100:GLU:O	7:G:104:ILE:HG23	2.11	0.50
12:L:129:MET:HB2	12:L:266:THR:HG23	1.92	0.50
14:N:74:SER:OG	14:N:256:ARG:NH2	2.44	0.50
21:f:15:ASP:N	24:m:165:HIS:HD1	2.09	0.50
6:F:84:ALA:HB1	6:F:98:MET:SD	2.52	0.50
14:N:357:ALA:HB1	14:N:437:MET:HG3	1.94	0.50
24:i:64:PHE:CZ	37:i:301:3PH:H241	2.47	0.50
22:k:456:SER:HA	22:k:459:ILE:HD12	1.94	0.50
19:d:91:TYR:CE2	19:d:92:MET:HG2	2.47	0.49
22:g:276:HIS:O	22:g:279:VAL:HG22	2.12	0.49
8:H:94:LEU:HD13	8:H:126:LEU:HB3	1.94	0.49
21:c:48:ASN:HD21	30:c:205:DU0:C19	2.25	0.49
22:k:176:GLY:O	22:k:249:ARG:NH2	2.45	0.49
8:H:196:LEU:HB3	8:H:197:PRO:HD3	1.95	0.49
32:a:511:U10:H553	32:d:506:U10:H103	1.95	0.49
19:d:144:PHE:HB2	32:d:506:U10:C1M	2.41	0.49
22:k:308:MET:HE1	22:k:358:TRP:CD1	2.48	0.49
6:F:229:PHE:CZ	6:F:239:GLY:HA3	2.48	0.49
22:g:220:PHE:HB2	22:g:292:HIS:CD2	2.48	0.48
24:m:245:HIS:CD2	24:m:249:GLU:OE1	2.66	0.48
7:G:263:VAL:O	7:G:392:ARG:NH1	2.45	0.48
14:N:24:MET:HE2	14:N:24:MET:HA	1.94	0.48
42:e:504:HEC:HMC1	42:e:504:HEC:HBC3	1.96	0.48
7:G:174:ILE:HG21	7:G:198:SER:HB2	1.95	0.48
3:C:34:GLU:OE2	3:C:93:ARG:NH2	2.43	0.48
19:d:133:MET:HE1	19:d:343:MET:HE3	1.96	0.48
19:d:380:VAL:HG11	19:d:393:ALA:HB2	1.96	0.47
22:k:267:TYR:CE2	22:k:271:LEU:HD22	2.48	0.47
6:F:329:ASP:CG	6:F:416:ARG:HH22	2.22	0.47
12:L:236:MET:HG3	12:L:241:GLN:HB2	1.95	0.47
3:C:141:ASP:OD2	3:C:172:TYR:OH	2.31	0.47
1:A:46:GLU:HG3	4:D:30:ASN:HD22	1.80	0.47
11:K:28:ASN:OD1	11:K:30:ILE:HG22	2.15	0.47
23:h:104:THR:N	23:h:105:PRO:HD2	2.30	0.47
13:M:53:LEU:HD22	13:M:90:LEU:CD2	2.45	0.46
37:P:402:3PH:H31	28:P:403:3PE:H11	1.97	0.46
33:H:402:PC1:H133	9:I:36:ASN:HB2	1.97	0.46
10:J:176:VAL:HG12	10:J:180:MET:HE2	1.97	0.46
2:B:169:ARG:HG3	2:B:170:THR:HG23	1.97	0.46
4:D:44:MET:HE2	4:D:46:LEU:HD21	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:137:CYS:O	6:F:126:ARG:NH2	2.44	0.46
6:F:88:GLU:O	6:F:91:THR:OG1	2.32	0.46
19:a:162:ILE:HD11	32:a:512:U10:C5	2.46	0.46
22:g:165:VAL:HB	22:g:271:LEU:HD21	1.98	0.46
22:g:382:LEU:HD13	22:g:418:LEU:HB3	1.98	0.46
32:B:1002:U10:H4M3	8:H:38:ARG:HD2	1.97	0.46
22:k:151:ALA:HA	28:m:310:3PE:H11	1.98	0.46
20:e:285:GLU:CD	20:e:285:GLU:H	2.24	0.46
22:g:21:ARG:O	22:g:25:SER:HB3	2.15	0.46
24:i:82:VAL:HG22	25:j:17:ILE:HG22	1.98	0.46
24:m:239:GLN:O	33:m:311:PC1:H121	2.15	0.46
21:f:142:CYS:HG	21:f:159:CYS:HG	1.62	0.46
24:i:214:THR:HG23	24:i:269:ILE:HD11	1.96	0.46
12:L:83:MET:HE1	12:L:269:THR:HG21	1.98	0.46
22:k:297:PHE:CE2	22:k:372:PRO:HB2	2.50	0.46
22:k:103:VAL:HG21	44:k:604:HEA:HBC2	1.96	0.45
13:M:82:ASP:OD1	13:M:83:GLY:N	2.48	0.45
13:M:12:PRO:HG3	13:M:45:THR:HG21	1.97	0.45
42:e:504:HEC:HBB3	42:e:504:HEC:HMB3	1.98	0.45
6:F:313:ARG:HG2	6:F:313:ARG:HH11	1.82	0.45
10:J:5:PHE:CZ	11:K:6:HIS:HB3	2.52	0.45
13:M:200:ASP:OD1	13:M:200:ASP:N	2.49	0.45
22:k:187:HIS:NE2	22:k:242:ILE:HG13	2.31	0.45
1:A:13:VAL:HG21	8:H:15:MET:SD	2.57	0.45
32:B:1002:U10:H1M3	32:B:1002:U10:C8	2.47	0.45
33:D:1001:PC1:H133	10:J:180:MET:HE1	1.97	0.45
7:G:357:ARG:HA	7:G:360:TYR:CE2	2.52	0.45
18:Z:54:ASP:N	18:Z:54:ASP:OD1	2.50	0.45
19:a:270:MET:O	19:a:270:MET:HG2	2.16	0.45
20:b:408:GLU:OE2	20:b:414:ARG:NH1	2.39	0.45
19:a:133:MET:HE1	19:a:343:MET:HE3	1.99	0.45
23:l:173:LEU:HD11	23:l:183:TYR:HA	1.99	0.45
12:L:78:ARG:HD3	12:L:503:TYR:CE2	2.52	0.44
13:M:167:PHE:CD1	14:N:422:LEU:HD11	2.52	0.44
24:i:115:TYR:CD1	33:i:313:PC1:H153	2.52	0.44
22:k:98:MET:HB3	44:k:604:HEA:HAC	1.98	0.44
13:M:237:PRO:C	13:M:239:HIS:H	2.24	0.44
42:b:502:HEC:HMC1	42:b:502:HEC:HBC3	1.98	0.44
20:e:218:ILE:HD11	20:e:220:PHE:CZ	2.52	0.44
6:F:316:PHE:CZ	6:F:319:ALA:HB2	2.52	0.44
2:B:71:ARG:HA	8:H:50:PRO:HA	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:185:SER:OG	5:E:186:ALA:N	2.50	0.44
10:J:158:ILE:HD11	14:N:23:LEU:HD11	1.98	0.44
13:M:27:ASP:OD1	13:M:28:GLU:N	2.51	0.44
22:g:174:GLU:O	22:g:249:ARG:NH2	2.50	0.44
12:L:170:MET:HE1	13:M:436:TRP:HB2	1.99	0.44
37:L:811:3PH:H222	24:i:50:TRP:CD1	2.53	0.44
13:M:53:LEU:HD22	13:M:90:LEU:HD22	2.00	0.44
15:P:92:ASP:OD1	15:P:93:ALA:N	2.51	0.44
33:k:609:PC1:H31	33:k:609:PC1:H121	1.99	0.44
7:G:123:ASP:OD2	16:Q:14:GLN:NE2	2.48	0.43
21:c:16:HIS:CG	21:c:17:GLY:N	2.82	0.43
19:d:154:MET:HG2	19:d:278:ASP:HB2	2.01	0.43
44:g:606:HEA:OMA	44:g:606:HEA:HHB	2.18	0.43
7:G:532:ASP:CG	7:G:533:ARG:H	2.27	0.43
33:b:501:PC1:H32	33:b:501:PC1:H121	2.00	0.43
22:g:342:LEU:HD11	23:h:126:LEU:HD11	2.00	0.43
24:m:88:GLN:HA	24:m:91:PHE:CE2	2.54	0.43
26:p:2:PHE:CG	26:p:3:ASP:N	2.86	0.43
13:M:276:MET:C	13:M:278:PRO:HD3	2.44	0.43
18:Z:166:ARG:HD2	18:Z:167:GLU:O	2.18	0.43
19:a:193:ARG:HG3	19:a:193:ARG:HH11	1.84	0.43
7:G:34:PRO:HG3	7:G:128:TYR:CE2	2.54	0.43
32:B:1002:U10:H202	8:H:27:MET:HE3	2.00	0.43
21:c:63:VAL:HG11	21:c:192:ILE:HD12	2.00	0.43
22:g:104:ILE:HB	22:g:105:PRO:HD3	2.00	0.43
13:M:19:MET:HE1	13:M:114:MET:HB2	1.99	0.43
13:M:310:LYS:HG3	13:M:357:VAL:HG11	2.00	0.43
19:a:51:LEU:HD21	19:a:108:VAL:HG13	2.01	0.43
24:m:234:ARG:NH2	33:m:311:PC1:O12	2.52	0.43
22:k:257:ASP:HA	22:k:258:PRO:HD3	1.90	0.43
1:A:64:TYR:OH	11:K:86:ARG:NH2	2.52	0.43
4:D:83:LEU:HG	4:D:98:TRP:HB2	2.01	0.43
22:g:269:HIS:CD2	22:g:327:MET:HE1	2.53	0.43
26:p:52:ILE:N	26:p:52:ILE:HD12	2.34	0.43
22:k:103:VAL:HG21	44:k:604:HEA:CBC	2.48	0.42
24:i:60:LEU:HD23	24:i:63:MET:HE2	2.00	0.42
4:D:179:VAL:HG22	4:D:306:VAL:CG1	2.50	0.42
10:J:77:ASP:OD1	10:J:78:PHE:N	2.52	0.42
6:F:191:ARG:HD2	16:Q:93:PHE:CZ	2.54	0.42
6:F:379:LEU:O	6:F:383:THR:HG23	2.18	0.42
13:M:71:TRP:CG	13:M:72:ILE:H	2.37	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:268:ILE:HD12	15:P:268:ILE:H	1.85	0.42
22:g:417:SER:O	22:g:418:LEU:HD23	2.19	0.42
4:D:10:TYR:HA	10:J:168:ARG:HA	2.01	0.42
22:g:234:SER:O	22:g:237:VAL:HG22	2.20	0.42
44:k:605:HEA:OMA	44:k:605:HEA:HHB	2.19	0.42
23:l:33:LEU:HD22	23:l:263:VAL:HG11	2.02	0.42
5:E:140:ALA:HB3	5:E:146:MET:SD	2.59	0.42
12:L:203:PHE:HA	12:L:206:VAL:HG23	2.01	0.42
19:d:294:PRO:HG3	32:d:506:U10:H3M1	2.00	0.42
19:d:302:TYR:HA	32:d:506:U10:H4M1	2.01	0.42
6:F:29:TRP:CE2	6:F:148:LEU:HD13	2.54	0.42
20:e:388:THR:HG23	20:e:389:PRO:HD2	2.02	0.42
6:F:339:LYS:HA	6:F:360:MET:HG3	2.02	0.42
13:M:430:SER:HA	13:M:433:TYR:CE2	2.54	0.42
22:g:324:ALA:HB3	22:g:340:PHE:CG	2.54	0.42
6:F:390:THR:HB	31:F:501:SF4:S4	2.60	0.41
14:N:133:LEU:HD21	14:N:217:LYS:HE3	2.01	0.41
24:m:240:MET:HA	33:m:311:PC1:H142	2.02	0.41
2:B:49:THR:HG22	2:B:78:ALA:HA	2.02	0.41
13:M:53:LEU:HD21	37:M:604:3PH:C22	2.50	0.41
22:k:371:THR:HB	22:k:440:TYR:OH	2.20	0.41
33:l:304:PC1:O12	33:l:304:PC1:H32	2.20	0.41
20:b:320:PHE:CE2	20:b:333:ASN:HB3	2.55	0.41
22:k:412:PHE:CE1	22:k:413:HIS:CE1	3.08	0.41
33:H:402:PC1:H152	9:I:36:ASN:HB2	2.03	0.41
19:a:250:ILE:HD11	30:c:202:DU0:C78	2.50	0.41
4:D:381:LEU:HD13	4:D:405:ILE:HD13	2.02	0.41
22:k:324:ALA:HB3	22:k:340:PHE:CG	2.55	0.41
22:k:386:GLY:HA3	22:k:415:VAL:HG13	2.03	0.41
44:k:604:HEA:HHB	44:k:604:HEA:OMA	2.21	0.41
21:c:88:GLU:O	21:c:92:GLN:NE2	2.53	0.41
5:E:142:THR:HG23	6:F:92:CYS:SG	2.61	0.41
37:f:205:3PH:O13	28:m:315:3PE:N	2.50	0.41
23:l:146:ILE:HD11	23:l:206:THR:HG23	2.02	0.41
24:m:10:GLN:HG3	24:m:78:GLU:HG3	2.03	0.41
19:a:162:ILE:HD11	32:a:512:U10:C4	2.51	0.41
6:F:99:ARG:HG3	6:F:100:HIS:CD2	2.56	0.40
7:G:300:TRP:HE1	7:G:573:GLU:HB3	1.86	0.40
13:M:137:TYR:CE2	13:M:141:GLU:HG3	2.56	0.40
22:k:104:ILE:HB	22:k:105:PRO:HD3	2.02	0.40
15:P:314:SER:HB3	15:P:318:GLU:HG2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:c:142:CYS:HG	21:c:159:CYS:HG	1.68	0.40
21:f:152:PHE:CD2	21:f:171:ARG:HB2	2.56	0.40
21:f:193:LYS:NZ	21:f:195:GLY:O	2.50	0.40
44:g:610:HEA:OMA	44:g:610:HEA:HHB	2.20	0.40
2:B:152:THR:HG22	2:B:154:GLU:H	1.85	0.40
13:M:187:MET:HE1	13:M:221:LEU:HD11	2.03	0.40
22:k:163:GLY:C	22:k:165:VAL:H	2.29	0.40

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%)	115 (97%)	4 (3%)	0	100	100
2	B	160/175 (91%)	153 (96%)	6 (4%)	1 (1%)	21	56
3	C	192/208 (92%)	188 (98%)	4 (2%)	0	100	100
4	D	408/412 (99%)	397 (97%)	11 (3%)	0	100	100
5	E	235/239 (98%)	225 (96%)	9 (4%)	1 (0%)	30	65
6	F	420/431 (97%)	404 (96%)	16 (4%)	0	100	100
7	G	663/674 (98%)	639 (96%)	23 (4%)	1 (0%)	43	76
8	H	339/345 (98%)	330 (97%)	9 (3%)	0	100	100
9	I	160/163 (98%)	157 (98%)	3 (2%)	0	100	100
10	J	197/199 (99%)	192 (98%)	5 (2%)	0	100	100
11	K	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	12	45
12	L	657/703 (94%)	626 (95%)	31 (5%)	0	100	100
13	M	501/513 (98%)	493 (98%)	7 (1%)	1 (0%)	43	76
14	N	478/499 (96%)	468 (98%)	10 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	P	326/330 (99%)	318 (98%)	8 (2%)	0	100	100
16	Q	101/103 (98%)	101 (100%)	0	0	100	100
17	R	59/62 (95%)	54 (92%)	5 (8%)	0	100	100
18	Z	214/217 (99%)	208 (97%)	6 (3%)	0	100	100
19	a	431/440 (98%)	424 (98%)	7 (2%)	0	100	100
19	d	432/440 (98%)	422 (98%)	10 (2%)	0	100	100
20	b	237/450 (53%)	235 (99%)	1 (0%)	1 (0%)	30	65
20	e	237/450 (53%)	231 (98%)	6 (2%)	0	100	100
21	c	178/195 (91%)	172 (97%)	6 (3%)	0	100	100
21	f	179/195 (92%)	175 (98%)	4 (2%)	0	100	100
22	g	542/558 (97%)	528 (97%)	14 (3%)	0	100	100
22	k	542/558 (97%)	526 (97%)	16 (3%)	0	100	100
23	h	250/298 (84%)	240 (96%)	10 (4%)	0	100	100
23	l	250/298 (84%)	239 (96%)	11 (4%)	0	100	100
24	i	271/274 (99%)	262 (97%)	9 (3%)	0	100	100
24	m	271/274 (99%)	259 (96%)	12 (4%)	0	100	100
25	j	41/66 (62%)	39 (95%)	2 (5%)	0	100	100
25	n	41/66 (62%)	40 (98%)	1 (2%)	0	100	100
26	o	40/176 (23%)	38 (95%)	2 (5%)	0	100	100
26	p	41/176 (23%)	41 (100%)	0	0	100	100
27	q	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
All	All	9432/10533 (90%)	9151 (97%)	275 (3%)	6 (0%)	49	80

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	137	CYS
13	M	238	VAL
20	b	369	ASN
7	G	263	VAL
2	B	122	GLY
11	K	96	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	97/97 (100%)	97 (100%)	0	100	100
2	B	136/145 (94%)	133 (98%)	3 (2%)	45	74
3	C	172/183 (94%)	172 (100%)	0	100	100
4	D	341/342 (100%)	341 (100%)	0	100	100
5	E	189/190 (100%)	189 (100%)	0	100	100
6	F	331/335 (99%)	330 (100%)	1 (0%)	86	91
7	G	530/535 (99%)	527 (99%)	3 (1%)	78	88
8	H	277/279 (99%)	277 (100%)	0	100	100
9	I	136/137 (99%)	136 (100%)	0	100	100
10	J	158/158 (100%)	158 (100%)	0	100	100
11	K	81/81 (100%)	80 (99%)	1 (1%)	63	82
12	L	520/543 (96%)	520 (100%)	0	100	100
13	M	410/416 (99%)	408 (100%)	2 (0%)	81	89
14	N	357/369 (97%)	356 (100%)	1 (0%)	86	91
15	P	248/250 (99%)	248 (100%)	0	100	100
16	Q	87/87 (100%)	87 (100%)	0	100	100
17	R	51/52 (98%)	51 (100%)	0	100	100
18	Z	167/168 (99%)	167 (100%)	0	100	100
19	a	360/366 (98%)	359 (100%)	1 (0%)	86	91
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
21	c	139/151 (92%)	138 (99%)	1 (1%)	76	86
21	f	140/151 (93%)	140 (100%)	0	100	100
22	g	447/454 (98%)	446 (100%)	1 (0%)	87	92
22	k	447/454 (98%)	447 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	h	211/243 (87%)	210 (100%)	1 (0%)	81	89
23	l	211/243 (87%)	210 (100%)	1 (0%)	81	89
24	i	220/221 (100%)	220 (100%)	0	100	100
24	m	220/221 (100%)	219 (100%)	1 (0%)	81	89
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	34/126 (27%)	34 (100%)	0	100	100
27	q	103/104 (99%)	103 (100%)	0	100	100
All	All	7666/8337 (92%)	7649 (100%)	17 (0%)	85	92

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	54	CYS
2	B	91	THR
2	B	92	LEU
6	F	260	SER
7	G	31	ILE
7	G	90	MET
7	G	376	GLN
11	K	25	ASN
13	M	365	HIS
13	M	471	MET
14	N	188	GLU
19	a	282	GLU
21	c	92	GLN
22	g	165	VAL
23	h	102	HIS
23	l	88	ARG
24	m	258	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	29	GLN
3	C	38	ASN
6	F	103	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	137	GLN
7	G	259	ASN
7	G	562	GLN
7	G	619	GLN
10	J	102	GLN
10	J	167	HIS
10	J	179	GLN
12	L	404	HIS
12	L	498	HIS
12	L	675	GLN
13	M	105	GLN
13	M	246	HIS
13	M	248	GLN
13	M	495	GLN
13	M	498	ASN
13	M	499	GLN
14	N	65	HIS
14	N	291	GLN
14	N	323	ASN
14	N	445	GLN
15	P	27	GLN
15	P	95	HIS
16	Q	48	GLN
18	Z	6	GLN
18	Z	78	ASN
19	a	192	ASN
19	a	358	GLN
20	b	231	GLN
20	b	342	HIS
20	b	436	ASN
21	c	60	GLN
19	d	8	HIS
20	e	372	GLN
20	e	416	GLN
20	e	436	ASN
21	f	92	GLN
22	g	83	ASN
22	g	113	ASN
22	g	131	ASN
22	g	157	GLN
22	g	206	ASN
22	g	526	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	h	30	GLN
23	h	48	ASN
23	h	102	HIS
23	h	137	ASN
23	h	158	ASN
23	h	244	GLN
24	i	244	GLN
24	i	256	HIS
22	k	119	HIS
22	k	269	HIS
22	k	457	ASN
22	k	463	GLN
23	l	94	ASN
23	l	158	ASN
23	l	252	ASN
27	q	14	GLN
27	q	65	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	$\# Z > 2$
13	FME	M	1	13	8,9,10	0.89	0	7,9,11	1.05	0
4	2MR	D	65	4	10,12,13	2.26	3 (30%)	5,13,15	0.87	0
12	FME	L	1	12	8,9,10	0.95	0	7,9,11	0.77	0
10	FME	J	1	10	8,9,10	0.98	0	7,9,11	0.66	0
27	FME	q	1	27	8,9,10	0.91	0	7,9,11	1.06	1 (14%)
1	FME	A	1	1	8,9,10	0.94	0	7,9,11	0.99	1 (14%)

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
13	FME	M	1	13	-	2/7/9/11	-
4	2MR	D	65	4	-	0/10/13/15	-
12	FME	L	1	12	-	1/7/9/11	-
10	FME	J	1	10	-	1/7/9/11	-
27	FME	q	1	27	-	0/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	65	2MR	CZ-NH2	4.67	1.43	1.33
4	D	65	2MR	CZ-NE	4.33	1.43	1.34
4	D	65	2MR	CQ1-NH1	-2.20	1.42	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	FME	C-CA-N	2.03	113.40	109.73
27	q	1	FME	C-CA-N	2.02	113.38	109.73

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	C-CA-CB-CG
10	J	1	FME	CB-CG-SD-CE
1	A	1	FME	N-CA-CB-CG
12	L	1	FME	C-CA-CB-CG
13	M	1	FME	CB-CG-SD-CE
1	A	1	FME	CB-CA-N-CN
13	M	1	FME	CB-CA-N-CN

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 194 ligands modelled in this entry, 12 are monoatomic - leaving 182 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	$\# Z > 2$
30	DU0	m	302	-	42,42,42	0.65	0	66,66,66	0.81	2 (3%)
37	3PH	M	603	-	47,47,47	1.36	5 (10%)	51,52,52	0.99	4 (7%)
47	CUA	l	302	23	0,1,1	-	-	-		
30	DU0	J	204	-	42,42,42	0.64	0	66,66,66	0.89	4 (6%)
37	3PH	a	504	-	47,47,47	1.37	5 (10%)	51,52,52	1.08	6 (11%)
33	PC1	f	201	-	53,53,53	0.93	3 (5%)	59,61,61	0.91	3 (5%)
28	3PE	H	408	-	50,50,50	0.95	4 (8%)	53,55,55	0.95	3 (5%)
29	PGT	a	514	-	50,50,50	0.91	3 (6%)	53,56,56	0.84	2 (3%)
30	DU0	k	608	-	42,42,42	0.62	0	66,66,66	0.81	1 (1%)
35	FES	f	204	21	0,4,4	-	-	-		
30	DU0	h	306	-	42,42,42	0.61	0	66,66,66	0.67	0
37	3PH	d	513	-	47,47,47	1.36	5 (10%)	51,52,52	1.02	4 (7%)
31	SF4	B	1001	2	0,12,12	-	-	-		
33	PC1	D	1001	-	53,53,53	0.95	3 (5%)	59,61,61	0.89	2 (3%)
36	FMN	F	502	-	33,33,33	1.07	2 (6%)	48,50,50	1.29	7 (14%)
37	3PH	L	810	-	47,47,47	1.36	5 (10%)	51,52,52	1.03	4 (7%)
28	3PE	c	201	-	50,50,50	0.96	4 (8%)	53,55,55	1.06	3 (5%)
30	DU0	a	516	-	42,42,42	0.64	0	66,66,66	0.88	1 (1%)
33	PC1	h	302	-	53,53,53	0.96	3 (5%)	59,61,61	0.91	3 (5%)
37	3PH	L	801	-	47,47,47	1.36	5 (10%)	51,52,52	1.00	4 (7%)
37	3PH	d	502	-	47,47,47	1.35	5 (10%)	51,52,52	1.04	4 (7%)
33	PC1	i	310	-	53,53,53	0.95	3 (5%)	59,61,61	0.89	1 (1%)
28	3PE	L	805	-	50,50,50	0.94	4 (8%)	53,55,55	1.01	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	3PH	i	304	-	47,47,47	1.35	5 (10%)	51,52,52	0.98	3 (5%)
28	3PE	a	502	-	50,50,50	0.96	4 (8%)	53,55,55	1.06	4 (7%)
33	PC1	M	601	-	53,53,53	0.96	3 (5%)	59,61,61	0.83	1 (1%)
28	3PE	n	1002	-	50,50,50	0.96	4 (8%)	53,55,55	0.90	2 (3%)
30	DU0	i	315	-	42,42,42	0.62	0	66,66,66	0.83	1 (1%)
37	3PH	i	303	-	47,47,47	1.37	5 (10%)	51,52,52	0.98	3 (5%)
33	PC1	L	803	-	53,53,53	0.96	3 (5%)	59,61,61	0.93	3 (5%)
28	3PE	m	310	-	50,50,50	0.96	4 (8%)	53,55,55	1.04	4 (7%)
42	HEC	e	504	20	50,50,50	1.61	3 (6%)	68,82,82	1.59	10 (14%)
38	P5S	a	513	-	52,53,53	0.92	3 (5%)	56,60,60	0.92	4 (7%)
30	DU0	e	503	-	42,42,42	0.61	0	66,66,66	0.64	0
29	PGT	M	602	-	50,50,50	0.93	4 (8%)	53,56,56	0.85	4 (7%)
28	3PE	i	309	-	50,50,50	0.94	4 (8%)	53,55,55	0.92	2 (3%)
28	3PE	L	802	-	50,50,50	0.94	4 (8%)	53,55,55	0.97	3 (5%)
28	3PE	m	306	-	50,50,50	0.96	4 (8%)	53,55,55	0.99	2 (3%)
29	PGT	L	804	-	50,50,50	0.93	4 (8%)	53,56,56	1.11	6 (11%)
37	3PH	f	203	-	47,47,47	1.37	6 (12%)	51,52,52	0.97	3 (5%)
33	PC1	m	314	-	53,53,53	0.94	3 (5%)	59,61,61	0.85	1 (1%)
28	3PE	L	808	-	50,50,50	0.98	4 (8%)	53,55,55	0.95	3 (5%)
28	3PE	m	305	-	50,50,50	0.95	4 (8%)	53,55,55	0.96	3 (5%)
29	PGT	J	205	-	50,50,50	0.93	4 (8%)	53,56,56	0.79	2 (3%)
31	SF4	F	501	6	0,12,12	-	-	-	-	-
33	PC1	a	507	-	53,53,53	0.95	3 (5%)	59,61,61	0.86	3 (5%)
33	PC1	d	509	-	53,53,53	0.95	3 (5%)	59,61,61	0.79	1 (1%)
28	3PE	a	503	-	50,50,50	0.96	4 (8%)	53,55,55	0.92	4 (7%)
29	PGT	H	406	-	50,50,50	0.91	4 (8%)	53,56,56	1.14	3 (5%)
33	PC1	N	504	-	53,53,53	0.96	3 (5%)	59,61,61	0.86	2 (3%)
30	DU0	j	1002	-	42,42,42	0.62	0	66,66,66	0.81	2 (3%)
33	PC1	l	303	-	53,53,53	0.95	3 (5%)	59,61,61	0.87	2 (3%)
33	PC1	m	303	-	53,53,53	0.92	3 (5%)	59,61,61	0.96	2 (3%)
28	3PE	i	307	-	50,50,50	0.96	4 (8%)	53,55,55	1.15	3 (5%)
33	PC1	m	311	-	53,53,53	0.95	3 (5%)	59,61,61	0.84	2 (3%)
33	PC1	N	501	-	53,53,53	0.96	3 (5%)	59,61,61	0.86	2 (3%)
30	DU0	m	313	-	42,42,42	0.62	0	66,66,66	0.89	1 (1%)
28	3PE	e	502	-	50,50,50	0.96	4 (8%)	53,55,55	0.95	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	3PH	f	205	-	47,47,47	1.36	5 (10%)	51,52,52	1.06	4 (7%)
37	3PH	c	206	-	47,47,47	1.36	5 (10%)	51,52,52	1.04	6 (11%)
28	3PE	g	601	-	50,50,50	0.95	4 (8%)	53,55,55	0.97	3 (5%)
28	3PE	d	515	-	50,50,50	0.97	4 (8%)	53,55,55	0.92	4 (7%)
37	3PH	M	606	-	47,47,47	1.35	5 (10%)	51,52,52	0.97	3 (5%)
39	T7X	J	202	-	61,61,61	0.96	4 (6%)	71,73,73	0.95	4 (5%)
28	3PE	h	307	-	50,50,50	0.94	4 (8%)	53,55,55	0.95	3 (5%)
37	3PH	M	604	-	47,47,47	1.37	5 (10%)	51,52,52	1.05	5 (9%)
30	DU0	i	305	-	42,42,42	0.59	0	66,66,66	0.74	0
30	DU0	M	607	-	42,42,42	0.64	0	66,66,66	0.72	1 (1%)
44	HEA	g	606	22	66,67,67	1.33	7 (10%)	78,103,103	2.30	27 (34%)
30	DU0	c	205	-	42,42,42	0.65	0	66,66,66	1.08	5 (7%)
30	DU0	i	302	-	42,42,42	0.65	0	66,66,66	0.79	0
32	U10	a	512	-	63,63,63	0.66	0	76,79,79	1.02	2 (2%)
31	SF4	I	202	9	0,12,12	-	-	-	-	-
33	PC1	H	403	-	53,53,53	0.95	3 (5%)	59,61,61	0.81	1 (1%)
43	CDL	d	501	-	99,99,99	0.91	7 (7%)	105,111,111	0.95	5 (4%)
29	PGT	N	505	-	50,50,50	0.92	4 (8%)	53,56,56	0.91	2 (3%)
28	3PE	d	503	-	50,50,50	0.94	4 (8%)	53,55,55	0.96	3 (5%)
30	DU0	c	202	-	42,42,42	0.64	0	66,66,66	0.78	2 (3%)
38	P5S	L	809	-	52,53,53	0.93	3 (5%)	56,60,60	0.83	2 (3%)
28	3PE	a	508	-	50,50,50	0.96	4 (8%)	53,55,55	0.99	2 (3%)
32	U10	d	504	-	63,63,63	0.65	0	76,79,79	0.96	2 (2%)
28	3PE	A	201	-	50,50,50	0.96	4 (8%)	53,55,55	1.02	4 (7%)
33	PC1	g	612	-	53,53,53	0.94	3 (5%)	59,61,61	0.87	4 (6%)
32	U10	B	1002	-	63,63,63	0.67	0	76,79,79	1.17	4 (5%)
33	PC1	n	1001	-	53,53,53	0.95	3 (5%)	59,61,61	0.86	2 (3%)
33	PC1	M	609	-	53,53,53	0.95	3 (5%)	59,61,61	0.86	2 (3%)
44	HEA	k	605	22	66,67,67	1.32	6 (9%)	78,103,103	2.29	28 (35%)
28	3PE	g	607	-	50,50,50	0.96	4 (8%)	53,55,55	0.94	1 (1%)
35	FES	E	401	5	0,4,4	-	-	-	-	-
33	PC1	N	502	-	53,53,53	0.95	3 (5%)	59,61,61	0.82	2 (3%)
28	3PE	m	307	-	50,50,50	0.96	4 (8%)	53,55,55	0.95	2 (3%)
35	FES	G	701	7	0,4,4	-	-	-	-	-
39	T7X	g	615	-	61,61,61	0.94	4 (6%)	71,73,73	0.81	2 (2%)
37	3PH	k	601	-	47,47,47	1.39	5 (10%)	51,52,52	1.01	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	DU0	d	511	-	42,42,42	0.59	0	66,66,66	0.77	2 (3%)
37	3PH	k	607	-	47,47,47	1.35	5 (10%)	51,52,52	1.04	4 (7%)
47	CUA	h	305	23	0,1,1	-	-	-		
28	3PE	g	613	-	50,50,50	0.97	4 (8%)	53,55,55	1.07	3 (5%)
28	3PE	e	505	-	50,50,50	0.95	4 (8%)	53,55,55	0.95	2 (3%)
41	HEM	d	514	19	50,50,50	1.27	7 (14%)	66,82,82	1.25	8 (12%)
37	3PH	M	605	-	47,47,47	1.37	5 (10%)	51,52,52	0.97	5 (9%)
32	U10	d	506	-	63,63,63	0.69	1 (1%)	76,79,79	1.25	3 (3%)
29	PGT	A	202	-	50,50,50	0.94	4 (8%)	53,56,56	0.81	1 (1%)
33	PC1	b	504	-	53,53,53	0.94	3 (5%)	59,61,61	0.85	3 (5%)
28	3PE	H	404	-	50,50,50	0.95	4 (8%)	53,55,55	0.95	2 (3%)
28	3PE	m	315	-	50,50,50	0.95	4 (8%)	53,55,55	0.96	1 (1%)
28	3PE	P	403	-	50,50,50	0.97	4 (8%)	53,55,55	1.01	2 (3%)
30	DU0	i	316	-	42,42,42	0.59	0	66,66,66	0.78	0
30	DU0	h	304	-	42,42,42	0.67	1 (2%)	66,66,66	1.38	11 (16%)
33	PC1	k	606	-	53,53,53	0.95	3 (5%)	59,61,61	0.83	2 (3%)
28	3PE	m	304	-	50,50,50	0.97	4 (8%)	53,55,55	0.96	2 (3%)
37	3PH	i	314	-	47,47,47	1.37	6 (12%)	51,52,52	1.04	5 (9%)
30	DU0	h	303	-	42,42,42	0.59	0	66,66,66	0.68	0
33	PC1	m	312	-	53,53,53	0.95	3 (5%)	59,61,61	0.84	3 (5%)
37	3PH	L	811	-	47,47,47	1.35	5 (10%)	51,52,52	1.07	6 (11%)
30	DU0	d	505	-	42,42,42	0.64	0	66,66,66	0.69	1 (1%)
37	3PH	j	1003	-	47,47,47	1.35	5 (10%)	51,52,52	1.11	5 (9%)
30	DU0	g	604	-	42,42,42	0.69	0	66,66,66	0.85	1 (1%)
38	P5S	I	201	-	52,53,53	0.93	3 (5%)	56,60,60	0.97	2 (3%)
37	3PH	i	301	-	47,47,47	1.36	5 (10%)	51,52,52	0.99	4 (7%)
30	DU0	g	617	-	42,42,42	0.64	0	66,66,66	1.03	5 (7%)
29	PGT	J	201	-	50,50,50	0.92	4 (8%)	53,56,56	0.90	4 (7%)
35	FES	c	204	21	0,4,4	-	-	-		
33	PC1	l	301	-	53,53,53	0.98	3 (5%)	59,61,61	0.85	2 (3%)
33	PC1	i	313	-	53,53,53	0.95	3 (5%)	59,61,61	0.96	4 (6%)
37	3PH	i	318	-	47,47,47	1.34	5 (10%)	51,52,52	1.04	6 (11%)
33	PC1	M	608	-	53,53,53	0.95	3 (5%)	59,61,61	0.87	3 (5%)
33	PC1	c	203	-	53,53,53	0.95	3 (5%)	59,61,61	0.84	2 (3%)
33	PC1	d	516	-	53,53,53	0.94	3 (5%)	59,61,61	0.85	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	HEM	a	515	19	50,50,50	1.28	6 (12%)	66,82,82	1.16	5 (7%)
30	DU0	g	605	-	42,42,42	0.61	0	66,66,66	0.82	1 (1%)
28	3PE	a	509	-	50,50,50	0.95	4 (8%)	53,55,55	0.91	1 (1%)
28	3PE	H	407	-	50,50,50	0.97	4 (8%)	53,55,55	0.89	3 (5%)
30	DU0	M	610	-	42,42,42	0.63	0	66,66,66	0.77	0
37	3PH	H	409	-	47,47,47	1.35	5 (10%)	51,52,52	1.00	4 (7%)
37	3PH	g	603	-	47,47,47	1.37	6 (12%)	51,52,52	1.07	5 (9%)
44	HEA	g	610	22	66,67,67	1.30	7 (10%)	78,103,103	2.31	27 (34%)
28	3PE	h	301	-	50,50,50	0.96	4 (8%)	53,55,55	0.91	3 (5%)
33	PC1	a	517	-	53,53,53	0.97	3 (5%)	59,61,61	0.85	2 (3%)
29	PGT	q	1000	-	50,50,50	0.93	4 (8%)	53,56,56	0.83	1 (1%)
30	DU0	J	203	-	42,42,42	0.64	0	66,66,66	0.63	0
28	3PE	i	311	-	50,50,50	0.97	4 (8%)	53,55,55	0.98	2 (3%)
31	SF4	G	703	7	0,12,12	-	-	-	-	-
37	3PH	P	402	-	47,47,47	1.36	5 (10%)	51,52,52	1.09	5 (9%)
37	3PH	a	510	-	47,47,47	1.37	5 (10%)	51,52,52	0.99	4 (7%)
44	HEA	k	604	22	66,67,67	1.35	7 (10%)	78,103,103	2.29	26 (33%)
30	DU0	A	203	-	42,42,42	0.61	0	66,66,66	0.82	3 (4%)
37	3PH	d	508	-	47,47,47	1.36	5 (10%)	51,52,52	1.01	5 (9%)
29	PGT	g	602	-	50,50,50	0.93	4 (8%)	53,56,56	1.11	5 (9%)
30	DU0	f	202	-	42,42,42	0.66	0	66,66,66	0.80	1 (1%)
37	3PH	o	201	-	47,47,47	1.35	5 (10%)	51,52,52	0.99	4 (7%)
33	PC1	k	609	-	53,53,53	0.95	3 (5%)	59,61,61	0.82	2 (3%)
32	U10	a	511	-	63,63,63	0.66	0	76,79,79	1.02	5 (6%)
29	PGT	K	201	-	50,50,50	0.90	4 (8%)	53,56,56	0.83	2 (3%)
41	HEM	a	505	19	50,50,50	1.29	6 (12%)	66,82,82	1.20	8 (12%)
37	3PH	a	506	-	47,47,47	1.35	5 (10%)	51,52,52	1.00	4 (7%)
31	SF4	I	203	9	0,12,12	-	-	-	-	-
31	SF4	G	702	7	0,12,12	-	-	-	-	-
28	3PE	p	1001	-	50,50,50	0.97	4 (8%)	53,55,55	0.97	3 (5%)
30	DU0	d	512	-	42,42,42	0.61	0	66,66,66	0.70	0
30	DU0	g	616	-	42,42,42	0.61	0	66,66,66	1.05	4 (6%)
28	3PE	k	603	-	50,50,50	0.96	4 (8%)	53,55,55	0.94	2 (3%)
28	3PE	d	510	-	50,50,50	0.95	4 (8%)	53,55,55	0.99	2 (3%)
33	PC1	i	308	-	53,53,53	0.95	3 (5%)	59,61,61	0.91	2 (3%)
37	3PH	g	611	-	47,47,47	1.35	5 (10%)	51,52,52	1.04	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	3PH	m	301	-	47,47,47	1.36	5 (10%)	51,52,52	1.03	4 (7%)
28	3PE	i	317	-	50,50,50	0.96	4 (8%)	53,55,55	0.96	3 (5%)
30	DU0	H	401	-	42,42,42	0.62	0	66,66,66	0.74	1 (1%)
28	3PE	L	806	-	50,50,50	0.95	4 (8%)	53,55,55	1.00	3 (5%)
37	3PH	m	309	-	47,47,47	1.36	5 (10%)	51,52,52	1.02	5 (9%)
33	PC1	j	1001	-	53,53,53	0.95	3 (5%)	59,61,61	0.90	4 (6%)
28	3PE	i	306	-	50,50,50	0.97	4 (8%)	53,55,55	0.95	3 (5%)
41	HEM	d	507	19	50,50,50	1.29	6 (12%)	66,82,82	1.15	6 (9%)
29	PGT	P	401	-	50,50,50	0.93	4 (8%)	53,56,56	0.81	2 (3%)
33	PC1	a	501	-	53,53,53	0.96	3 (5%)	59,61,61	0.79	1 (1%)
42	HEC	b	502	20	50,50,50	1.62	5 (10%)	68,82,82	1.63	9 (13%)
37	3PH	L	807	-	47,47,47	1.33	5 (10%)	51,52,52	1.08	5 (9%)
33	PC1	l	304	-	53,53,53	0.96	3 (5%)	59,61,61	0.93	3 (5%)
37	3PH	N	503	-	47,47,47	1.37	6 (12%)	51,52,52	1.01	4 (7%)
28	3PE	H	405	-	50,50,50	0.95	4 (8%)	53,55,55	1.01	4 (7%)
33	PC1	b	501	-	53,53,53	0.95	3 (5%)	59,61,61	0.85	2 (3%)
33	PC1	H	402	-	53,53,53	0.95	3 (5%)	59,61,61	0.88	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	DU0	m	302	-	-	1/10/98/98	0/6/6/6
37	3PH	M	603	-	-	7/49/49/49	-
30	DU0	J	204	-	-	1/10/98/98	0/6/6/6
37	3PH	a	504	-	-	7/49/49/49	-
33	PC1	f	201	-	-	20/57/57/57	-
28	3PE	H	408	-	-	9/54/54/54	-
29	PGT	a	514	-	-	5/55/55/55	-
30	DU0	k	608	-	-	1/10/98/98	0/6/6/6
37	3PH	d	513	-	-	11/49/49/49	-
30	DU0	h	306	-	-	2/10/98/98	0/6/6/6
35	FES	f	204	21	-	-	0/1/1/1
31	SF4	B	1001	2	-	-	0/6/5/5
33	PC1	D	1001	-	-	9/57/57/57	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	FMN	F	502	-	-	2/18/18/18	0/3/3/3
37	3PH	L	810	-	-	13/49/49/49	-
28	3PE	c	201	-	-	14/54/54/54	-
30	DU0	a	516	-	-	2/10/98/98	0/6/6/6
33	PC1	h	302	-	-	16/57/57/57	-
37	3PH	L	801	-	-	9/49/49/49	-
37	3PH	d	502	-	-	7/49/49/49	-
33	PC1	i	310	-	-	13/57/57/57	-
28	3PE	L	805	-	-	13/54/54/54	-
37	3PH	i	304	-	-	7/49/49/49	-
28	3PE	a	502	-	-	10/54/54/54	-
33	PC1	M	601	-	-	7/57/57/57	-
28	3PE	n	1002	-	-	9/54/54/54	-
30	DU0	i	315	-	-	0/10/98/98	0/6/6/6
37	3PH	i	303	-	-	7/49/49/49	-
33	PC1	L	803	-	-	16/57/57/57	-
28	3PE	m	310	-	-	10/54/54/54	-
42	HEC	e	504	20	-	8/14/54/54	-
38	P5S	a	513	-	-	9/59/59/59	-
30	DU0	e	503	-	-	0/10/98/98	0/6/6/6
29	PGT	M	602	-	-	10/55/55/55	-
28	3PE	i	309	-	-	15/54/54/54	-
28	3PE	L	802	-	-	9/54/54/54	-
28	3PE	m	306	-	-	11/54/54/54	-
29	PGT	L	804	-	-	12/55/55/55	-
37	3PH	f	203	-	-	9/49/49/49	-
33	PC1	m	314	-	-	12/57/57/57	-
28	3PE	L	808	-	-	17/54/54/54	-
28	3PE	m	305	-	-	11/54/54/54	-
29	PGT	J	205	-	-	13/55/55/55	-
31	SF4	F	501	6	-	-	0/6/5/5
33	PC1	a	507	-	-	16/57/57/57	-
33	PC1	d	509	-	-	7/57/57/57	-
28	3PE	a	503	-	-	14/54/54/54	-
29	PGT	H	406	-	-	9/55/55/55	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	PC1	N	504	-	-	10/57/57/57	-
30	DU0	j	1002	-	-	0/10/98/98	0/6/6/6
33	PC1	l	303	-	-	9/57/57/57	-
33	PC1	m	303	-	-	11/57/57/57	-
28	3PE	i	307	-	-	18/54/54/54	-
33	PC1	m	311	-	-	13/57/57/57	-
33	PC1	N	501	-	-	11/57/57/57	-
30	DU0	m	313	-	-	1/10/98/98	0/6/6/6
28	3PE	e	502	-	-	8/54/54/54	-
37	3PH	f	205	-	-	12/49/49/49	-
37	3PH	c	206	-	-	6/49/49/49	-
28	3PE	g	601	-	-	13/54/54/54	-
28	3PE	d	515	-	-	8/54/54/54	-
37	3PH	M	606	-	-	11/49/49/49	-
39	T7X	J	202	-	-	10/56/80/80	0/1/1/1
28	3PE	h	307	-	-	14/54/54/54	-
37	3PH	M	604	-	-	13/49/49/49	-
30	DU0	i	305	-	-	1/10/98/98	0/6/6/6
30	DU0	M	607	-	-	0/10/98/98	0/6/6/6
44	HEA	g	606	22	-	5/36/76/76	-
30	DU0	c	205	-	-	3/10/98/98	0/6/6/6
30	DU0	i	302	-	-	0/10/98/98	0/6/6/6
32	U10	a	512	-	-	9/63/87/87	0/1/1/1
33	PC1	H	403	-	-	7/57/57/57	-
43	CDL	d	501	-	-	29/110/110/110	-
31	SF4	I	202	9	-	-	0/6/5/5
29	PGT	N	505	-	-	12/55/55/55	-
28	3PE	d	503	-	-	17/54/54/54	-
30	DU0	c	202	-	-	2/10/98/98	0/6/6/6
38	P5S	L	809	-	-	6/59/59/59	-
28	3PE	a	508	-	-	13/54/54/54	-
32	U10	d	504	-	-	8/63/87/87	0/1/1/1
28	3PE	A	201	-	-	16/54/54/54	-
33	PC1	g	612	-	-	9/57/57/57	-
32	U10	B	1002	-	-	13/63/87/87	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	PC1	n	1001	-	-	18/57/57/57	-
33	PC1	M	609	-	-	10/57/57/57	-
44	HEA	k	605	22	-	6/36/76/76	-
28	3PE	g	607	-	-	7/54/54/54	-
35	FES	E	401	5	-	-	0/1/1/1
33	PC1	N	502	-	-	13/57/57/57	-
28	3PE	m	307	-	-	17/54/54/54	-
35	FES	G	701	7	-	-	0/1/1/1
39	T7X	g	615	-	-	14/56/80/80	0/1/1/1
37	3PH	k	601	-	-	11/49/49/49	-
30	DU0	d	511	-	-	1/10/98/98	0/6/6/6
37	3PH	k	607	-	-	8/49/49/49	-
28	3PE	g	613	-	-	13/54/54/54	-
28	3PE	e	505	-	-	15/54/54/54	-
41	HEM	d	514	19	-	8/14/54/54	-
37	3PH	M	605	-	-	5/49/49/49	-
32	U10	d	506	-	-	6/63/87/87	0/1/1/1
29	PGT	A	202	-	-	13/55/55/55	-
33	PC1	b	504	-	-	12/57/57/57	-
28	3PE	H	404	-	-	10/54/54/54	-
28	3PE	m	315	-	-	12/54/54/54	-
28	3PE	P	403	-	-	11/54/54/54	-
30	DU0	i	316	-	-	0/10/98/98	0/6/6/6
30	DU0	h	304	-	-	0/10/98/98	0/6/6/6
33	PC1	k	606	-	-	11/57/57/57	-
28	3PE	m	304	-	-	7/54/54/54	-
37	3PH	i	314	-	-	10/49/49/49	-
30	DU0	h	303	-	-	1/10/98/98	0/6/6/6
33	PC1	m	312	-	-	12/57/57/57	-
37	3PH	L	811	-	-	9/49/49/49	-
30	DU0	d	505	-	-	1/10/98/98	0/6/6/6
37	3PH	j	1003	-	-	6/49/49/49	-
30	DU0	g	604	-	-	0/10/98/98	0/6/6/6
38	P5S	I	201	-	-	16/59/59/59	-
37	3PH	i	301	-	-	10/49/49/49	-
30	DU0	g	617	-	-	5/10/98/98	0/6/6/6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PGT	J	201	-	-	11/55/55/55	-
35	FES	c	204	21	-	-	0/1/1/1
33	PC1	l	301	-	-	11/57/57/57	-
33	PC1	i	313	-	-	17/57/57/57	-
37	3PH	i	318	-	-	9/49/49/49	-
33	PC1	M	608	-	-	12/57/57/57	-
33	PC1	c	203	-	-	13/57/57/57	-
33	PC1	d	516	-	-	10/57/57/57	-
41	HEM	a	515	19	-	5/14/54/54	-
30	DU0	g	605	-	-	0/10/98/98	0/6/6/6
28	3PE	a	509	-	-	9/54/54/54	-
28	3PE	H	407	-	-	13/54/54/54	-
30	DU0	M	610	-	-	0/10/98/98	0/6/6/6
37	3PH	H	409	-	-	4/49/49/49	-
37	3PH	g	603	-	-	12/49/49/49	-
44	HEA	g	610	22	-	7/36/76/76	-
28	3PE	h	301	-	-	15/54/54/54	-
33	PC1	a	517	-	-	16/57/57/57	-
29	PGT	q	1000	-	-	13/55/55/55	-
30	DU0	J	203	-	-	0/10/98/98	0/6/6/6
28	3PE	i	311	-	-	6/54/54/54	-
37	3PH	P	402	-	-	14/49/49/49	-
37	3PH	a	510	-	-	6/49/49/49	-
44	HEA	k	604	22	-	6/36/76/76	-
31	SF4	G	703	7	-	-	0/6/5/5
30	DU0	A	203	-	-	0/10/98/98	0/6/6/6
37	3PH	d	508	-	-	7/49/49/49	-
29	PGT	g	602	-	-	13/55/55/55	-
30	DU0	f	202	-	-	1/10/98/98	0/6/6/6
37	3PH	o	201	-	-	6/49/49/49	-
33	PC1	k	609	-	-	15/57/57/57	-
32	U10	a	511	-	-	10/63/87/87	0/1/1/1
29	PGT	K	201	-	-	9/55/55/55	-
41	HEM	a	505	19	-	6/14/54/54	-
37	3PH	a	506	-	-	9/49/49/49	-
31	SF4	I	203	9	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	SF4	G	702	7	-	-	0/6/5/5
28	3PE	p	1001	-	-	8/54/54/54	-
30	DU0	d	512	-	-	0/10/98/98	0/6/6/6
30	DU0	g	616	-	-	1/10/98/98	0/6/6/6
28	3PE	k	603	-	-	9/54/54/54	-
28	3PE	d	510	-	-	10/54/54/54	-
33	PC1	i	308	-	-	12/57/57/57	-
37	3PH	g	611	-	-	10/49/49/49	-
37	3PH	m	301	-	-	5/49/49/49	-
28	3PE	i	317	-	-	19/54/54/54	-
30	DU0	H	401	-	-	1/10/98/98	0/6/6/6
28	3PE	L	806	-	-	11/54/54/54	-
37	3PH	m	309	-	-	6/49/49/49	-
33	PC1	j	1001	-	-	13/57/57/57	-
28	3PE	i	306	-	-	15/54/54/54	-
41	HEM	d	507	19	-	7/14/54/54	-
29	PGT	P	401	-	-	18/55/55/55	-
33	PC1	a	501	-	-	11/57/57/57	-
42	HEC	b	502	20	1/1/3/7	8/14/54/54	-
37	3PH	L	807	-	-	5/49/49/49	-
33	PC1	l	304	-	-	17/57/57/57	-
37	3PH	N	503	-	-	6/49/49/49	-
28	3PE	H	405	-	-	15/54/54/54	-
33	PC1	b	501	-	-	12/57/57/57	-
33	PC1	H	402	-	-	11/57/57/57	-

All (565) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	b	502	HEC	C3D-C2D	7.67	1.53	1.36
42	e	504	HEC	C3D-C2D	7.60	1.52	1.36
37	k	601	3PH	P-O11	7.56	1.84	1.60
37	M	605	3PH	P-O11	7.38	1.84	1.60
37	i	301	3PH	P-O11	7.35	1.83	1.60
37	M	604	3PH	P-O11	7.34	1.83	1.60
37	f	203	3PH	P-O11	7.34	1.83	1.60
37	i	303	3PH	P-O11	7.29	1.83	1.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	a	510	3PH	P-O11	7.28	1.83	1.60
37	N	503	3PH	P-O11	7.28	1.83	1.60
37	m	309	3PH	P-O11	7.27	1.83	1.60
37	P	402	3PH	P-O11	7.26	1.83	1.60
37	a	504	3PH	P-O11	7.26	1.83	1.60
37	c	206	3PH	P-O11	7.26	1.83	1.60
37	M	603	3PH	P-O11	7.26	1.83	1.60
37	L	801	3PH	P-O11	7.26	1.83	1.60
37	i	314	3PH	P-O11	7.25	1.83	1.60
37	f	205	3PH	P-O11	7.24	1.83	1.60
37	L	811	3PH	P-O11	7.23	1.83	1.60
37	g	603	3PH	P-O11	7.23	1.83	1.60
37	L	810	3PH	P-O11	7.22	1.83	1.60
37	m	301	3PH	P-O11	7.21	1.83	1.60
37	M	606	3PH	P-O11	7.21	1.83	1.60
37	i	304	3PH	P-O11	7.21	1.83	1.60
37	d	508	3PH	P-O11	7.20	1.83	1.60
37	d	513	3PH	P-O11	7.19	1.83	1.60
37	j	1003	3PH	P-O11	7.18	1.83	1.60
37	k	607	3PH	P-O11	7.18	1.83	1.60
37	d	502	3PH	P-O11	7.17	1.83	1.60
37	i	318	3PH	P-O11	7.16	1.83	1.60
37	g	611	3PH	P-O11	7.16	1.83	1.60
37	o	201	3PH	P-O11	7.14	1.83	1.60
37	H	409	3PH	P-O11	7.13	1.83	1.60
37	a	506	3PH	P-O11	7.11	1.83	1.60
37	L	807	3PH	P-O11	7.04	1.82	1.60
44	k	604	HEA	C3B-C2B	4.45	1.44	1.34
44	k	605	HEA	C3B-C2B	4.19	1.44	1.34
44	g	606	HEA	C3B-C2B	4.14	1.44	1.34
44	g	610	HEA	C3B-C2B	3.97	1.43	1.34
44	k	604	HEA	C3D-C2D	3.85	1.44	1.36
44	g	610	HEA	C3D-C2D	3.77	1.44	1.36
44	k	605	HEA	C3D-C2D	3.75	1.44	1.36
44	g	606	HEA	C3D-C2D	3.74	1.44	1.36
28	i	306	3PE	P-O14	-3.70	1.37	1.50
28	a	508	3PE	P-O14	-3.68	1.37	1.50
28	m	307	3PE	P-O14	-3.59	1.38	1.50
28	m	304	3PE	P-O14	-3.58	1.38	1.50
42	e	504	HEC	FE-ND	3.58	2.05	1.94
28	L	808	3PE	P-O14	-3.57	1.38	1.50
28	k	603	3PE	P-O14	-3.56	1.38	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	i	311	3PE	P-O14	-3.55	1.38	1.50
28	i	307	3PE	P-O14	-3.55	1.38	1.50
28	L	802	3PE	P-O14	-3.55	1.38	1.50
28	d	510	3PE	P-O14	-3.54	1.38	1.50
28	P	403	3PE	P-O14	-3.53	1.38	1.50
28	h	301	3PE	P-O14	-3.53	1.38	1.50
28	a	509	3PE	P-O14	-3.53	1.38	1.50
28	c	201	3PE	P-O14	-3.53	1.38	1.50
28	H	408	3PE	P-O14	-3.52	1.38	1.50
28	d	515	3PE	P-O14	-3.51	1.38	1.50
28	e	502	3PE	P-O14	-3.51	1.38	1.50
28	n	1002	3PE	P-O14	-3.51	1.38	1.50
28	H	405	3PE	P-O14	-3.51	1.38	1.50
28	p	1001	3PE	P-O14	-3.50	1.38	1.50
28	L	805	3PE	P-O14	-3.50	1.38	1.50
28	H	407	3PE	P-O14	-3.50	1.38	1.50
28	H	404	3PE	P-O14	-3.49	1.38	1.50
28	m	315	3PE	P-O14	-3.49	1.38	1.50
39	J	202	T7X	P1-O1	3.49	1.69	1.60
28	m	306	3PE	P-O14	-3.49	1.38	1.50
28	g	607	3PE	P-O14	-3.49	1.38	1.50
28	d	503	3PE	P-O14	-3.48	1.38	1.50
28	i	317	3PE	P-O14	-3.48	1.38	1.50
28	h	307	3PE	P-O14	-3.47	1.38	1.50
44	k	604	HEA	C3A-C2A	3.47	1.44	1.36
28	m	305	3PE	P-O14	-3.45	1.38	1.50
28	L	806	3PE	P-O14	-3.45	1.38	1.50
28	i	309	3PE	P-O14	-3.45	1.38	1.50
28	A	201	3PE	P-O14	-3.45	1.38	1.50
33	H	402	PC1	P-O14	-3.45	1.38	1.50
33	l	301	PC1	P-O13	3.44	1.73	1.59
33	h	302	PC1	P-O13	3.44	1.73	1.59
28	a	503	3PE	P-O14	-3.44	1.38	1.50
28	a	502	3PE	P-O14	-3.43	1.38	1.50
28	e	505	3PE	P-O14	-3.43	1.38	1.50
36	F	502	FMN	C4A-N5	3.43	1.37	1.30
28	m	310	3PE	P-O14	-3.43	1.38	1.50
33	D	1001	PC1	P-O14	-3.43	1.38	1.50
33	m	311	PC1	P-O14	-3.42	1.38	1.50
33	i	308	PC1	P-O14	-3.42	1.38	1.50
28	g	613	3PE	P-O14	-3.42	1.38	1.50
33	i	313	PC1	P-O14	-3.42	1.38	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	g	601	3PE	P-O14	-3.41	1.38	1.50
33	b	501	PC1	P-O14	-3.41	1.38	1.50
33	a	501	PC1	P-O14	-3.41	1.38	1.50
33	c	203	PC1	P-O14	-3.41	1.38	1.50
33	l	301	PC1	P-O14	-3.40	1.38	1.50
33	b	504	PC1	P-O14	-3.40	1.38	1.50
29	J	201	PGT	P-O2P	-3.39	1.39	1.55
33	a	501	PC1	P-O13	3.39	1.73	1.59
33	a	517	PC1	P-O13	3.38	1.73	1.59
33	L	803	PC1	P-O14	-3.38	1.38	1.50
29	A	202	PGT	P-O2P	-3.37	1.39	1.55
29	P	401	PGT	P-O2P	-3.37	1.39	1.55
33	M	601	PC1	P-O14	-3.37	1.38	1.50
33	N	504	PC1	P-O14	-3.36	1.39	1.50
33	i	310	PC1	P-O14	-3.36	1.39	1.50
33	M	608	PC1	P-O14	-3.35	1.39	1.50
33	f	201	PC1	P-O14	-3.35	1.39	1.50
33	l	304	PC1	P-O14	-3.35	1.39	1.50
33	d	516	PC1	P-O14	-3.35	1.39	1.50
33	M	601	PC1	P-O13	3.35	1.72	1.59
33	k	606	PC1	P-O14	-3.35	1.39	1.50
33	H	403	PC1	P-O14	-3.34	1.39	1.50
33	M	609	PC1	P-O14	-3.34	1.39	1.50
33	N	502	PC1	P-O14	-3.34	1.39	1.50
33	N	501	PC1	P-O14	-3.34	1.39	1.50
33	d	509	PC1	P-O14	-3.34	1.39	1.50
33	m	303	PC1	P-O14	-3.34	1.39	1.50
33	n	1001	PC1	P-O14	-3.33	1.39	1.50
29	J	205	PGT	P-O2P	-3.33	1.39	1.55
29	N	505	PGT	P-O2P	-3.32	1.39	1.55
33	h	302	PC1	P-O14	-3.32	1.39	1.50
29	M	602	PGT	P-O2P	-3.32	1.39	1.55
33	n	1001	PC1	P-O13	3.31	1.72	1.59
33	a	507	PC1	P-O14	-3.31	1.39	1.50
33	k	609	PC1	P-O14	-3.30	1.39	1.50
29	a	514	PGT	P-O2P	-3.30	1.39	1.55
29	H	406	PGT	P-O2P	-3.30	1.39	1.55
29	L	804	PGT	P-O2P	-3.30	1.39	1.55
33	j	1001	PC1	P-O14	-3.30	1.39	1.50
29	g	602	PGT	P-O2P	-3.30	1.39	1.55
33	l	303	PC1	P-O14	-3.29	1.39	1.50
44	k	605	HEA	C3A-C2A	3.29	1.43	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	q	1000	PGT	P-O2P	-3.29	1.39	1.55
33	a	517	PC1	P-O14	-3.29	1.39	1.50
33	k	606	PC1	P-O13	3.28	1.72	1.59
33	m	312	PC1	P-O14	-3.28	1.39	1.50
33	N	504	PC1	P-O13	3.28	1.72	1.59
29	K	201	PGT	P-O2P	-3.27	1.40	1.55
33	k	609	PC1	P-O13	3.27	1.72	1.59
33	M	608	PC1	P-O13	3.26	1.72	1.59
39	g	615	T7X	P1-O1	3.26	1.69	1.60
33	g	612	PC1	P-O13	3.26	1.72	1.59
33	l	303	PC1	P-O13	3.26	1.72	1.59
33	m	314	PC1	P-O14	-3.25	1.39	1.50
33	H	403	PC1	P-O13	3.24	1.72	1.59
33	g	612	PC1	P-O14	-3.23	1.39	1.50
38	L	809	P5S	P12-O15	-3.23	1.40	1.55
42	b	502	HEC	FE-ND	3.23	2.04	1.94
33	i	310	PC1	P-O13	3.21	1.72	1.59
33	m	312	PC1	P-O13	3.21	1.72	1.59
33	b	501	PC1	P-O13	3.21	1.72	1.59
33	b	504	PC1	P-O13	3.21	1.72	1.59
39	J	202	T7X	P1-O12	-3.20	1.40	1.55
44	g	606	HEA	C3A-C2A	3.20	1.43	1.36
33	m	314	PC1	P-O13	3.19	1.72	1.59
33	j	1001	PC1	P-O13	3.18	1.72	1.59
33	d	509	PC1	P-O13	3.18	1.72	1.59
33	L	803	PC1	P-O13	3.17	1.72	1.59
33	N	501	PC1	P-O13	3.17	1.72	1.59
38	I	201	P5S	P12-O15	-3.17	1.40	1.55
38	a	513	P5S	P12-O15	-3.16	1.40	1.55
33	c	203	PC1	P-O13	3.16	1.72	1.59
33	H	402	PC1	P-O12	-3.15	1.40	1.55
33	D	1001	PC1	P-O12	-3.15	1.40	1.55
33	i	308	PC1	P-O13	3.13	1.72	1.59
39	g	615	T7X	P1-O12	-3.11	1.40	1.55
33	a	507	PC1	P-O13	3.11	1.71	1.59
33	D	1001	PC1	P-O13	3.09	1.71	1.59
33	m	311	PC1	P-O13	3.09	1.71	1.59
33	d	516	PC1	P-O13	3.08	1.71	1.59
33	l	304	PC1	P-O13	3.07	1.71	1.59
33	N	502	PC1	P-O13	3.07	1.71	1.59
33	i	308	PC1	P-O12	-3.07	1.40	1.55
33	i	313	PC1	P-O13	3.07	1.71	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	M	601	PC1	P-O12	-3.07	1.40	1.55
33	i	313	PC1	P-O12	-3.07	1.40	1.55
33	m	311	PC1	P-O12	-3.06	1.40	1.55
33	M	609	PC1	P-O13	3.06	1.71	1.59
33	H	403	PC1	P-O12	-3.05	1.41	1.55
33	d	516	PC1	P-O12	-3.04	1.41	1.55
33	c	203	PC1	P-O12	-3.03	1.41	1.55
33	a	501	PC1	P-O12	-3.03	1.41	1.55
33	f	201	PC1	P-O12	-3.03	1.41	1.55
33	a	517	PC1	P-O12	-3.03	1.41	1.55
33	M	608	PC1	P-O12	-3.03	1.41	1.55
33	n	1001	PC1	P-O12	-3.03	1.41	1.55
33	N	502	PC1	P-O12	-3.02	1.41	1.55
33	l	304	PC1	P-O12	-3.02	1.41	1.55
33	L	803	PC1	P-O12	-3.01	1.41	1.55
33	m	312	PC1	P-O12	-3.01	1.41	1.55
33	j	1001	PC1	P-O12	-3.01	1.41	1.55
33	a	507	PC1	P-O12	-3.01	1.41	1.55
39	J	202	T7X	P1-O11	-3.00	1.40	1.50
33	m	303	PC1	P-O12	-3.00	1.41	1.55
33	b	501	PC1	P-O12	-3.00	1.41	1.55
33	M	609	PC1	P-O12	-3.00	1.41	1.55
33	f	201	PC1	P-O13	2.99	1.71	1.59
44	g	610	HEA	C3A-C2A	2.99	1.43	1.36
33	N	501	PC1	P-O12	-2.98	1.41	1.55
33	m	303	PC1	P-O13	2.98	1.71	1.59
33	N	504	PC1	P-O12	-2.98	1.41	1.55
33	l	301	PC1	P-O12	-2.98	1.41	1.55
33	m	314	PC1	P-O12	-2.97	1.41	1.55
33	i	310	PC1	P-O12	-2.97	1.41	1.55
33	H	402	PC1	P-O13	2.97	1.71	1.59
33	d	509	PC1	P-O12	-2.97	1.41	1.55
33	g	612	PC1	P-O12	-2.95	1.41	1.55
33	l	303	PC1	P-O12	-2.95	1.41	1.55
33	b	504	PC1	P-O12	-2.95	1.41	1.55
28	i	306	3PE	P-O12	-2.95	1.41	1.55
33	k	609	PC1	P-O12	-2.93	1.41	1.55
33	h	302	PC1	P-O12	-2.93	1.41	1.55
33	k	606	PC1	P-O12	-2.92	1.41	1.55
28	L	808	3PE	P-O12	-2.88	1.41	1.55
39	g	615	T7X	P1-O11	-2.88	1.40	1.50
41	a	505	HEM	FE-NA	2.85	2.04	1.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	L	802	3PE	P-O12	-2.85	1.41	1.55
29	L	804	PGT	P-O1P	-2.85	1.40	1.50
28	H	405	3PE	P-O12	-2.84	1.42	1.55
28	H	407	3PE	P-O12	-2.83	1.42	1.55
29	A	202	PGT	P-O1P	-2.83	1.40	1.50
28	m	315	3PE	P-O12	-2.82	1.42	1.55
28	m	304	3PE	P-O12	-2.82	1.42	1.55
28	g	607	3PE	P-O12	-2.82	1.42	1.55
28	d	510	3PE	P-O12	-2.82	1.42	1.55
28	m	307	3PE	P-O12	-2.81	1.42	1.55
28	a	503	3PE	P-O12	-2.81	1.42	1.55
28	k	603	3PE	P-O12	-2.81	1.42	1.55
44	k	605	HEA	C4B-C3B	2.80	1.49	1.44
28	c	201	3PE	P-O12	-2.80	1.42	1.55
28	d	503	3PE	P-O12	-2.80	1.42	1.55
28	g	613	3PE	P-O12	-2.80	1.42	1.55
28	a	508	3PE	P-O12	-2.79	1.42	1.55
28	e	505	3PE	P-O12	-2.79	1.42	1.55
28	e	502	3PE	P-O12	-2.79	1.42	1.55
28	A	201	3PE	P-O12	-2.79	1.42	1.55
28	P	403	3PE	P-O12	-2.77	1.42	1.55
28	H	408	3PE	P-O12	-2.76	1.42	1.55
29	J	201	PGT	P-O1P	-2.76	1.41	1.50
28	h	301	3PE	P-O12	-2.76	1.42	1.55
28	L	806	3PE	P-O12	-2.76	1.42	1.55
28	n	1002	3PE	P-O12	-2.76	1.42	1.55
28	i	309	3PE	P-O12	-2.76	1.42	1.55
28	h	307	3PE	P-O12	-2.76	1.42	1.55
28	p	1001	3PE	P-O12	-2.76	1.42	1.55
28	H	404	3PE	P-O12	-2.76	1.42	1.55
28	a	509	3PE	P-O12	-2.75	1.42	1.55
28	L	805	3PE	P-O12	-2.75	1.42	1.55
28	i	307	3PE	P-O12	-2.75	1.42	1.55
28	i	317	3PE	P-O12	-2.75	1.42	1.55
28	i	311	3PE	P-O12	-2.74	1.42	1.55
29	J	205	PGT	P-O1P	-2.74	1.41	1.50
28	m	306	3PE	P-O12	-2.74	1.42	1.55
28	m	305	3PE	P-O12	-2.74	1.42	1.55
29	q	1000	PGT	P-O1P	-2.74	1.41	1.50
28	d	515	3PE	P-O12	-2.74	1.42	1.55
28	m	310	3PE	P-O12	-2.73	1.42	1.55
29	P	401	PGT	P-O1P	-2.73	1.41	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	a	515	HEM	FE-NB	2.73	2.03	1.94
28	a	502	3PE	P-O12	-2.73	1.42	1.55
29	H	406	PGT	P-O1P	-2.72	1.41	1.50
28	g	601	3PE	P-O12	-2.72	1.42	1.55
29	a	514	PGT	P-O1P	-2.72	1.41	1.50
38	L	809	P5S	P12-O13	-2.72	1.41	1.50
41	d	507	HEM	FE-NB	2.71	2.03	1.94
29	N	505	PGT	P-O1P	-2.70	1.41	1.50
29	M	602	PGT	P-O1P	-2.70	1.41	1.50
44	g	610	HEA	C4B-C3B	2.69	1.49	1.44
29	K	201	PGT	P-O1P	-2.68	1.41	1.50
38	I	201	P5S	P12-O16	2.67	1.70	1.59
29	g	602	PGT	P-O1P	-2.67	1.41	1.50
44	g	606	HEA	C1D-ND	-2.66	1.35	1.40
38	I	201	P5S	P12-O13	-2.65	1.41	1.50
41	a	505	HEM	CAC-C3C	2.64	1.54	1.47
38	a	513	P5S	P12-O16	2.64	1.70	1.59
38	a	513	P5S	P12-O13	-2.64	1.41	1.50
41	d	514	HEM	FE-NC	2.63	2.04	1.95
41	d	507	HEM	CAB-C3B	2.61	1.54	1.47
44	k	604	HEA	C1D-ND	-2.59	1.35	1.40
37	f	205	3PH	P-O13	-2.58	1.44	1.54
37	g	611	3PH	P-O13	-2.58	1.44	1.54
37	a	506	3PH	P-O13	-2.57	1.44	1.54
41	d	514	HEM	FE-ND	2.56	2.02	1.94
41	d	507	HEM	FE-NA	2.56	2.03	1.95
41	d	514	HEM	CAC-C3C	2.55	1.54	1.47
38	L	809	P5S	P12-O16	2.55	1.69	1.59
37	a	510	3PH	P-O14	-2.54	1.45	1.54
43	d	501	CDL	OB8-CB7	2.54	1.40	1.33
41	a	505	HEM	CAB-C3B	2.54	1.54	1.47
37	a	506	3PH	P-O14	-2.54	1.45	1.54
41	a	515	HEM	CAB-C3B	2.54	1.54	1.47
43	d	501	CDL	OA8-CA7	2.53	1.40	1.33
42	b	502	HEC	FE-NB	2.53	2.02	1.94
37	M	604	3PH	P-O14	-2.53	1.45	1.54
44	g	606	HEA	C4B-C3B	2.53	1.48	1.44
37	c	206	3PH	P-O14	-2.52	1.45	1.54
43	d	501	CDL	OA6-CA5	2.52	1.41	1.34
37	m	309	3PH	P-O13	-2.52	1.45	1.54
37	M	604	3PH	P-O13	-2.52	1.45	1.54
37	m	301	3PH	P-O14	-2.52	1.45	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	g	603	3PH	P-O14	-2.52	1.45	1.54
37	H	409	3PH	P-O14	-2.51	1.45	1.54
37	i	304	3PH	P-O14	-2.51	1.45	1.54
28	a	503	3PE	P-O11	2.51	1.69	1.59
28	n	1002	3PE	P-O11	2.50	1.69	1.59
37	M	605	3PH	P-O14	-2.50	1.45	1.54
37	i	304	3PH	P-O13	-2.50	1.45	1.54
37	a	504	3PH	P-O14	-2.50	1.45	1.54
37	j	1003	3PH	P-O14	-2.50	1.45	1.54
37	M	606	3PH	P-O14	-2.49	1.45	1.54
37	M	603	3PH	P-O14	-2.49	1.45	1.54
37	L	811	3PH	P-O14	-2.49	1.45	1.54
37	i	314	3PH	P-O14	-2.49	1.45	1.54
28	m	306	3PE	P-O13	2.49	1.69	1.59
37	M	605	3PH	P-O13	-2.48	1.45	1.54
28	H	407	3PE	P-O11	2.48	1.69	1.59
37	H	409	3PH	P-O13	-2.48	1.45	1.54
37	f	205	3PH	P-O14	-2.48	1.45	1.54
37	o	201	3PH	P-O14	-2.48	1.45	1.54
41	d	507	HEM	CAC-C3C	2.48	1.54	1.47
37	L	801	3PH	P-O14	-2.47	1.45	1.54
37	N	503	3PH	P-O14	-2.47	1.45	1.54
37	L	807	3PH	P-O13	-2.47	1.45	1.54
37	k	601	3PH	P-O13	-2.47	1.45	1.54
37	L	811	3PH	P-O13	-2.47	1.45	1.54
37	L	810	3PH	P-O14	-2.47	1.45	1.54
37	N	503	3PH	P-O13	-2.47	1.45	1.54
37	f	203	3PH	P-O14	-2.47	1.45	1.54
37	L	807	3PH	P-O14	-2.47	1.45	1.54
41	d	514	HEM	CAB-C3B	2.47	1.54	1.47
28	g	613	3PE	P-O11	2.47	1.69	1.59
28	i	309	3PE	P-O11	2.47	1.69	1.59
37	i	303	3PH	P-O13	-2.47	1.45	1.54
37	k	607	3PH	P-O13	-2.46	1.45	1.54
37	d	513	3PH	P-O13	-2.46	1.45	1.54
37	m	301	3PH	P-O13	-2.46	1.45	1.54
37	i	301	3PH	P-O14	-2.46	1.45	1.54
37	m	309	3PH	P-O14	-2.46	1.45	1.54
37	f	203	3PH	P-O13	-2.46	1.45	1.54
37	i	303	3PH	P-O14	-2.45	1.45	1.54
37	d	513	3PH	P-O14	-2.45	1.45	1.54
41	a	515	HEM	CAC-C3C	2.45	1.54	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	d	501	CDL	OB6-CB4	-2.45	1.40	1.46
37	g	611	3PH	P-O14	-2.45	1.45	1.54
37	i	318	3PH	P-O14	-2.45	1.45	1.54
37	M	603	3PH	P-O13	-2.45	1.45	1.54
37	c	206	3PH	P-O13	-2.45	1.45	1.54
37	i	314	3PH	P-O13	-2.45	1.45	1.54
37	d	502	3PH	P-O14	-2.45	1.45	1.54
37	d	508	3PH	P-O14	-2.44	1.45	1.54
37	i	318	3PH	P-O13	-2.44	1.45	1.54
37	g	603	3PH	P-O13	-2.44	1.45	1.54
28	L	808	3PE	P-O11	2.44	1.69	1.59
28	P	403	3PE	P-O13	2.44	1.69	1.59
37	P	402	3PH	P-O14	-2.43	1.45	1.54
44	k	604	HEA	C4B-C3B	2.43	1.48	1.44
37	a	504	3PH	P-O13	-2.43	1.45	1.54
37	P	402	3PH	P-O13	-2.43	1.45	1.54
28	g	607	3PE	P-O11	2.43	1.69	1.59
37	o	201	3PH	P-O13	-2.43	1.45	1.54
37	d	502	3PH	P-O13	-2.43	1.45	1.54
28	d	515	3PE	P-O11	2.43	1.69	1.59
29	L	804	PGT	P-O3P	2.43	1.69	1.59
28	p	1001	3PE	P-O13	2.42	1.69	1.59
37	d	508	3PH	P-O13	-2.42	1.45	1.54
37	j	1003	3PH	P-O13	-2.42	1.45	1.54
37	k	607	3PH	P-O14	-2.42	1.45	1.54
37	i	301	3PH	P-O13	-2.42	1.45	1.54
28	c	201	3PE	P-O11	2.42	1.69	1.59
28	i	311	3PE	P-O11	2.42	1.69	1.59
28	m	304	3PE	P-O13	2.41	1.69	1.59
37	L	810	3PH	O11-C1	-2.41	1.35	1.44
37	a	510	3PH	P-O13	-2.40	1.45	1.54
28	i	317	3PE	P-O11	2.40	1.69	1.59
28	e	502	3PE	P-O13	2.40	1.69	1.59
37	k	601	3PH	P-O14	-2.40	1.45	1.54
37	L	801	3PH	P-O13	-2.40	1.45	1.54
28	m	307	3PE	P-O11	2.40	1.69	1.59
28	a	509	3PE	P-O13	2.39	1.69	1.59
37	H	409	3PH	O11-C1	-2.39	1.35	1.44
28	a	502	3PE	P-O11	2.39	1.69	1.59
28	P	403	3PE	P-O11	2.39	1.69	1.59
37	M	606	3PH	P-O13	-2.39	1.45	1.54
37	L	807	3PH	O11-C1	-2.39	1.35	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	L	810	3PH	P-O13	-2.39	1.45	1.54
28	m	310	3PE	P-O11	2.38	1.68	1.59
28	d	510	3PE	P-O13	2.38	1.68	1.59
28	d	515	3PE	P-O13	2.37	1.68	1.59
28	H	405	3PE	P-O11	2.37	1.68	1.59
28	A	201	3PE	P-O13	2.37	1.68	1.59
28	i	317	3PE	P-O13	2.36	1.68	1.59
37	o	201	3PH	O11-C1	-2.36	1.35	1.44
37	N	503	3PH	O11-C1	-2.36	1.35	1.44
37	L	801	3PH	O11-C1	-2.36	1.35	1.44
28	i	306	3PE	P-O13	2.35	1.68	1.59
28	p	1001	3PE	P-O11	2.35	1.68	1.59
42	e	504	HEC	FE-NB	2.35	2.02	1.94
41	a	515	HEM	FE-NC	2.35	2.03	1.95
28	H	404	3PE	P-O11	2.35	1.68	1.59
28	g	601	3PE	P-O11	2.35	1.68	1.59
28	L	806	3PE	P-O11	2.34	1.68	1.59
29	J	205	PGT	P-O3P	2.34	1.68	1.59
28	m	305	3PE	P-O13	2.34	1.68	1.59
28	m	304	3PE	P-O11	2.34	1.68	1.59
37	d	508	3PH	O11-C1	-2.34	1.35	1.44
37	d	513	3PH	O11-C1	-2.33	1.35	1.44
28	L	802	3PE	P-O13	2.33	1.68	1.59
28	H	408	3PE	P-O11	2.33	1.68	1.59
28	g	601	3PE	P-O13	2.33	1.68	1.59
37	g	611	3PH	O11-C1	-2.33	1.35	1.44
28	a	503	3PE	P-O13	2.33	1.68	1.59
37	k	607	3PH	O11-C1	-2.32	1.35	1.44
37	a	506	3PH	O11-C1	-2.32	1.35	1.44
37	L	811	3PH	O11-C1	-2.32	1.35	1.44
28	e	505	3PE	P-O11	2.32	1.68	1.59
37	M	606	3PH	O11-C1	-2.32	1.35	1.44
28	H	407	3PE	P-O13	2.32	1.68	1.59
41	a	505	HEM	FE-NC	2.32	2.03	1.95
41	d	507	HEM	FE-ND	2.31	2.02	1.94
28	h	307	3PE	P-O11	2.31	1.68	1.59
28	i	306	3PE	P-O11	2.31	1.68	1.59
29	N	505	PGT	P-O3P	2.31	1.68	1.59
37	M	603	3PH	O11-C1	-2.31	1.35	1.44
28	a	509	3PE	P-O11	2.31	1.68	1.59
37	d	502	3PH	O11-C1	-2.30	1.35	1.44
28	h	301	3PE	P-O13	2.30	1.68	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	k	603	3PE	P-O11	2.30	1.68	1.59
29	g	602	PGT	P-O3P	2.30	1.68	1.59
28	i	311	3PE	P-O13	2.30	1.68	1.59
28	c	201	3PE	P-O13	2.30	1.68	1.59
29	P	401	PGT	P-O3P	2.29	1.68	1.59
28	g	607	3PE	P-O13	2.29	1.68	1.59
37	P	402	3PH	O11-C1	-2.29	1.35	1.44
37	f	205	3PH	O11-C1	-2.29	1.36	1.44
37	a	504	3PH	O11-C1	-2.29	1.36	1.44
28	e	502	3PE	P-O11	2.29	1.68	1.59
28	m	315	3PE	P-O11	2.29	1.68	1.59
37	a	510	3PH	O11-C1	-2.29	1.36	1.44
28	A	201	3PE	P-O11	2.29	1.68	1.59
37	m	301	3PH	O11-C1	-2.29	1.36	1.44
28	i	307	3PE	P-O11	2.29	1.68	1.59
37	m	309	3PH	O11-C1	-2.28	1.36	1.44
28	m	305	3PE	P-O11	2.28	1.68	1.59
28	H	408	3PE	P-O13	2.28	1.68	1.59
44	g	610	HEA	C3C-C4C	2.27	1.48	1.42
37	M	604	3PH	O11-C1	-2.27	1.36	1.44
37	i	303	3PH	O11-C1	-2.27	1.36	1.44
29	q	1000	PGT	P-O3P	2.27	1.68	1.59
36	F	502	FMN	C10-N1	2.27	1.37	1.33
37	f	203	3PH	O11-C1	-2.27	1.36	1.44
37	M	603	3PH	P-O12	-2.27	1.43	1.50
28	e	505	3PE	P-O13	2.26	1.68	1.59
44	g	610	HEA	C1D-ND	-2.26	1.36	1.40
44	k	604	HEA	C4D-C3D	2.26	1.48	1.45
28	a	508	3PE	P-O11	2.26	1.68	1.59
28	L	806	3PE	P-O13	2.26	1.68	1.59
29	L	804	PGT	P-O4P	2.26	1.68	1.59
37	j	1003	3PH	P-O12	-2.26	1.43	1.50
41	a	505	HEM	FE-ND	2.26	2.01	1.94
37	c	206	3PH	O11-C1	-2.25	1.36	1.44
28	d	510	3PE	P-O11	2.25	1.68	1.59
28	n	1002	3PE	P-O13	2.25	1.68	1.59
28	d	503	3PE	P-O13	2.25	1.68	1.59
28	a	508	3PE	P-O13	2.25	1.68	1.59
37	i	318	3PH	O11-C1	-2.25	1.36	1.44
37	i	301	3PH	O11-C1	-2.25	1.36	1.44
37	d	508	3PH	P-O12	-2.25	1.43	1.50
28	h	307	3PE	P-O13	2.25	1.68	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	g	603	3PH	O11-C1	-2.25	1.36	1.44
28	m	315	3PE	P-O13	2.24	1.68	1.59
41	d	514	HEM	C3B-C2B	-2.24	1.32	1.37
29	A	202	PGT	P-O3P	2.24	1.68	1.59
37	a	504	3PH	P-O12	-2.24	1.43	1.50
28	H	404	3PE	P-O13	2.24	1.68	1.59
28	L	805	3PE	P-O13	2.23	1.68	1.59
43	d	501	CDL	OB8-CB6	-2.23	1.40	1.45
28	g	613	3PE	P-O13	2.23	1.68	1.59
28	h	301	3PE	P-O11	2.22	1.68	1.59
28	a	502	3PE	P-O13	2.22	1.68	1.59
28	m	310	3PE	P-O13	2.22	1.68	1.59
44	k	605	HEA	C1D-ND	-2.22	1.36	1.40
29	q	1000	PGT	P-O4P	2.22	1.68	1.59
39	J	202	T7X	P1-O13	2.22	1.68	1.59
37	j	1003	3PH	O11-C1	-2.21	1.36	1.44
28	m	306	3PE	P-O11	2.21	1.68	1.59
29	M	602	PGT	P-O4P	2.21	1.68	1.59
42	b	502	HEC	FE-NA	2.21	2.02	1.95
39	g	615	T7X	P1-O13	2.21	1.68	1.59
37	L	801	3PH	P-O12	-2.20	1.43	1.50
37	i	314	3PH	O11-C1	-2.20	1.36	1.44
28	k	603	3PE	P-O13	2.20	1.68	1.59
37	c	206	3PH	P-O12	-2.20	1.43	1.50
37	P	402	3PH	P-O12	-2.20	1.43	1.50
28	m	307	3PE	P-O13	2.20	1.68	1.59
28	L	808	3PE	P-O13	2.19	1.68	1.59
28	L	805	3PE	P-O11	2.19	1.68	1.59
28	i	309	3PE	P-O13	2.19	1.68	1.59
28	L	802	3PE	P-O11	2.19	1.68	1.59
37	L	810	3PH	P-O12	-2.19	1.43	1.50
37	a	506	3PH	P-O12	-2.19	1.43	1.50
37	i	318	3PH	P-O12	-2.18	1.43	1.50
37	i	301	3PH	P-O12	-2.18	1.43	1.50
32	d	506	U10	C1M-C1	-2.18	1.46	1.50
37	m	301	3PH	P-O12	-2.18	1.43	1.50
37	i	304	3PH	O11-C1	-2.18	1.36	1.44
44	k	604	HEA	C1C-C2C	2.17	1.48	1.43
37	d	513	3PH	P-O12	-2.17	1.43	1.50
37	i	304	3PH	P-O12	-2.17	1.43	1.50
28	i	307	3PE	P-O13	2.17	1.68	1.59
37	N	503	3PH	P-O12	-2.17	1.43	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	M	605	3PH	O11-C1	-2.17	1.36	1.44
43	d	501	CDL	OB6-CB5	2.16	1.40	1.34
37	i	314	3PH	P-O12	-2.16	1.43	1.50
37	M	605	3PH	P-O12	-2.16	1.43	1.50
37	g	603	3PH	P-O12	-2.16	1.43	1.50
28	H	405	3PE	P-O13	2.16	1.68	1.59
29	A	202	PGT	P-O4P	2.16	1.68	1.59
37	H	409	3PH	P-O12	-2.16	1.43	1.50
37	m	309	3PH	P-O12	-2.16	1.43	1.50
37	L	807	3PH	P-O12	-2.15	1.43	1.50
37	M	606	3PH	P-O12	-2.15	1.43	1.50
37	k	607	3PH	P-O12	-2.15	1.43	1.50
41	d	507	HEM	FE-NC	2.15	2.02	1.95
37	f	203	3PH	P-O12	-2.14	1.43	1.50
37	i	303	3PH	P-O12	-2.14	1.43	1.50
37	f	205	3PH	P-O12	-2.13	1.43	1.50
41	a	515	HEM	C2A-C3A	-2.13	1.33	1.38
37	M	604	3PH	P-O12	-2.13	1.43	1.50
44	g	610	HEA	C1D-C2D	2.13	1.48	1.44
29	M	602	PGT	P-O3P	2.13	1.67	1.59
37	k	601	3PH	P-O12	-2.13	1.43	1.50
29	P	401	PGT	P-O4P	2.12	1.67	1.59
37	o	201	3PH	P-O12	-2.12	1.43	1.50
28	d	503	3PE	P-O11	2.12	1.67	1.59
29	K	201	PGT	P-O3P	2.12	1.67	1.59
37	i	314	3PH	O31-C31	2.12	1.39	1.33
37	L	811	3PH	P-O12	-2.12	1.43	1.50
37	g	611	3PH	P-O12	-2.12	1.43	1.50
37	k	601	3PH	O11-C1	-2.11	1.36	1.44
44	g	606	HEA	C4D-C3D	2.11	1.48	1.45
29	a	514	PGT	P-O3P	2.09	1.67	1.59
29	J	205	PGT	P-O4P	2.09	1.67	1.59
37	d	502	3PH	P-O12	-2.08	1.43	1.50
42	b	502	HEC	FE-NC	2.08	2.02	1.95
29	g	602	PGT	P-O4P	2.08	1.67	1.59
37	a	510	3PH	P-O12	-2.07	1.43	1.50
41	a	515	HEM	FE-ND	2.07	2.01	1.94
30	h	304	DU0	C09-C07	2.07	1.57	1.53
29	N	505	PGT	P-O4P	2.06	1.67	1.59
37	g	603	3PH	O31-C31	2.05	1.39	1.33
29	H	406	PGT	P-O3P	2.05	1.67	1.59
44	g	606	HEA	C4A-NA	-2.04	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	d	501	CDL	OA6-CA4	-2.04	1.41	1.46
29	J	201	PGT	P-O3P	2.04	1.67	1.59
29	H	406	PGT	P-O4P	2.04	1.67	1.59
41	a	505	HEM	C2A-C3A	-2.04	1.33	1.38
29	K	201	PGT	P-O4P	2.03	1.67	1.59
29	J	201	PGT	P-O4P	2.02	1.67	1.59
44	k	605	HEA	C3C-C4C	2.01	1.47	1.42
37	N	503	3PH	O31-C31	2.01	1.39	1.33
41	d	514	HEM	C2A-C3A	-2.01	1.33	1.38
37	f	203	3PH	O31-C31	2.01	1.39	1.33
41	d	514	HEM	FE-NA	2.00	2.01	1.95

All (606) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	d	506	U10	C6-C1-C2	7.39	125.02	119.18
44	k	604	HEA	C3A-C2A-C1A	-6.26	101.10	107.08
44	g	606	HEA	C3A-C2A-C1A	-6.20	101.15	107.08
44	k	605	HEA	C3A-C2A-C1A	-5.87	101.47	107.08
44	g	610	HEA	CAA-CBA-CGA	-5.79	101.14	113.60
44	g	610	HEA	C3A-C2A-C1A	-5.74	101.59	107.08
42	b	502	HEC	C1D-ND-C4D	5.56	110.82	105.07
42	e	504	HEC	C1D-ND-C4D	5.55	110.81	105.07
44	k	605	HEA	CAA-CBA-CGA	-5.10	102.63	113.60
29	H	406	PGT	C2-O2-C31	5.09	130.32	117.79
44	g	606	HEA	CAA-CBA-CGA	-5.02	102.80	113.60
32	d	504	U10	C6-C1-C2	4.92	123.07	119.18
44	k	604	HEA	CAA-CBA-CGA	-4.88	103.10	113.60
44	k	605	HEA	CAD-CBD-CGD	-4.78	103.33	113.60
44	g	610	HEA	C3D-C4D-ND	4.74	114.95	110.36
32	B	1002	U10	C8-C7-C6	4.71	124.76	112.05
32	a	512	U10	C6-C1-C2	4.67	122.87	119.18
44	k	605	HEA	CMC-C2C-C3C	4.66	137.88	126.59
44	k	604	HEA	CMD-C2D-C1D	-4.64	117.97	125.04
44	g	610	HEA	CMC-C2C-C3C	4.55	137.61	126.59
44	k	605	HEA	CMC-C2C-C1C	-4.54	118.45	125.37
44	g	606	HEA	C13-C12-C11	-4.53	107.54	114.35
44	g	610	HEA	C13-C12-C11	-4.49	107.61	114.35
44	k	604	HEA	C3D-C4D-ND	4.46	114.67	110.36
28	g	613	3PE	C2-O21-C21	4.36	128.52	117.79
33	f	201	PC1	O12-P-O14	4.34	133.69	112.24
44	g	606	HEA	CMD-C2D-C1D	-4.33	118.44	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	m	314	PC1	O12-P-O14	4.33	133.63	112.24
32	B	1002	U10	C7-C8-C9	-4.32	119.59	126.79
44	k	605	HEA	C3D-C4D-ND	4.32	114.54	110.36
44	g	610	HEA	CMC-C2C-C1C	-4.30	118.81	125.37
33	H	402	PC1	O12-P-O14	4.30	133.51	112.24
33	m	303	PC1	O12-P-O14	4.30	133.49	112.24
33	i	310	PC1	O12-P-O14	4.29	133.46	112.24
42	b	502	HEC	CAB-C3B-C4B	-4.28	119.25	124.81
33	i	308	PC1	O12-P-O14	4.28	133.40	112.24
44	g	606	HEA	CMC-C2C-C3C	4.28	136.95	126.59
33	c	203	PC1	O12-P-O14	4.25	133.27	112.24
33	b	504	PC1	O12-P-O14	4.25	133.25	112.24
33	d	516	PC1	O12-P-O14	4.25	133.25	112.24
33	M	609	PC1	O12-P-O14	4.24	133.22	112.24
44	k	604	HEA	CMC-C2C-C3C	4.24	136.85	126.59
44	g	610	HEA	C26-C15-C16	4.23	122.39	115.27
33	m	311	PC1	O12-P-O14	4.23	133.14	112.24
28	d	503	3PE	O12-P-O14	4.22	133.10	112.24
33	i	313	PC1	O12-P-O14	4.21	133.07	112.24
44	k	604	HEA	CMB-C2B-C1B	-4.21	118.63	125.04
28	L	805	3PE	O12-P-O14	4.21	133.03	112.24
44	k	604	HEA	C2A-C1A-NA	4.20	114.41	110.32
33	k	606	PC1	O12-P-O14	4.19	132.97	112.24
33	l	303	PC1	O12-P-O14	4.19	132.97	112.24
30	c	205	DU0	C22-C21-C20	4.19	118.03	111.52
28	h	307	3PE	O12-P-O14	4.19	132.96	112.24
33	a	507	PC1	O12-P-O14	4.17	132.85	112.24
38	I	201	P5S	OG-CB-CA	4.17	111.69	108.06
28	a	508	3PE	O12-P-O14	4.16	132.83	112.24
33	D	1001	PC1	O12-P-O14	4.15	132.76	112.24
28	e	505	3PE	O12-P-O14	4.15	132.75	112.24
28	h	301	3PE	O12-P-O14	4.15	132.74	112.24
42	e	504	HEC	CAC-C3C-C4C	-4.14	119.17	124.92
33	d	509	PC1	O12-P-O14	4.14	132.72	112.24
28	k	603	3PE	O12-P-O14	4.14	132.69	112.24
28	i	307	3PE	O12-P-O14	4.13	132.68	112.24
33	N	501	PC1	O12-P-O14	4.13	132.68	112.24
28	m	315	3PE	O12-P-O14	4.13	132.64	112.24
44	g	610	HEA	C2A-C1A-NA	4.13	114.34	110.32
28	m	305	3PE	O12-P-O14	4.11	132.56	112.24
28	a	502	3PE	O12-P-O14	4.11	132.54	112.24
33	L	803	PC1	O12-P-O14	4.10	132.53	112.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	L	808	3PE	O12-P-O14	4.10	132.52	112.24
28	m	307	3PE	O12-P-O14	4.10	132.49	112.24
28	H	408	3PE	O12-P-O14	4.09	132.47	112.24
33	N	502	PC1	O12-P-O14	4.09	132.46	112.24
28	d	510	3PE	O12-P-O14	4.08	132.42	112.24
33	M	608	PC1	O12-P-O14	4.08	132.41	112.24
28	H	404	3PE	O12-P-O14	4.07	132.36	112.24
33	H	403	PC1	O12-P-O14	4.07	132.34	112.24
28	e	502	3PE	O12-P-O14	4.07	132.34	112.24
28	g	601	3PE	O12-P-O14	4.06	132.32	112.24
28	i	306	3PE	O12-P-O14	4.06	132.32	112.24
33	M	601	PC1	O12-P-O14	4.05	132.28	112.24
33	j	1001	PC1	O12-P-O14	4.05	132.27	112.24
28	L	806	3PE	O12-P-O14	4.05	132.25	112.24
28	A	201	3PE	O12-P-O14	4.05	132.25	112.24
33	n	1001	PC1	O12-P-O14	4.05	132.24	112.24
33	g	612	PC1	O12-P-O14	4.04	132.24	112.24
28	g	613	3PE	O12-P-O14	4.04	132.21	112.24
33	h	302	PC1	O12-P-O14	4.04	132.20	112.24
44	k	605	HEA	C2A-C1A-NA	4.03	114.25	110.32
28	m	310	3PE	O12-P-O14	4.03	132.15	112.24
33	l	304	PC1	O12-P-O14	4.02	132.10	112.24
28	m	304	3PE	O12-P-O14	4.00	132.03	112.24
28	m	310	3PE	C2-O21-C21	4.00	127.65	117.79
28	i	309	3PE	O12-P-O14	4.00	132.02	112.24
28	c	201	3PE	O12-P-O14	3.99	131.96	112.24
28	g	607	3PE	O12-P-O14	3.99	131.94	112.24
44	g	606	HEA	C3D-C4D-ND	3.99	114.22	110.36
42	b	502	HEC	CMC-C2C-C1C	-3.98	119.31	125.37
28	n	1002	3PE	O12-P-O14	3.97	131.86	112.24
44	g	606	HEA	C2A-C1A-NA	3.96	114.18	110.32
28	H	405	3PE	O12-P-O14	3.95	131.77	112.24
44	g	606	HEA	CMB-C2B-C1B	-3.94	119.04	125.04
33	N	504	PC1	O12-P-O14	3.94	131.71	112.24
28	a	509	3PE	O12-P-O14	3.93	131.67	112.24
28	d	515	3PE	O12-P-O14	3.92	131.63	112.24
28	i	311	3PE	O12-P-O14	3.92	131.62	112.24
28	L	802	3PE	O12-P-O14	3.92	131.61	112.24
33	k	609	PC1	O12-P-O14	3.91	131.55	112.24
28	i	317	3PE	O12-P-O14	3.90	131.51	112.24
33	a	517	PC1	O12-P-O14	3.89	131.48	112.24
33	a	501	PC1	O12-P-O14	3.88	131.44	112.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	503	3PE	O12-P-O14	3.86	131.35	112.24
44	g	606	HEA	CMC-C2C-C1C	-3.85	119.50	125.37
44	g	606	HEA	CAD-C3D-C4D	3.84	131.37	124.66
44	k	605	HEA	C13-C12-C11	-3.83	108.59	114.35
30	g	617	DU0	C22-C21-C20	3.82	117.45	111.52
33	m	312	PC1	O12-P-O14	3.81	131.06	112.24
28	p	1001	3PE	O12-P-O14	3.80	131.05	112.24
42	b	502	HEC	CAC-C3C-C4C	-3.79	119.66	124.92
29	N	505	PGT	O3-C3-C2	3.79	119.46	108.43
28	m	306	3PE	O12-P-O14	3.77	130.89	112.24
44	k	604	HEA	C4D-C3D-C2D	-3.76	101.42	106.90
28	P	403	3PE	O12-P-O14	3.76	130.83	112.24
44	g	610	HEA	CHA-C4D-C3D	-3.72	119.38	124.84
33	b	501	PC1	O12-P-O14	3.69	130.46	112.24
42	e	504	HEC	CAC-C3C-C2C	3.68	132.76	126.86
28	H	407	3PE	O12-P-O14	3.68	130.43	112.24
28	i	307	3PE	O31-C3-C2	3.67	119.11	108.43
37	f	205	3PH	O13-P-O11	-3.67	96.98	106.73
44	g	610	HEA	C4D-C3D-C2D	-3.61	101.63	106.90
44	g	610	HEA	CMB-C2B-C1B	-3.60	119.56	125.04
44	k	604	HEA	CMC-C2C-C1C	-3.59	119.89	125.37
42	b	502	HEC	CAA-CBA-CGA	-3.59	105.89	113.60
44	g	606	HEA	CAA-C2A-C1A	3.58	131.63	124.89
42	e	504	HEC	CAB-C3B-C4B	-3.57	120.18	124.81
33	l	301	PC1	O12-P-O14	3.56	129.83	112.24
44	g	606	HEA	C4D-C3D-C2D	-3.51	101.78	106.90
37	M	606	3PH	O13-P-O11	-3.51	97.40	106.73
44	k	605	HEA	CHA-C1A-C2A	-3.49	119.28	124.94
37	d	502	3PH	O13-P-O11	-3.49	97.44	106.73
37	k	607	3PH	O13-P-O11	-3.49	97.46	106.73
44	k	604	HEA	CHA-C1A-C2A	-3.48	119.30	124.94
37	L	801	3PH	O13-P-O11	-3.48	97.48	106.73
32	B	1002	U10	C7-C6-C5	-3.47	114.30	118.48
42	b	502	HEC	CAB-C3B-C2B	3.47	133.46	127.53
44	k	604	HEA	CMD-C2D-C3D	3.47	135.53	126.12
44	g	610	HEA	CMD-C2D-C1D	-3.46	119.78	125.04
44	k	605	HEA	CHA-C4D-C3D	-3.45	119.78	124.84
44	k	604	HEA	C27-C19-C20	3.44	121.06	115.27
44	g	610	HEA	CHA-C1A-C2A	-3.44	119.37	124.94
37	M	603	3PH	O13-P-O11	-3.42	97.62	106.73
37	g	603	3PH	O13-P-O11	-3.42	97.63	106.73
44	g	610	HEA	CAD-CBD-CGD	-3.41	106.27	113.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	k	605	HEA	CAD-C3D-C4D	3.40	130.60	124.66
44	k	605	HEA	C26-C15-C16	3.38	120.96	115.27
39	g	615	T7X	O12-P1-O11	3.38	128.94	112.24
44	g	610	HEA	C27-C19-C20	3.38	120.95	115.27
32	B	1002	U10	C6-C1-C2	3.38	121.85	119.18
41	a	515	HEM	CAD-CBD-CGD	-3.37	106.36	113.60
44	k	604	HEA	CAA-C2A-C1A	3.36	131.23	124.89
42	e	504	HEC	CMC-C2C-C1C	-3.36	120.26	125.37
29	H	406	PGT	O2P-P-O1P	3.35	128.80	112.24
33	l	304	PC1	C2-O21-C21	3.33	125.99	117.79
29	K	201	PGT	O2P-P-O1P	3.32	128.64	112.24
44	g	606	HEA	CMD-C2D-C3D	3.32	135.12	126.12
44	k	605	HEA	C4D-C3D-C2D	-3.31	102.07	106.90
29	a	514	PGT	O2P-P-O1P	3.30	128.55	112.24
37	m	301	3PH	O13-P-O11	-3.29	97.97	106.73
44	k	605	HEA	CMD-C2D-C1D	-3.28	120.04	125.04
44	k	605	HEA	CMB-C2B-C1B	-3.28	120.05	125.04
37	P	402	3PH	O13-P-O11	-3.26	98.05	106.73
28	c	201	3PE	C2-O21-C21	3.26	125.82	117.79
29	g	602	PGT	O2P-P-O1P	3.26	128.35	112.24
36	F	502	FMN	C4-N3-C2	-3.26	119.63	125.64
28	H	405	3PE	C2-O21-C21	3.25	125.79	117.79
37	o	201	3PH	O13-P-O11	-3.24	98.10	106.73
44	k	604	HEA	C3C-C2C-C1C	-3.24	103.25	107.16
37	H	409	3PH	O13-P-O11	-3.24	98.12	106.73
37	a	506	3PH	O13-P-O11	-3.23	98.14	106.73
37	i	303	3PH	O13-P-O11	-3.22	98.17	106.73
30	h	304	DU0	C77-C79-C17	-3.21	107.92	112.73
37	L	810	3PH	O13-P-O11	-3.20	98.21	106.73
29	L	804	PGT	C3-C2-C1	3.20	119.36	111.79
43	d	501	CDL	OA8-CA6-CA4	3.20	117.75	108.43
44	k	604	HEA	CBA-CAA-C2A	3.20	121.51	112.63
44	k	604	HEA	CAD-C3D-C4D	3.19	130.23	124.66
37	L	807	3PH	O13-P-O11	-3.19	98.26	106.73
28	i	311	3PE	C2-O21-C21	3.19	125.63	117.79
28	m	306	3PE	C2-O21-C21	3.18	125.62	117.79
28	i	307	3PE	C2-O21-C21	3.18	125.61	117.79
33	l	301	PC1	C2-O21-C21	3.18	125.61	117.79
28	A	201	3PE	C2-O21-C21	3.17	125.61	117.79
30	h	304	DU0	O10-C09-O16	-3.17	100.93	109.78
29	J	201	PGT	O2P-P-O1P	3.17	127.91	112.24
37	d	513	3PH	O13-P-O11	-3.15	98.35	106.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	i	314	3PH	O13-P-O11	-3.15	98.36	106.73
41	d	507	HEM	CAD-CBD-CGD	-3.14	106.85	113.60
44	g	606	HEA	C13-C14-C15	-3.13	120.13	127.66
44	k	604	HEA	CMB-C2B-C3B	3.12	136.28	130.34
37	i	304	3PH	O13-P-O11	-3.12	98.44	106.73
44	g	606	HEA	CBD-CAD-C3D	-3.11	103.99	112.63
44	k	604	HEA	C26-C15-C16	3.11	120.50	115.27
33	f	201	PC1	C2-O21-C21	3.11	125.44	117.79
33	a	517	PC1	C2-O21-C21	3.10	125.42	117.79
29	J	205	PGT	O2P-P-O1P	3.10	127.55	112.24
33	L	803	PC1	C2-O21-C21	3.09	125.40	117.79
44	g	606	HEA	CHA-C1A-C2A	-3.08	119.94	124.94
37	a	504	3PH	O13-P-O11	-3.08	98.53	106.73
37	i	318	3PH	O13-P-O11	-3.06	98.58	106.73
42	e	504	HEC	CAA-CBA-CGA	-3.06	107.02	113.60
36	F	502	FMN	C4A-C10-N10	3.05	120.95	116.48
32	a	511	U10	C37-C38-C39	3.05	135.00	127.66
29	M	602	PGT	O2P-P-O1P	3.04	127.28	112.24
37	f	205	3PH	O31-C31-O32	-3.03	115.95	123.59
39	J	202	T7X	O1-C1-C6	3.02	115.70	108.66
44	k	604	HEA	CHA-C4D-C3D	-3.02	120.41	124.84
44	g	606	HEA	CMB-C2B-C3B	3.01	136.09	130.34
30	J	204	DU0	O10-C11-C12	-3.00	107.85	112.18
44	g	606	HEA	C3C-C2C-C1C	-2.99	103.55	107.16
38	a	513	P5S	OG-CB-CA	2.99	110.66	108.06
30	g	616	DU0	C18-C17-C03	-2.98	106.58	110.91
29	L	804	PGT	O2P-P-O1P	2.98	126.97	112.24
44	g	610	HEA	C3C-C2C-C1C	-2.97	103.58	107.16
33	n	1001	PC1	C2-O21-C21	2.96	125.08	117.79
33	N	504	PC1	C2-O21-C21	2.95	125.06	117.79
32	a	511	U10	C36-C37-C38	2.95	121.58	111.88
29	g	602	PGT	C2-O2-C31	2.95	125.04	117.79
43	d	501	CDL	OB6-CB5-C51	2.94	117.84	111.50
30	M	607	DU0	O10-C09-O16	-2.94	101.58	109.78
37	L	811	3PH	O31-C31-O32	-2.93	116.20	123.59
37	f	203	3PH	O13-P-O11	-2.93	98.94	106.73
29	P	401	PGT	O2P-P-O1P	2.93	126.70	112.24
37	d	508	3PH	O13-P-O11	-2.92	98.95	106.73
37	a	504	3PH	O31-C31-O32	-2.91	116.24	123.59
44	k	605	HEA	C3C-C2C-C1C	-2.90	103.66	107.16
44	g	606	HEA	C27-C19-C20	2.90	120.15	115.27
29	A	202	PGT	O2P-P-O1P	2.90	126.56	112.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	d	514	HEM	CAA-CBA-CGA	-2.90	107.37	113.60
30	J	204	DU0	O10-C09-C15	2.90	113.46	110.77
37	g	611	3PH	O31-C31-O32	-2.89	116.29	123.59
44	g	606	HEA	CHA-C4D-C3D	-2.89	120.60	124.84
29	q	1000	PGT	O2P-P-O1P	2.87	126.44	112.24
29	N	505	PGT	O2P-P-O1P	2.85	126.34	112.24
32	a	511	U10	C6-C1-C2	2.85	121.43	119.18
28	p	1001	3PE	C2-O21-C21	2.85	124.80	117.79
29	g	602	PGT	C34-C33-C32	2.85	123.42	113.19
37	j	1003	3PH	O31-C31-O32	-2.83	116.44	123.59
41	d	514	HEM	C3B-C2B-C1B	2.83	108.59	106.49
44	g	606	HEA	CHB-C1B-C2B	-2.83	120.56	124.98
44	g	610	HEA	CHB-C1B-C2B	-2.82	120.57	124.98
30	h	304	DU0	C17-C18-C19	-2.82	108.68	112.73
28	P	403	3PE	C2-O21-C21	2.82	124.73	117.79
37	c	206	3PH	O31-C3-C2	2.81	116.62	108.43
37	N	503	3PH	O13-P-O11	-2.81	99.25	106.73
44	k	605	HEA	CMD-C2D-C3D	2.80	133.72	126.12
37	a	510	3PH	O31-C31-O32	-2.80	116.53	123.59
29	L	804	PGT	O2-C31-O31	-2.80	116.94	123.70
37	M	604	3PH	O31-C31-O32	-2.79	116.54	123.59
42	b	502	HEC	CAC-C3C-C2C	2.79	131.33	126.86
44	g	610	HEA	CMD-C2D-C3D	2.79	133.68	126.12
44	k	605	HEA	CAA-C2A-C1A	2.78	130.15	124.89
37	L	807	3PH	O31-C31-O32	-2.78	116.57	123.59
30	h	304	DU0	C76-C77-C79	2.77	112.60	108.73
39	J	202	T7X	O12-P1-O11	2.76	125.88	112.24
37	d	513	3PH	O31-C31-O32	-2.76	116.63	123.59
28	a	502	3PE	O31-C3-C2	2.76	116.46	108.43
42	e	504	HEC	CAB-C3B-C2B	2.76	132.24	127.53
30	m	302	DU0	C22-C21-C20	2.75	115.80	111.52
37	j	1003	3PH	O13-P-O11	-2.75	99.42	106.73
37	c	206	3PH	O13-P-O11	-2.74	99.44	106.73
44	g	610	HEA	CAA-C2A-C1A	2.74	130.05	124.89
37	i	314	3PH	O31-C3-C2	2.73	116.38	108.43
44	g	610	HEA	C16-C15-C14	-2.73	115.59	121.12
29	J	201	PGT	O3-C3-C2	2.73	116.37	108.43
37	L	811	3PH	O31-C3-C2	2.72	116.36	108.43
30	g	617	DU0	C76-C75-C22	2.72	114.97	110.33
37	M	603	3PH	O31-C31-O32	-2.71	116.75	123.59
41	d	514	HEM	C1B-NB-C4B	2.71	107.88	105.07
37	i	301	3PH	O13-P-O11	-2.70	99.54	106.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	g	603	3PH	O31-C3-C2	2.70	116.30	108.43
37	i	318	3PH	O31-C31-O32	-2.70	116.77	123.59
41	a	505	HEM	C1B-NB-C4B	2.68	107.84	105.07
37	L	811	3PH	O13-P-O11	-2.68	99.60	106.73
37	L	801	3PH	O31-C31-O32	-2.68	116.83	123.59
37	f	203	3PH	O31-C31-O32	-2.68	116.84	123.59
37	g	611	3PH	O13-P-O11	-2.67	99.62	106.73
37	m	309	3PH	O31-C31-O32	-2.65	116.89	123.59
37	i	304	3PH	O31-C31-O32	-2.63	116.96	123.59
44	k	605	HEA	C27-C19-C20	2.62	119.68	115.27
37	M	605	3PH	O31-C31-O32	-2.62	116.97	123.59
33	j	1001	PC1	C2-O21-C21	2.62	124.24	117.79
36	F	502	FMN	C4A-C4-N3	2.62	119.83	113.19
37	P	402	3PH	O31-C3-C2	2.61	116.04	108.43
32	d	504	U10	C7-C6-C5	-2.61	115.34	118.48
29	g	602	PGT	O2-C31-O31	-2.61	117.40	123.70
37	L	807	3PH	O14-P-O11	-2.61	99.80	106.73
29	J	201	PGT	O2-C31-O31	-2.60	117.42	123.70
33	l	303	PC1	C2-O21-C21	2.59	124.18	117.79
44	g	610	HEA	CAD-C3D-C4D	2.58	129.18	124.66
41	a	515	HEM	C1B-NB-C4B	2.58	107.74	105.07
37	L	810	3PH	O31-C31-O32	-2.57	117.10	123.59
38	L	809	P5S	O15-P12-O13	2.57	124.92	112.24
37	a	510	3PH	O13-P-O11	-2.56	99.92	106.73
38	a	513	P5S	O15-P12-O13	2.56	124.88	112.24
30	h	304	DU0	C22-C21-C20	2.56	115.49	111.52
37	N	503	3PH	O14-P-O11	-2.55	99.95	106.73
30	h	304	DU0	C81-C80-C79	2.54	117.51	113.11
37	m	301	3PH	O31-C31-O32	-2.53	117.20	123.59
37	c	206	3PH	O31-C31-O32	-2.53	117.20	123.59
30	i	315	DU0	O10-C11-C12	-2.53	108.54	112.18
37	a	510	3PH	O31-C3-C2	2.52	115.76	108.43
41	d	507	HEM	C1B-NB-C4B	2.51	107.67	105.07
37	k	601	3PH	O31-C31-O32	-2.51	117.25	123.59
33	h	302	PC1	O31-C3-C2	2.51	115.74	108.43
37	i	301	3PH	O31-C31-O32	-2.51	117.26	123.59
44	k	605	HEA	C17-C18-C19	-2.50	121.65	127.66
30	c	205	DU0	C76-C75-C22	2.49	114.57	110.33
39	J	202	T7X	C9-C8-C7	2.49	117.68	111.79
44	g	610	HEA	CMB-C2B-C3B	2.49	135.09	130.34
32	d	506	U10	C41-C39-C38	2.48	126.14	121.12
37	M	605	3PH	O14-P-O11	-2.48	100.14	106.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	a	504	3PH	C2-O21-C21	2.48	123.89	117.79
30	h	304	DU0	C11-O10-C09	2.47	118.40	113.72
41	d	507	HEM	C3B-C2B-C1B	2.47	108.32	106.49
32	a	512	U10	C40-C39-C41	2.47	119.42	115.27
29	a	514	PGT	O3-C3-C2	2.47	115.61	108.43
37	M	606	3PH	O31-C31-O32	-2.47	117.37	123.59
37	L	811	3PH	O21-C21-O22	-2.45	117.77	123.70
37	j	1003	3PH	O14-P-O11	-2.45	100.20	106.73
37	o	201	3PH	O31-C31-O32	-2.45	117.41	123.59
37	i	303	3PH	O31-C31-O32	-2.45	117.41	123.59
28	m	307	3PE	O31-C31-O32	-2.44	117.42	123.59
44	g	610	HEA	CHC-C1C-C2C	-2.44	120.33	127.24
37	H	409	3PH	O31-C31-O32	-2.44	117.43	123.59
36	F	502	FMN	O4-C4-C4A	-2.44	120.13	126.60
28	p	1001	3PE	O31-C31-O32	-2.44	117.44	123.59
28	L	808	3PE	O31-C31-O32	-2.43	117.47	123.59
44	g	610	HEA	C25-C23-C24	2.43	119.96	114.60
30	k	608	DU0	C22-C21-C20	2.42	115.28	111.52
28	a	503	3PE	O31-C31-O32	-2.42	117.48	123.59
37	d	508	3PH	O31-C31-O32	-2.42	117.48	123.59
30	g	617	DU0	C75-C22-C21	2.42	114.59	110.99
28	H	404	3PE	O21-C21-O22	-2.42	117.86	123.70
37	a	506	3PH	O31-C31-O32	-2.41	117.51	123.59
30	g	616	DU0	C22-C21-C20	2.41	115.26	111.52
43	d	501	CDL	OA6-CA5-C11	2.40	116.68	111.50
33	i	313	PC1	C23-C22-C21	-2.40	104.88	113.62
28	m	304	3PE	O31-C31-O32	-2.40	117.53	123.59
44	k	604	HEA	CHB-C1B-C2B	-2.40	121.23	124.98
37	d	502	3PH	O31-C31-O32	-2.40	117.53	123.59
28	A	201	3PE	O31-C31-O32	-2.40	117.54	123.59
28	d	510	3PE	O31-C31-O32	-2.40	117.54	123.59
38	I	201	P5S	O15-P12-O13	2.40	124.09	112.24
44	g	610	HEA	CHB-C1B-NB	2.39	127.02	124.42
37	m	309	3PH	O13-P-O11	-2.39	100.38	106.73
37	i	318	3PH	O14-P-O11	-2.39	100.39	106.73
42	e	504	HEC	CAD-CBD-CGD	-2.38	108.47	113.60
30	g	616	DU0	C02-C03-C17	2.38	117.91	114.38
44	k	605	HEA	C25-C23-C24	2.38	119.86	114.60
37	g	603	3PH	C2-O21-C21	2.38	123.64	117.79
44	k	605	HEA	CHC-C1C-C2C	-2.37	120.53	127.24
29	L	804	PGT	C2-O2-C31	-2.37	111.95	117.79
37	m	309	3PH	O14-P-O11	-2.37	100.44	106.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	H	409	3PH	O14-P-O11	-2.36	100.44	106.73
37	M	603	3PH	O14-P-O13	2.36	116.66	107.64
41	d	507	HEM	C4A-NA-C1A	2.36	107.66	105.35
44	k	605	HEA	CHB-C1B-C2B	-2.36	121.30	124.98
33	b	501	PC1	O31-C31-O32	-2.35	117.66	123.59
30	h	304	DU0	C76-C75-C22	2.35	114.33	110.33
37	d	502	3PH	O31-C3-C2	2.35	115.27	108.43
30	f	202	DU0	C77-C79-C17	-2.35	109.21	112.73
33	i	313	PC1	O31-C3-C2	2.34	115.24	108.43
37	d	508	3PH	O14-P-O11	-2.34	100.51	106.73
37	g	611	3PH	O14-P-O11	-2.34	100.51	106.73
33	j	1001	PC1	O31-C31-O32	-2.34	117.69	123.59
38	L	809	P5S	O19-C17-O18	-2.33	117.71	123.59
36	F	502	FMN	C4A-C10-N1	-2.33	119.33	124.73
37	M	605	3PH	O14-P-O13	2.33	116.53	107.64
37	j	1003	3PH	C2-O21-C21	2.32	123.51	117.79
30	H	401	DU0	C75-C22-C21	-2.32	107.53	110.99
44	g	606	HEA	C2B-C1B-NB	2.32	112.66	109.88
33	i	313	PC1	O31-C31-O32	-2.31	117.75	123.59
41	a	505	HEM	C3B-C2B-C1B	2.31	108.20	106.49
37	P	402	3PH	O14-P-O11	-2.31	100.58	106.73
29	M	602	PGT	C2-O2-C31	2.31	123.48	117.79
28	a	508	3PE	O31-C31-O32	-2.31	117.76	123.59
30	h	304	DU0	O10-C09-C07	2.31	115.48	107.38
28	g	601	3PE	C2-O21-C21	2.31	123.47	117.79
37	M	604	3PH	O13-P-O11	-2.30	100.61	106.73
28	d	503	3PE	O31-C31-O32	-2.30	117.78	123.59
33	m	312	PC1	C2-O21-C21	2.30	123.46	117.79
41	d	514	HEM	C4A-NA-C1A	2.29	107.59	105.35
37	m	301	3PH	O14-P-O11	-2.29	100.63	106.73
41	a	505	HEM	C4A-NA-C1A	2.29	107.59	105.35
29	L	804	PGT	O3-C11-O11	-2.29	117.82	123.59
37	a	506	3PH	O14-P-O11	-2.28	100.67	106.73
30	g	617	DU0	C14-C12-C11	-2.28	105.40	108.56
36	F	502	FMN	C10-C4A-N5	-2.27	120.04	124.86
33	M	608	PC1	O12-P-O13	-2.27	97.21	107.75
33	m	303	PC1	O12-P-O13	-2.27	97.21	107.75
41	a	505	HEM	C4D-ND-C1D	2.27	107.42	105.07
30	d	511	DU0	C24-C25-C26	-2.27	111.01	113.88
28	A	201	3PE	O12-P-O11	-2.27	97.22	107.75
37	L	807	3PH	O14-P-O13	2.27	116.30	107.64
37	P	402	3PH	O31-C31-O32	-2.26	117.88	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	g	610	HEA	C20-C19-C18	-2.26	116.54	121.12
38	a	513	P5S	O19-C17-O18	-2.26	117.89	123.59
30	c	202	DU0	C77-C79-C17	-2.26	109.35	112.73
33	d	516	PC1	O12-P-O13	-2.26	97.26	107.75
44	k	604	HEA	C3C-C4C-NC	2.25	111.63	110.25
28	L	802	3PE	O12-P-O11	-2.25	97.28	107.75
30	m	313	DU0	O10-C09-C15	-2.25	108.68	110.77
37	L	810	3PH	O14-P-O13	2.25	116.22	107.64
28	g	601	3PE	O31-C31-O32	-2.24	117.93	123.59
37	k	607	3PH	O31-C31-O32	-2.24	117.93	123.59
37	P	402	3PH	O14-P-O13	2.24	116.21	107.64
44	k	605	HEA	CMB-C2B-C3B	2.24	134.61	130.34
28	L	806	3PE	O31-C3-C2	2.24	114.95	108.43
41	a	505	HEM	CBD-CAD-C3D	-2.24	106.41	112.63
37	L	801	3PH	O21-C21-O22	-2.24	118.30	123.70
33	m	311	PC1	O12-P-O13	-2.24	97.36	107.75
41	a	505	HEM	CAA-CBA-CGA	-2.24	108.79	113.60
29	K	201	PGT	O3-C11-O11	-2.24	117.95	123.59
37	m	309	3PH	O14-P-O13	2.23	116.17	107.64
41	d	514	HEM	CAD-CBD-CGD	-2.23	108.81	113.60
37	d	502	3PH	C2-O21-C21	2.23	123.28	117.79
28	a	503	3PE	O21-C21-O22	-2.23	118.32	123.70
28	i	306	3PE	O31-C31-O32	-2.22	117.98	123.59
33	b	504	PC1	O21-C21-O22	-2.22	118.33	123.70
33	k	609	PC1	O31-C31-O32	-2.22	117.98	123.59
42	e	504	HEC	C1D-C2D-C3D	-2.22	104.62	106.96
37	d	508	3PH	O31-C3-C2	2.22	114.90	108.43
33	a	507	PC1	O12-P-O13	-2.22	97.42	107.75
37	g	603	3PH	O31-C31-O32	-2.22	117.98	123.59
37	i	318	3PH	O31-C3-C2	2.22	114.89	108.43
33	h	302	PC1	C3-C2-C1	-2.22	106.54	111.79
32	a	511	U10	C4M-O4-C4	2.21	124.31	116.47
44	k	605	HEA	C3B-C4B-NB	2.21	112.46	109.84
37	o	201	3PH	O14-P-O11	-2.21	100.86	106.73
29	J	201	PGT	O3-C11-O11	-2.21	118.02	123.59
37	N	503	3PH	O31-C31-O32	-2.20	118.03	123.59
29	M	602	PGT	O3-C11-O11	-2.20	118.03	123.59
28	i	317	3PE	O31-C31-O32	-2.20	118.04	123.59
37	a	506	3PH	O14-P-O13	2.20	116.05	107.64
41	d	514	HEM	C4D-ND-C1D	2.20	107.34	105.07
37	H	409	3PH	O14-P-O13	2.20	116.03	107.64
41	a	515	HEM	C3B-C2B-C1B	2.19	108.11	106.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	m	305	3PE	O12-P-O11	-2.19	97.57	107.75
37	i	301	3PH	O14-P-O13	2.19	116.01	107.64
41	a	515	HEM	C4A-NA-C1A	2.19	107.49	105.35
28	i	306	3PE	O12-P-O11	-2.19	97.57	107.75
41	d	507	HEM	C4D-ND-C1D	2.19	107.33	105.07
28	d	515	3PE	O31-C31-O32	-2.18	118.08	123.59
30	h	304	DU0	C79-C17-C03	2.18	112.01	109.09
30	j	1002	DU0	C22-C21-C20	2.18	114.90	111.52
30	m	302	DU0	C76-C75-C22	2.18	114.04	110.33
37	f	203	3PH	O14-P-O13	2.17	115.95	107.64
37	i	314	3PH	O14-P-O13	2.17	115.95	107.64
44	k	604	HEA	C12-C13-C14	2.17	117.97	112.23
44	g	606	HEA	CHB-C1B-NB	2.17	126.78	124.42
33	m	312	PC1	O12-P-O13	-2.17	97.67	107.75
44	g	606	HEA	C3C-C4C-NC	2.17	111.58	110.25
33	M	608	PC1	O31-C31-O32	-2.17	118.12	123.59
37	o	201	3PH	O14-P-O13	2.17	115.92	107.64
43	d	501	CDL	CA4-OA6-CA5	2.16	123.12	117.79
37	i	301	3PH	O14-P-O11	-2.16	100.97	106.73
33	M	609	PC1	O31-C31-O32	-2.16	118.14	123.59
33	a	507	PC1	O31-C31-O32	-2.16	118.14	123.59
37	c	206	3PH	O21-C21-O22	-2.16	118.48	123.70
28	m	310	3PE	O31-C31-O32	-2.16	118.14	123.59
29	M	602	PGT	O3-C3-C2	2.16	114.72	108.43
28	c	201	3PE	O12-P-O11	-2.16	97.73	107.75
28	i	309	3PE	O31-C31-O32	-2.16	118.15	123.59
37	i	304	3PH	O14-P-O13	2.15	115.87	107.64
33	H	402	PC1	O12-P-O13	-2.15	97.75	107.75
37	N	503	3PH	O14-P-O13	2.15	115.86	107.64
37	i	314	3PH	O31-C31-O32	-2.15	118.16	123.59
33	N	501	PC1	O31-C31-O32	-2.15	118.17	123.59
37	i	303	3PH	O14-P-O13	2.15	115.84	107.64
30	A	203	DU0	O10-C09-O16	-2.15	103.80	109.78
37	j	1003	3PH	O14-P-O13	2.14	115.83	107.64
39	g	615	T7X	O16-C10-O17	-2.14	118.53	123.70
37	d	508	3PH	O14-P-O13	2.14	115.82	107.64
37	g	611	3PH	O14-P-O13	2.14	115.81	107.64
28	g	613	3PE	O31-C31-O32	-2.14	118.20	123.59
36	F	502	FMN	C4-C4A-C10	2.13	120.38	116.79
42	e	504	HEC	C4B-NB-C1B	2.13	107.28	105.07
37	a	510	3PH	O14-P-O13	2.13	115.79	107.64
37	M	604	3PH	C2-O21-C21	2.13	123.04	117.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	J	202	T7X	O18-C11-O19	-2.13	118.21	123.59
33	g	612	PC1	C3-C2-C1	-2.13	106.75	111.79
37	L	801	3PH	O14-P-O13	2.13	115.77	107.64
44	k	605	HEA	C2B-C1B-NB	2.13	112.43	109.88
33	c	203	PC1	O31-C31-O32	-2.13	118.22	123.59
28	e	502	3PE	O12-P-O11	-2.13	97.87	107.75
37	M	604	3PH	O14-P-O11	-2.13	101.08	106.73
37	m	309	3PH	O31-C3-C2	2.13	114.62	108.43
33	L	803	PC1	O12-P-O13	-2.13	97.87	107.75
28	L	802	3PE	O21-C21-O22	-2.13	118.57	123.70
33	N	502	PC1	O12-P-O13	-2.12	97.88	107.75
41	d	507	HEM	C4C-NC-C1C	2.12	107.43	105.35
30	c	205	DU0	C76-C77-C79	2.12	111.69	108.73
37	k	607	3PH	O14-P-O11	-2.12	101.08	106.73
44	k	604	HEA	CBD-CAD-C3D	-2.12	106.73	112.63
28	h	307	3PE	O31-C31-O32	-2.12	118.24	123.59
37	k	601	3PH	O14-P-O13	2.12	115.74	107.64
37	c	206	3PH	O14-P-O13	2.12	115.74	107.64
44	k	605	HEA	C4B-C3B-C2B	-2.12	103.79	107.41
33	j	1001	PC1	O12-P-O13	-2.12	97.91	107.75
37	k	601	3PH	O21-C2-C3	-2.12	100.74	108.40
29	g	602	PGT	O3-C3-C2	-2.12	102.28	108.43
44	g	610	HEA	C2B-C1B-NB	2.11	112.42	109.88
44	g	606	HEA	C25-C23-C24	2.11	119.27	114.60
28	k	603	3PE	O31-C31-O32	-2.11	118.27	123.59
37	i	318	3PH	O21-C21-O22	-2.11	118.61	123.70
37	M	606	3PH	O14-P-O13	2.11	115.69	107.64
44	k	604	HEA	C2D-C1D-ND	2.11	112.34	109.84
30	g	617	DU0	O10-C11-C12	-2.11	109.14	112.18
28	n	1002	3PE	O31-C31-O32	-2.10	118.28	123.59
37	a	504	3PH	O14-P-O11	-2.10	101.15	106.73
37	a	504	3PH	O14-P-O13	2.10	115.66	107.64
43	d	501	CDL	OA8-CA7-C31	2.10	118.49	111.91
30	g	604	DU0	C08-C07-C06	-2.10	109.84	114.50
41	a	505	HEM	C3D-C4D-ND	-2.09	107.83	110.17
33	b	504	PC1	O12-P-O13	-2.09	98.02	107.75
28	H	405	3PE	O12-P-O11	-2.09	98.02	107.75
37	L	810	3PH	O21-C21-O22	-2.09	118.65	123.70
37	M	603	3PH	O21-C21-O22	-2.09	118.65	123.70
30	A	203	DU0	C04-C03-C02	-2.09	101.13	103.91
44	g	606	HEA	C26-C15-C16	2.09	118.78	115.27
28	a	502	3PE	O12-P-O11	-2.09	98.05	107.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	m	301	3PH	O14-P-O13	2.09	115.61	107.64
30	c	205	DU0	C80-C79-C17	-2.09	108.75	111.75
30	g	605	DU0	C75-C76-C77	2.09	117.26	112.74
29	P	401	PGT	O2-C31-O31	-2.08	118.67	123.70
37	c	206	3PH	O14-P-O11	-2.08	101.19	106.73
28	a	503	3PE	O12-P-O13	-2.08	98.08	107.75
29	J	205	PGT	O3-C11-O11	-2.08	118.34	123.59
41	d	514	HEM	C2B-C1B-NB	-2.08	107.38	109.84
30	c	205	DU0	C21-C20-C77	2.07	119.18	116.42
37	L	811	3PH	O14-P-O11	-2.07	101.21	106.73
30	a	516	DU0	O10-C09-O16	-2.07	104.00	109.78
30	h	304	DU0	C08-C07-C06	-2.07	109.90	114.50
37	M	605	3PH	O13-P-O11	-2.07	101.22	106.73
44	k	604	HEA	C25-C23-C24	2.07	119.18	114.60
37	k	607	3PH	O32-C31-C32	2.07	131.81	123.73
41	a	505	HEM	C4C-NC-C1C	2.07	107.37	105.35
37	f	205	3PH	O14-P-O13	2.07	115.54	107.64
28	H	408	3PE	O31-C31-O32	-2.06	118.38	123.59
33	d	516	PC1	O21-C21-O22	-2.06	118.72	123.70
30	A	203	DU0	C79-C17-C03	2.06	111.85	109.09
37	i	318	3PH	O14-P-O13	2.06	115.52	107.64
37	d	513	3PH	O21-C21-O22	-2.06	118.72	123.70
30	d	511	DU0	C22-C21-C20	2.06	114.72	111.52
33	f	201	PC1	O12-P-O13	-2.06	98.18	107.75
30	d	505	DU0	C22-C21-C20	2.06	114.71	111.52
37	f	205	3PH	O14-P-O11	-2.05	101.27	106.73
28	m	305	3PE	O31-C31-O32	-2.05	118.42	123.59
44	k	604	HEA	CHC-C1C-C2C	-2.05	121.45	127.24
37	g	603	3PH	O14-P-O13	2.05	115.47	107.64
28	m	310	3PE	O12-P-O11	-2.05	98.23	107.75
41	a	515	HEM	C4C-NC-C1C	2.05	107.35	105.35
37	L	807	3PH	O21-C21-O22	-2.05	118.75	123.70
28	H	405	3PE	O31-C31-O32	-2.05	118.42	123.59
29	L	804	PGT	O4P-P-O1P	-2.05	101.08	109.07
37	i	314	3PH	C2-O21-C21	2.04	122.82	117.79
44	g	606	HEA	CHC-C1C-C2C	-2.04	121.47	127.24
30	g	616	DU0	C80-C79-C77	2.04	115.77	113.08
33	k	606	PC1	C2-O21-C21	2.04	122.81	117.79
37	M	605	3PH	O21-C21-O22	-2.04	118.78	123.70
28	H	407	3PE	O31-C31-O32	-2.04	118.45	123.59
32	a	511	U10	C7-C6-C5	-2.04	116.03	118.48
42	b	502	HEC	CHC-C4B-NB	2.03	126.88	124.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	d	515	3PE	O21-C21-O22	-2.03	118.79	123.70
37	a	504	3PH	O31-C3-C2	2.03	114.35	108.43
33	D	1001	PC1	O31-C31-O32	-2.03	118.47	123.59
28	H	408	3PE	O21-C21-O22	-2.03	118.79	123.70
30	J	204	DU0	O10-C09-O16	-2.03	104.12	109.78
42	b	502	HEC	C4A-NA-C1A	2.03	107.33	105.35
33	g	612	PC1	C2-O21-C21	2.03	122.79	117.79
37	L	811	3PH	O14-P-O13	2.03	115.39	107.64
28	e	505	3PE	O12-P-O11	-2.03	98.33	107.75
30	J	204	DU0	C24-O23-C22	2.03	120.06	115.40
29	H	406	PGT	O3-C11-O11	-2.03	118.48	123.59
28	i	317	3PE	O12-P-O11	-2.03	98.34	107.75
28	a	502	3PE	O21-C21-O22	-2.03	118.81	123.70
33	g	612	PC1	O12-P-O13	-2.02	98.34	107.75
28	d	503	3PE	O12-P-O11	-2.02	98.35	107.75
28	h	301	3PE	O12-P-O11	-2.02	98.35	107.75
37	d	513	3PH	O14-P-O13	2.02	115.35	107.64
28	H	407	3PE	C2-O21-C21	2.02	122.76	117.79
28	L	806	3PE	O12-P-O11	-2.02	98.37	107.75
33	i	308	PC1	O12-P-O13	-2.02	98.38	107.75
30	j	1002	DU0	C08-C07-C09	-2.01	111.24	114.92
28	L	808	3PE	O12-P-O13	-2.01	98.39	107.75
30	c	202	DU0	O10-C09-O16	-2.01	104.16	109.78
32	d	506	U10	C41-C42-C43	2.01	118.50	111.88
38	a	513	P5S	CB-CA-C	-2.01	107.01	110.93
33	l	304	PC1	O12-P-O13	-2.01	98.41	107.75
37	M	604	3PH	O21-C2-C1	2.01	115.68	108.40
41	d	514	HEM	CBD-CAD-C3D	-2.01	107.05	112.63
28	d	515	3PE	O12-P-O11	-2.01	98.42	107.75
44	k	605	HEA	C13-C14-C15	-2.00	122.84	127.66
28	h	307	3PE	O12-P-O13	-2.00	98.45	107.75
28	L	805	3PE	O12-P-O11	-2.00	98.45	107.75
28	h	301	3PE	O31-C31-O32	-2.00	118.54	123.59

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
42	b	502	HEC	NA

All (1541) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	A	201	3PE	C1-O11-P-O14
28	A	201	3PE	C11-O13-P-O12
28	H	404	3PE	C1-O11-P-O12
28	H	404	3PE	C11-O13-P-O14
28	H	404	3PE	C2-C1-O11-P
28	H	407	3PE	C11-O13-P-O11
28	H	407	3PE	C11-O13-P-O12
28	H	407	3PE	C2-C1-O11-P
28	H	407	3PE	C12-C11-O13-P
28	L	802	3PE	C1-O11-P-O14
28	L	802	3PE	C12-C11-O13-P
28	L	805	3PE	C11-O13-P-O11
28	L	805	3PE	C11-O13-P-O12
28	L	805	3PE	C2-C1-O11-P
28	L	805	3PE	C12-C11-O13-P
28	L	806	3PE	C1-O11-P-O12
28	L	806	3PE	C11-O13-P-O12
28	L	806	3PE	C12-C11-O13-P
28	P	403	3PE	C11-O13-P-O12
28	P	403	3PE	C12-C11-O13-P
28	P	403	3PE	O21-C2-C3-O31
28	a	502	3PE	C11-O13-P-O11
28	a	502	3PE	C11-O13-P-O12
28	a	502	3PE	C2-C1-O11-P
28	a	502	3PE	C12-C11-O13-P
28	a	502	3PE	O21-C2-C3-O31
28	a	503	3PE	C2-C1-O11-P
28	a	503	3PE	C12-C11-O13-P
28	a	508	3PE	C1-O11-P-O12
28	a	508	3PE	C1-O11-P-O13
28	a	508	3PE	C11-O13-P-O11
28	a	508	3PE	C11-O13-P-O14
28	a	509	3PE	C11-O13-P-O12
28	a	509	3PE	C12-C11-O13-P
28	c	201	3PE	C12-C11-O13-P
28	d	510	3PE	C1-O11-P-O13
28	d	510	3PE	C1-O11-P-O14
28	d	510	3PE	C2-C1-O11-P
28	d	510	3PE	C12-C11-O13-P
28	d	510	3PE	O21-C2-C3-O31
28	e	505	3PE	C1-O11-P-O14
28	e	505	3PE	C11-O13-P-O12
28	e	505	3PE	C11-O13-P-O14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	e	505	3PE	O13-C11-C12-N
28	g	607	3PE	C11-O13-P-O11
28	g	607	3PE	C11-O13-P-O14
28	g	607	3PE	C12-C11-O13-P
28	g	613	3PE	C11-O13-P-O14
28	h	301	3PE	C1-O11-P-O12
28	h	301	3PE	C11-O13-P-O14
28	h	307	3PE	C1-O11-P-O14
28	i	306	3PE	C11-O13-P-O12
28	i	306	3PE	C12-C11-O13-P
28	i	307	3PE	C12-C11-O13-P
28	i	309	3PE	C11-O13-P-O11
28	i	309	3PE	C11-O13-P-O12
28	i	309	3PE	C12-C11-O13-P
28	i	311	3PE	C2-C1-O11-P
28	i	317	3PE	C1-O11-P-O12
28	i	317	3PE	C11-O13-P-O12
28	k	603	3PE	C1-O11-P-O12
28	k	603	3PE	O21-C2-C3-O31
28	m	304	3PE	C1-O11-P-O12
28	m	304	3PE	C1-O11-P-O14
28	m	305	3PE	C1-O11-P-O12
28	m	306	3PE	C11-O13-P-O12
28	m	306	3PE	C2-C1-O11-P
28	m	306	3PE	C12-C11-O13-P
28	m	307	3PE	C11-O13-P-O12
28	m	307	3PE	C11-O13-P-O14
28	m	315	3PE	C11-O13-P-O11
28	m	315	3PE	C11-O13-P-O12
28	m	315	3PE	C12-C11-O13-P
28	n	1002	3PE	C2-C1-O11-P
28	p	1001	3PE	C1-O11-P-O14
28	p	1001	3PE	C11-O13-P-O12
28	p	1001	3PE	C2-C1-O11-P
28	p	1001	3PE	C12-C11-O13-P
29	A	202	PGT	C2-C1-O3P-P
29	A	202	PGT	C5-C4-O4P-P
29	H	406	PGT	C1-O3P-P-O2P
29	J	201	PGT	C1-O3P-P-O2P
29	J	205	PGT	C2-C1-O3P-P
29	J	205	PGT	C5-C4-O4P-P
29	L	804	PGT	C5-C4-O4P-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	M	602	PGT	C5-C4-O4P-P
29	P	401	PGT	O2-C2-C3-O3
29	P	401	PGT	C4-O4P-P-O3P
29	P	401	PGT	C4-O4P-P-O1P
29	P	401	PGT	C4-O4P-P-O2P
29	P	401	PGT	C5-C4-O4P-P
29	a	514	PGT	C4-O4P-P-O2P
29	g	602	PGT	C32-C31-O2-C2
29	g	602	PGT	C1-O3P-P-O1P
29	q	1000	PGT	C5-C4-O4P-P
32	B	1002	U10	C1-C6-C7-C8
32	B	1002	U10	C5-C6-C7-C8
32	B	1002	U10	C16-C17-C18-C19
32	a	511	U10	C36-C37-C38-C39
32	d	506	U10	C29-C31-C32-C33
33	D	1001	PC1	C11-O13-P-O14
33	D	1001	PC1	C11-O13-P-O11
33	D	1001	PC1	C12-C11-O13-P
33	D	1001	PC1	O13-C11-C12-N
33	H	402	PC1	C11-O13-P-O12
33	H	402	PC1	C1-O11-P-O12
33	H	403	PC1	C11-O13-P-O12
33	H	403	PC1	C1-O11-P-O12
33	H	403	PC1	C12-C11-O13-P
33	L	803	PC1	C11-O13-P-O14
33	M	608	PC1	C12-C11-O13-P
33	M	609	PC1	C11-O13-P-O14
33	N	501	PC1	C1-O11-P-O12
33	N	502	PC1	C1-O11-P-O12
33	N	504	PC1	C12-C11-O13-P
33	N	504	PC1	O13-C11-C12-N
33	a	501	PC1	C12-C11-O13-P
33	a	507	PC1	C11-O13-P-O12
33	a	507	PC1	C11-O13-P-O14
33	a	507	PC1	C11-O13-P-O11
33	a	507	PC1	C1-O11-P-O14
33	a	507	PC1	C12-C11-O13-P
33	a	507	PC1	C2-C1-O11-P
33	a	517	PC1	C1-O11-P-O12
33	a	517	PC1	C1-O11-P-O14
33	a	517	PC1	C12-C11-O13-P
33	a	517	PC1	O13-C11-C12-N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	a	517	PC1	C2-C1-O11-P
33	b	501	PC1	C11-O13-P-O12
33	b	501	PC1	C11-O13-P-O14
33	b	504	PC1	C2-C1-O11-P
33	c	203	PC1	C11-O13-P-O12
33	c	203	PC1	C11-O13-P-O14
33	c	203	PC1	C11-O13-P-O11
33	d	509	PC1	C11-O13-P-O14
33	d	509	PC1	C11-O13-P-O11
33	d	509	PC1	O13-C11-C12-N
33	d	516	PC1	C1-O11-P-O14
33	f	201	PC1	C11-O13-P-O12
33	f	201	PC1	C1-O11-P-O12
33	g	612	PC1	O13-C11-C12-N
33	h	302	PC1	C11-O13-P-O12
33	h	302	PC1	C1-O11-P-O12
33	h	302	PC1	C1-O11-P-O13
33	h	302	PC1	C12-C11-O13-P
33	i	308	PC1	C11-O13-P-O14
33	i	308	PC1	C1-O11-P-O14
33	i	310	PC1	C11-O13-P-O14
33	i	310	PC1	C11-O13-P-O11
33	i	310	PC1	C1-O11-P-O12
33	i	310	PC1	C12-C11-O13-P
33	i	313	PC1	C11-O13-P-O12
33	i	313	PC1	C1-O11-P-O14
33	i	313	PC1	O21-C2-C3-O31
33	j	1001	PC1	C12-C11-O13-P
33	k	606	PC1	C2-C1-O11-P
33	k	609	PC1	C11-O13-P-O12
33	k	609	PC1	C12-C11-O13-P
33	k	609	PC1	O13-C11-C12-N
33	l	301	PC1	C12-C11-O13-P
33	l	301	PC1	O13-C11-C12-N
33	l	301	PC1	C2-C1-O11-P
33	l	303	PC1	C11-O13-P-O12
33	l	303	PC1	C1-O11-P-O14
33	l	304	PC1	C11-O13-P-O14
33	l	304	PC1	C2-C1-O11-P
33	m	303	PC1	O13-C11-C12-N
33	m	303	PC1	C2-C1-O11-P
33	m	303	PC1	O21-C2-C3-O31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	m	311	PC1	C11-O13-P-O14
33	m	311	PC1	C1-O11-P-O14
33	m	312	PC1	C11-O13-P-O14
33	m	312	PC1	C12-C11-O13-P
33	m	314	PC1	C11-O13-P-O14
33	n	1001	PC1	C11-O13-P-O12
33	n	1001	PC1	C1-O11-P-O14
33	n	1001	PC1	C12-C11-O13-P
37	L	801	3PH	C1-O11-P-O12
37	M	605	3PH	C2-C1-O11-P
37	M	606	3PH	C1-O11-P-O13
37	M	606	3PH	C1-O11-P-O14
37	M	606	3PH	C1-O11-P-O12
37	P	402	3PH	C1-O11-P-O13
37	P	402	3PH	C1-O11-P-O14
37	a	504	3PH	C2-C1-O11-P
37	a	510	3PH	C2-C1-O11-P
37	d	502	3PH	C2-C1-O11-P
37	f	203	3PH	C1-O11-P-O13
37	f	203	3PH	C1-O11-P-O14
37	f	203	3PH	C2-C1-O11-P
37	f	205	3PH	C1-O11-P-O13
37	f	205	3PH	C1-O11-P-O14
37	g	603	3PH	C2-C1-O11-P
37	g	611	3PH	O21-C2-C3-O31
37	i	303	3PH	C2-C1-O11-P
37	i	304	3PH	C2-C1-O11-P
37	i	314	3PH	C2-C1-O11-P
37	i	318	3PH	C1-O11-P-O12
37	i	318	3PH	C2-C1-O11-P
37	i	318	3PH	O21-C2-C3-O31
37	j	1003	3PH	C2-C1-O11-P
37	k	601	3PH	C2-C1-O11-P
38	I	201	P5S	C2-C3-O16-P12
38	I	201	P5S	CB-OG-P12-O15
39	g	615	T7X	C1-O1-P1-O12
39	g	615	T7X	C8-C7-O13-P1
39	g	615	T7X	C19-C20-C21-C22
41	a	515	HEM	C2C-C3C-CAC-CBC
41	a	515	HEM	C4C-C3C-CAC-CBC
41	d	507	HEM	C2C-C3C-CAC-CBC
41	d	507	HEM	C4C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
41	d	514	HEM	C2B-C3B-CAB-CBB
41	d	514	HEM	C4B-C3B-CAB-CBB
42	b	502	HEC	C2C-C3C-CAC-CBC
43	d	501	CDL	CB3-OB5-PB2-OB3
43	d	501	CDL	CB3-OB5-PB2-OB4
43	d	501	CDL	CB4-CB3-OB5-PB2
42	b	502	HEC	C2B-C3B-CAB-CBB
42	b	502	HEC	C4B-C3B-CAB-CBB
42	e	504	HEC	C2B-C3B-CAB-CBB
42	e	504	HEC	C2C-C3C-CAC-CBC
42	e	504	HEC	C4B-C3B-CAB-CBB
42	e	504	HEC	C4C-C3C-CAC-CBC
29	g	602	PGT	O31-C31-O2-C2
28	L	808	3PE	C2-C1-O11-P
28	a	509	3PE	C2-C1-O11-P
33	M	608	PC1	C2-C1-O11-P
33	c	203	PC1	C2-C1-O11-P
33	k	609	PC1	C2-C1-O11-P
33	m	312	PC1	C2-C1-O11-P
41	d	507	HEM	C2A-CAA-CBA-CGA
32	B	1002	U10	C14-C16-C17-C18
32	d	504	U10	C19-C21-C22-C23
29	A	202	PGT	O4P-C4-C5-C6
29	J	205	PGT	O4P-C4-C5-C6
30	g	617	DU0	O23-C24-C25-C26
42	b	502	HEC	C4C-C3C-CAC-CBC
28	m	315	3PE	O11-C1-C2-O21
29	A	202	PGT	O4P-C4-C5-O5
43	d	501	CDL	O1-C1-CB2-OB2
33	M	601	PC1	C31-C32-C33-C34
29	J	205	PGT	O2-C2-C3-O3
44	g	610	HEA	C18-C19-C20-C21
37	M	606	3PH	C38-C39-C3A-C3B
33	N	502	PC1	C21-C22-C23-C24
28	i	306	3PE	C21-C22-C23-C24
28	m	307	3PE	C21-C22-C23-C24
28	g	613	3PE	C2-C1-O11-P
33	a	501	PC1	C21-C22-C23-C24
32	d	504	U10	C49-C51-C52-C53
32	d	506	U10	C9-C11-C12-C13
32	d	506	U10	C39-C41-C42-C43
28	m	304	3PE	C29-C2A-C2B-C2C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	c	201	3PE	C11-O13-P-O11
28	d	515	3PE	C11-O13-P-O11
28	e	505	3PE	C11-O13-P-O11
28	g	613	3PE	C11-O13-P-O11
28	h	307	3PE	C1-O11-P-O13
28	i	317	3PE	C1-O11-P-O13
28	i	317	3PE	C11-O13-P-O11
28	m	304	3PE	C1-O11-P-O13
28	m	307	3PE	C11-O13-P-O11
28	p	1001	3PE	C1-O11-P-O13
29	H	406	PGT	C1-O3P-P-O4P
29	M	602	PGT	C1-O3P-P-O4P
29	a	514	PGT	C4-O4P-P-O3P
33	H	403	PC1	C1-O11-P-O13
33	L	803	PC1	C11-O13-P-O11
33	L	803	PC1	C1-O11-P-O13
33	a	517	PC1	C1-O11-P-O13
33	b	501	PC1	C11-O13-P-O11
33	f	201	PC1	C11-O13-P-O11
33	i	310	PC1	C1-O11-P-O13
33	l	303	PC1	C1-O11-P-O13
33	m	311	PC1	C11-O13-P-O11
33	m	314	PC1	C11-O13-P-O11
38	I	201	P5S	CB-OG-P12-O16
43	d	501	CDL	CB3-OB5-PB2-OB2
38	I	201	P5S	C17-C20-C21-C22
28	n	1002	3PE	C33-C34-C35-C36
33	i	313	PC1	C2E-C2F-C2G-C2H
33	k	609	PC1	C3C-C3D-C3E-C3F
37	d	508	3PH	C3C-C3D-C3E-C3F
29	M	602	PGT	C42-C43-C44-C45
33	h	302	PC1	C3B-C3C-C3D-C3E
43	d	501	CDL	C18-C19-C20-C21
29	H	406	PGT	C3-C2-O2-C31
37	j	1003	3PH	C31-C32-C33-C34
28	c	201	3PE	C23-C24-C25-C26
29	q	1000	PGT	C41-C42-C43-C44
28	H	405	3PE	C2-C1-O11-P
28	e	502	3PE	C2-C1-O11-P
28	m	315	3PE	C2-C1-O11-P
29	P	401	PGT	C2-C1-O3P-P
28	m	305	3PE	C3A-C3B-C3C-C3D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	i	301	3PH	C3B-C3C-C3D-C3E
37	k	601	3PH	C2B-C2C-C2D-C2E
29	J	205	PGT	O4P-C4-C5-O5
29	P	401	PGT	O4P-C4-C5-O5
28	H	407	3PE	C3A-C3B-C3C-C3D
37	f	205	3PH	C37-C38-C39-C3A
33	L	803	PC1	O21-C2-C3-O31
28	c	201	3PE	C3D-C3E-C3F-C3G
37	L	801	3PH	C3B-C3C-C3D-C3E
37	i	318	3PH	C37-C38-C39-C3A
39	J	202	T7X	C2-C1-O1-P1
39	J	202	T7X	C6-C1-O1-P1
28	c	201	3PE	C29-C2A-C2B-C2C
33	m	312	PC1	C22-C23-C24-C25
33	m	312	PC1	C3D-C3E-C3F-C3G
37	f	205	3PH	C25-C26-C27-C28
39	g	615	T7X	C11-C31-C32-C33
28	L	802	3PE	C35-C36-C37-C38
28	d	515	3PE	C39-C3A-C3B-C3C
37	N	503	3PH	C36-C37-C38-C39
30	h	306	DU0	C25-C24-O23-C22
30	m	313	DU0	C25-C24-O23-C22
28	a	503	3PE	C2D-C2E-C2F-C2G
28	i	307	3PE	C2C-C2D-C2E-C2F
33	b	501	PC1	C3A-C3B-C3C-C3D
33	b	504	PC1	C27-C28-C29-C2A
33	i	308	PC1	C32-C33-C34-C35
37	m	309	3PH	C33-C34-C35-C36
29	L	804	PGT	C11-C12-C13-C14
28	A	201	3PE	C23-C24-C25-C26
28	H	407	3PE	C2C-C2D-C2E-C2F
28	L	808	3PE	C28-C29-C2A-C2B
28	d	503	3PE	C26-C27-C28-C29
29	J	205	PGT	C21-C22-C23-C24
29	g	602	PGT	C39-C40-C41-C42
28	i	306	3PE	C2D-C2E-C2F-C2G
33	a	517	PC1	C26-C27-C28-C29
37	L	811	3PH	C3B-C3C-C3D-C3E
29	J	201	PGT	C43-C44-C45-C46
37	M	603	3PH	C3D-C3E-C3F-C3G
33	M	609	PC1	C21-C22-C23-C24
33	k	609	PC1	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	a	504	3PH	C3C-C3D-C3E-C3F
37	i	301	3PH	C2D-C2E-C2F-C2G
28	H	408	3PE	C24-C25-C26-C27
28	i	307	3PE	C27-C28-C29-C2A
29	g	602	PGT	C33-C34-C35-C36
29	q	1000	PGT	C38-C39-C40-C41
33	N	501	PC1	C2D-C2E-C2F-C2G
28	L	806	3PE	C2A-C2B-C2C-C2D
28	m	310	3PE	C3A-C3B-C3C-C3D
29	L	804	PGT	C33-C34-C35-C36
33	j	1001	PC1	C3E-C3F-C3G-C3H
33	l	304	PC1	C32-C33-C34-C35
33	m	303	PC1	C3C-C3D-C3E-C3F
37	d	513	3PH	C2C-C2D-C2E-C2F
37	i	303	3PH	C3C-C3D-C3E-C3F
28	h	307	3PE	C1-C2-C3-O31
29	g	602	PGT	C16-C17-C18-C19
37	N	503	3PH	C32-C33-C34-C35
37	f	203	3PH	C38-C39-C3A-C3B
28	H	407	3PE	C31-C32-C33-C34
28	g	601	3PE	C21-C22-C23-C24
28	A	201	3PE	C28-C29-C2A-C2B
28	h	307	3PE	C38-C39-C3A-C3B
33	M	609	PC1	C22-C23-C24-C25
33	M	609	PC1	C39-C3A-C3B-C3C
32	B	1002	U10	C45-C44-C46-C47
32	a	512	U10	C30-C29-C31-C32
32	B	1002	U10	C43-C44-C46-C47
33	M	609	PC1	C33-C34-C35-C36
33	l	303	PC1	C29-C2A-C2B-C2C
33	M	601	PC1	C21-C22-C23-C24
33	l	304	PC1	C25-C26-C27-C28
33	m	311	PC1	C2D-C2E-C2F-C2G
28	m	310	3PE	C3E-C3F-C3G-C3H
37	L	810	3PH	C3C-C3D-C3E-C3F
37	M	606	3PH	C25-C26-C27-C28
37	d	502	3PH	C32-C33-C34-C35
28	P	403	3PE	C3C-C3D-C3E-C3F
33	k	606	PC1	C39-C3A-C3B-C3C
28	h	307	3PE	C39-C3A-C3B-C3C
29	K	201	PGT	C17-C18-C19-C20
37	f	203	3PH	C3A-C3B-C3C-C3D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	a	502	3PE	C23-C24-C25-C26
28	g	601	3PE	C35-C36-C37-C38
33	a	501	PC1	C39-C3A-C3B-C3C
28	A	201	3PE	C2-C1-O11-P
29	g	602	PGT	C5-C4-O4P-P
37	M	604	3PH	C2-C1-O11-P
33	D	1001	PC1	C2A-C2B-C2C-C2D
29	H	406	PGT	C41-C42-C43-C44
37	M	606	3PH	C2D-C2E-C2F-C2G
28	i	317	3PE	C28-C29-C2A-C2B
28	k	603	3PE	C38-C39-C3A-C3B
33	k	609	PC1	C25-C26-C27-C28
33	m	312	PC1	C3A-C3B-C3C-C3D
37	g	603	3PH	C3D-C3E-C3F-C3G
28	a	509	3PE	C3D-C3E-C3F-C3G
32	d	504	U10	C25-C24-C26-C27
32	a	512	U10	C28-C29-C31-C32
32	d	504	U10	C23-C24-C26-C27
28	i	307	3PE	C2D-C2E-C2F-C2G
29	H	406	PGT	C11-C12-C13-C14
33	d	516	PC1	C21-C22-C23-C24
37	a	506	3PH	C2E-C2F-C2G-C2H
37	d	502	3PH	C2C-C2D-C2E-C2F
37	L	801	3PH	C22-C23-C24-C25
33	N	501	PC1	C2B-C2C-C2D-C2E
33	f	201	PC1	C3E-C3F-C3G-C3H
37	N	503	3PH	C37-C38-C39-C3A
37	M	603	3PH	C38-C39-C3A-C3B
41	a	505	HEM	C2C-C3C-CAC-CBC
28	L	806	3PE	C2-C3-O31-C31
33	b	501	PC1	C26-C27-C28-C29
37	g	611	3PH	C26-C27-C28-C29
28	n	1002	3PE	C29-C2A-C2B-C2C
37	j	1003	3PH	C27-C28-C29-C2A
37	g	603	3PH	C31-C32-C33-C34
28	L	802	3PE	C36-C37-C38-C39
37	P	402	3PH	C23-C24-C25-C26
41	a	505	HEM	C4C-C3C-CAC-CBC
28	H	408	3PE	C26-C27-C28-C29
33	M	608	PC1	C33-C34-C35-C36
33	a	517	PC1	C22-C23-C24-C25
37	o	201	3PH	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	h	307	3PE	O21-C2-C3-O31
28	n	1002	3PE	O21-C2-C3-O31
33	m	314	PC1	O21-C2-C3-O31
43	d	501	CDL	C13-C14-C15-C16
33	D	1001	PC1	C3B-C3C-C3D-C3E
37	N	503	3PH	C2B-C2C-C2D-C2E
44	g	610	HEA	C27-C19-C20-C21
32	d	504	U10	C13-C14-C16-C17
33	i	308	PC1	C2E-C2F-C2G-C2H
33	a	501	PC1	C3B-C3C-C3D-C3E
33	n	1001	PC1	C33-C34-C35-C36
28	h	307	3PE	C29-C2A-C2B-C2C
33	N	501	PC1	C29-C2A-C2B-C2C
33	f	201	PC1	C22-C23-C24-C25
37	m	309	3PH	C39-C3A-C3B-C3C
43	d	501	CDL	C22-C23-C24-C25
28	i	317	3PE	C38-C39-C3A-C3B
29	P	401	PGT	C22-C23-C24-C25
33	m	311	PC1	C3C-C3D-C3E-C3F
28	L	802	3PE	C1-O11-P-O13
29	J	201	PGT	C1-O3P-P-O4P
33	a	507	PC1	C1-O11-P-O13
33	h	302	PC1	C11-O13-P-O11
33	i	313	PC1	C1-O11-P-O13
33	l	304	PC1	C1-O11-P-O13
33	m	311	PC1	C1-O11-P-O13
28	d	503	3PE	C2-C1-O11-P
28	g	601	3PE	C2-C1-O11-P
29	L	804	PGT	C2-C1-O3P-P
33	j	1001	PC1	C2-C1-O11-P
37	f	205	3PH	C2-C1-O11-P
37	i	301	3PH	C2-C1-O11-P
37	m	309	3PH	C2-C1-O11-P
28	e	505	3PE	C2C-C2D-C2E-C2F
28	i	306	3PE	C25-C26-C27-C28
29	M	602	PGT	C16-C17-C18-C19
33	b	504	PC1	C37-C38-C39-C3A
33	l	303	PC1	C33-C34-C35-C36
28	L	808	3PE	O11-C1-C2-C3
28	a	503	3PE	O11-C1-C2-C3
28	m	315	3PE	O11-C1-C2-C3
28	n	1002	3PE	O11-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	A	202	PGT	O3P-C1-C2-C3
29	J	205	PGT	O3P-C1-C2-C3
33	h	302	PC1	O11-C1-C2-C3
38	I	201	P5S	C1-C2-C3-O16
37	m	309	3PH	C3D-C3E-C3F-C3G
28	A	201	3PE	C2A-C2B-C2C-C2D
29	P	401	PGT	C32-C33-C34-C35
33	l	304	PC1	C3D-C3E-C3F-C3G
38	L	809	P5S	C42-C43-C44-C45
28	i	307	3PE	C3C-C3D-C3E-C3F
29	P	401	PGT	O4P-C4-C5-C6
29	H	406	PGT	C18-C19-C20-C21
33	k	609	PC1	C3A-C3B-C3C-C3D
37	i	301	3PH	C38-C39-C3A-C3B
38	I	201	P5S	C45-C46-C48-C49
28	P	403	3PE	C1-C2-C3-O31
28	e	502	3PE	C1-C2-C3-O31
28	g	607	3PE	C1-C2-C3-O31
28	i	317	3PE	C1-C2-C3-O31
28	m	306	3PE	C1-C2-C3-O31
29	J	205	PGT	C1-C2-C3-O3
33	f	201	PC1	C1-C2-C3-O31
33	i	313	PC1	C1-C2-C3-O31
33	m	314	PC1	C37-C38-C39-C3A
37	L	810	3PH	C1-C2-C3-O31
37	i	303	3PH	C1-C2-C3-O31
37	i	318	3PH	C1-C2-C3-O31
37	j	1003	3PH	C1-C2-C3-O31
28	e	505	3PE	C38-C39-C3A-C3B
28	L	802	3PE	C2A-C2B-C2C-C2D
38	a	513	P5S	C26-C27-C28-C29
28	a	503	3PE	C21-C22-C23-C24
37	o	201	3PH	C31-C32-C33-C34
33	l	303	PC1	C2C-C2D-C2E-C2F
44	g	610	HEA	C15-C16-C17-C18
39	g	615	T7X	C24-C25-C26-C27
28	d	503	3PE	C21-C22-C23-C24
28	i	307	3PE	C3F-C3G-C3H-C3I
32	d	504	U10	C15-C14-C16-C17
38	I	201	P5S	C42-C43-C44-C45
37	P	402	3PH	C2-C3-O31-C31
33	k	606	PC1	C3D-C3E-C3F-C3G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	a	511	U10	C5-C6-C7-C8
33	c	203	PC1	C2C-C2D-C2E-C2F
28	L	808	3PE	C3A-C3B-C3C-C3D
29	N	505	PGT	C5-C4-O4P-P
33	h	302	PC1	C2-C1-O11-P
37	d	508	3PH	C1-O11-P-O12
37	f	203	3PH	C1-O11-P-O12
37	M	604	3PH	C37-C38-C39-C3A
37	M	604	3PH	C38-C39-C3A-C3B
37	i	314	3PH	C2-C3-O31-C31
28	A	201	3PE	O11-C1-C2-O21
28	H	405	3PE	O11-C1-C2-O21
28	i	309	3PE	O11-C1-C2-O21
28	m	306	3PE	O11-C1-C2-O21
29	q	1000	PGT	O3P-C1-C2-O2
33	d	509	PC1	O11-C1-C2-O21
33	i	313	PC1	O11-C1-C2-O21
33	m	312	PC1	C3B-C3C-C3D-C3E
28	m	310	3PE	C35-C36-C37-C38
37	i	304	3PH	C26-C27-C28-C29
28	g	607	3PE	O21-C2-C3-O31
28	h	301	3PE	O21-C2-C3-O31
28	m	306	3PE	O21-C2-C3-O31
37	L	810	3PH	O21-C2-C3-O31
43	d	501	CDL	OA6-CA4-CA6-OA8
37	a	510	3PH	C2C-C2D-C2E-C2F
39	J	202	T7X	C35-C36-C37-C38
29	L	804	PGT	C19-C20-C21-C22
33	i	310	PC1	C29-C2A-C2B-C2C
33	l	304	PC1	C2C-C2D-C2E-C2F
37	M	603	3PH	C3A-C3B-C3C-C3D
32	a	511	U10	C30-C29-C31-C32
33	b	501	PC1	C34-C35-C36-C37
37	L	811	3PH	C32-C33-C34-C35
37	M	603	3PH	C3F-C3G-C3H-C3I
32	a	511	U10	C28-C29-C31-C32
33	f	201	PC1	C32-C33-C34-C35
37	P	402	3PH	C22-C23-C24-C25
33	m	312	PC1	C32-C33-C34-C35
38	a	513	P5S	C25-C26-C27-C28
33	M	601	PC1	C3A-C3B-C3C-C3D
33	a	517	PC1	C2F-C2G-C2H-C2I

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	a	506	3PH	C32-C33-C34-C35
28	i	309	3PE	C3D-C3E-C3F-C3G
33	l	301	PC1	C24-C25-C26-C27
30	J	204	DU0	C25-C24-O23-C22
30	a	516	DU0	C25-C24-O23-C22
28	m	305	3PE	C3B-C3C-C3D-C3E
37	k	607	3PH	C22-C23-C24-C25
33	h	302	PC1	C27-C28-C29-C2A
28	e	502	3PE	C3B-C3C-C3D-C3E
28	H	404	3PE	O11-C1-C2-C3
28	H	407	3PE	O11-C1-C2-C3
29	g	602	PGT	O3P-C1-C2-C3
33	H	402	PC1	O11-C1-C2-C3
33	L	803	PC1	O11-C1-C2-C3
33	f	201	PC1	O11-C1-C2-C3
33	i	313	PC1	O11-C1-C2-C3
37	P	402	3PH	O11-C1-C2-C3
37	i	304	3PH	O11-C1-C2-C3
37	i	314	3PH	O11-C1-C2-C3
37	k	601	3PH	O11-C1-C2-C3
37	L	811	3PH	C3C-C3D-C3E-C3F
37	H	409	3PH	C31-C32-C33-C34
28	h	301	3PE	O13-C11-C12-N
33	M	608	PC1	C26-C27-C28-C29
37	c	206	3PH	C36-C37-C38-C39
28	H	405	3PE	C3F-C3G-C3H-C3I
33	a	507	PC1	C25-C26-C27-C28
33	l	303	PC1	C2B-C2C-C2D-C2E
28	h	301	3PE	C23-C24-C25-C26
28	L	806	3PE	C2-C1-O11-P
28	c	201	3PE	C2-C1-O11-P
28	g	607	3PE	C2-C1-O11-P
28	i	309	3PE	C2-C1-O11-P
29	K	201	PGT	C5-C4-O4P-P
29	q	1000	PGT	C2-C1-O3P-P
33	g	612	PC1	C2-C1-O11-P
37	M	606	3PH	C2-C1-O11-P
37	P	402	3PH	C2-C1-O11-P
37	g	611	3PH	C2-C1-O11-P
28	L	805	3PE	C35-C36-C37-C38
33	D	1001	PC1	C2C-C2D-C2E-C2F
33	j	1001	PC1	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	m	311	PC1	C32-C33-C34-C35
33	N	501	PC1	C3E-C3F-C3G-C3H
28	k	603	3PE	C33-C34-C35-C36
28	H	405	3PE	C1-C2-C3-O31
28	h	301	3PE	C1-C2-C3-O31
28	k	603	3PE	C1-C2-C3-O31
28	m	305	3PE	C1-C2-C3-O31
28	n	1002	3PE	C1-C2-C3-O31
33	L	803	PC1	C1-C2-C3-O31
33	m	314	PC1	C1-C2-C3-O31
37	d	508	3PH	C1-C2-C3-O31
37	f	205	3PH	C1-C2-C3-O31
37	g	611	3PH	C1-C2-C3-O31
33	L	803	PC1	C35-C36-C37-C38
33	b	504	PC1	C2A-C2B-C2C-C2D
37	m	301	3PH	C39-C3A-C3B-C3C
33	i	313	PC1	C36-C37-C38-C39
28	H	408	3PE	C36-C37-C38-C39
39	g	615	T7X	C1-O1-P1-O11
29	K	201	PGT	C33-C34-C35-C36
37	L	811	3PH	C2B-C2C-C2D-C2E
37	a	506	3PH	C2A-C2B-C2C-C2D
28	i	317	3PE	C3B-C3C-C3D-C3E
29	A	202	PGT	C43-C44-C45-C46
33	g	612	PC1	C3B-C3C-C3D-C3E
37	L	801	3PH	C3A-C3B-C3C-C3D
37	N	503	3PH	C2D-C2E-C2F-C2G
28	h	301	3PE	C1-O11-P-O13
33	l	304	PC1	C11-O13-P-O11
39	g	615	T7X	C15-C16-C17-C18
37	f	203	3PH	C33-C34-C35-C36
30	g	617	DU0	C24-C25-C26-C51
28	c	201	3PE	C32-C33-C34-C35
28	H	404	3PE	O11-C1-C2-O21
28	H	407	3PE	O11-C1-C2-O21
28	n	1002	3PE	O11-C1-C2-O21
29	A	202	PGT	O3P-C1-C2-O2
29	J	205	PGT	O3P-C1-C2-O2
29	g	602	PGT	O3P-C1-C2-O2
33	N	504	PC1	O11-C1-C2-O21
33	h	302	PC1	O11-C1-C2-O21
37	a	506	3PH	O11-C1-C2-O21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	g	611	3PH	C28-C29-C2A-C2B
33	m	312	PC1	C39-C3A-C3B-C3C
28	a	508	3PE	C3D-C3E-C3F-C3G
33	M	608	PC1	C2A-C2B-C2C-C2D
33	b	501	PC1	C25-C26-C27-C28
37	c	206	3PH	C27-C28-C29-C2A
28	H	407	3PE	O21-C2-C3-O31
28	e	502	3PE	O21-C2-C3-O31
28	m	305	3PE	O21-C2-C3-O31
29	N	505	PGT	O2-C2-C3-O3
29	g	602	PGT	O2-C2-C3-O3
33	n	1001	PC1	O21-C2-C3-O31
37	f	205	3PH	O21-C2-C3-O31
37	g	603	3PH	O21-C2-C3-O31
32	B	1002	U10	C31-C32-C33-C34
28	i	309	3PE	C36-C37-C38-C39
32	a	511	U10	C14-C16-C17-C18
28	L	808	3PE	C3C-C3D-C3E-C3F
33	a	501	PC1	C2F-C2G-C2H-C2I
29	H	406	PGT	O31-C31-O2-C2
28	m	305	3PE	C33-C34-C35-C36
37	k	601	3PH	C21-C22-C23-C24
28	L	805	3PE	C25-C26-C27-C28
28	P	403	3PE	C2C-C2D-C2E-C2F
28	d	503	3PE	C24-C25-C26-C27
28	i	309	3PE	C2E-C2F-C2G-C2H
33	a	501	PC1	C2C-C2D-C2E-C2F
37	M	605	3PH	C38-C39-C3A-C3B
28	d	503	3PE	C28-C29-C2A-C2B
29	L	804	PGT	C35-C36-C37-C38
28	H	408	3PE	C2-C1-O11-P
28	h	307	3PE	C2-C1-O11-P
28	i	317	3PE	C2-C1-O11-P
29	J	201	PGT	C2-C1-O3P-P
29	N	505	PGT	C2-C1-O3P-P
33	L	803	PC1	C2-C1-O11-P
33	b	501	PC1	C2-C1-O11-P
33	n	1001	PC1	C2-C1-O11-P
37	a	506	3PH	C2-C1-O11-P
37	d	513	3PH	C2-C1-O11-P
29	J	205	PGT	C40-C41-C42-C43
33	k	606	PC1	C2C-C2D-C2E-C2F

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	A	201	3PE	C2C-C2D-C2E-C2F
28	h	301	3PE	C39-C3A-C3B-C3C
37	o	201	3PH	C2B-C2C-C2D-C2E
28	m	306	3PE	C32-C33-C34-C35
37	a	504	3PH	C37-C38-C39-C3A
30	a	516	DU0	O23-C24-C25-C26
30	h	306	DU0	O23-C24-C25-C26
28	a	509	3PE	C2D-C2E-C2F-C2G
28	g	601	3PE	C34-C35-C36-C37
29	L	804	PGT	C32-C33-C34-C35
33	d	509	PC1	O11-C1-C2-C3
37	a	506	3PH	O11-C1-C2-C3
39	g	615	T7X	O13-C7-C8-C9
28	P	403	3PE	C2A-C2B-C2C-C2D
39	g	615	T7X	C1-O1-P1-O13
39	g	615	T7X	C13-C14-C15-C16
37	N	503	3PH	C2E-C2F-C2G-C2H
37	i	303	3PH	C2C-C2D-C2E-C2F
33	M	608	PC1	C3A-C3B-C3C-C3D
33	c	203	PC1	C2B-C2C-C2D-C2E
28	i	307	3PE	C28-C29-C2A-C2B
28	k	603	3PE	C22-C23-C24-C25
28	k	603	3PE	C26-C27-C28-C29
33	N	501	PC1	C3B-C3C-C3D-C3E
33	m	303	PC1	C2B-C2C-C2D-C2E
37	L	801	3PH	C1-O11-P-O13
37	i	318	3PH	C1-O11-P-O13
33	D	1001	PC1	C3C-C3D-C3E-C3F
37	k	607	3PH	C34-C35-C36-C37
29	N	505	PGT	C41-C42-C43-C44
37	L	810	3PH	C26-C27-C28-C29
28	c	201	3PE	C1-C2-O21-C21
28	g	613	3PE	C1-C2-O21-C21
29	A	202	PGT	C1-C2-O2-C31
29	M	602	PGT	C1-C2-O2-C31
29	g	602	PGT	C3-C2-O2-C31
33	l	301	PC1	C1-C2-O21-C21
41	d	514	HEM	C2C-C3C-CAC-CBC
28	i	307	3PE	C29-C2A-C2B-C2C
37	M	604	3PH	C28-C29-C2A-C2B
33	i	313	PC1	C3B-C3C-C3D-C3E
33	j	1001	PC1	C27-C28-C29-C2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	a	512	U10	C2-C3-O3-C3M
28	d	510	3PE	C1-C2-C3-O31
28	g	601	3PE	C1-C2-C3-O31
28	m	304	3PE	C2-C1-O11-P
29	J	201	PGT	C5-C4-O4P-P
29	P	401	PGT	C1-C2-C3-O3
29	g	602	PGT	C1-C2-C3-O3
33	l	301	PC1	C1-C2-C3-O31
33	m	303	PC1	C1-C2-C3-O31
36	F	502	FMN	C4'-C5'-O5'-P
37	a	510	3PH	C1-C2-C3-O31
43	d	501	CDL	C1-CA2-OA2-PA1
43	d	501	CDL	CA3-CA4-CA6-OA8
43	d	501	CDL	C1-CB2-OB2-PB2
28	L	808	3PE	O11-C1-C2-O21
28	a	503	3PE	O11-C1-C2-O21
28	h	301	3PE	O11-C1-C2-O21
29	N	505	PGT	O3P-C1-C2-O2
33	L	803	PC1	O11-C1-C2-O21
33	f	201	PC1	O11-C1-C2-O21
33	j	1001	PC1	O11-C1-C2-O21
37	L	811	3PH	O11-C1-C2-O21
37	d	513	3PH	O11-C1-C2-O21
37	g	603	3PH	O11-C1-C2-O21
37	i	304	3PH	O11-C1-C2-O21
37	k	601	3PH	O11-C1-C2-O21
39	g	615	T7X	O13-C7-C8-O16
28	d	503	3PE	C29-C2A-C2B-C2C
28	g	613	3PE	C24-C25-C26-C27
29	K	201	PGT	C19-C20-C21-C22
33	c	203	PC1	C29-C2A-C2B-C2C
33	l	301	PC1	C3C-C3D-C3E-C3F
39	J	202	T7X	C36-C37-C38-C39
28	g	601	3PE	O21-C2-C3-O31
33	c	203	PC1	O21-C2-C3-O31
37	a	510	3PH	O21-C2-C3-O31
37	d	508	3PH	O21-C2-C3-O31
37	i	303	3PH	O21-C2-C3-O31
37	j	1003	3PH	O21-C2-C3-O31
37	L	811	3PH	C2-C3-O31-C31
28	i	307	3PE	C37-C38-C39-C3A
33	m	314	PC1	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
38	a	513	P5S	CA-CB-OG-P12
33	L	803	PC1	C39-C3A-C3B-C3C
28	g	601	3PE	C2D-C2E-C2F-C2G
33	a	507	PC1	C3B-C3C-C3D-C3E
29	N	505	PGT	C2-C3-O3-C11
37	a	504	3PH	C38-C39-C3A-C3B
28	d	503	3PE	O32-C31-O31-C3
29	P	401	PGT	C31-C32-C33-C34
33	l	301	PC1	C29-C2A-C2B-C2C
37	k	601	3PH	C3C-C3D-C3E-C3F
30	c	205	DU0	C21-C22-O23-C24
30	g	617	DU0	C21-C22-O23-C24
30	g	617	DU0	C75-C22-O23-C24
30	m	302	DU0	C25-C24-O23-C22
38	a	513	P5S	N-CA-CB-OG
28	A	201	3PE	C1-O11-P-O13
28	L	806	3PE	C11-O13-P-O11
28	e	505	3PE	C1-O11-P-O13
28	h	301	3PE	C11-O13-P-O11
28	m	310	3PE	C11-O13-P-O11
33	H	402	PC1	C1-O11-P-O13
33	d	516	PC1	C11-O13-P-O11
33	d	516	PC1	C1-O11-P-O13
33	i	308	PC1	C11-O13-P-O11
33	i	308	PC1	C1-O11-P-O13
33	k	609	PC1	C11-O13-P-O11
33	n	1001	PC1	C11-O13-P-O11
33	n	1001	PC1	C1-O11-P-O13
38	a	513	P5S	CB-OG-P12-O16
28	i	309	3PE	C27-C28-C29-C2A
33	M	608	PC1	C2C-C2D-C2E-C2F
43	d	501	CDL	C58-C59-C60-C61
28	i	307	3PE	C2-C1-O11-P
37	M	603	3PH	C2-C1-O11-P
37	m	301	3PH	C2-C1-O11-P
38	a	513	P5S	C2-C3-O16-P12
39	J	202	T7X	C8-C7-O13-P1
28	g	601	3PE	C38-C39-C3A-C3B
28	m	307	3PE	C38-C39-C3A-C3B
28	m	315	3PE	C38-C39-C3A-C3B
28	L	805	3PE	C1-O11-P-O12
28	P	403	3PE	C1-O11-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	c	201	3PE	C11-O13-P-O14
28	d	515	3PE	C11-O13-P-O14
28	g	601	3PE	C11-O13-P-O12
28	g	613	3PE	C11-O13-P-O12
28	h	301	3PE	C1-O11-P-O14
28	h	307	3PE	C11-O13-P-O12
28	i	307	3PE	C11-O13-P-O12
28	i	311	3PE	C1-O11-P-O12
28	i	317	3PE	C1-O11-P-O14
28	m	310	3PE	C11-O13-P-O12
29	M	602	PGT	C1-O3P-P-O1P
29	a	514	PGT	C4-O4P-P-O1P
33	H	402	PC1	C1-O11-P-O14
33	L	803	PC1	C11-O13-P-O12
33	L	803	PC1	C1-O11-P-O14
33	d	516	PC1	C11-O13-P-O12
33	i	310	PC1	C11-O13-P-O12
33	l	303	PC1	C1-O11-P-O12
33	l	304	PC1	C11-O13-P-O12
33	l	304	PC1	C1-O11-P-O14
33	m	303	PC1	C1-O11-P-O12
33	m	314	PC1	C11-O13-P-O12
28	A	201	3PE	O11-C1-C2-C3
28	c	201	3PE	O11-C1-C2-C3
28	h	301	3PE	O11-C1-C2-C3
29	q	1000	PGT	O3P-C1-C2-C3
33	j	1001	PC1	O11-C1-C2-C3
37	g	603	3PH	O11-C1-C2-C3
37	m	309	3PH	C23-C24-C25-C26
28	i	307	3PE	O13-C11-C12-N
37	a	506	3PH	C28-C29-C2A-C2B
28	A	201	3PE	C12-C11-O13-P
28	H	405	3PE	C12-C11-O13-P
28	H	408	3PE	C12-C11-O13-P
28	d	503	3PE	C12-C11-O13-P
28	e	502	3PE	C12-C11-O13-P
28	e	505	3PE	C12-C11-O13-P
28	g	601	3PE	C12-C11-O13-P
28	g	613	3PE	C12-C11-O13-P
28	h	301	3PE	C12-C11-O13-P
28	h	307	3PE	C12-C11-O13-P
28	i	317	3PE	C12-C11-O13-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	m	305	3PE	C12-C11-O13-P
28	m	310	3PE	C12-C11-O13-P
33	L	803	PC1	C12-C11-O13-P
33	N	501	PC1	C12-C11-O13-P
33	N	502	PC1	C12-C11-O13-P
33	b	501	PC1	C12-C11-O13-P
33	b	504	PC1	C12-C11-O13-P
33	c	203	PC1	C12-C11-O13-P
33	d	509	PC1	C12-C11-O13-P
33	g	612	PC1	C12-C11-O13-P
33	i	308	PC1	C12-C11-O13-P
33	k	606	PC1	C12-C11-O13-P
33	l	303	PC1	C12-C11-O13-P
33	m	311	PC1	C12-C11-O13-P
28	d	503	3PE	C27-C28-C29-C2A
28	i	317	3PE	C3D-C3E-C3F-C3G
28	i	307	3PE	C24-C25-C26-C27
33	m	303	PC1	C3B-C3C-C3D-C3E
33	m	314	PC1	C2F-C2G-C2H-C2I
43	d	501	CDL	CA2-C1-CB2-OB2
28	e	505	3PE	C28-C29-C2A-C2B
33	H	402	PC1	O11-C1-C2-O21
37	P	402	3PH	O11-C1-C2-O21
37	k	607	3PH	O11-C1-C2-O21
38	I	201	P5S	O37-C2-C3-O16
28	e	505	3PE	C36-C37-C38-C39
28	i	307	3PE	C26-C27-C28-C29
33	M	601	PC1	C23-C24-C25-C26
28	d	503	3PE	C37-C38-C39-C3A
28	d	515	3PE	C28-C29-C2A-C2B
33	i	310	PC1	C3A-C3B-C3C-C3D
37	P	402	3PH	C27-C28-C29-C2A
32	d	506	U10	C4-C3-O3-C3M
38	L	809	P5S	C38-C39-C40-C41
37	c	206	3PH	C22-C21-O21-C2
28	H	404	3PE	C23-C24-C25-C26
29	L	804	PGT	C34-C35-C36-C37
37	i	304	3PH	C23-C24-C25-C26
37	k	601	3PH	C32-C33-C34-C35
28	a	502	3PE	C1-C2-C3-O31
33	L	803	PC1	O13-C11-C12-N
33	M	608	PC1	O13-C11-C12-N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	M	609	PC1	O13-C11-C12-N
33	N	502	PC1	O13-C11-C12-N
33	a	501	PC1	O13-C11-C12-N
33	a	507	PC1	O13-C11-C12-N
33	b	501	PC1	O13-C11-C12-N
33	b	504	PC1	O13-C11-C12-N
33	c	203	PC1	O13-C11-C12-N
33	d	516	PC1	O13-C11-C12-N
33	f	201	PC1	O13-C11-C12-N
33	i	308	PC1	O13-C11-C12-N
33	i	313	PC1	O13-C11-C12-N
33	j	1001	PC1	O13-C11-C12-N
33	k	606	PC1	O13-C11-C12-N
33	m	311	PC1	O13-C11-C12-N
33	m	312	PC1	O13-C11-C12-N
33	n	1001	PC1	O13-C11-C12-N
28	i	317	3PE	O21-C2-C3-O31
33	f	201	PC1	O21-C2-C3-O31
33	l	301	PC1	O21-C2-C3-O31
37	i	301	3PH	O21-C2-C3-O31
29	K	201	PGT	C14-C15-C16-C17
37	g	603	3PH	C32-C33-C34-C35
37	L	810	3PH	C22-C23-C24-C25
38	L	809	P5S	C30-C31-C32-C33
43	d	501	CDL	C15-C16-C17-C18
37	i	304	3PH	C27-C28-C29-C2A
32	a	511	U10	C1-C6-C7-C8
29	q	1000	PGT	C31-C32-C33-C34
33	b	504	PC1	C34-C35-C36-C37
33	f	201	PC1	C3D-C3E-C3F-C3G
33	l	301	PC1	C3A-C3B-C3C-C3D
28	d	503	3PE	C32-C31-O31-C3
28	e	505	3PE	C33-C34-C35-C36
28	n	1002	3PE	C22-C23-C24-C25
37	g	603	3PH	C37-C38-C39-C3A
28	i	317	3PE	C24-C25-C26-C27
28	L	808	3PE	C2C-C2D-C2E-C2F
33	N	501	PC1	C28-C29-C2A-C2B
33	a	507	PC1	C38-C39-C3A-C3B
32	B	1002	U10	C34-C36-C37-C38
28	L	805	3PE	C23-C24-C25-C26
33	l	301	PC1	C2E-C2F-C2G-C2H

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	c	202	DU0	C24-C25-C26-C27
33	b	504	PC1	C33-C34-C35-C36
28	m	310	3PE	C2A-C2B-C2C-C2D
28	L	808	3PE	C31-C32-C33-C34
33	b	504	PC1	C2C-C2D-C2E-C2F
29	L	804	PGT	C18-C19-C20-C21
28	i	307	3PE	C31-C32-C33-C34
37	L	811	3PH	C37-C38-C39-C3A
28	L	805	3PE	C3D-C3E-C3F-C3G
28	m	315	3PE	C28-C29-C2A-C2B
33	k	606	PC1	C3B-C3C-C3D-C3E
37	i	314	3PH	C2F-C2G-C2H-C2I
28	H	405	3PE	C1-C2-O21-C21
28	i	311	3PE	C1-C2-O21-C21
28	m	310	3PE	C3-C2-O21-C21
29	N	505	PGT	C1-C2-O2-C31
29	g	602	PGT	C1-C2-O2-C31
28	H	405	3PE	O11-C1-C2-C3
28	m	306	3PE	O11-C1-C2-C3
29	P	401	PGT	O3P-C1-C2-C3
33	a	501	PC1	O11-C1-C2-C3
37	g	603	3PH	C2-C3-O31-C31
37	M	604	3PH	C29-C2A-C2B-C2C
28	H	407	3PE	C25-C26-C27-C28
33	m	311	PC1	C2E-C2F-C2G-C2H
37	L	807	3PH	C37-C38-C39-C3A
28	a	508	3PE	C2-C1-O11-P
37	L	810	3PH	C1-O11-P-O12
37	d	513	3PH	C1-O11-P-O12
28	h	307	3PE	C36-C37-C38-C39
33	a	517	PC1	C24-C25-C26-C27
37	k	607	3PH	C23-C24-C25-C26
33	i	313	PC1	C2-C3-O31-C31
28	c	201	3PE	O11-C1-C2-O21
33	N	502	PC1	O11-C1-C2-O21
33	a	501	PC1	O11-C1-C2-O21
37	i	314	3PH	O11-C1-C2-O21
33	i	310	PC1	C28-C29-C2A-C2B
28	g	613	3PE	O21-C2-C3-O31
37	M	606	3PH	O21-C2-C3-O31
37	k	607	3PH	O21-C2-C3-O31
28	m	307	3PE	C3C-C3D-C3E-C3F

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	m	307	3PE	C3F-C3G-C3H-C3I
29	J	205	PGT	C15-C16-C17-C18
33	H	402	PC1	C3E-C3F-C3G-C3H
33	g	612	PC1	C26-C27-C28-C29
28	H	405	3PE	C11-O13-P-O11
28	H	408	3PE	C1-O11-P-O13
28	H	408	3PE	C11-O13-P-O11
28	L	808	3PE	C1-O11-P-O13
28	P	403	3PE	C1-O11-P-O13
28	a	503	3PE	C11-O13-P-O11
28	d	503	3PE	C1-O11-P-O13
28	g	601	3PE	C11-O13-P-O11
28	h	307	3PE	C11-O13-P-O11
28	i	307	3PE	C11-O13-P-O11
28	m	304	3PE	C11-O13-P-O11
28	m	305	3PE	C11-O13-P-O11
33	M	608	PC1	C1-O11-P-O13
33	M	609	PC1	C11-O13-P-O11
33	b	504	PC1	C1-O11-P-O13
33	k	606	PC1	C11-O13-P-O11
33	m	303	PC1	C1-O11-P-O13
39	g	615	T7X	C7-O13-P1-O1
33	g	612	PC1	C22-C23-C24-C25
37	M	606	3PH	C3D-C3E-C3F-C3G
33	n	1001	PC1	C24-C25-C26-C27
37	o	201	3PH	C36-C37-C38-C39
28	a	508	3PE	C1-C2-C3-O31
28	m	315	3PE	C1-C2-C3-O31
33	n	1001	PC1	C1-C2-C3-O31
32	a	512	U10	C25-C24-C26-C27
37	L	810	3PH	C2D-C2E-C2F-C2G
43	d	501	CDL	C32-C33-C34-C35
29	K	201	PGT	C34-C35-C36-C37
32	a	511	U10	C46-C47-C48-C49
33	i	308	PC1	C33-C34-C35-C36
38	L	809	P5S	C41-C42-C43-C44
28	m	307	3PE	C2E-C2F-C2G-C2H
33	N	502	PC1	C2D-C2E-C2F-C2G
30	c	205	DU0	C75-C22-O23-C24
28	e	502	3PE	C3D-C3E-C3F-C3G
28	i	311	3PE	C29-C2A-C2B-C2C
33	i	313	PC1	C2-C1-O11-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	L	801	3PH	C2-C1-O11-P
37	i	304	3PH	O21-C21-C22-C23
28	P	403	3PE	C37-C38-C39-C3A
28	a	502	3PE	C25-C26-C27-C28
30	g	617	DU0	C25-C24-O23-C22
29	L	804	PGT	O31-C31-O2-C2
43	d	501	CDL	C21-C22-C23-C24
33	N	501	PC1	C3D-C3E-C3F-C3G
28	d	515	3PE	C29-C2A-C2B-C2C
37	P	402	3PH	O21-C21-C22-C23
28	L	808	3PE	C34-C35-C36-C37
28	a	508	3PE	C25-C26-C27-C28
37	i	301	3PH	C21-C22-C23-C24
28	d	503	3PE	C25-C26-C27-C28
28	d	503	3PE	C2F-C2G-C2H-C2I
33	i	310	PC1	C24-C25-C26-C27
37	k	601	3PH	C3D-C3E-C3F-C3G
28	i	317	3PE	O11-C1-C2-C3
33	m	311	PC1	C37-C38-C39-C3A
33	n	1001	PC1	C32-C33-C34-C35
28	a	509	3PE	O11-C1-C2-O21
28	m	307	3PE	C2A-C2B-C2C-C2D
33	M	601	PC1	C2A-C2B-C2C-C2D
33	a	507	PC1	C35-C36-C37-C38
33	M	608	PC1	C39-C3A-C3B-C3C
33	f	201	PC1	C3A-C3B-C3C-C3D
39	g	615	T7X	C43-C44-C45-C46
44	k	604	HEA	C26-C15-C16-C17
28	a	503	3PE	C38-C39-C3A-C3B
32	d	504	U10	C12-C11-C9-C8
28	A	201	3PE	C3A-C3B-C3C-C3D
38	a	513	P5S	C24-C25-C26-C27
33	h	302	PC1	C2-C3-O31-C31
37	a	504	3PH	C29-C2A-C2B-C2C
28	a	509	3PE	C25-C26-C27-C28
33	N	504	PC1	C3E-C3F-C3G-C3H
33	M	609	PC1	C28-C29-C2A-C2B
43	d	501	CDL	C17-C18-C19-C20
41	d	514	HEM	CAD-CBD-CGD-O1D
28	d	515	3PE	O21-C2-C3-O31
29	K	201	PGT	O2-C2-C3-O3
38	I	201	P5S	O19-C1-C2-O37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	P	403	3PE	C26-C27-C28-C29
33	H	403	PC1	C32-C33-C34-C35
37	L	810	3PH	C34-C35-C36-C37
33	N	502	PC1	C2-C1-O11-P
33	f	201	PC1	C2-C1-O11-P
37	L	810	3PH	C2-C1-O11-P
37	f	205	3PH	C2C-C2D-C2E-C2F
37	M	604	3PH	C2B-C2C-C2D-C2E
37	a	506	3PH	C2B-C2C-C2D-C2E
41	d	507	HEM	CAA-CBA-CGA-O1A
32	B	1002	U10	C25-C24-C26-C27
32	d	504	U10	C12-C11-C9-C10
37	k	601	3PH	C3E-C3F-C3G-C3H
41	d	507	HEM	C3A-C2A-CAA-CBA
28	i	306	3PE	C27-C28-C29-C2A
28	m	306	3PE	C25-C26-C27-C28
43	d	501	CDL	C53-C54-C55-C56
37	P	402	3PH	C2B-C2C-C2D-C2E
28	g	613	3PE	C1-C2-C3-O31
28	m	307	3PE	C1-C2-C3-O31
28	p	1001	3PE	C38-C39-C3A-C3B
33	M	609	PC1	C2A-C2B-C2C-C2D
33	i	310	PC1	C2A-C2B-C2C-C2D
41	d	514	HEM	CAA-CBA-CGA-O2A
28	g	613	3PE	C26-C27-C28-C29
42	e	504	HEC	CAD-CBD-CGD-O1D
28	d	510	3PE	C21-C22-C23-C24
33	h	302	PC1	C2C-C2D-C2E-C2F
37	i	301	3PH	C35-C36-C37-C38
28	m	306	3PE	C3-C2-O21-C21
28	p	1001	3PE	C3-C2-O21-C21
29	q	1000	PGT	C3-C2-O2-C31
33	N	504	PC1	C3-C2-O21-C21
33	a	517	PC1	C3-C2-O21-C21
33	f	201	PC1	C1-C2-O21-C21
33	j	1001	PC1	C3-C2-O21-C21
37	M	604	3PH	C1-C2-O21-C21
37	a	504	3PH	C3-C2-O21-C21
37	d	502	3PH	C1-C2-O21-C21
43	d	501	CDL	CA3-CA4-OA6-CA5
28	i	309	3PE	C2F-C2G-C2H-C2I
37	M	604	3PH	C35-C36-C37-C38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	a	517	PC1	C35-C36-C37-C38
37	a	510	3PH	C3E-C3F-C3G-C3H
33	f	201	PC1	C1-O11-P-O13
33	i	308	PC1	C28-C29-C2A-C2B
44	k	605	HEA	CAD-CBD-CGD-O1D
28	a	509	3PE	C28-C29-C2A-C2B
28	m	305	3PE	C28-C29-C2A-C2B
37	a	506	3PH	C39-C3A-C3B-C3C
28	d	510	3PE	C33-C34-C35-C36
33	M	608	PC1	C2E-C2F-C2G-C2H
37	k	607	3PH	C2-C1-O11-P
30	c	202	DU0	C24-C25-C26-C51
28	a	509	3PE	C37-C38-C39-C3A
29	P	401	PGT	O3P-C1-C2-O2
33	a	517	PC1	O21-C21-C22-C23
32	a	512	U10	C6-C7-C8-C9
37	c	206	3PH	O22-C21-O21-C2
37	d	513	3PH	C37-C38-C39-C3A
28	i	309	3PE	O11-C1-C2-C3
33	N	504	PC1	O11-C1-C2-C3
37	f	205	3PH	O11-C1-C2-C3
43	d	501	CDL	OB5-CB3-CB4-CB6
29	N	505	PGT	C37-C38-C39-C40
41	d	507	HEM	CAA-CBA-CGA-O2A
33	k	609	PC1	C32-C33-C34-C35
33	m	311	PC1	C2C-C2D-C2E-C2F
37	H	409	3PH	C37-C38-C39-C3A
28	m	306	3PE	C31-C32-C33-C34
32	B	1002	U10	C23-C24-C26-C27
32	a	512	U10	C23-C24-C26-C27
41	d	514	HEM	CAA-CBA-CGA-O1A
29	J	201	PGT	C31-C32-C33-C34
41	a	505	HEM	CAA-CBA-CGA-O2A
33	c	203	PC1	C3C-C3D-C3E-C3F
28	L	805	3PE	O21-C2-C3-O31
28	g	613	3PE	C38-C39-C3A-C3B
37	i	314	3PH	C35-C36-C37-C38
41	a	505	HEM	CAA-CBA-CGA-O1A
43	d	501	CDL	C54-C55-C56-C57
33	b	501	PC1	C3E-C3F-C3G-C3H
38	I	201	P5S	C20-C21-C22-C23
28	a	508	3PE	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	m	307	3PE	C22-C23-C24-C25
33	f	201	PC1	C24-C25-C26-C27
41	d	514	HEM	CAD-CBD-CGD-O2D
32	B	1002	U10	C35-C34-C36-C37
44	k	605	HEA	C27-C19-C20-C21
44	k	604	HEA	C14-C15-C16-C17
33	b	501	PC1	O31-C31-C32-C33
37	H	409	3PH	C23-C24-C25-C26
29	H	406	PGT	C32-C31-O2-C2
28	i	306	3PE	C37-C38-C39-C3A
33	l	304	PC1	C3C-C3D-C3E-C3F
37	L	801	3PH	C2D-C2E-C2F-C2G
37	i	314	3PH	C33-C34-C35-C36
37	k	601	3PH	C29-C2A-C2B-C2C
28	d	510	3PE	C3E-C3F-C3G-C3H
33	b	504	PC1	O21-C21-C22-C23
28	H	407	3PE	C1-C2-C3-O31
39	J	202	T7X	C38-C39-C40-C41
42	b	502	HEC	CAA-CBA-CGA-O2A
37	k	607	3PH	C33-C34-C35-C36
33	a	517	PC1	C38-C39-C3A-C3B
33	m	314	PC1	C35-C36-C37-C38
37	L	807	3PH	C3A-C3B-C3C-C3D
28	i	306	3PE	C2B-C2C-C2D-C2E
30	c	205	DU0	C25-C24-O23-C22
30	d	505	DU0	C25-C24-O23-C22
30	d	511	DU0	C25-C24-O23-C22
30	h	303	DU0	C25-C24-O23-C22
30	k	608	DU0	C25-C24-O23-C22
33	d	516	PC1	C32-C33-C34-C35
28	d	503	3PE	C36-C37-C38-C39
33	N	502	PC1	C26-C27-C28-C29
41	a	505	HEM	CAD-CBD-CGD-O2D
44	k	605	HEA	CAD-CBD-CGD-O2D
28	m	315	3PE	C29-C2A-C2B-C2C
29	J	201	PGT	C21-C22-C23-C24
29	M	602	PGT	C22-C23-C24-C25
37	i	318	3PH	C22-C23-C24-C25
28	L	806	3PE	C36-C37-C38-C39
28	a	502	3PE	C22-C23-C24-C25
33	N	502	PC1	C24-C25-C26-C27
28	i	317	3PE	O11-C1-C2-O21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	i	308	PC1	O11-C1-C2-O21
37	f	205	3PH	O11-C1-C2-O21
37	a	504	3PH	C21-C22-C23-C24
33	l	304	PC1	C29-C2A-C2B-C2C
41	a	515	HEM	CAA-CBA-CGA-O2A
33	l	304	PC1	C3A-C3B-C3C-C3D
33	m	312	PC1	C3F-C3G-C3H-C3I
37	g	611	3PH	C3D-C3E-C3F-C3G
28	m	305	3PE	O31-C31-C32-C33
32	B	1002	U10	C5-C4-O4-C4M
37	f	205	3PH	C38-C39-C3A-C3B
28	e	505	3PE	C24-C25-C26-C27
41	a	505	HEM	CAD-CBD-CGD-O1D
42	b	502	HEC	CAA-CBA-CGA-O1A
33	l	304	PC1	C38-C39-C3A-C3B
37	d	513	3PH	C36-C37-C38-C39
29	J	205	PGT	C18-C19-C20-C21
33	n	1001	PC1	C28-C29-C2A-C2B
37	M	604	3PH	C26-C27-C28-C29
29	N	505	PGT	O3P-C1-C2-C3
33	N	502	PC1	O11-C1-C2-C3
37	d	513	3PH	O11-C1-C2-C3
37	i	318	3PH	O11-C1-C2-C3
37	k	607	3PH	O11-C1-C2-C3
37	L	807	3PH	C21-C22-C23-C24
32	d	506	U10	C30-C29-C31-C32
32	a	512	U10	C29-C31-C32-C33
33	h	302	PC1	C23-C24-C25-C26
33	k	606	PC1	C37-C38-C39-C3A
43	d	501	CDL	C34-C35-C36-C37
33	i	313	PC1	O21-C21-C22-C23
28	h	301	3PE	C29-C2A-C2B-C2C
33	N	504	PC1	C2E-C2F-C2G-C2H
42	e	504	HEC	CAA-CBA-CGA-O1A
44	g	610	HEA	CAA-CBA-CGA-O2A
44	g	610	HEA	CAD-CBD-CGD-O2D
28	a	508	3PE	O21-C2-C3-O31
28	c	201	3PE	O21-C2-C3-O31
28	m	307	3PE	O21-C2-C3-O31
33	D	1001	PC1	C2D-C2E-C2F-C2G
33	a	507	PC1	C37-C38-C39-C3A
37	i	301	3PH	C2A-C2B-C2C-C2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
44	k	604	HEA	CAD-CBD-CGD-O2D
29	K	201	PGT	C22-C23-C24-C25
33	H	402	PC1	C39-C3A-C3B-C3C
28	d	510	3PE	C24-C25-C26-C27
44	g	606	HEA	CAA-CBA-CGA-O2A
28	L	808	3PE	C36-C37-C38-C39
37	L	807	3PH	C1-O11-P-O14
37	M	605	3PH	C2A-C2B-C2C-C2D
37	d	508	3PH	C1-O11-P-O13
37	g	603	3PH	C1-O11-P-O13
28	L	802	3PE	O21-C21-C22-C23
43	d	501	CDL	C44-C45-C46-C47
32	a	512	U10	C15-C14-C16-C17
44	g	606	HEA	C27-C19-C20-C21
33	m	303	PC1	C3A-C3B-C3C-C3D
37	M	603	3PH	C3E-C3F-C3G-C3H
28	H	407	3PE	C1-O11-P-O13
32	B	1002	U10	C33-C34-C36-C37
33	g	612	PC1	C2E-C2F-C2G-C2H
29	q	1000	PGT	O2-C31-C32-C33
37	k	601	3PH	C2A-C2B-C2C-C2D
33	m	303	PC1	C28-C29-C2A-C2B
37	d	508	3PH	C32-C33-C34-C35
42	b	502	HEC	CAD-CBD-CGD-O1D
28	H	404	3PE	O21-C21-C22-C23
28	L	808	3PE	O31-C31-C32-C33
33	d	516	PC1	O21-C21-C22-C23
37	o	201	3PH	O31-C31-C32-C33
38	I	201	P5S	O19-C17-C20-C21
28	i	309	3PE	C26-C27-C28-C29
38	I	201	P5S	C43-C44-C45-C46
28	A	201	3PE	C1-C2-O21-C21
28	A	201	3PE	C3-C2-O21-C21
33	L	803	PC1	C3-C2-O21-C21
33	f	201	PC1	C3-C2-O21-C21
33	n	1001	PC1	C3-C2-O21-C21
28	L	806	3PE	C34-C35-C36-C37
37	f	203	3PH	C3B-C3C-C3D-C3E
36	F	502	FMN	O4'-C4'-C5'-O5'
28	H	405	3PE	O31-C31-C32-C33
28	i	306	3PE	O21-C21-C22-C23
37	M	604	3PH	O31-C31-C32-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	d	502	3PH	O31-C31-C32-C33
37	d	513	3PH	O21-C21-C22-C23
28	e	505	3PE	C34-C35-C36-C37
38	I	201	P5S	C22-C23-C24-C25
32	a	511	U10	C25-C24-C26-C27
42	e	504	HEC	CAD-CBD-CGD-O2D
44	g	606	HEA	CAD-CBD-CGD-O2D
28	a	508	3PE	C3E-C3F-C3G-C3H
33	d	509	PC1	C2F-C2G-C2H-C2I
44	k	605	HEA	C18-C19-C20-C21
28	L	806	3PE	O31-C31-C32-C33
28	m	307	3PE	O21-C21-C22-C23
28	c	201	3PE	C39-C3A-C3B-C3C
28	k	603	3PE	C3D-C3E-C3F-C3G
33	k	609	PC1	C2E-C2F-C2G-C2H
29	H	406	PGT	C12-C13-C14-C15
37	L	810	3PH	C25-C26-C27-C28
37	f	205	3PH	C1-O11-P-O12
41	a	515	HEM	CAA-CBA-CGA-O1A
44	g	610	HEA	CAD-CBD-CGD-O1D
37	m	301	3PH	O11-C1-C2-O21
32	a	511	U10	C11-C12-C13-C14
28	H	405	3PE	O21-C21-C22-C23
29	A	202	PGT	O3-C11-C12-C13
33	N	502	PC1	O21-C21-C22-C23
44	g	610	HEA	CAA-CBA-CGA-O1A
44	k	604	HEA	CAA-CBA-CGA-O1A
29	J	205	PGT	C14-C15-C16-C17
33	i	313	PC1	C26-C27-C28-C29
41	a	515	HEM	C4B-C3B-CAB-CBB
41	d	514	HEM	C4C-C3C-CAC-CBC
29	q	1000	PGT	C35-C36-C37-C38
33	M	601	PC1	C2E-C2F-C2G-C2H
37	a	510	3PH	C2E-C2F-C2G-C2H
33	g	612	PC1	O31-C31-C32-C33
33	m	314	PC1	O31-C31-C32-C33
44	k	604	HEA	CAA-CBA-CGA-O2A
44	g	606	HEA	CAA-CBA-CGA-O1A
28	h	307	3PE	O21-C21-C22-C23
29	J	201	PGT	O2-C31-C32-C33
28	m	307	3PE	C28-C29-C2A-C2B
37	i	301	3PH	C27-C28-C29-C2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	A	201	3PE	O31-C31-C32-C33
28	g	601	3PE	O31-C31-C32-C33
29	P	401	PGT	O3-C11-C12-C13
33	N	501	PC1	O31-C31-C32-C33
37	L	801	3PH	O21-C21-C22-C23
37	M	605	3PH	O21-C21-C22-C23
29	J	201	PGT	C19-C20-C21-C22
33	H	402	PC1	C36-C37-C38-C39
37	L	811	3PH	C3E-C3F-C3G-C3H
28	a	503	3PE	O21-C2-C3-O31
29	L	804	PGT	O2-C2-C3-O3
33	a	507	PC1	O21-C2-C3-O31
33	k	606	PC1	O21-C2-C3-O31
43	d	501	CDL	OB6-CB4-CB6-OB8
33	c	203	PC1	C21-C22-C23-C24
41	d	507	HEM	C1A-C2A-CAA-CBA
33	k	609	PC1	C38-C39-C3A-C3B
44	g	606	HEA	CAD-CBD-CGD-O1D
44	k	604	HEA	CAD-CBD-CGD-O1D
44	k	605	HEA	CAA-CBA-CGA-O1A
43	d	501	CDL	C80-C81-C82-C83
28	i	306	3PE	O31-C31-C32-C33
28	m	307	3PE	O31-C31-C32-C33
29	A	202	PGT	O2-C31-C32-C33
29	M	602	PGT	O2-C31-C32-C33
37	L	810	3PH	O21-C21-C22-C23
33	a	517	PC1	C3B-C3C-C3D-C3E
33	i	313	PC1	C29-C2A-C2B-C2C
30	f	202	DU0	C24-C25-C26-C27
38	I	201	P5S	CA-CB-OG-P12
29	q	1000	PGT	O3-C11-C12-C13
33	l	304	PC1	O31-C31-C32-C33
37	f	203	3PH	C2D-C2E-C2F-C2G
28	a	502	3PE	C2-C3-O31-C31
32	a	512	U10	C13-C14-C16-C17
38	L	809	P5S	OXT-C-CA-CB
28	p	1001	3PE	C2A-C2B-C2C-C2D
28	i	317	3PE	O31-C31-C32-C33
33	a	501	PC1	O31-C31-C32-C33
37	i	314	3PH	O31-C31-C32-C33
37	m	301	3PH	O31-C31-C32-C33
33	H	403	PC1	C2B-C2C-C2D-C2E

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	d	502	3PH	C2-C3-O31-C31
28	a	503	3PE	C2A-C2B-C2C-C2D
37	i	303	3PH	C2F-C2G-C2H-C2I
42	b	502	HEC	CAD-CBD-CGD-O2D
33	M	609	PC1	C3E-C3F-C3G-C3H
33	N	502	PC1	C2C-C2D-C2E-C2F
33	i	308	PC1	C3A-C3B-C3C-C3D
29	A	202	PGT	O11-C11-C12-C13
30	g	616	DU0	O23-C24-C25-C26
33	L	803	PC1	C22-C23-C24-C25
33	h	302	PC1	C22-C23-C24-C25
33	k	606	PC1	C28-C29-C2A-C2B
29	L	804	PGT	C32-C31-O2-C2
33	a	507	PC1	C2B-C2C-C2D-C2E
30	H	401	DU0	C21-C22-O23-C24
29	M	602	PGT	O3-C11-C12-C13
28	n	1002	3PE	C2B-C2C-C2D-C2E
29	P	401	PGT	C41-C42-C43-C44
33	n	1001	PC1	C3C-C3D-C3E-C3F
38	L	809	P5S	C43-C44-C45-C46
29	A	202	PGT	C18-C19-C20-C21
33	N	502	PC1	O22-C21-C22-C23
37	d	513	3PH	O22-C21-C22-C23
33	m	312	PC1	C2C-C2D-C2E-C2F
28	i	309	3PE	C38-C39-C3A-C3B
33	a	507	PC1	C34-C35-C36-C37
33	c	203	PC1	C28-C29-C2A-C2B
28	L	805	3PE	C3F-C3G-C3H-C3I
28	m	315	3PE	C34-C35-C36-C37
37	L	810	3PH	C23-C24-C25-C26
37	d	513	3PH	C27-C28-C29-C2A
28	g	601	3PE	O32-C31-C32-C33
33	i	313	PC1	O22-C21-C22-C23
28	d	503	3PE	C34-C35-C36-C37
28	H	405	3PE	C35-C36-C37-C38
28	m	310	3PE	C24-C25-C26-C27
29	K	201	PGT	C37-C38-C39-C40
37	i	314	3PH	O32-C31-C32-C33
28	i	307	3PE	C35-C36-C37-C38
28	m	310	3PE	C3C-C3D-C3E-C3F
43	d	501	CDL	C16-C17-C18-C19
28	L	802	3PE	O22-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	M	604	3PH	O32-C31-C32-C33
38	I	201	P5S	O18-C17-C20-C21
28	i	306	3PE	C22-C23-C24-C25
28	d	515	3PE	C1-C2-C3-O31
37	i	301	3PH	C1-C2-C3-O31
28	g	607	3PE	C2D-C2E-C2F-C2G
29	P	401	PGT	C39-C40-C41-C42
28	H	404	3PE	C11-O13-P-O11
33	H	403	PC1	C11-O13-P-O11
37	g	603	3PH	C2E-C2F-C2G-C2H
28	L	806	3PE	O32-C31-C32-C33
28	L	808	3PE	O32-C31-C32-C33
28	h	307	3PE	O22-C21-C22-C23
28	m	307	3PE	O22-C21-C22-C23
33	m	314	PC1	O32-C31-C32-C33
37	L	810	3PH	O22-C21-C22-C23
37	M	603	3PH	C3B-C3C-C3D-C3E
29	N	505	PGT	C16-C17-C18-C19
37	P	402	3PH	C2C-C2D-C2E-C2F
28	i	306	3PE	O22-C21-C22-C23
28	m	307	3PE	O32-C31-C32-C33
37	M	605	3PH	O22-C21-C22-C23
28	L	808	3PE	C27-C28-C29-C2A
42	e	504	HEC	CAA-CBA-CGA-O2A
33	h	302	PC1	C38-C39-C3A-C3B
28	H	405	3PE	C11-O13-P-O14
28	H	408	3PE	C1-O11-P-O14
28	H	408	3PE	C11-O13-P-O14
28	L	805	3PE	C1-O11-P-O14
28	L	808	3PE	C1-O11-P-O14
28	a	503	3PE	C11-O13-P-O14
28	d	503	3PE	C1-O11-P-O12
28	i	306	3PE	C1-O11-P-O12
28	i	311	3PE	C1-O11-P-O14
28	m	305	3PE	C11-O13-P-O14
29	J	201	PGT	C1-O3P-P-O1P
33	M	601	PC1	C11-O13-P-O12
33	M	608	PC1	C1-O11-P-O14
33	b	504	PC1	C1-O11-P-O14
33	f	201	PC1	C1-O11-P-O14
33	h	302	PC1	C11-O13-P-O14
33	k	609	PC1	C11-O13-P-O14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	m	311	PC1	C11-O13-P-O12
33	n	1001	PC1	C11-O13-P-O14
38	a	513	P5S	CB-OG-P12-O15
39	J	202	T7X	C7-O13-P1-O11
39	g	615	T7X	C7-O13-P1-O11
43	d	501	CDL	CA2-OA2-PA1-OA3
38	I	201	P5S	C44-C45-C46-C48
28	H	405	3PE	O32-C31-C32-C33
29	J	201	PGT	O31-C31-C32-C33
29	q	1000	PGT	O31-C31-C32-C33
33	d	516	PC1	O22-C21-C22-C23
37	L	811	3PH	O11-C1-C2-C3
28	h	301	3PE	C22-C23-C24-C25
33	H	402	PC1	C3A-C3B-C3C-C3D
33	N	504	PC1	C2A-C2B-C2C-C2D
28	H	405	3PE	O13-C11-C12-N
28	L	805	3PE	O13-C11-C12-N
33	N	501	PC1	O32-C31-C32-C33
33	g	612	PC1	O32-C31-C32-C33
37	o	201	3PH	O32-C31-C32-C33
39	J	202	T7X	O19-C11-C31-C32
33	i	310	PC1	C2D-C2E-C2F-C2G
37	c	206	3PH	C28-C29-C2A-C2B
39	J	202	T7X	C39-C40-C41-C42
29	N	505	PGT	O3-C11-C12-C13
37	c	206	3PH	O31-C31-C32-C33
28	i	306	3PE	C39-C3A-C3B-C3C
28	H	405	3PE	O22-C21-C22-C23
28	i	306	3PE	O32-C31-C32-C33
33	a	501	PC1	O32-C31-C32-C33
33	l	304	PC1	O32-C31-C32-C33
37	j	1003	3PH	C3A-C3B-C3C-C3D
33	f	201	PC1	C3B-C3C-C3D-C3E
28	e	502	3PE	O21-C21-C22-C23
28	H	404	3PE	C3C-C3D-C3E-C3F
37	H	409	3PH	C34-C35-C36-C37
28	L	802	3PE	C3E-C3F-C3G-C3H
28	a	503	3PE	C27-C28-C29-C2A
44	k	605	HEA	CAA-CBA-CGA-O2A
28	L	808	3PE	C12-C11-O13-P
28	L	808	3PE	C3-C2-O21-C21
28	d	515	3PE	C12-C11-O13-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	i	307	3PE	C1-C2-O21-C21
28	i	311	3PE	C12-C11-O13-P
28	m	304	3PE	C12-C11-O13-P
30	i	305	DU0	O23-C24-C25-C26
33	d	516	PC1	C12-C11-O13-P
33	m	314	PC1	C12-C11-O13-P
33	n	1001	PC1	C1-C2-O21-C21
37	M	604	3PH	C3-C2-O21-C21
37	P	402	3PH	C1-C2-O21-C21
37	g	603	3PH	C1-C2-O21-C21
37	i	314	3PH	C3-C2-O21-C21
37	m	301	3PH	C1-C2-O21-C21
43	d	501	CDL	CA6-CA4-OA6-CA5
29	M	602	PGT	O11-C11-C12-C13
29	a	514	PGT	O3-C11-C12-C13
37	M	604	3PH	O21-C21-C22-C23
39	J	202	T7X	O18-C11-C31-C32
28	e	505	3PE	C25-C26-C27-C28
33	k	609	PC1	C2C-C2D-C2E-C2F
38	a	513	P5S	C30-C31-C32-C33
33	H	402	PC1	C11-C12-N-C14
28	a	503	3PE	O21-C21-C22-C23
28	a	508	3PE	O21-C21-C22-C23
33	N	504	PC1	O21-C21-C22-C23
37	i	318	3PH	C25-C26-C27-C28
28	i	309	3PE	C32-C33-C34-C35
33	j	1001	PC1	O31-C31-C32-C33
37	M	606	3PH	O21-C21-C22-C23
37	g	611	3PH	O31-C31-C32-C33
29	N	505	PGT	O4P-C4-C5-C6
28	i	317	3PE	O22-C21-C22-C23
37	g	611	3PH	O22-C21-C22-C23
37	d	508	3PH	C37-C38-C39-C3A
32	d	506	U10	C45-C44-C46-C47
28	a	503	3PE	O22-C21-C22-C23
28	i	317	3PE	O32-C31-C32-C33
33	j	1001	PC1	O22-C21-C22-C23
37	m	309	3PH	C2A-C2B-C2C-C2D
28	c	201	3PE	O21-C21-C22-C23
37	P	402	3PH	O31-C31-C32-C33
28	e	502	3PE	C3C-C3D-C3E-C3F
28	A	201	3PE	O32-C31-C32-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	j	1001	PC1	O32-C31-C32-C33
33	k	609	PC1	O21-C21-C22-C23
37	g	611	3PH	O21-C21-C22-C23
37	d	513	3PH	C29-C2A-C2B-C2C
28	g	613	3PE	C39-C3A-C3B-C3C
28	H	404	3PE	O22-C21-C22-C23
29	A	202	PGT	O31-C31-C32-C33
29	P	401	PGT	O11-C11-C12-C13
37	L	801	3PH	O22-C21-C22-C23
37	d	502	3PH	O32-C31-C32-C33
37	g	611	3PH	O32-C31-C32-C33
32	a	511	U10	C39-C41-C42-C43
29	a	514	PGT	C20-C21-C22-C23
28	k	603	3PE	C24-C25-C26-C27
33	N	504	PC1	C23-C24-C25-C26
33	i	310	PC1	C34-C35-C36-C37
33	j	1001	PC1	O21-C21-C22-C23
37	L	807	3PH	O21-C21-C22-C23
28	g	613	3PE	C3C-C3D-C3E-C3F
28	i	309	3PE	C34-C35-C36-C37
33	l	304	PC1	C22-C23-C24-C25
28	a	508	3PE	O22-C21-C22-C23
29	q	1000	PGT	O11-C11-C12-C13
37	M	606	3PH	O22-C21-C22-C23
28	m	315	3PE	C39-C3A-C3B-C3C
33	a	517	PC1	C32-C33-C34-C35
37	i	303	3PH	C29-C2A-C2B-C2C
33	n	1001	PC1	O31-C31-C32-C33

There are no ring outliers.

33 monomers are involved in 53 short contacts:

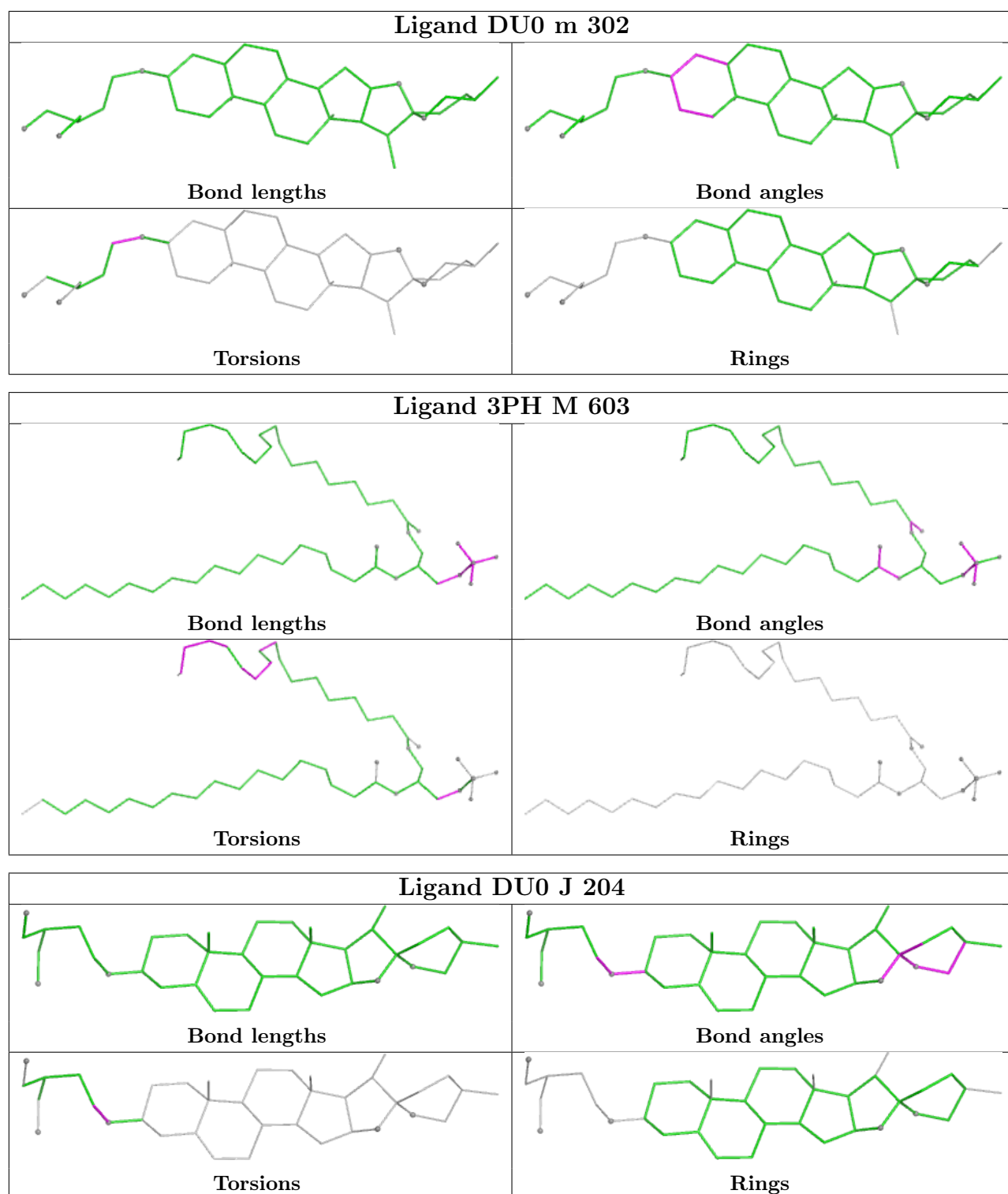
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	D	1001	PC1	2	0
36	F	502	FMN	1	0
28	m	310	3PE	1	0
42	e	504	HEC	2	0
31	F	501	SF4	1	0
29	H	406	PGT	1	0
33	m	311	PC1	4	0
37	f	205	3PH	1	0
37	M	604	3PH	2	0

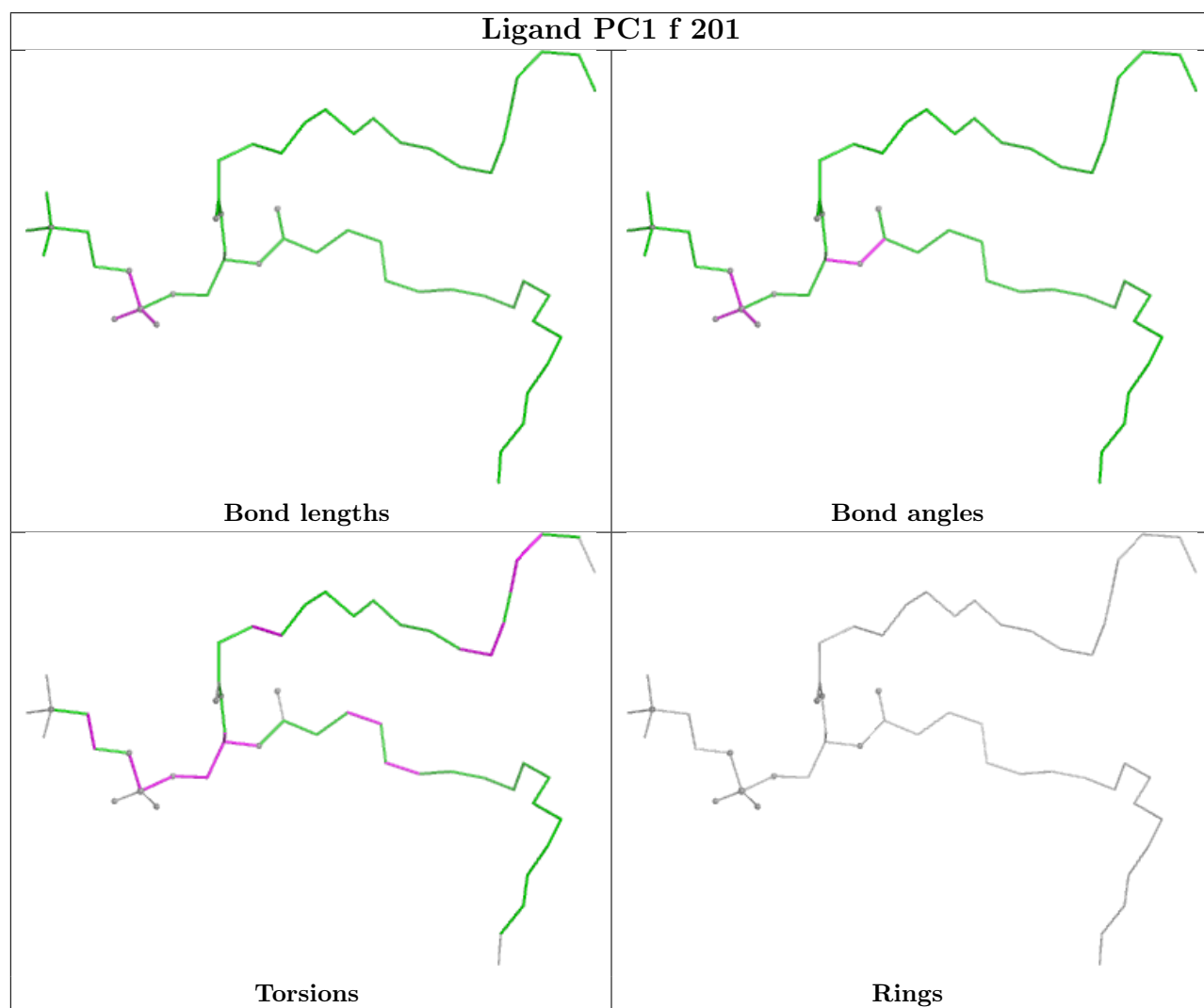
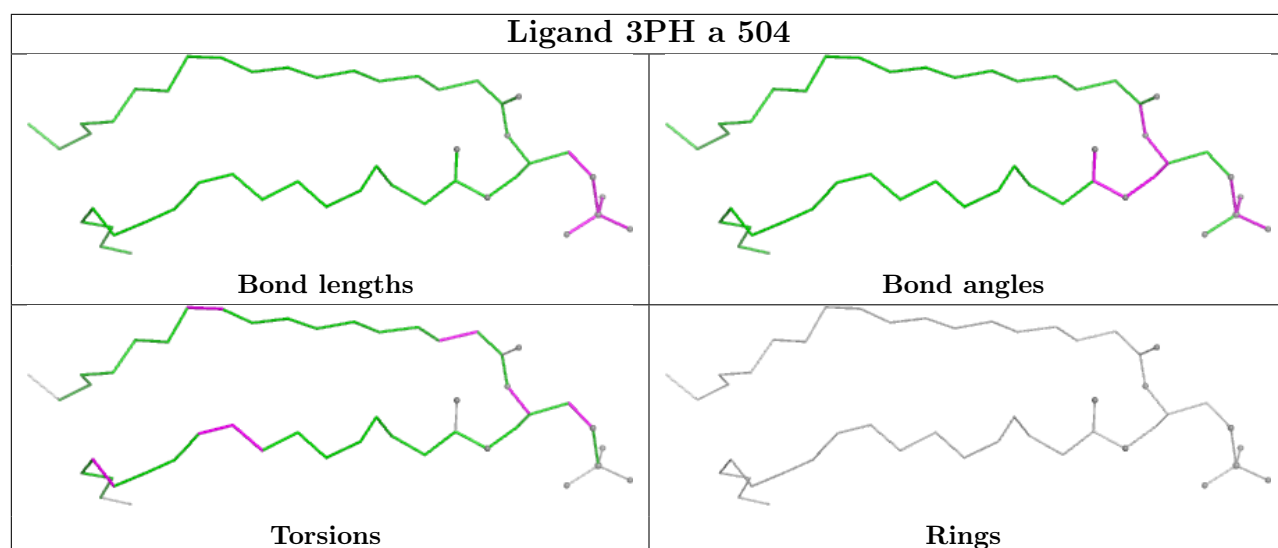
Continued on next page...

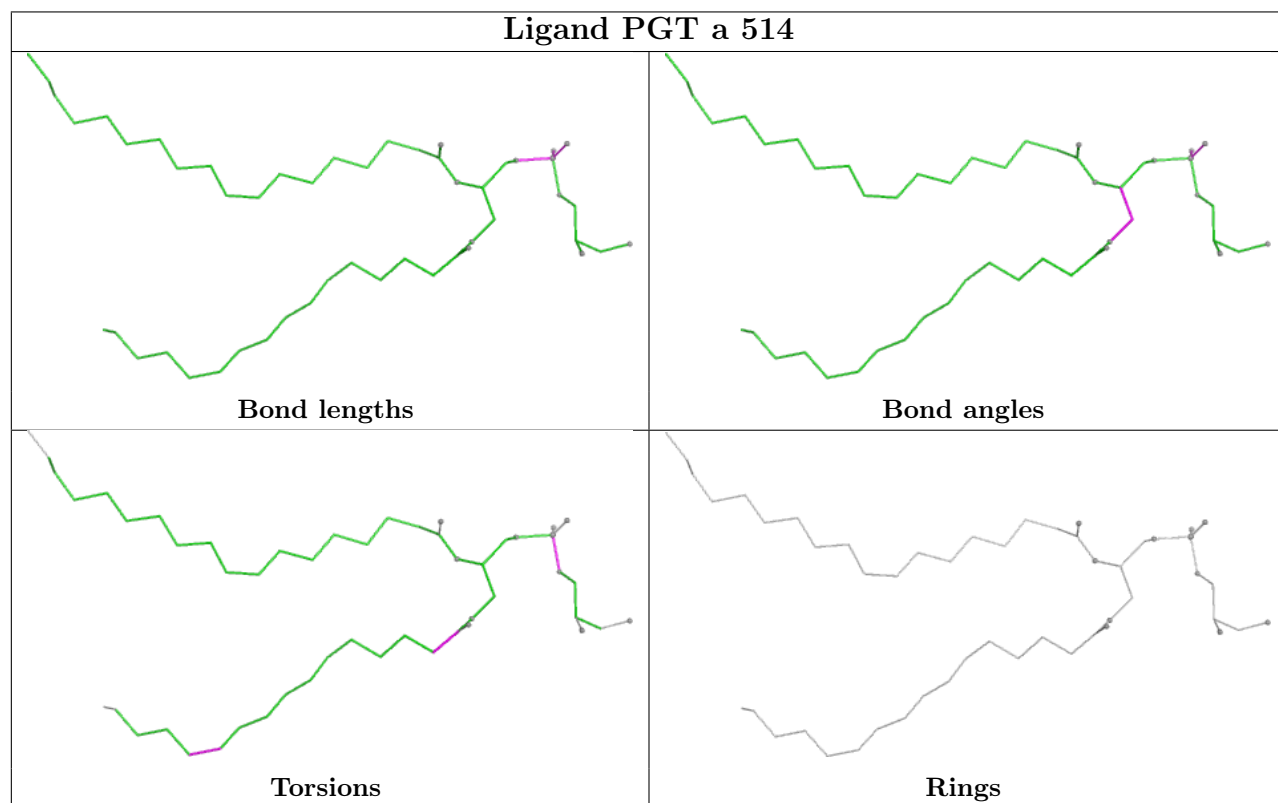
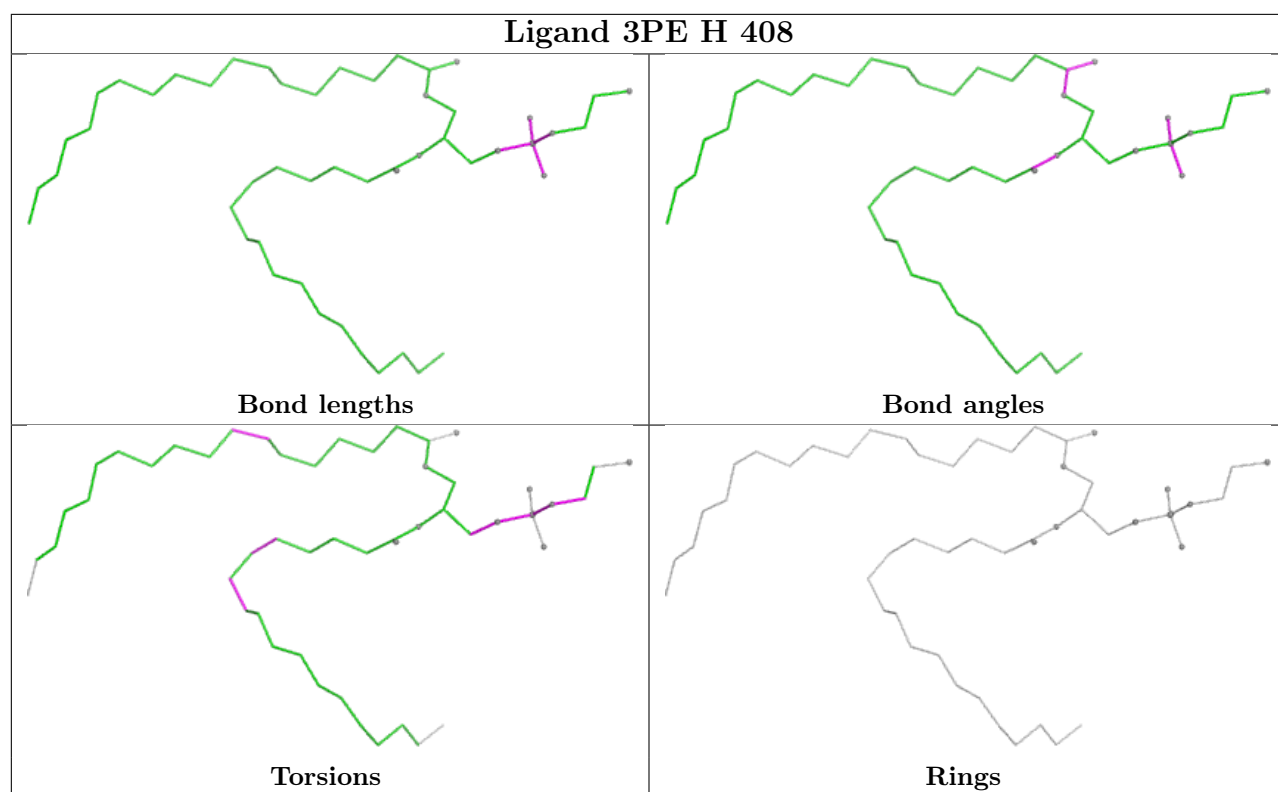
Continued from previous page...

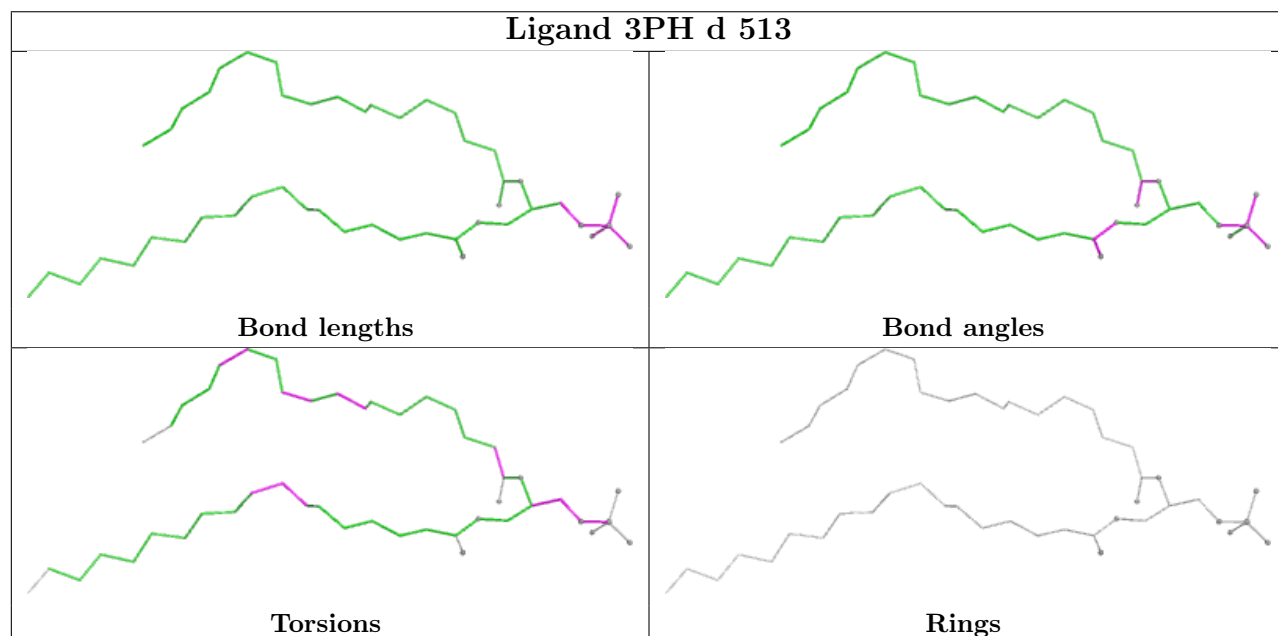
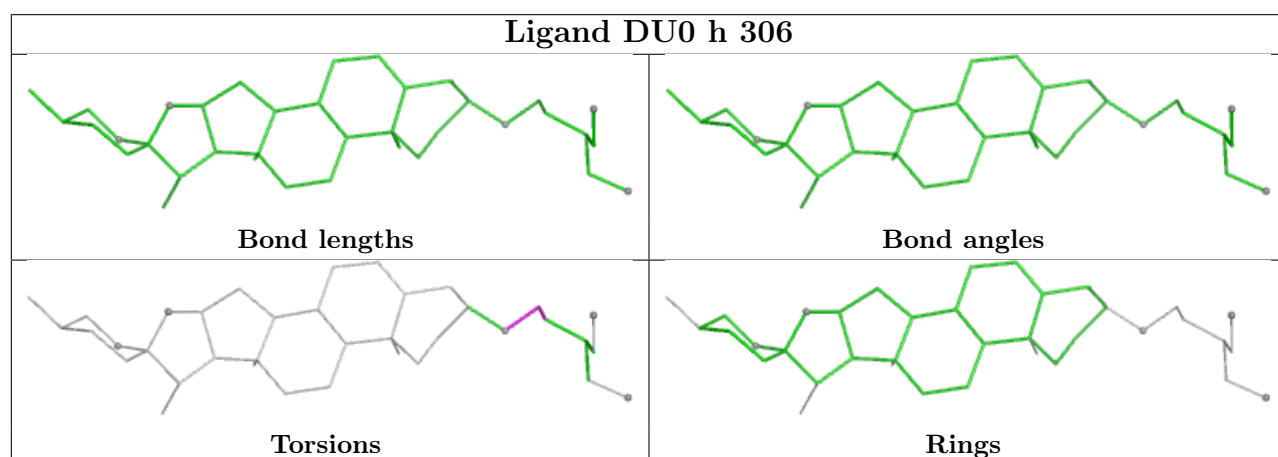
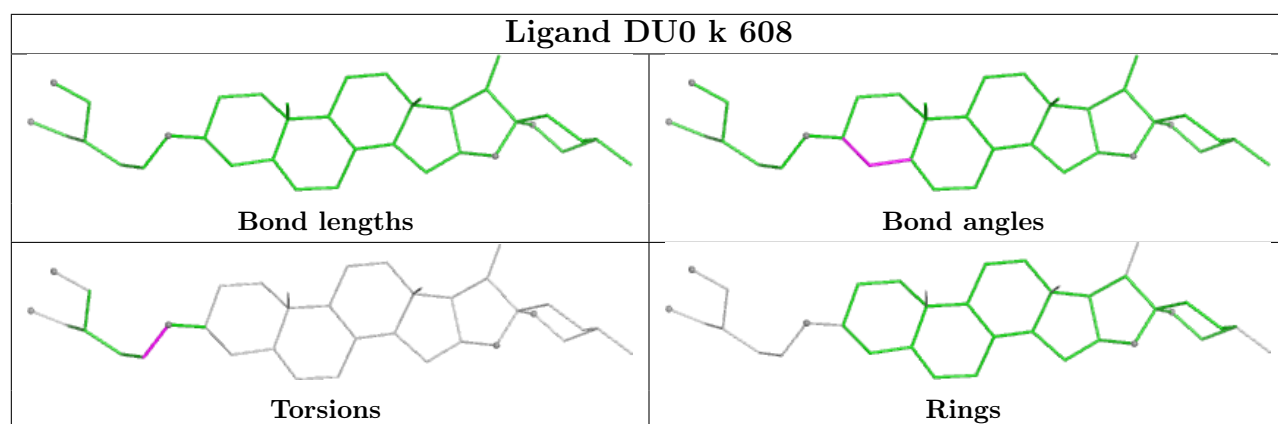
Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	g	606	HEA	2	0
30	c	205	DU0	1	0
32	a	512	U10	3	0
30	c	202	DU0	1	0
32	d	504	U10	1	0
28	A	201	3PE	1	0
32	B	1002	U10	3	0
44	k	605	HEA	1	0
32	d	506	U10	9	0
28	m	315	3PE	1	0
28	P	403	3PE	1	0
37	L	811	3PH	2	0
37	i	301	3PH	1	0
29	J	201	PGT	1	0
33	i	313	PC1	1	0
44	g	610	HEA	1	0
37	P	402	3PH	1	0
44	k	604	HEA	5	0
33	k	609	PC1	1	0
32	a	511	U10	1	0
42	b	502	HEC	1	0
33	l	304	PC1	1	0
33	b	501	PC1	1	0
33	H	402	PC1	2	0

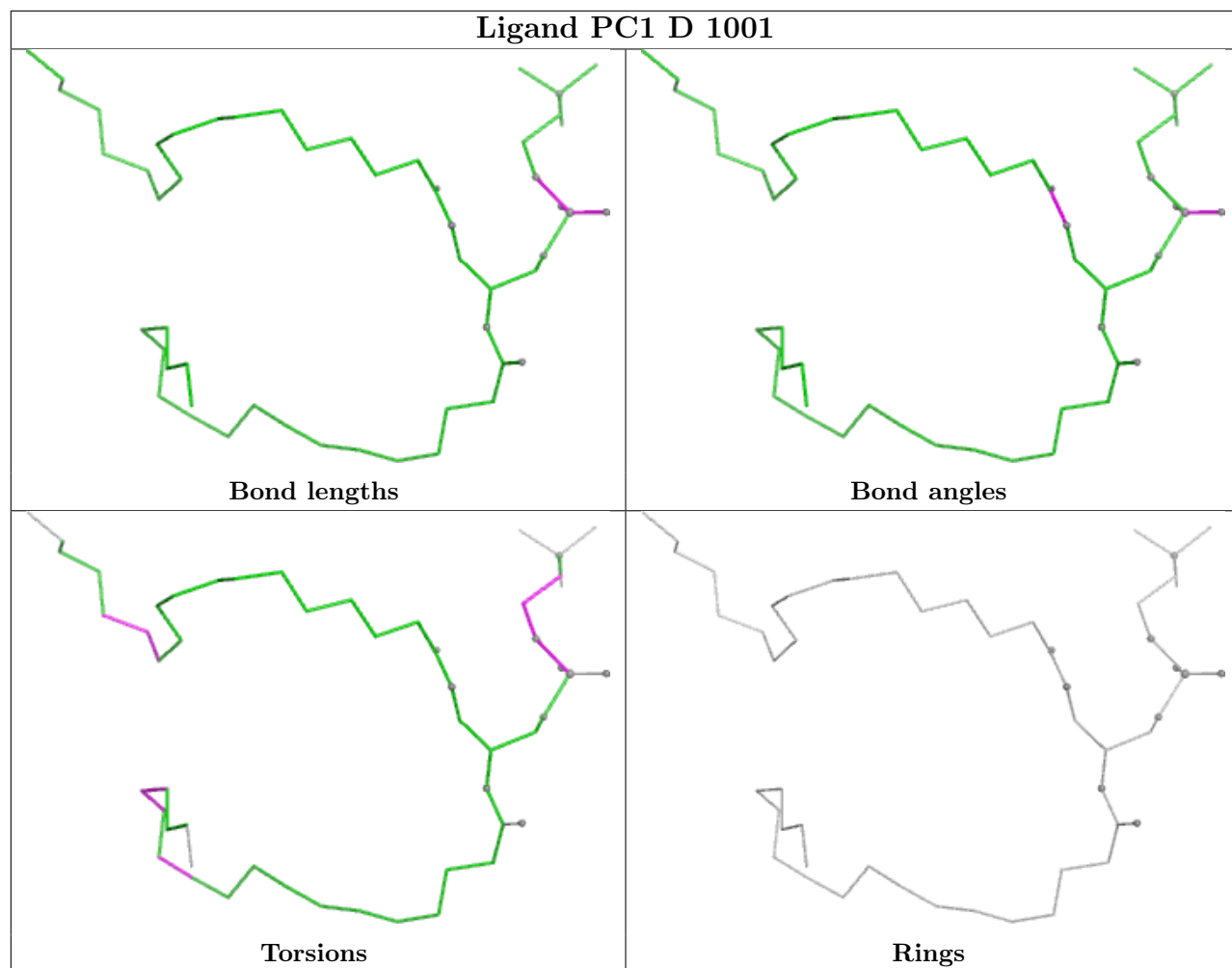
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

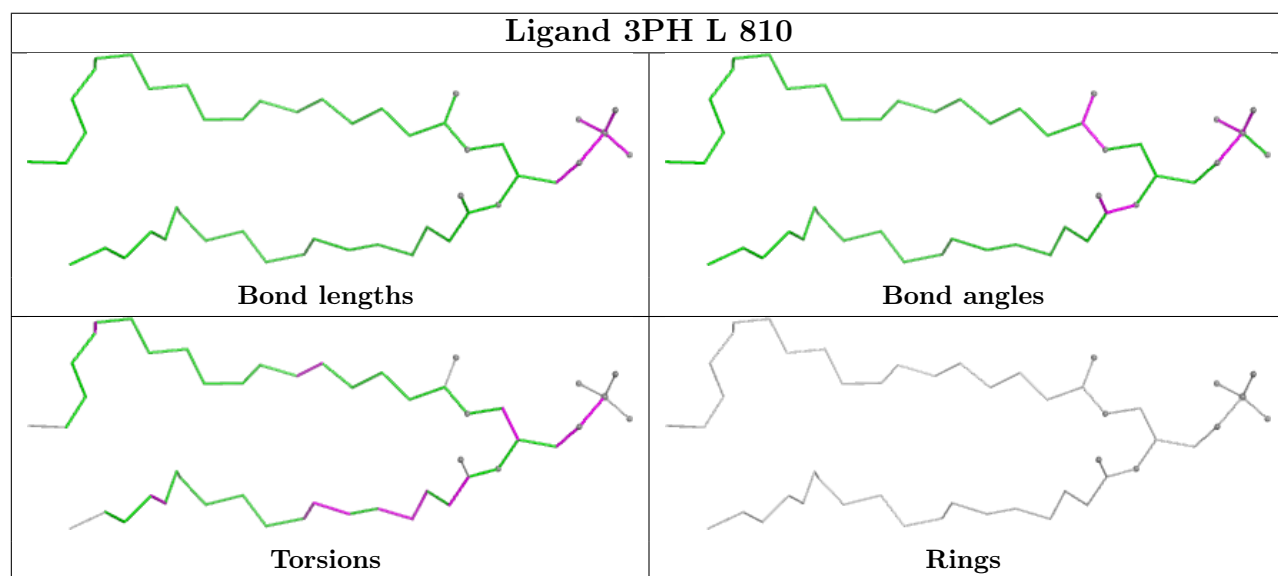
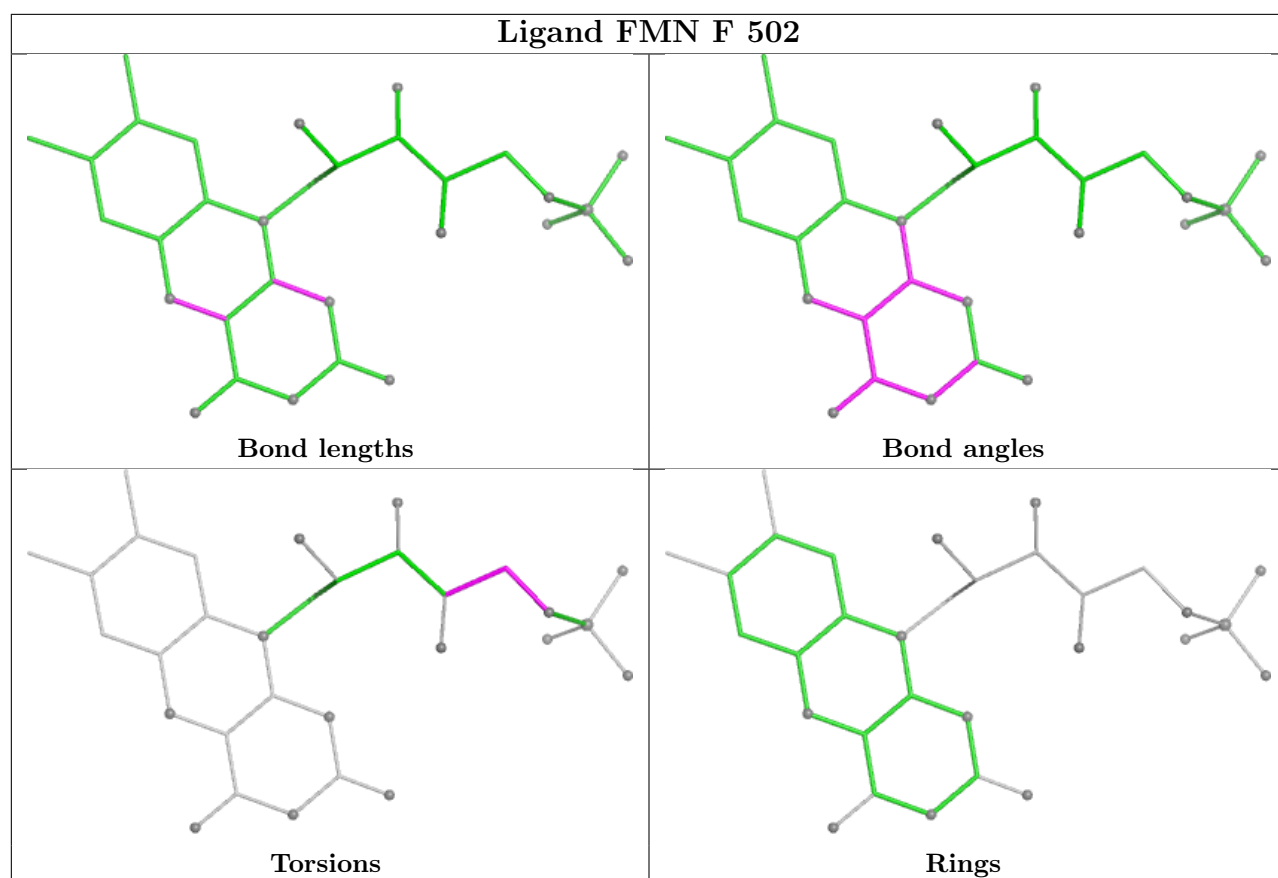


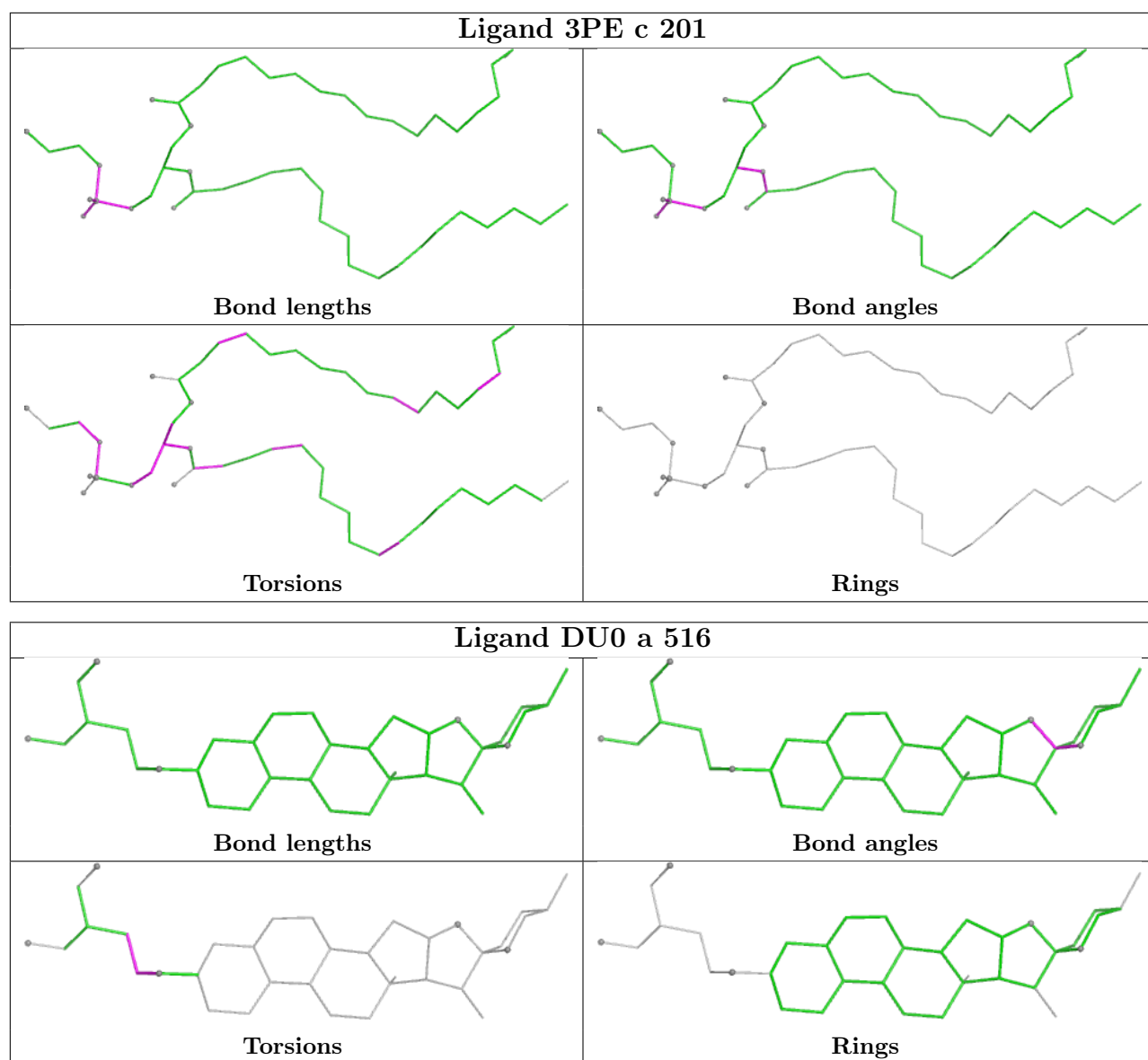


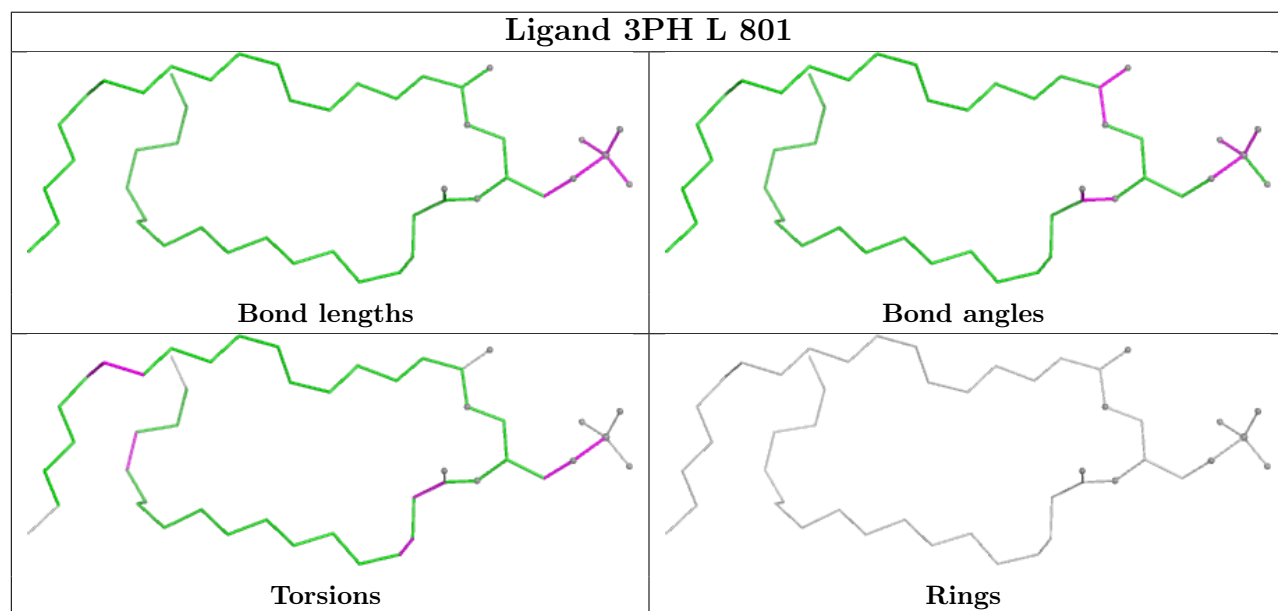
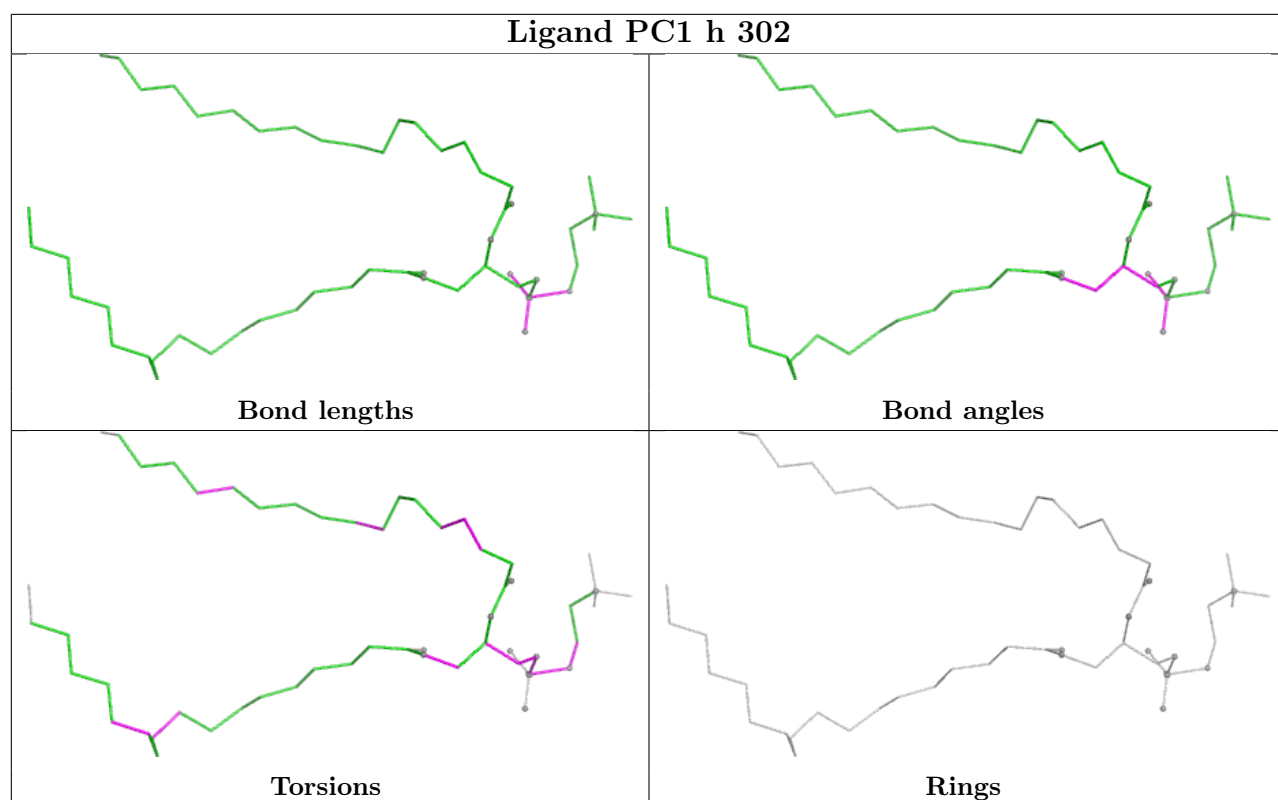


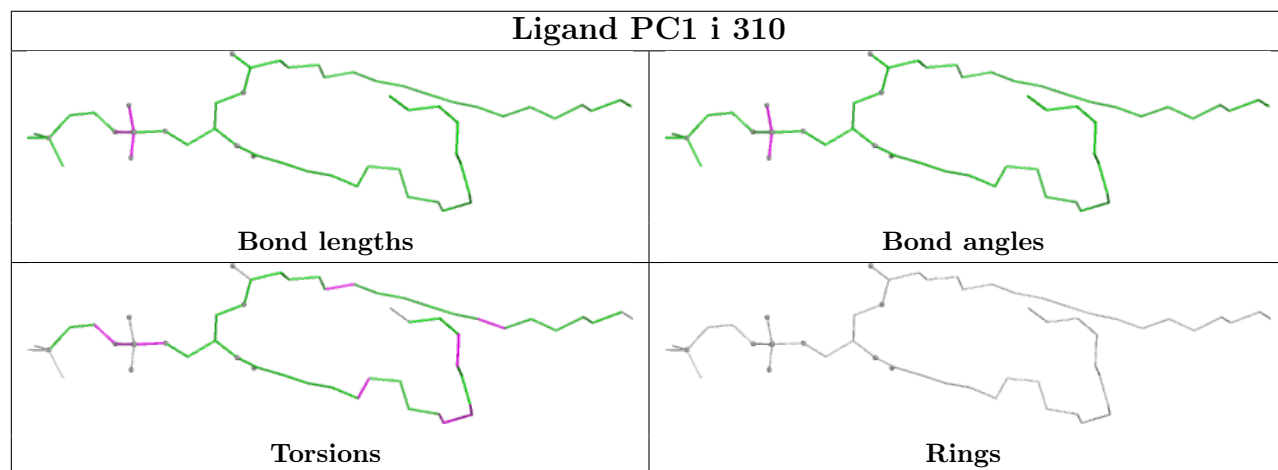
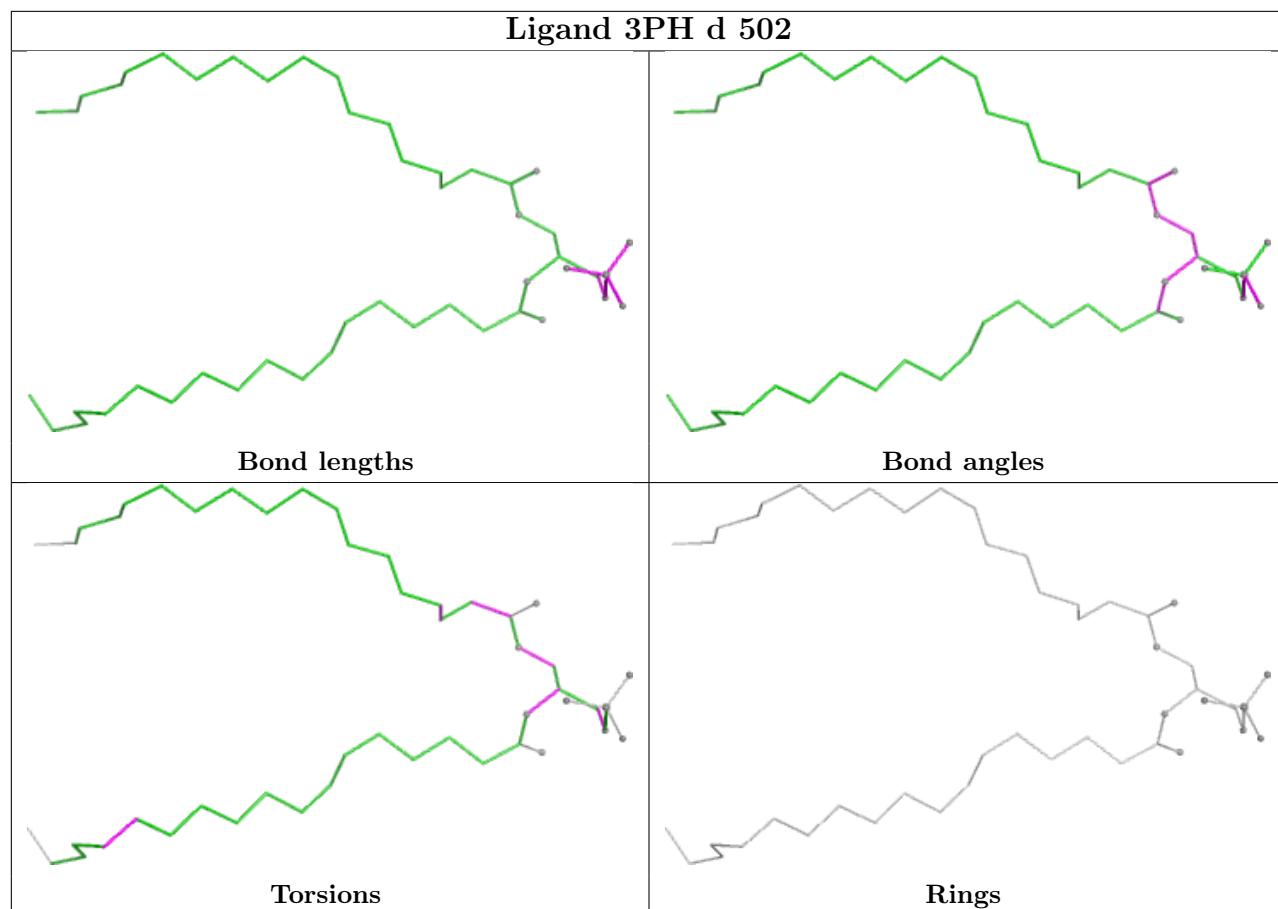


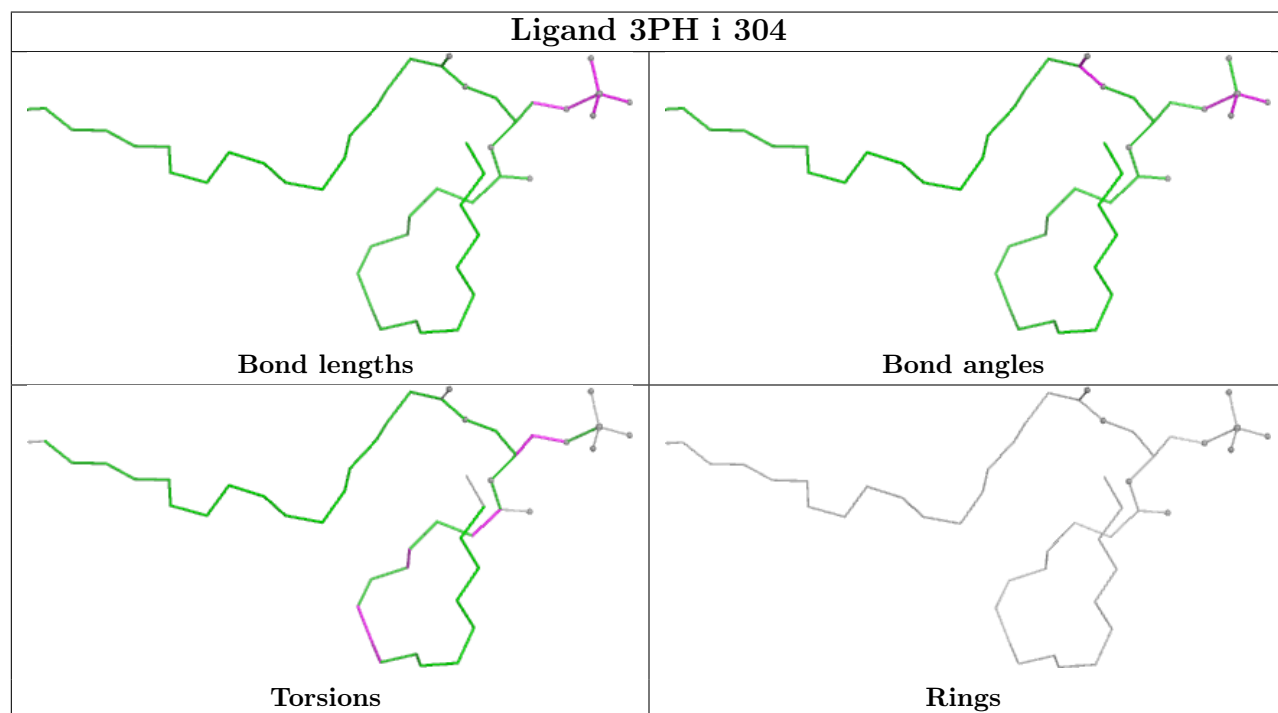
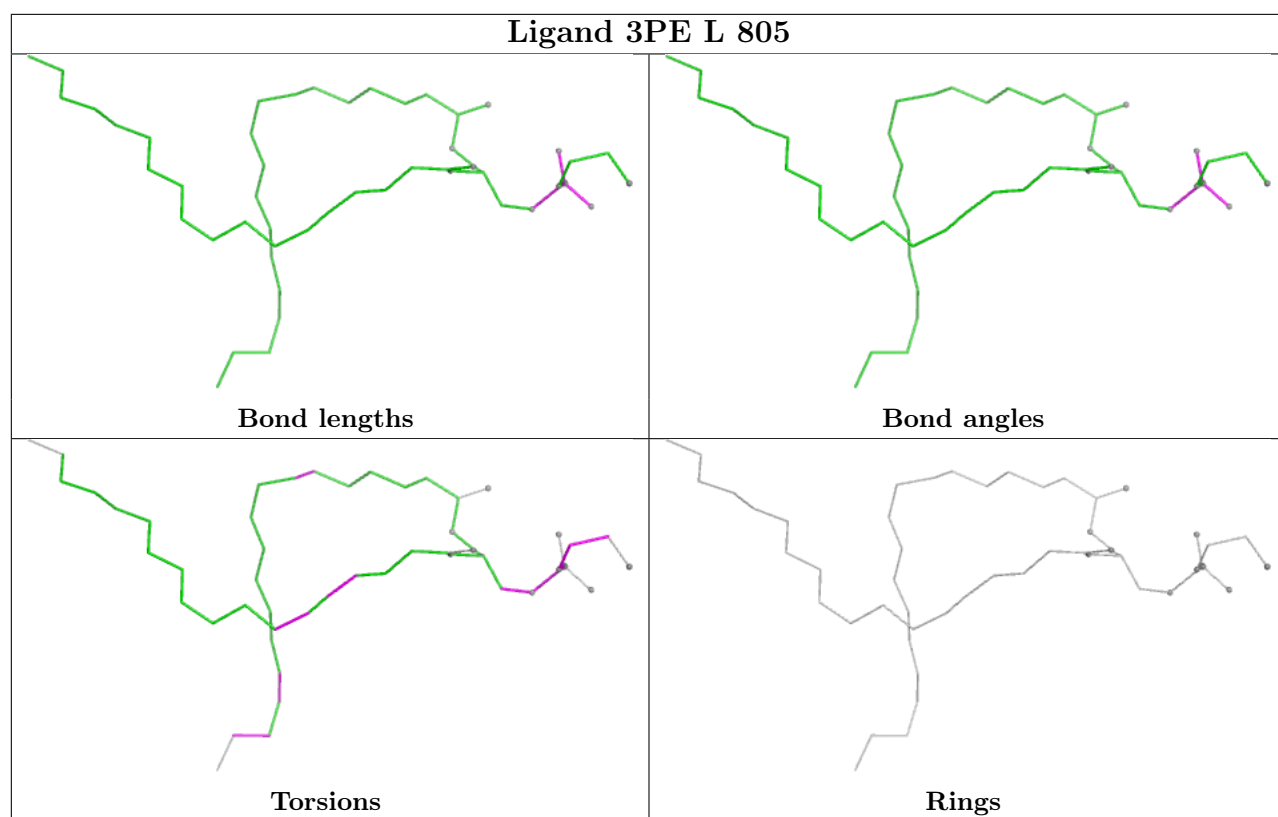


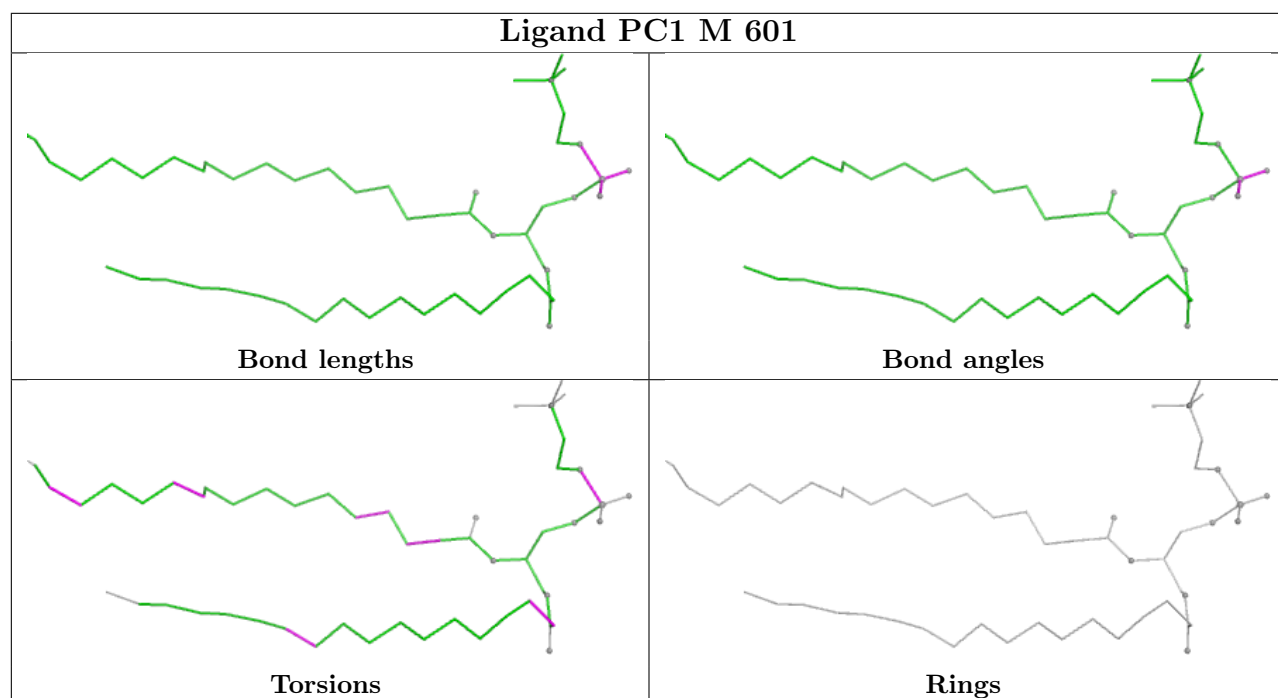
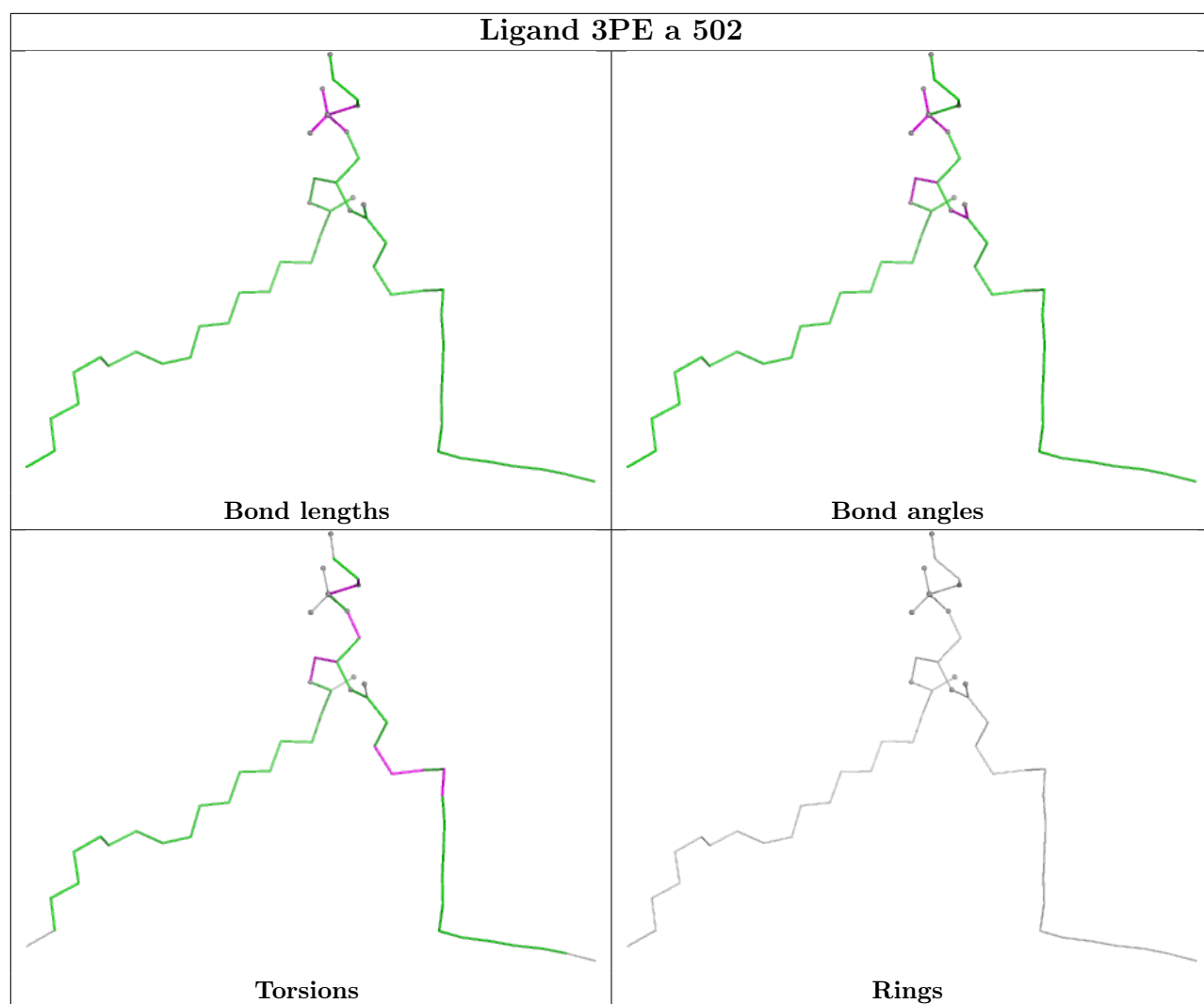


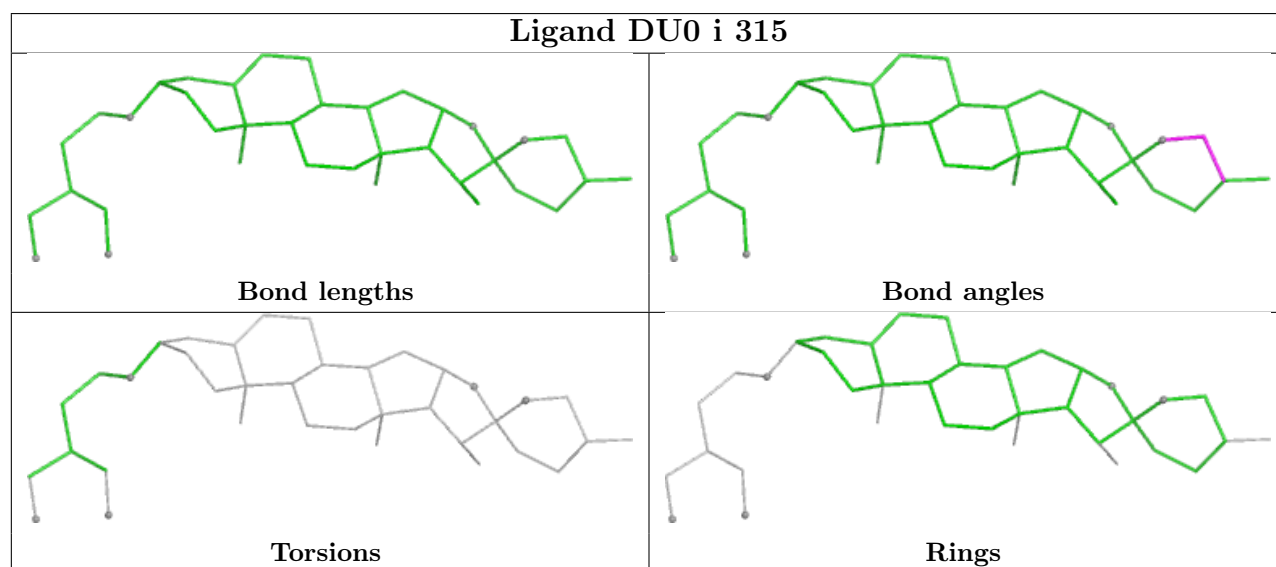
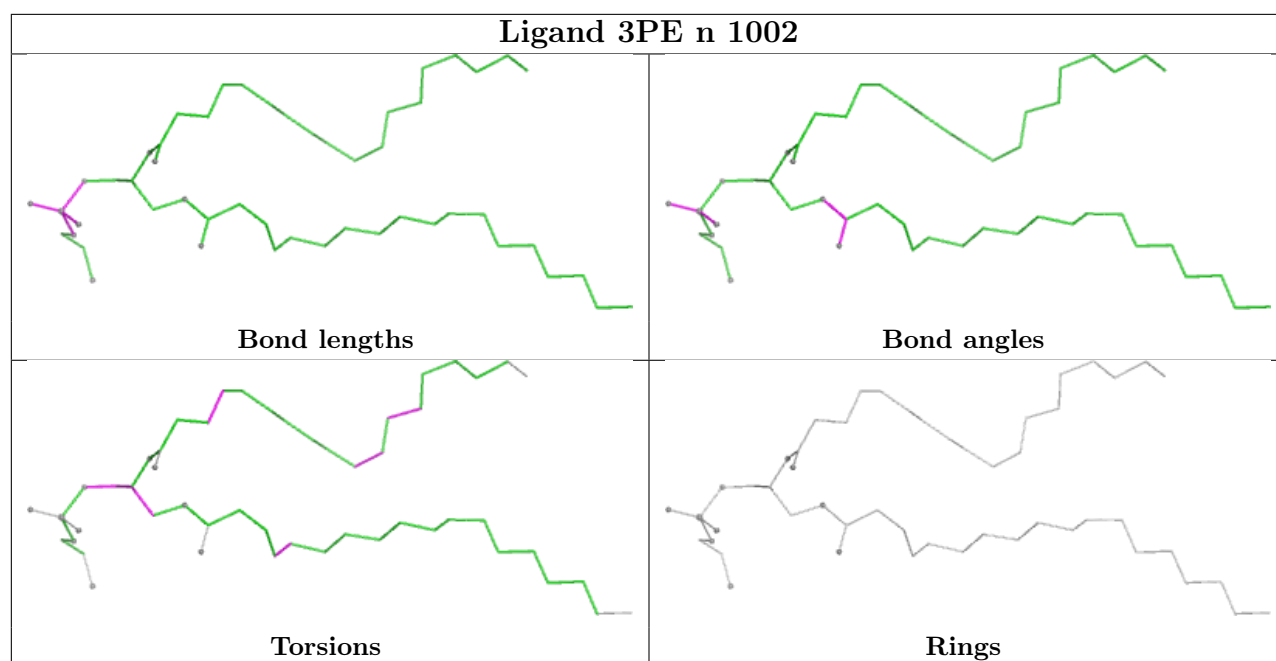


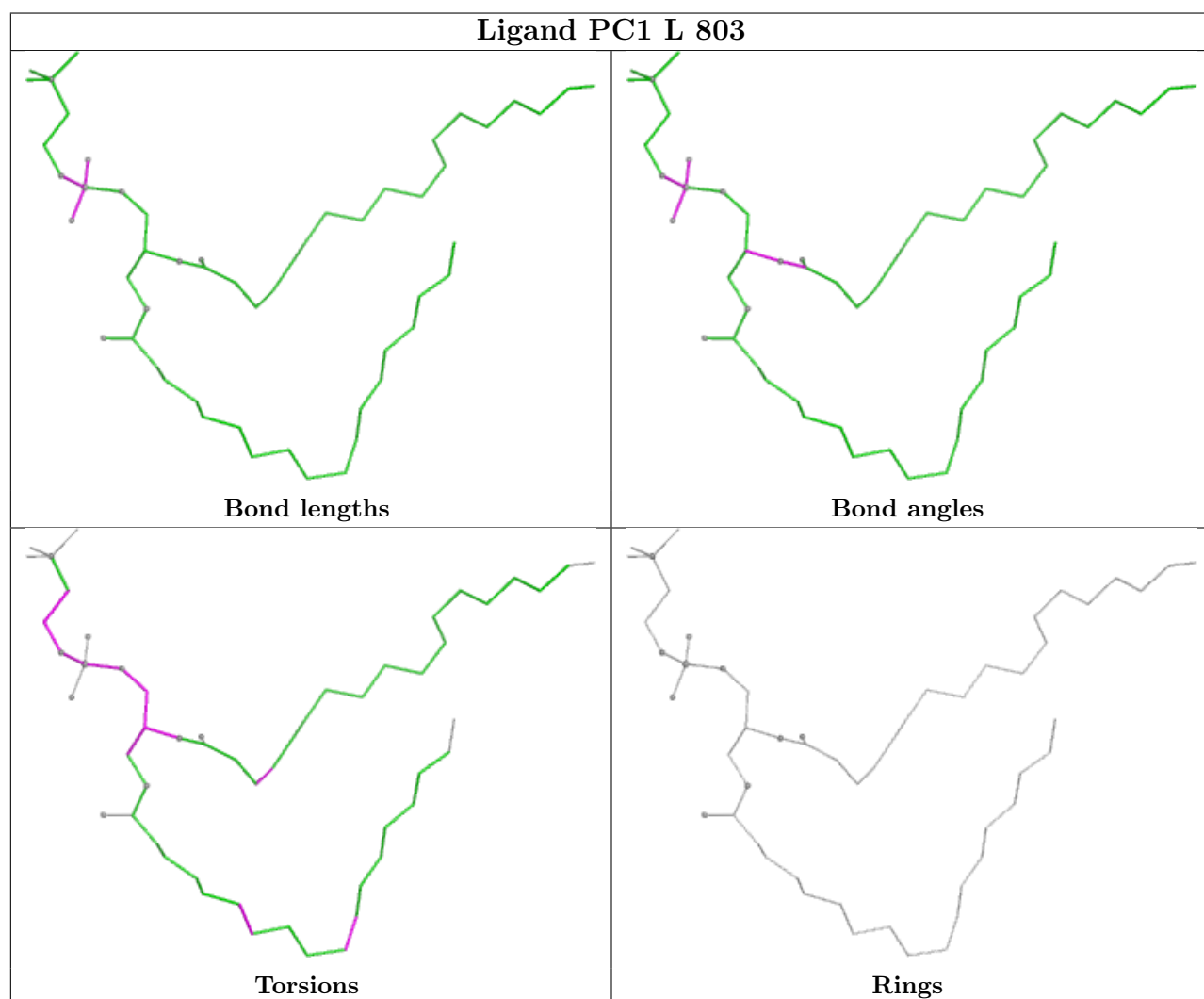
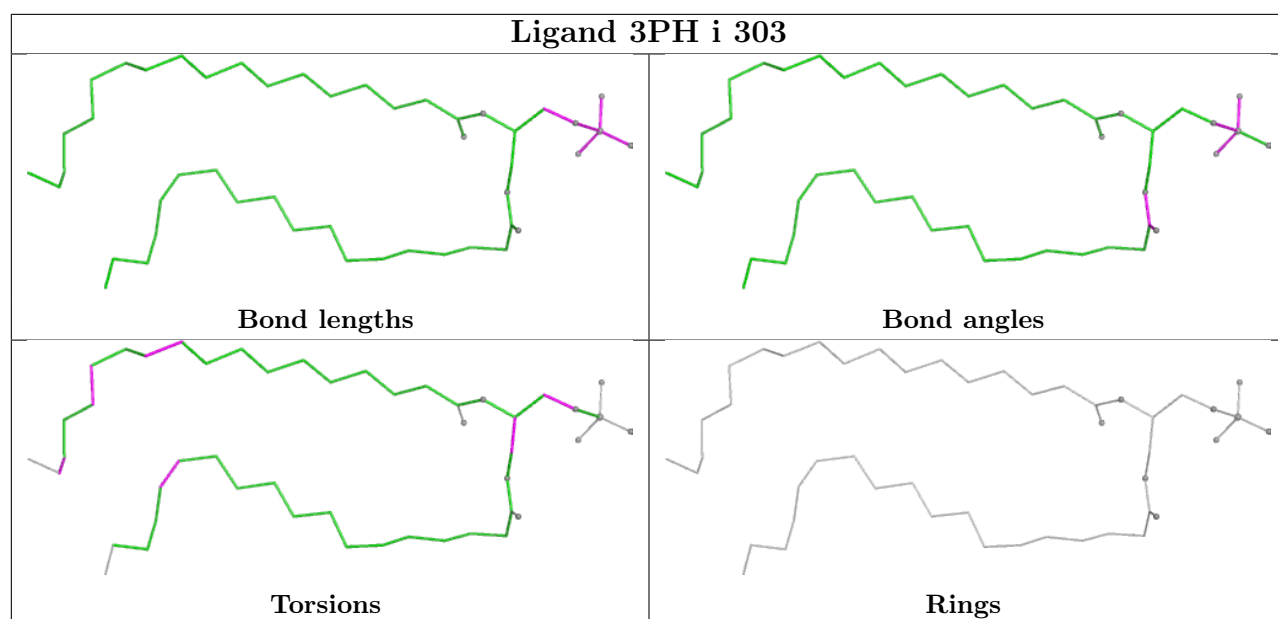


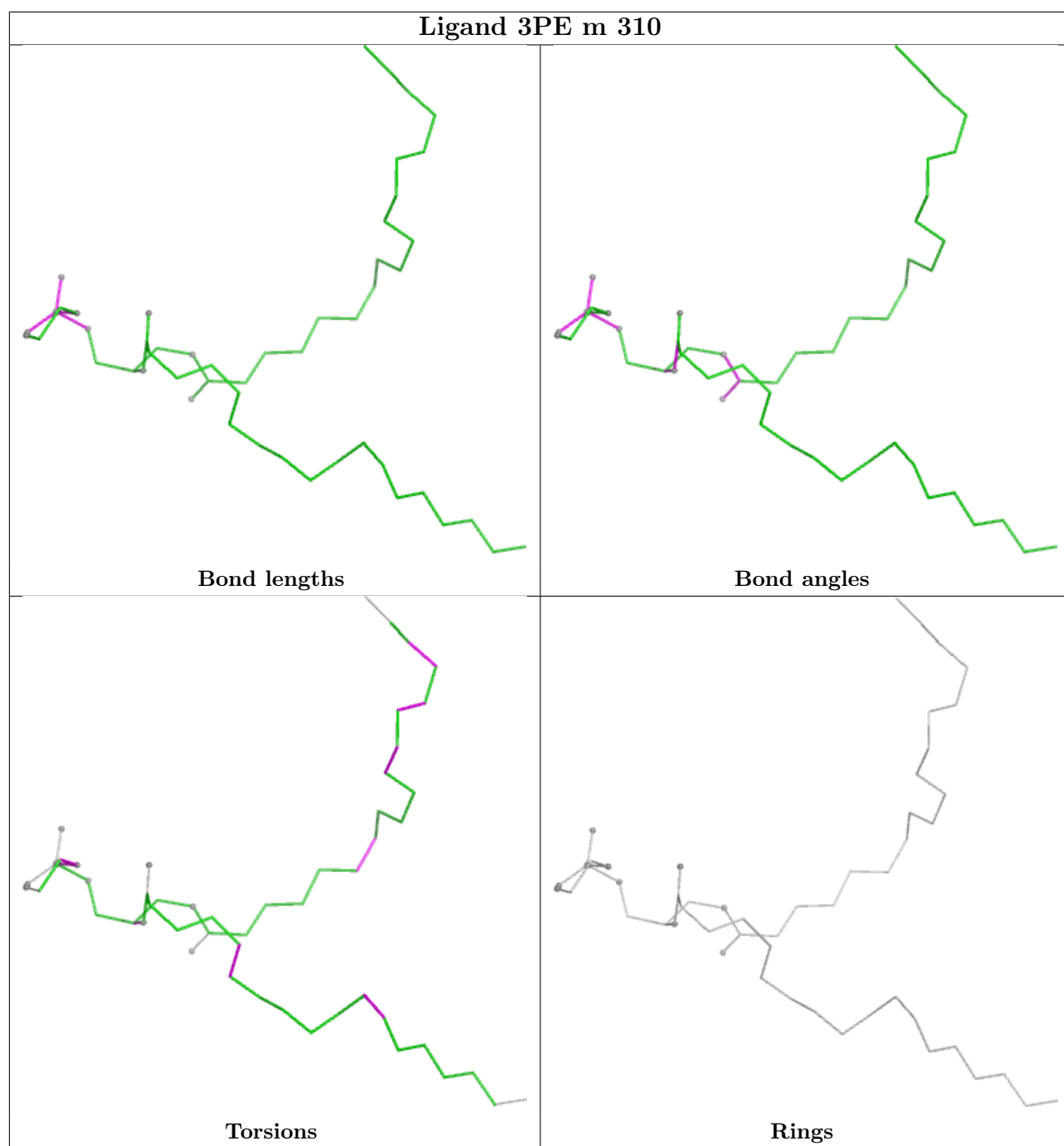




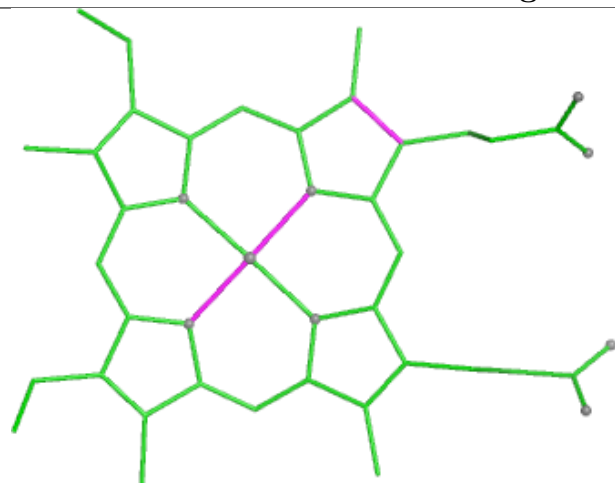




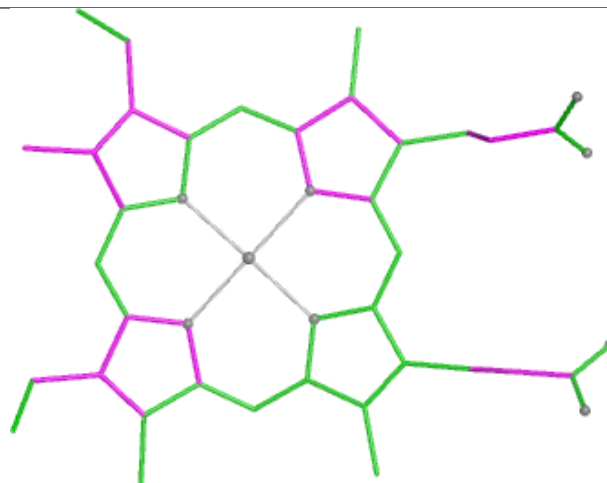




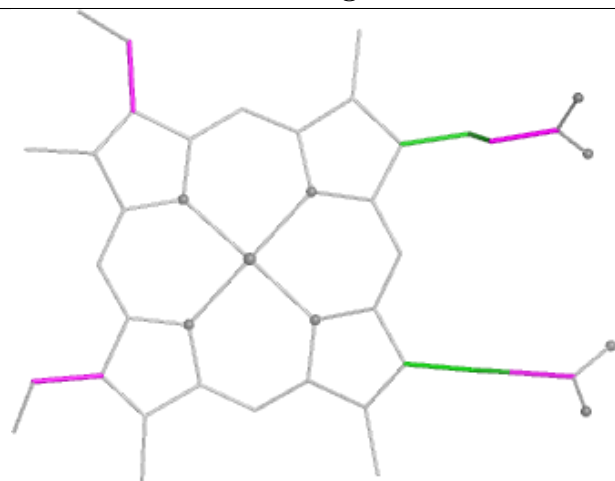
Ligand HEC e 504



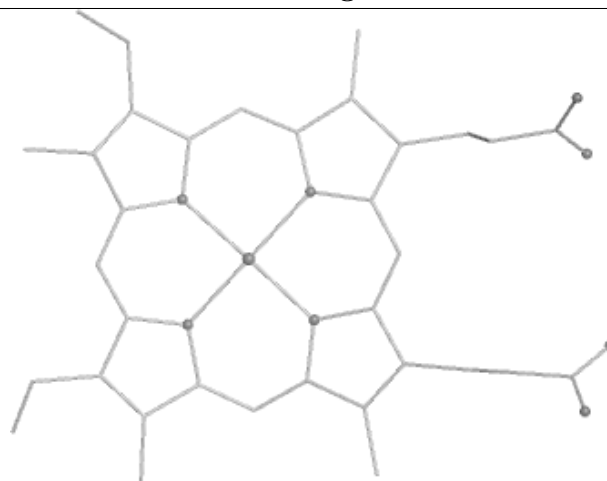
Bond lengths



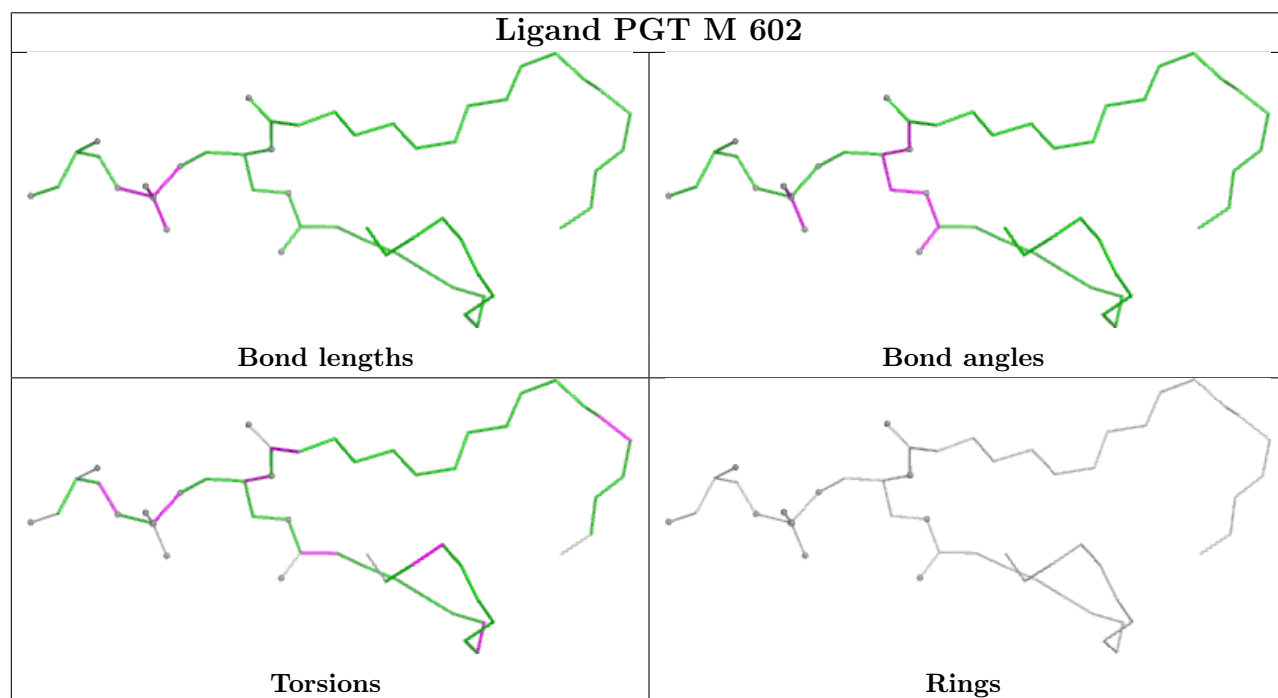
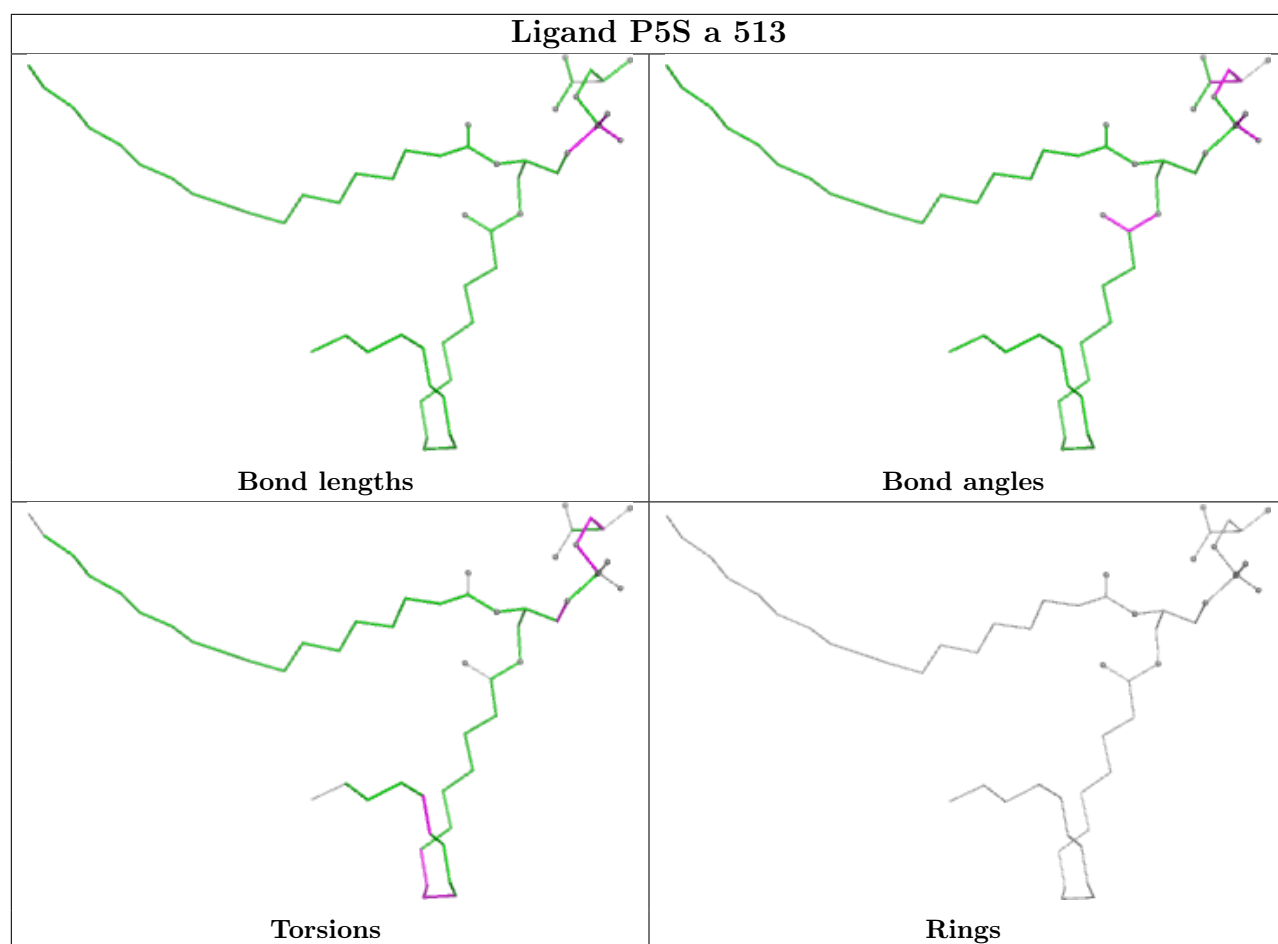
Bond angles

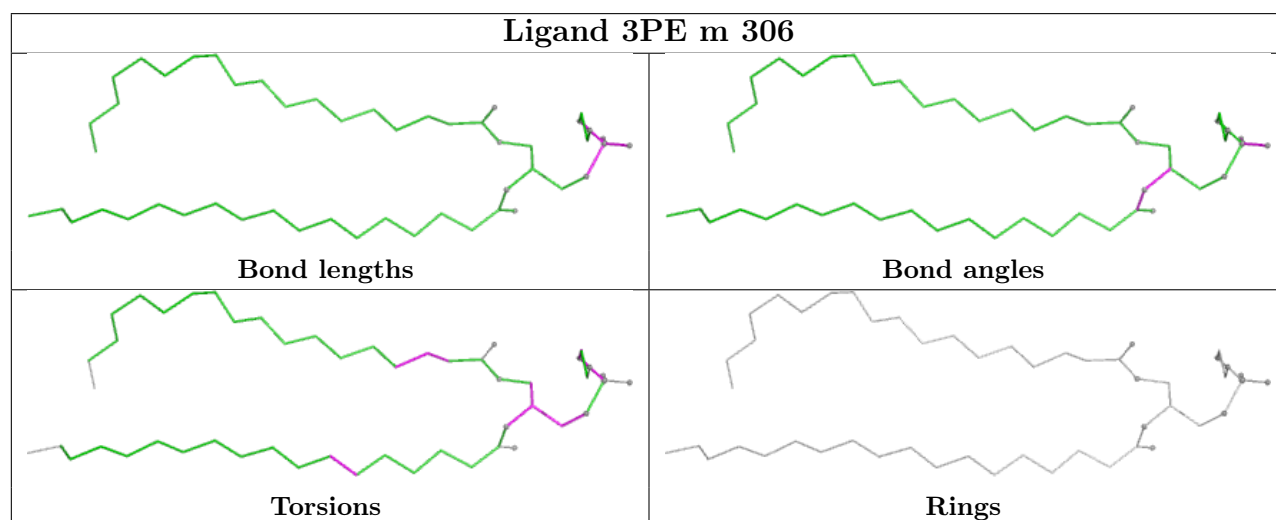
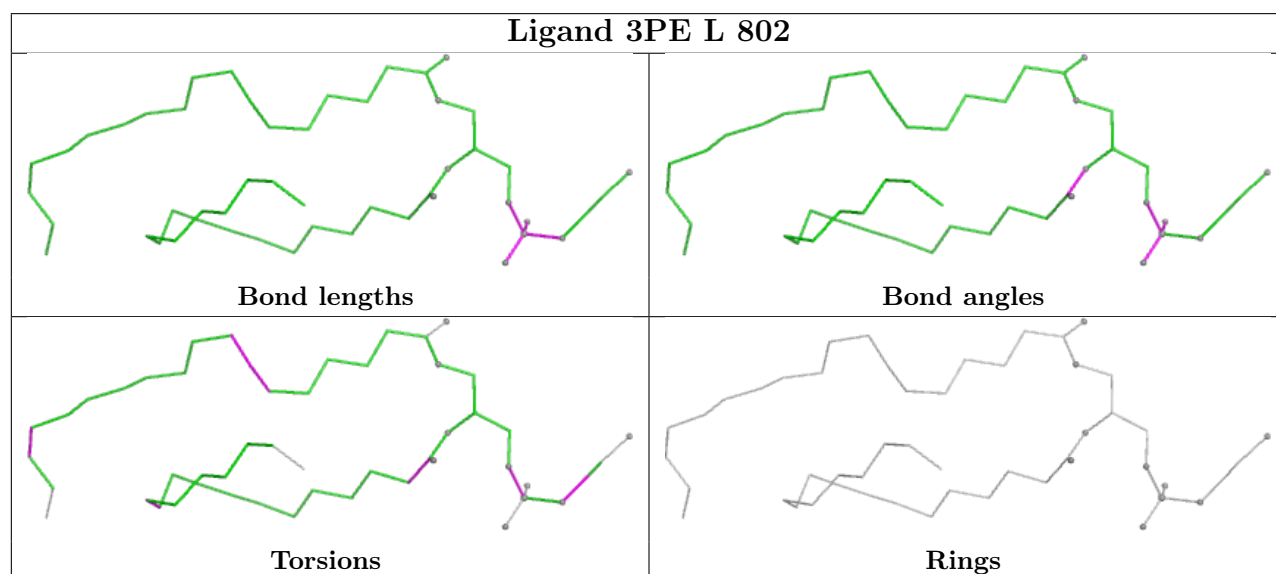
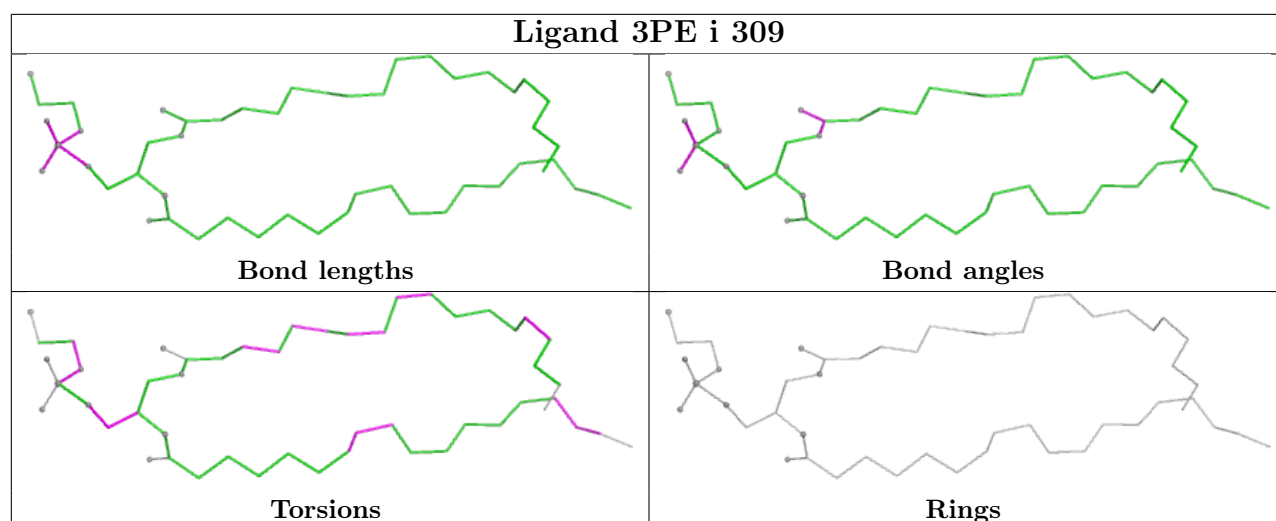


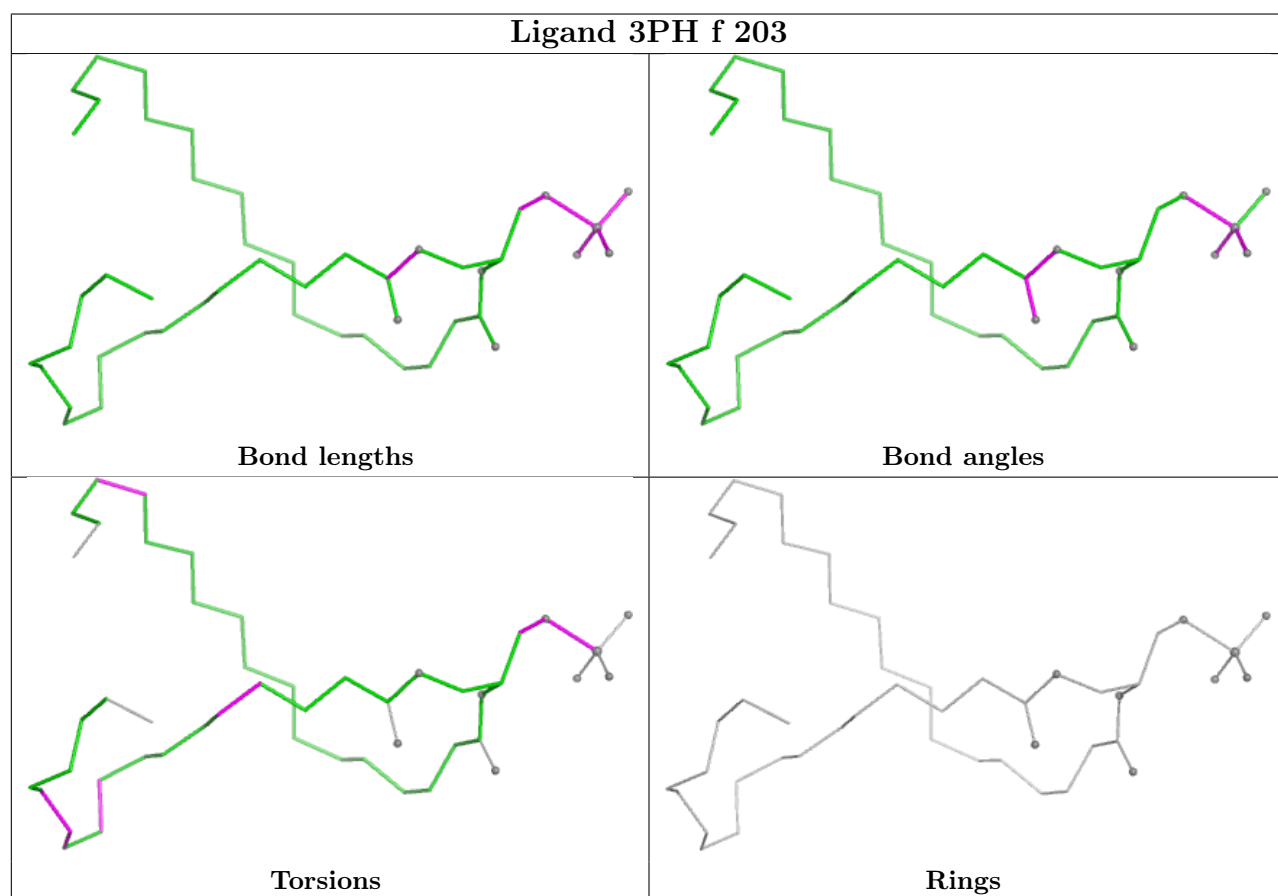
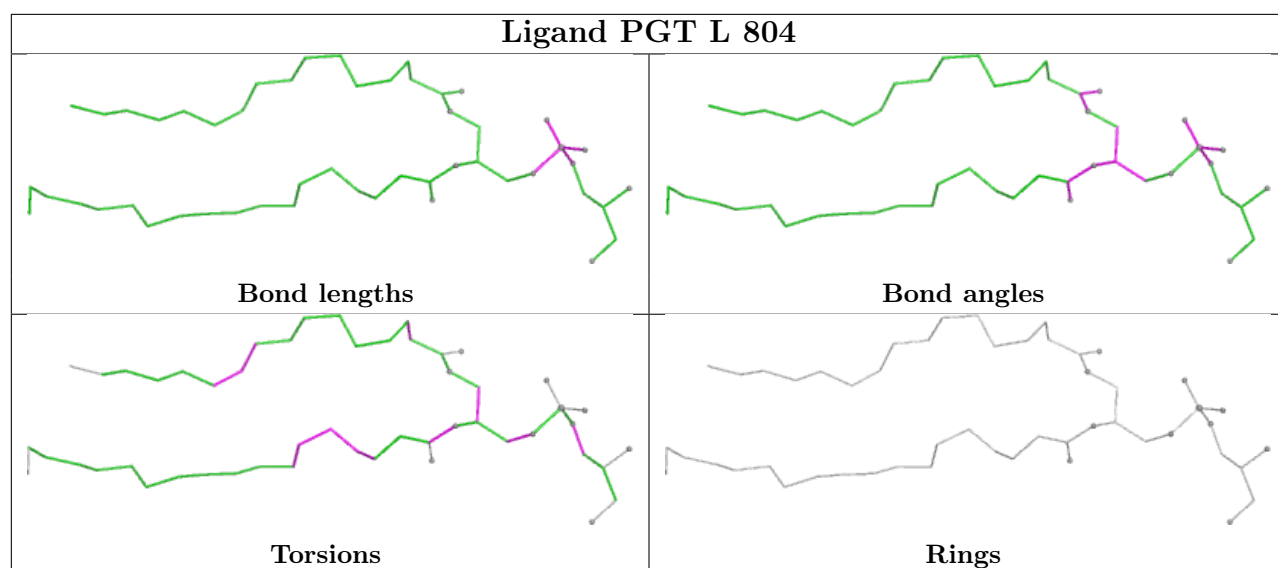
Torsions

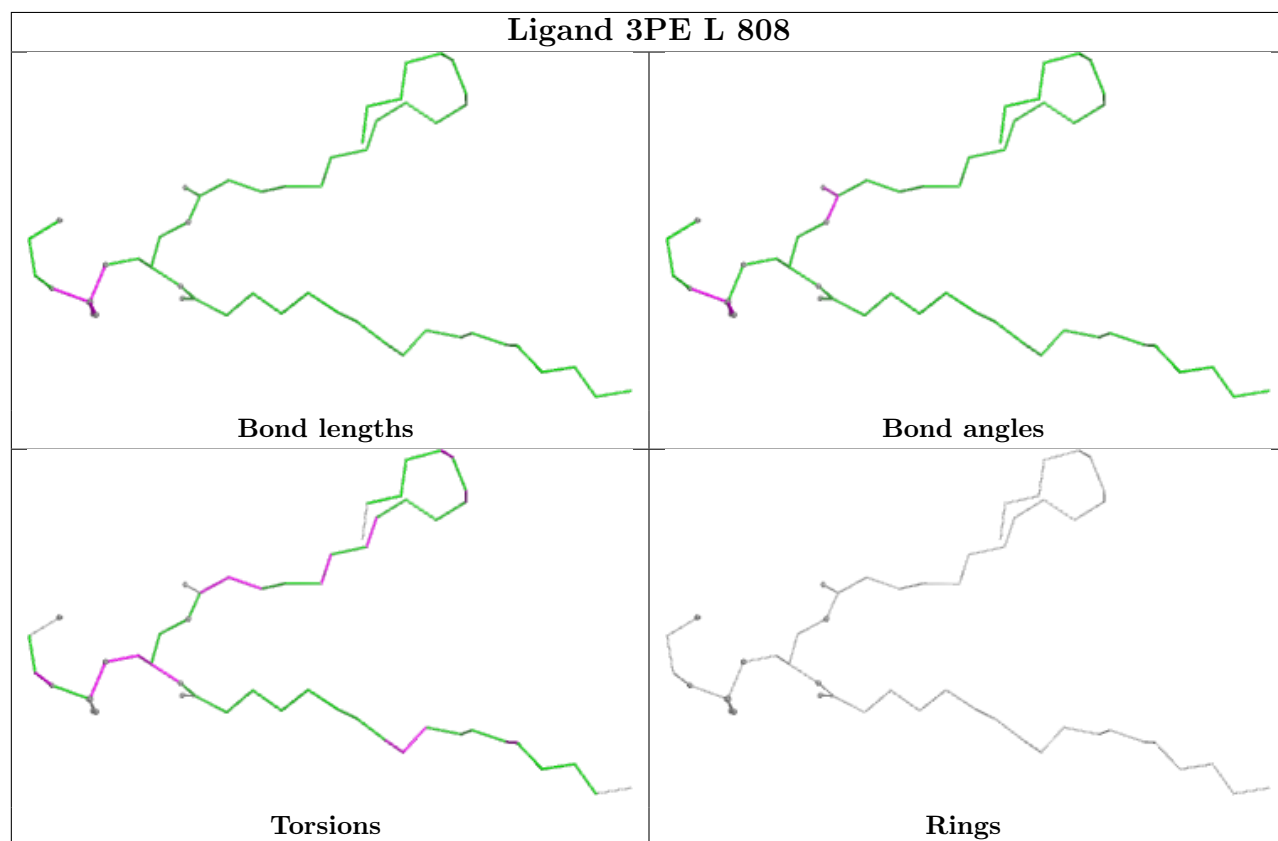
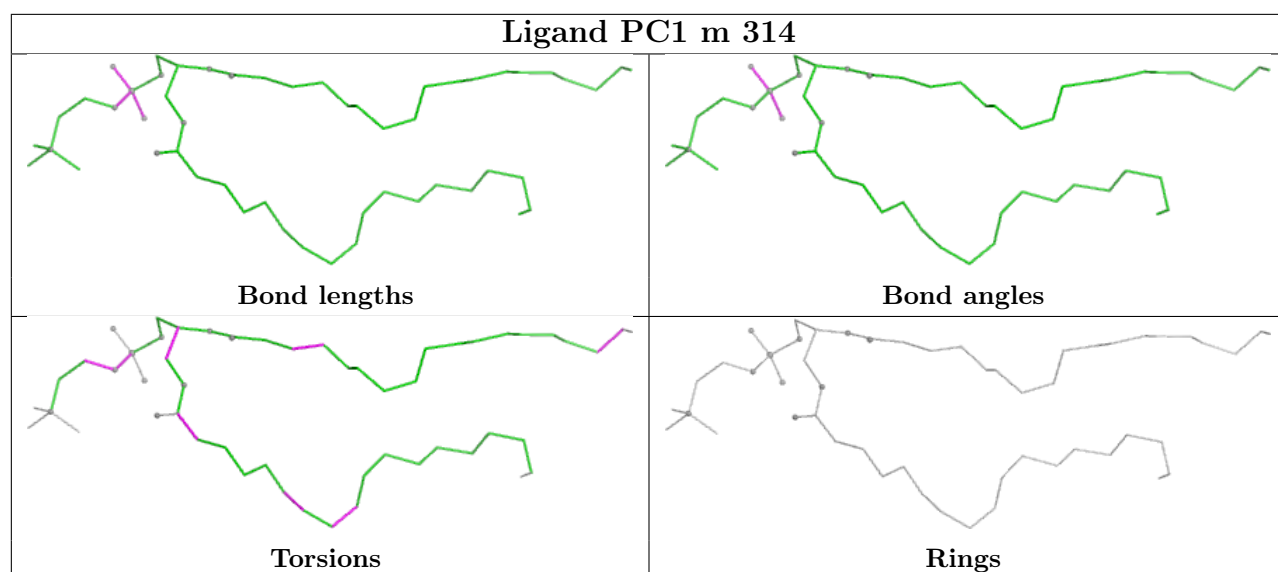


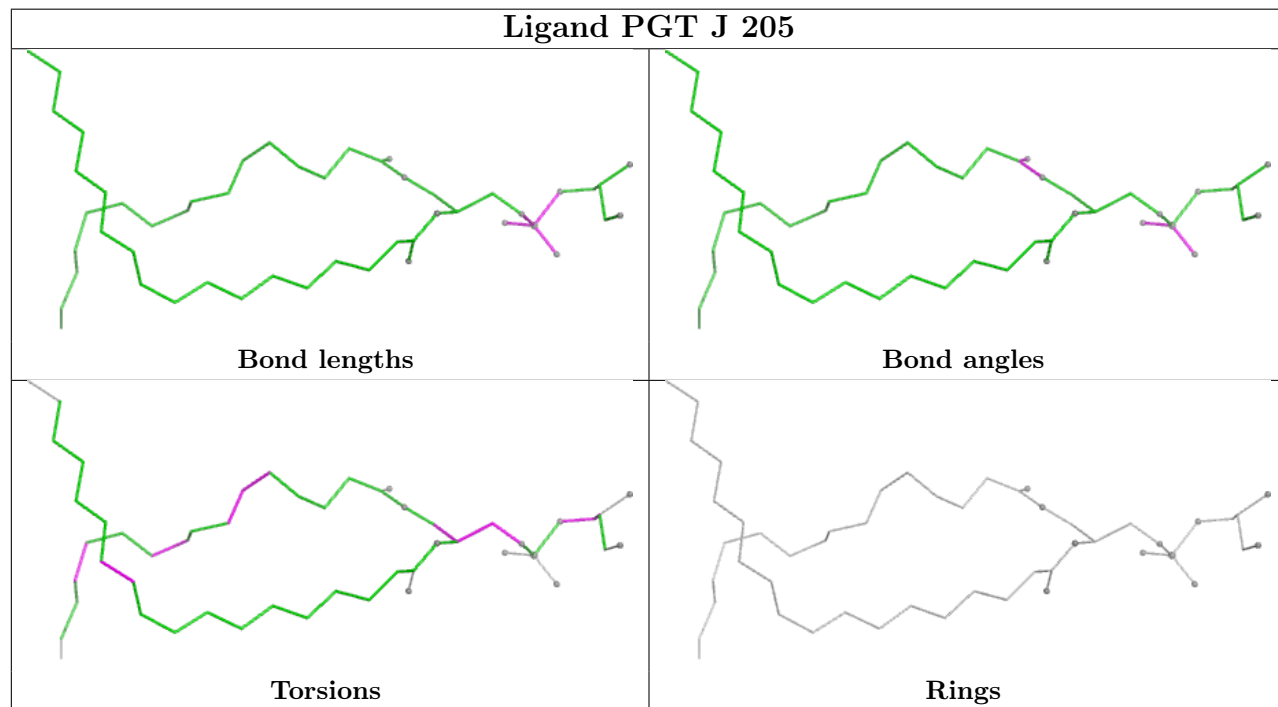
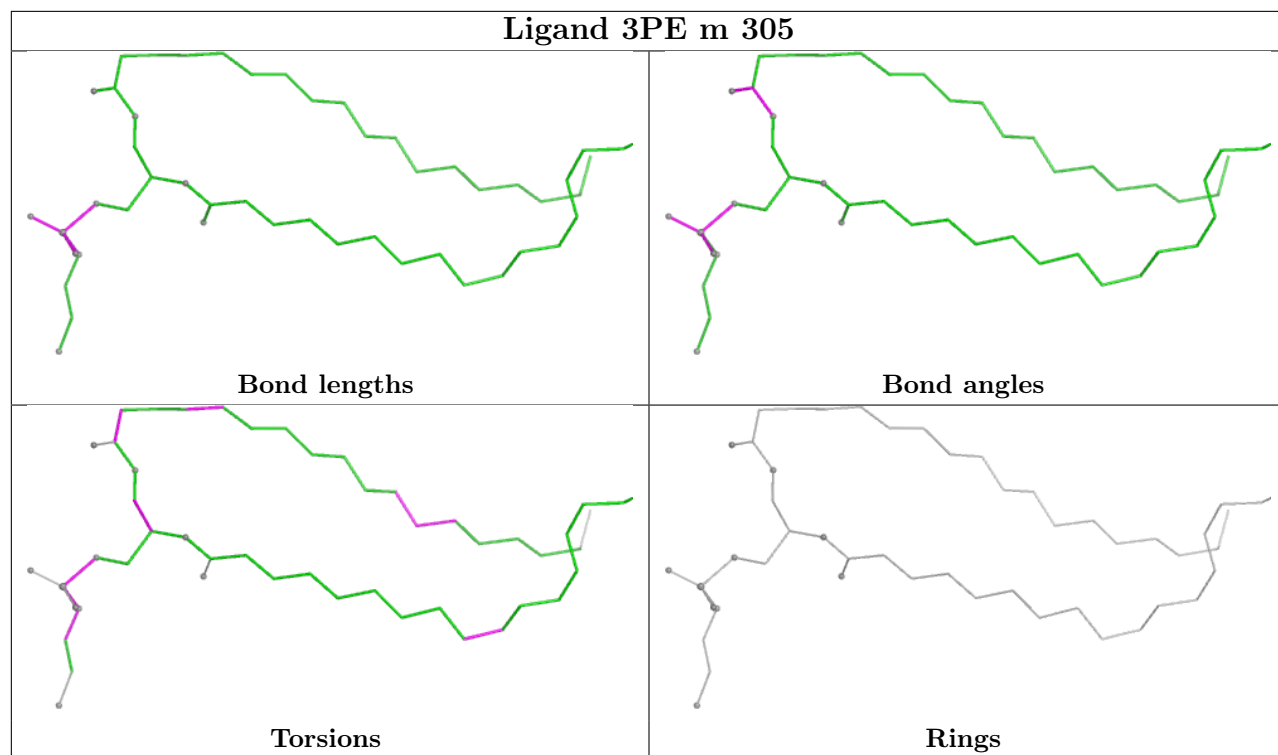
Rings

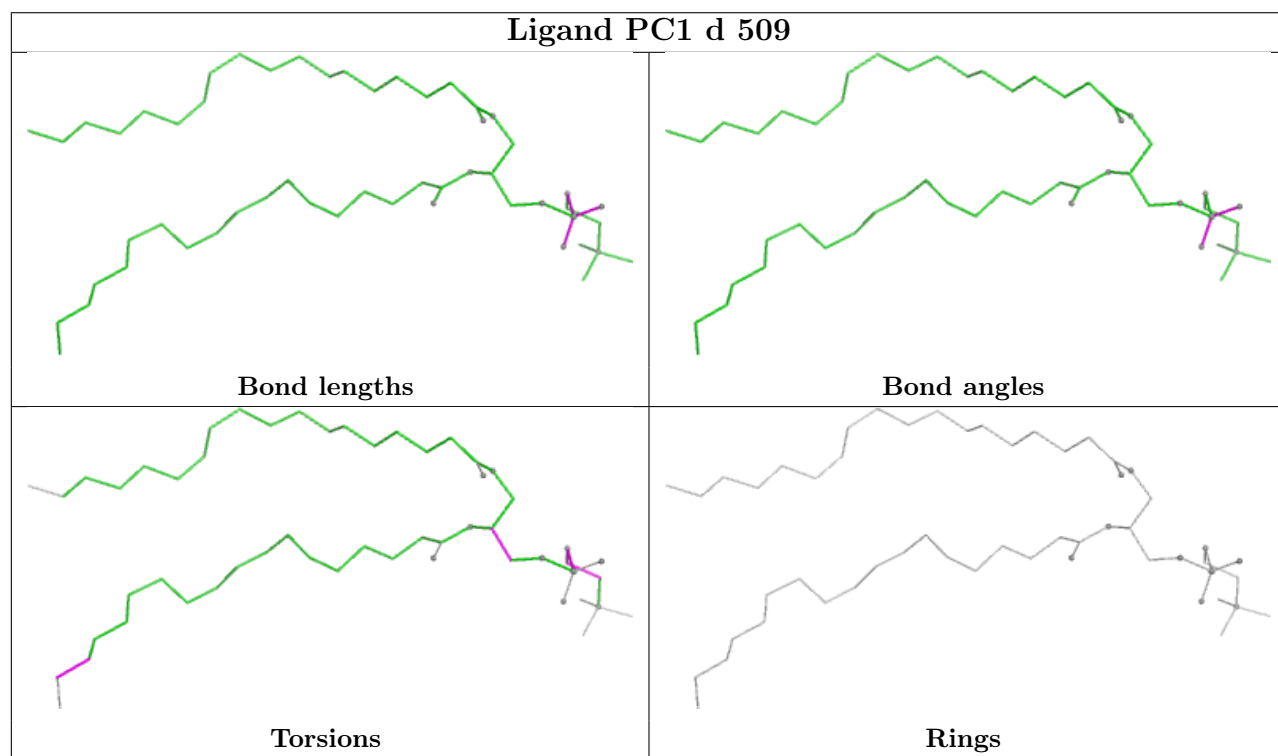
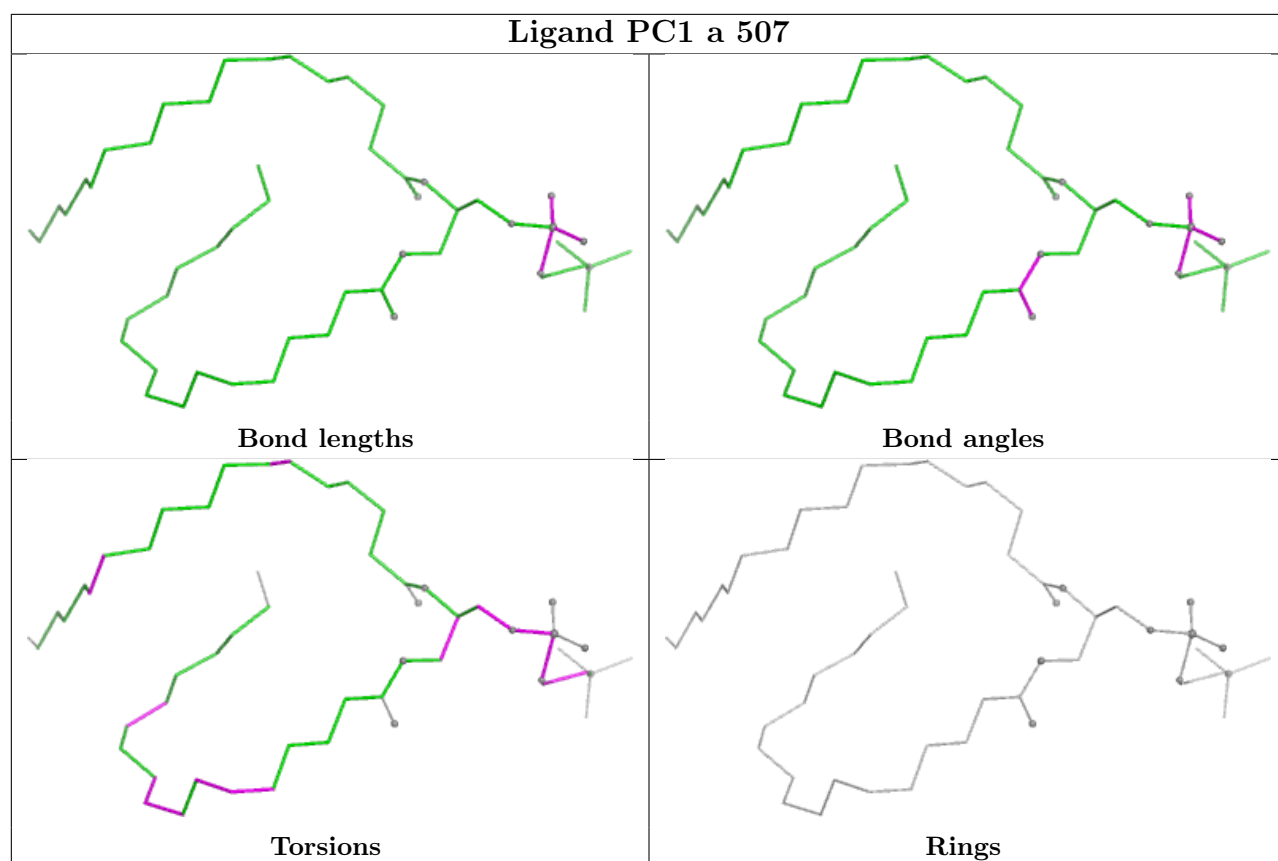


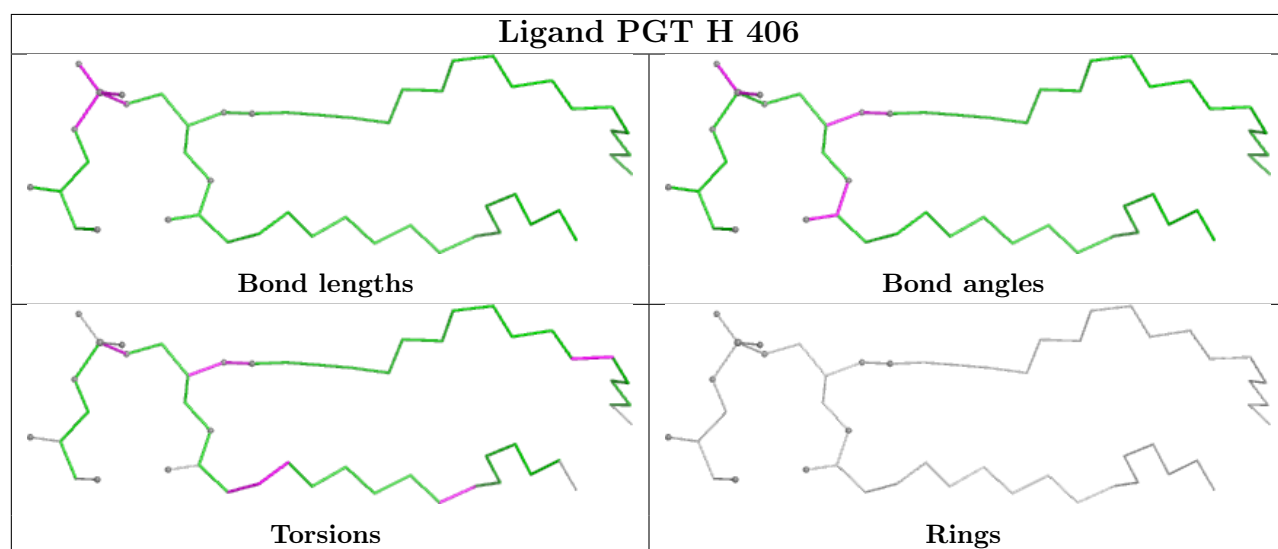
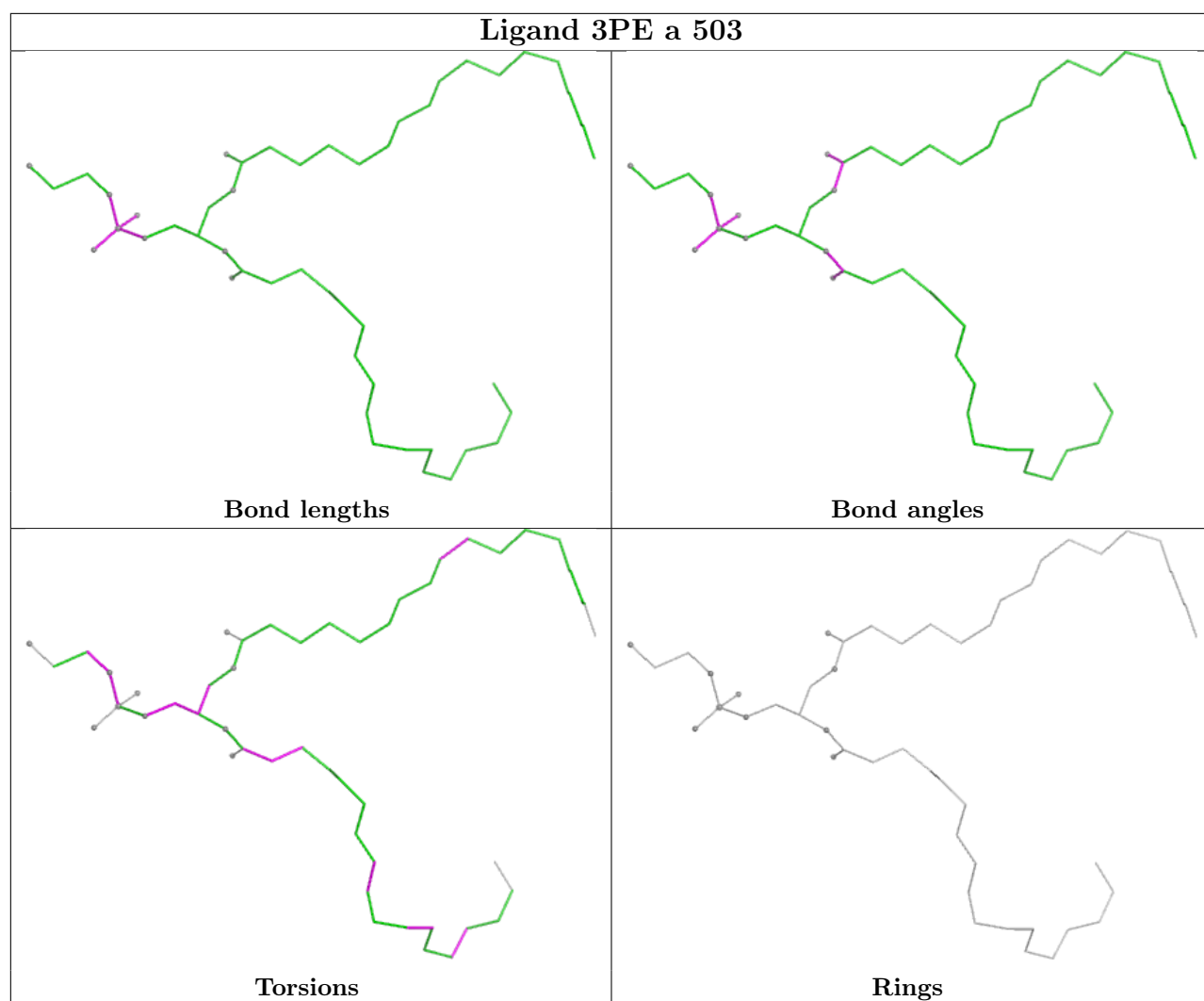


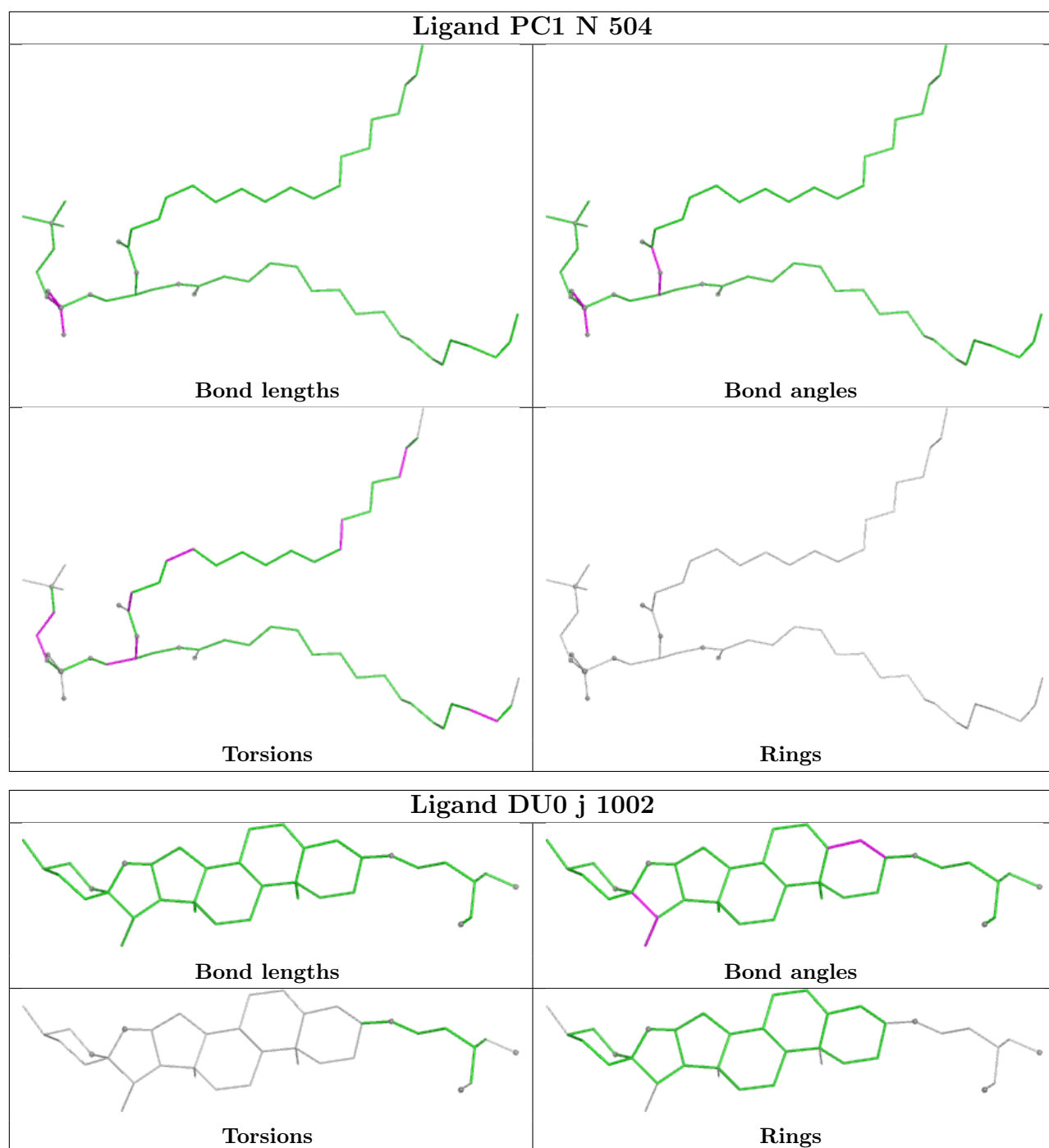


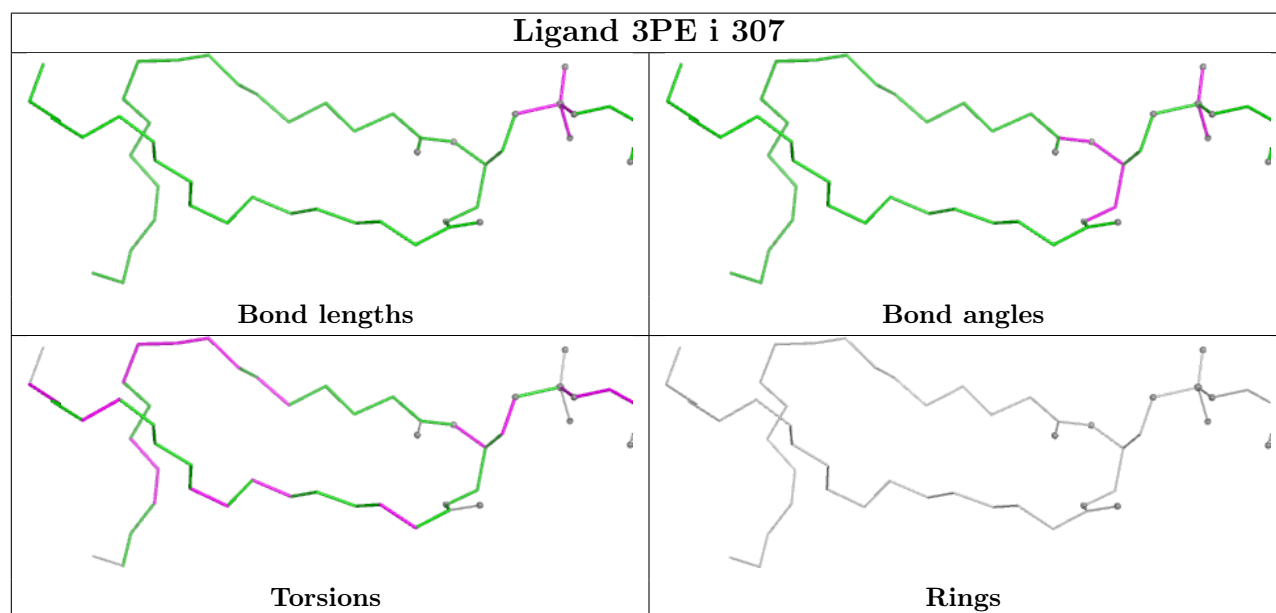
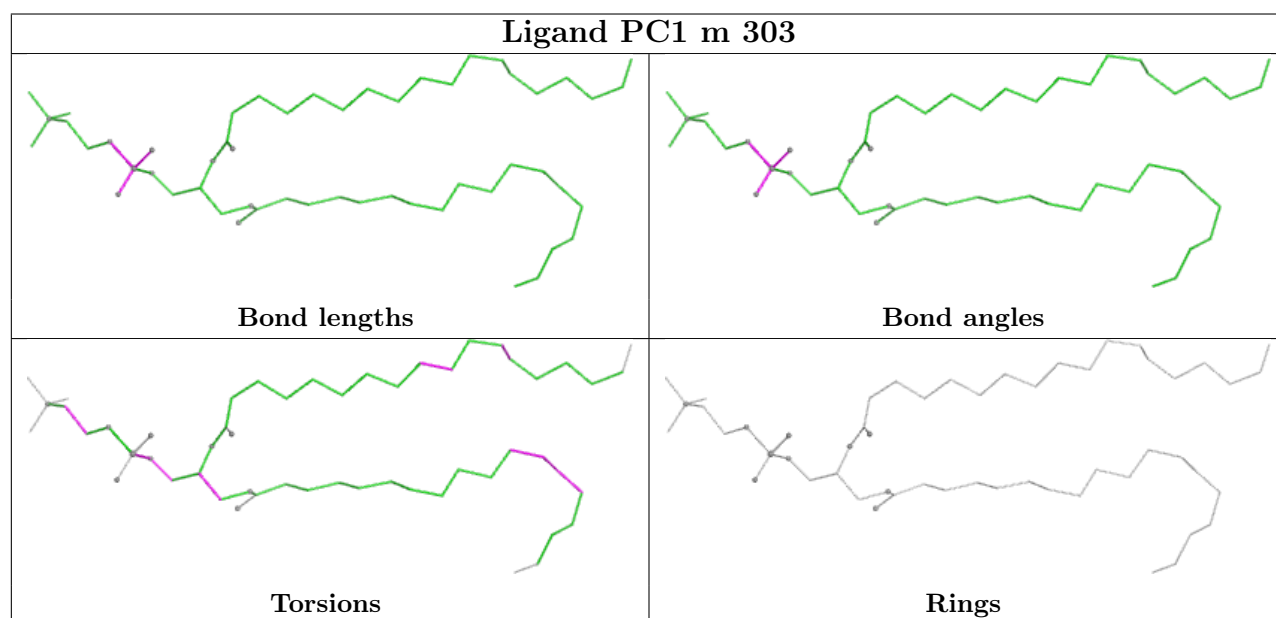
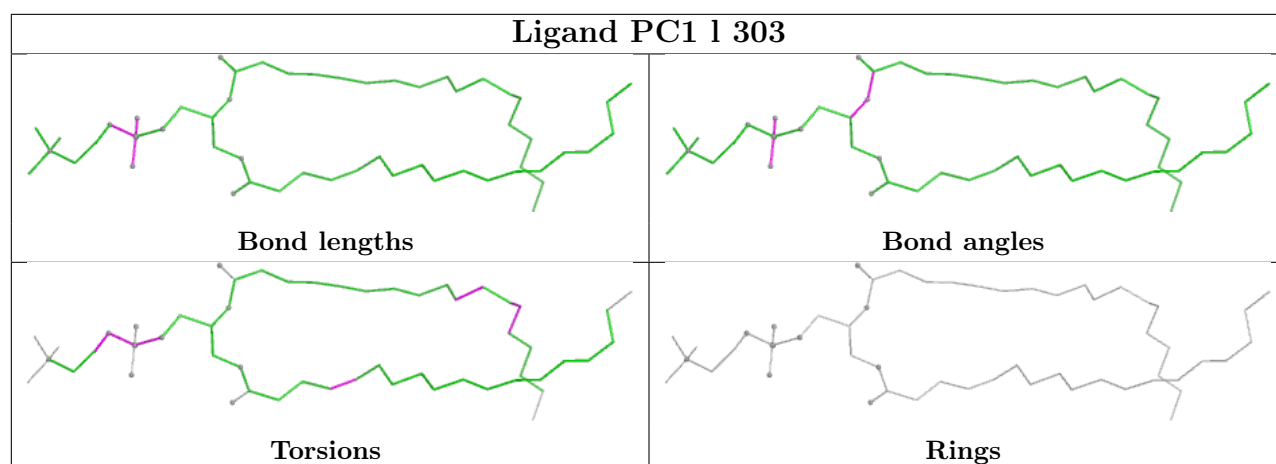


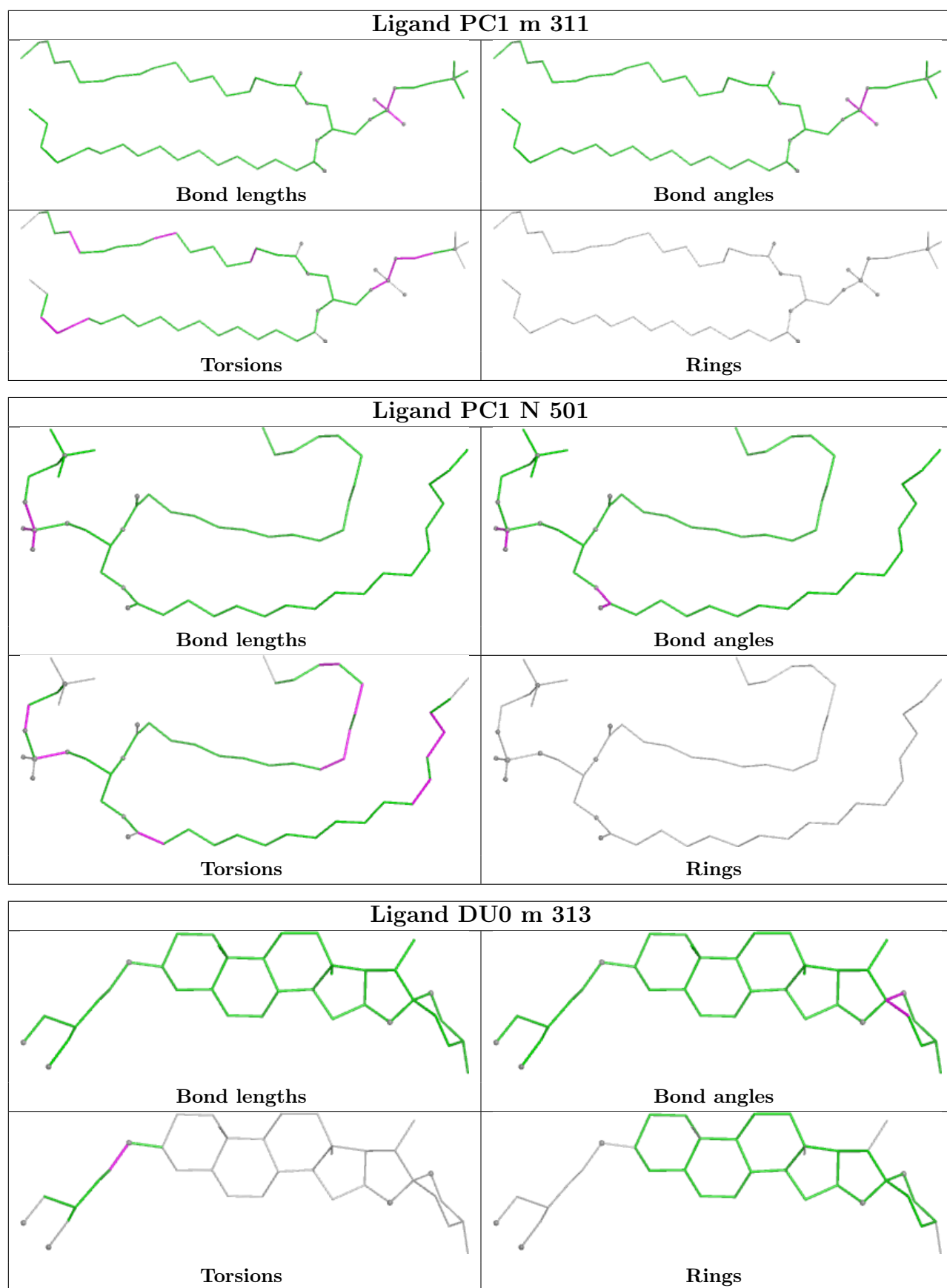


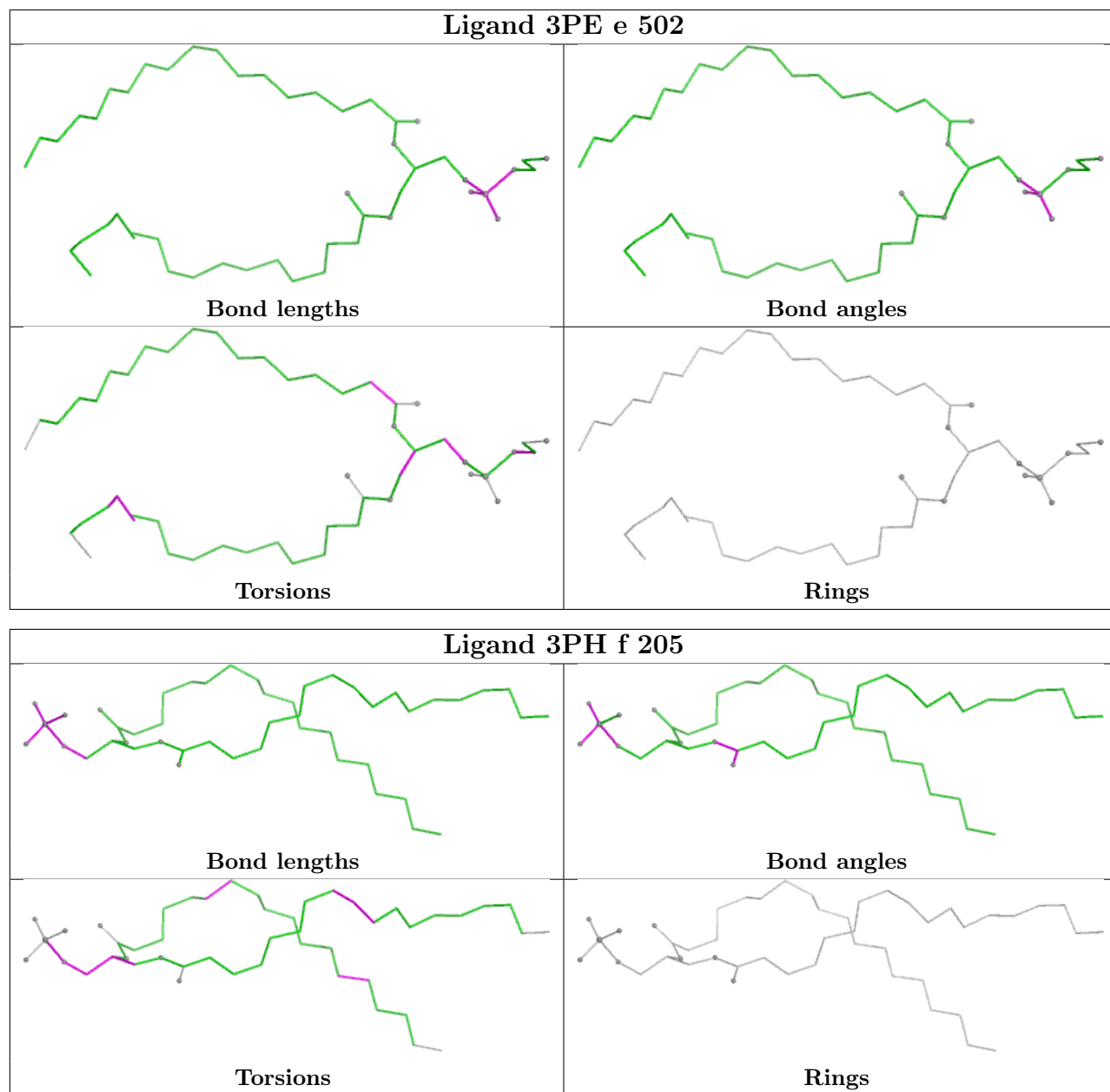


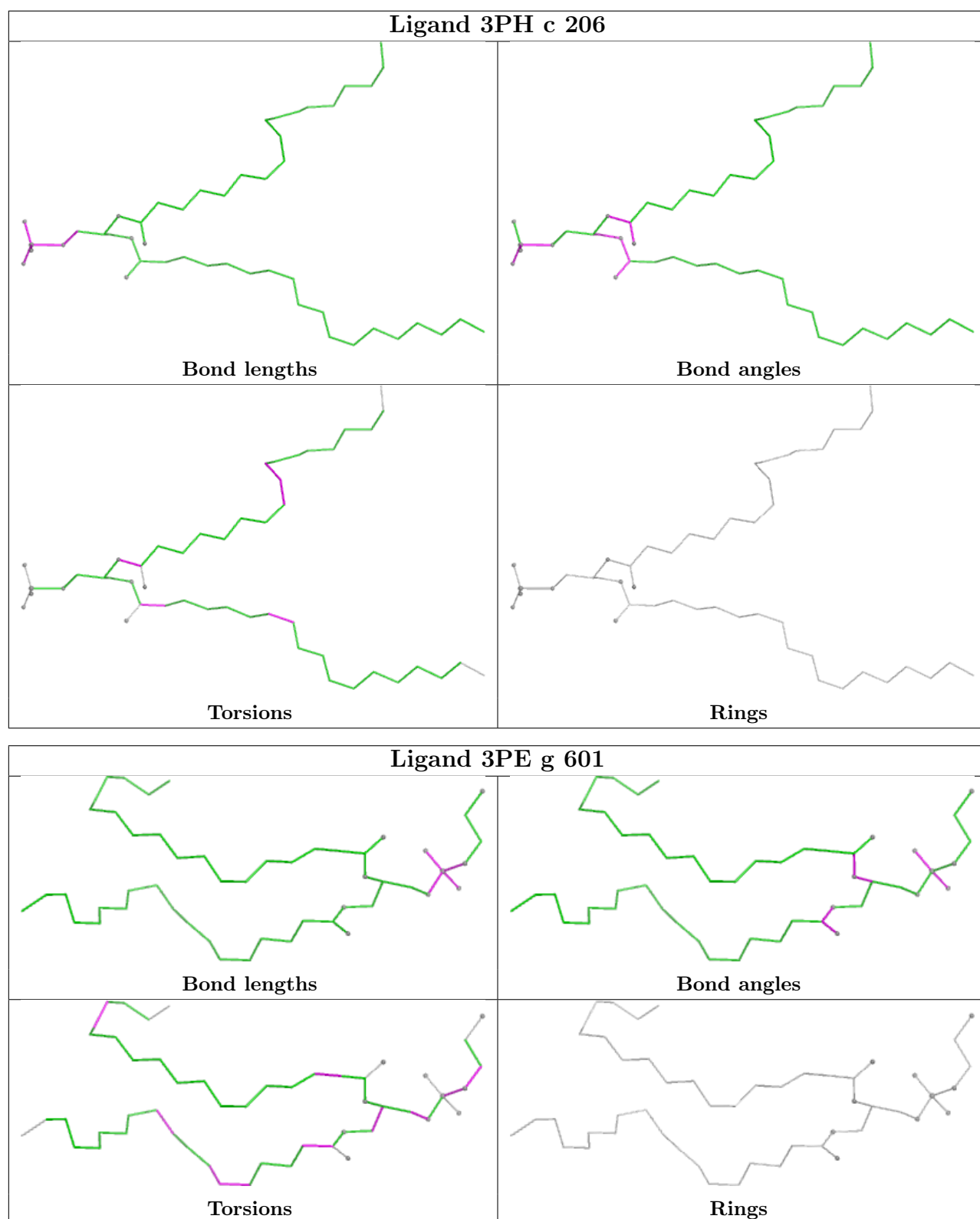


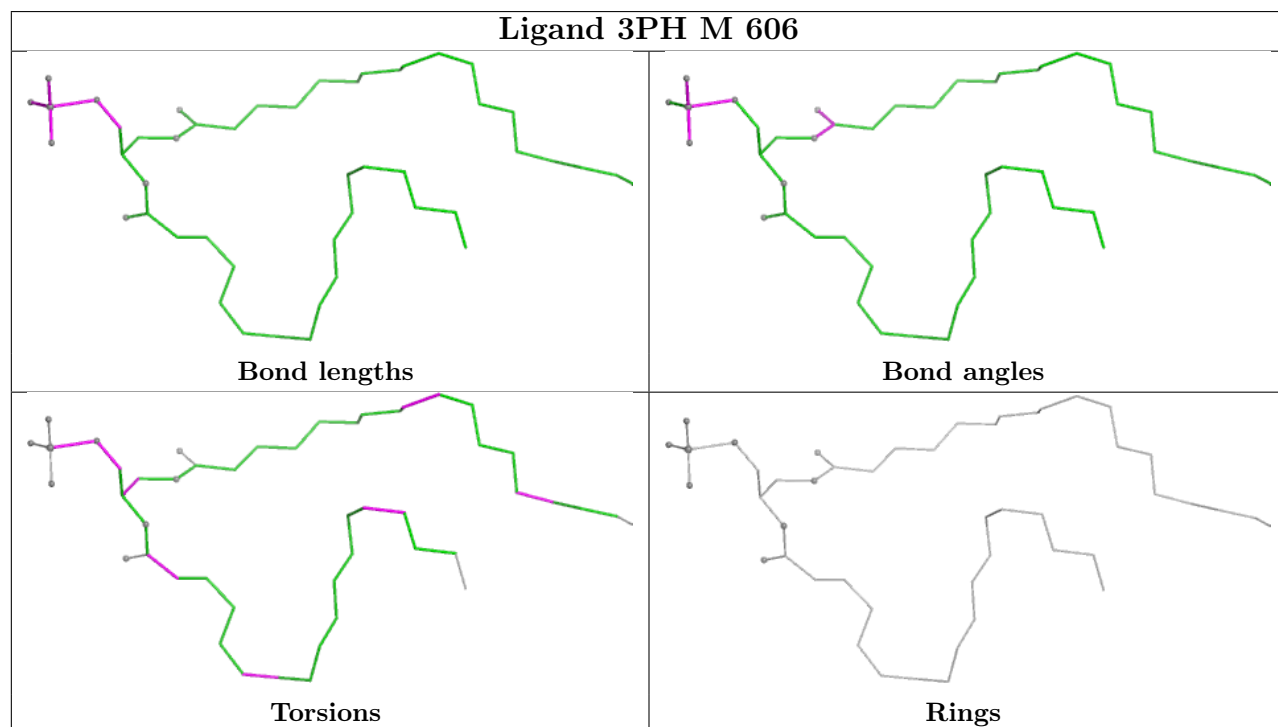
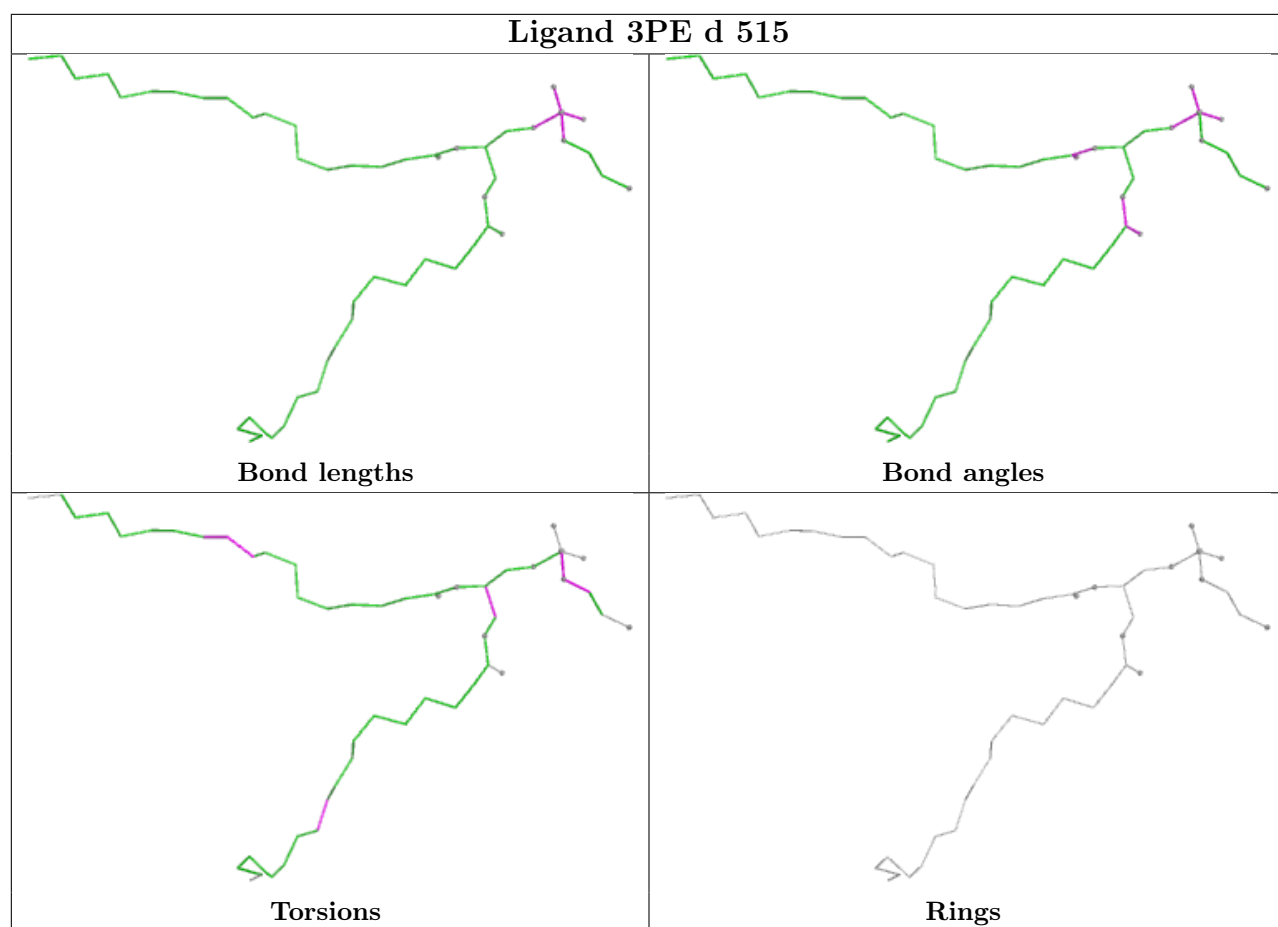


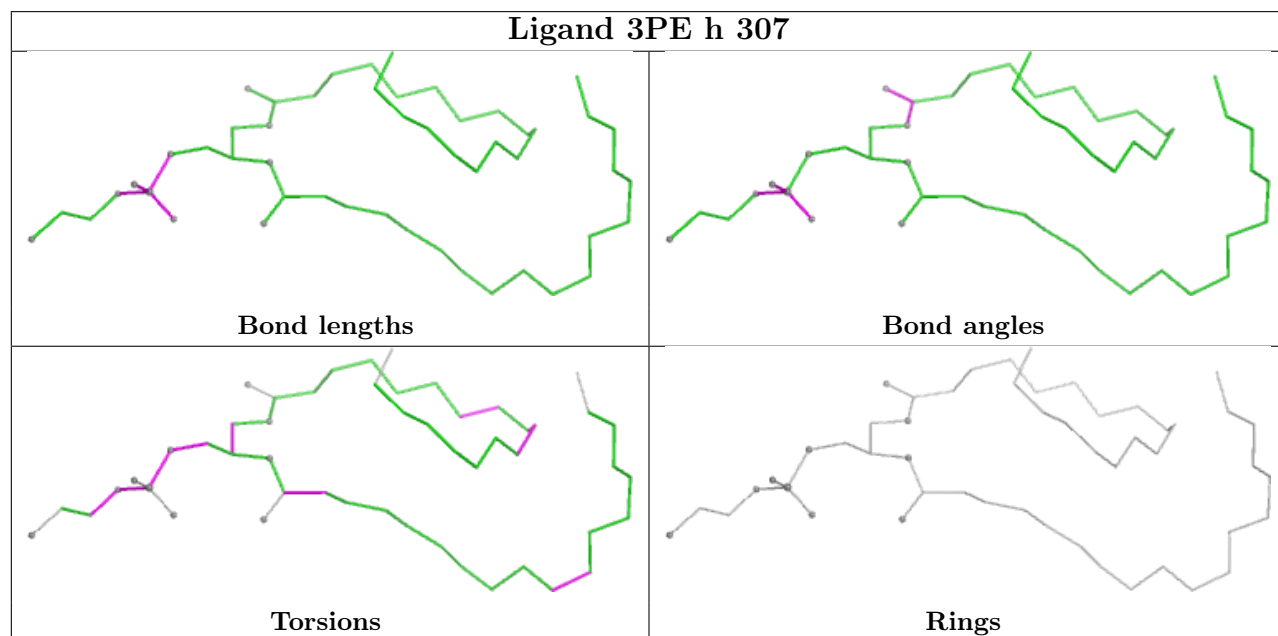
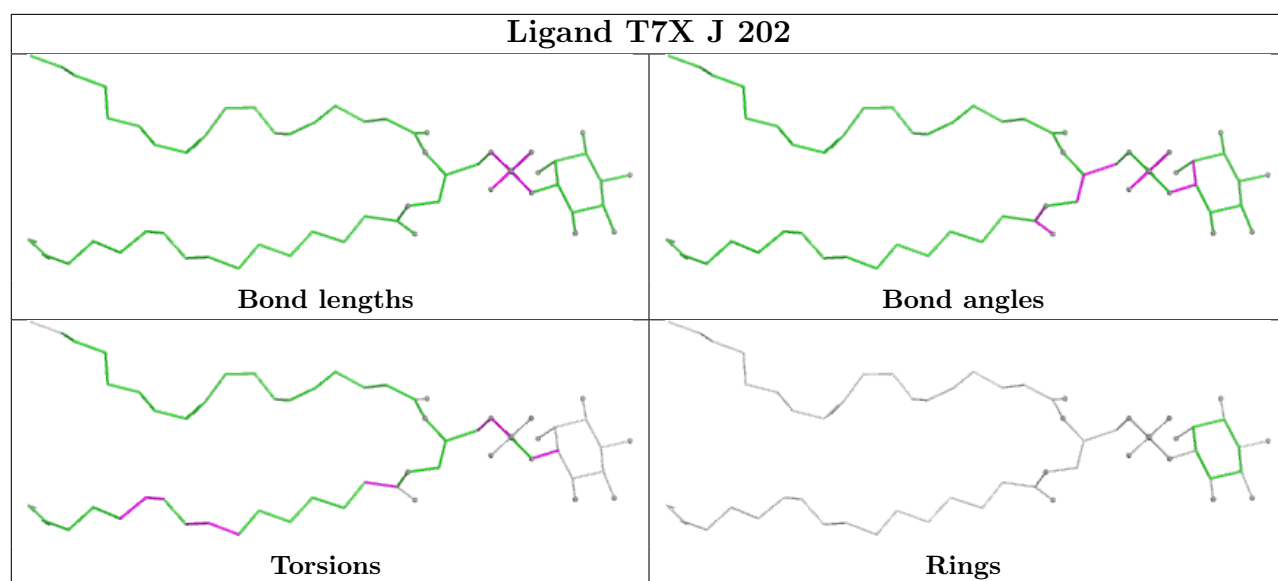


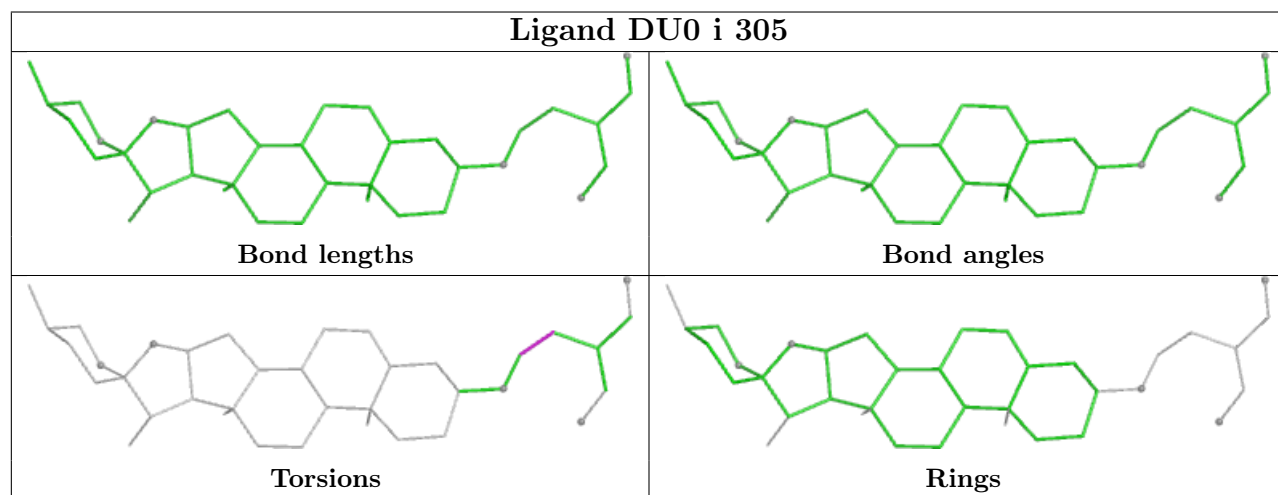
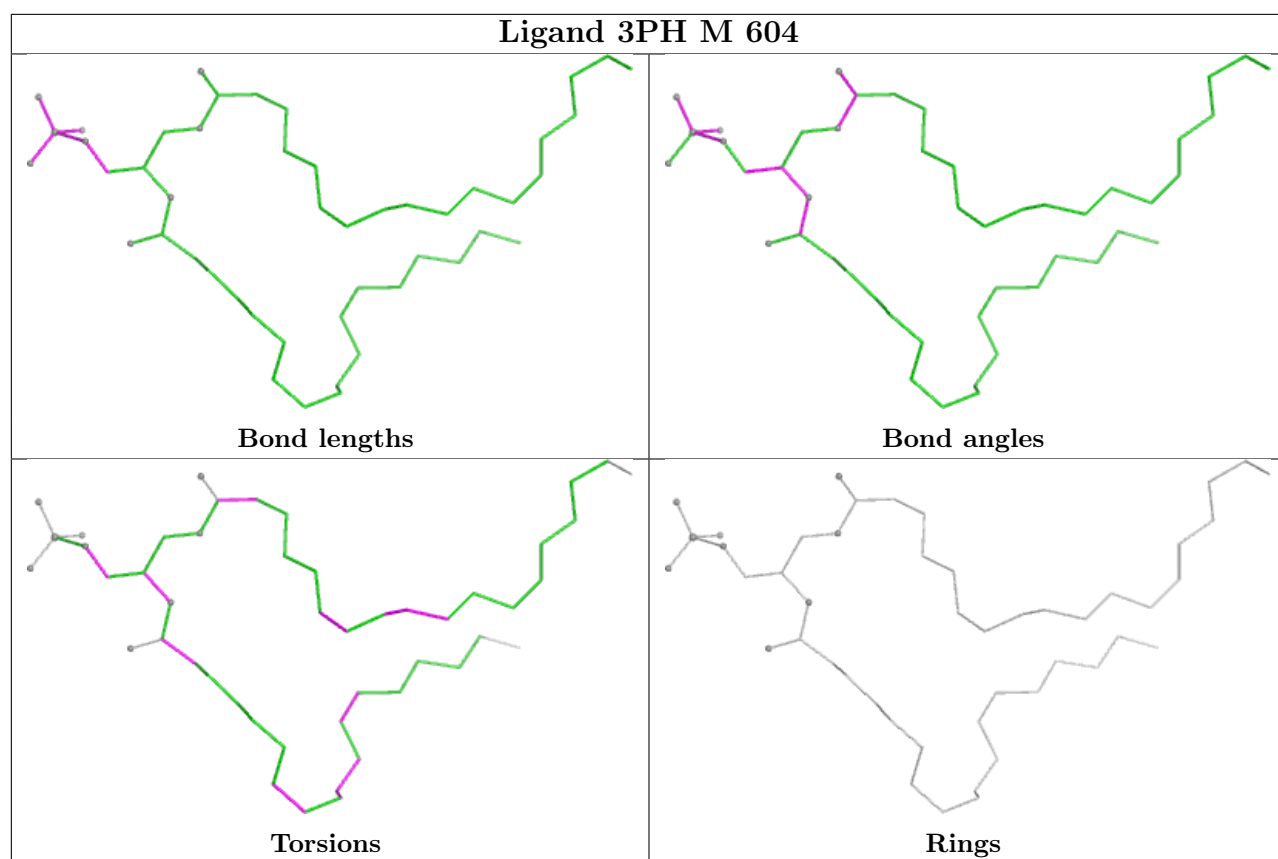


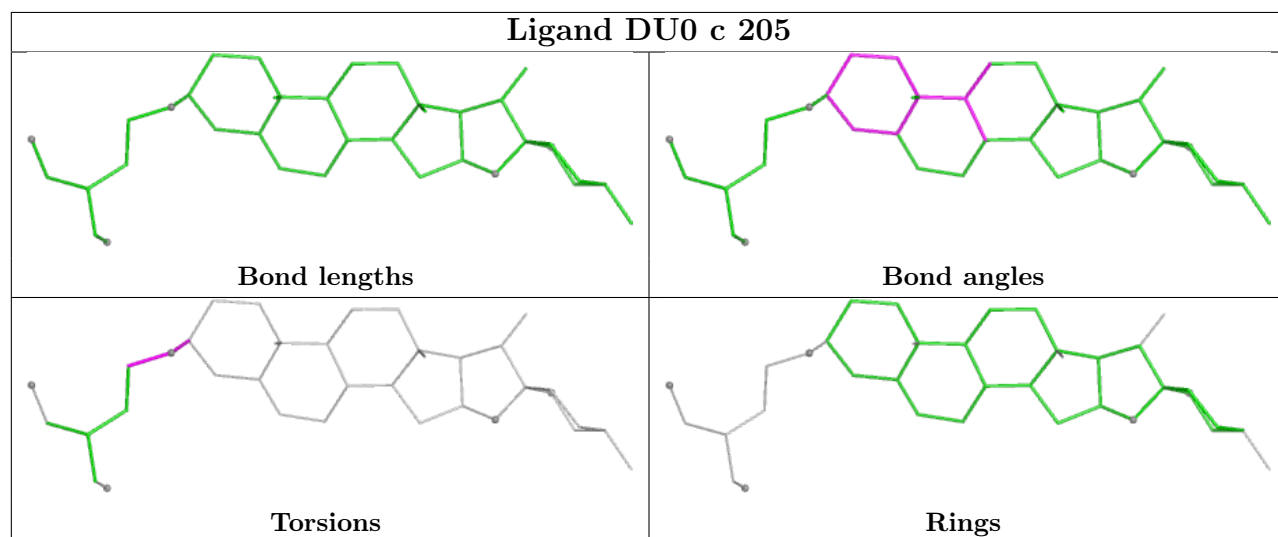
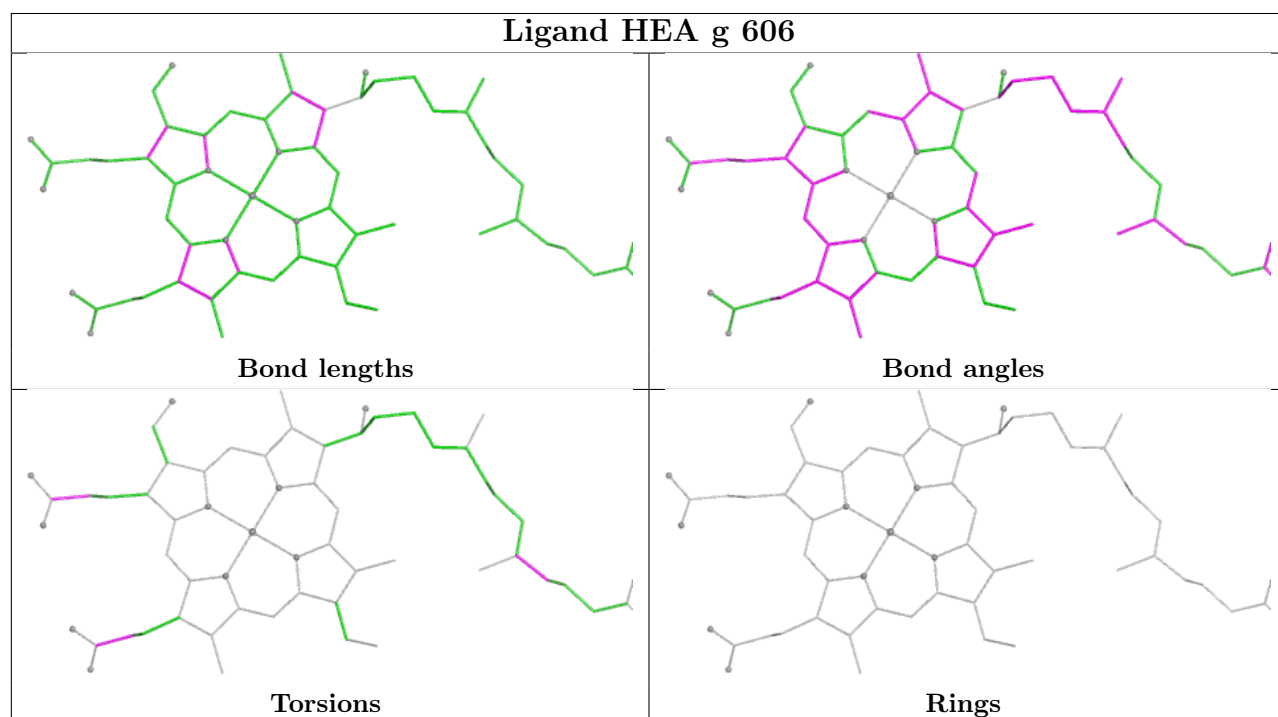
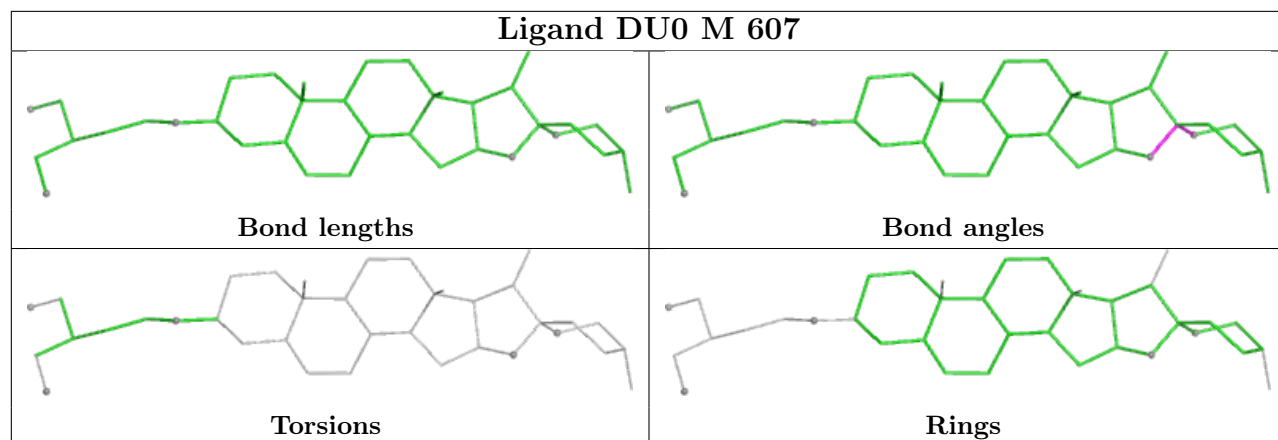


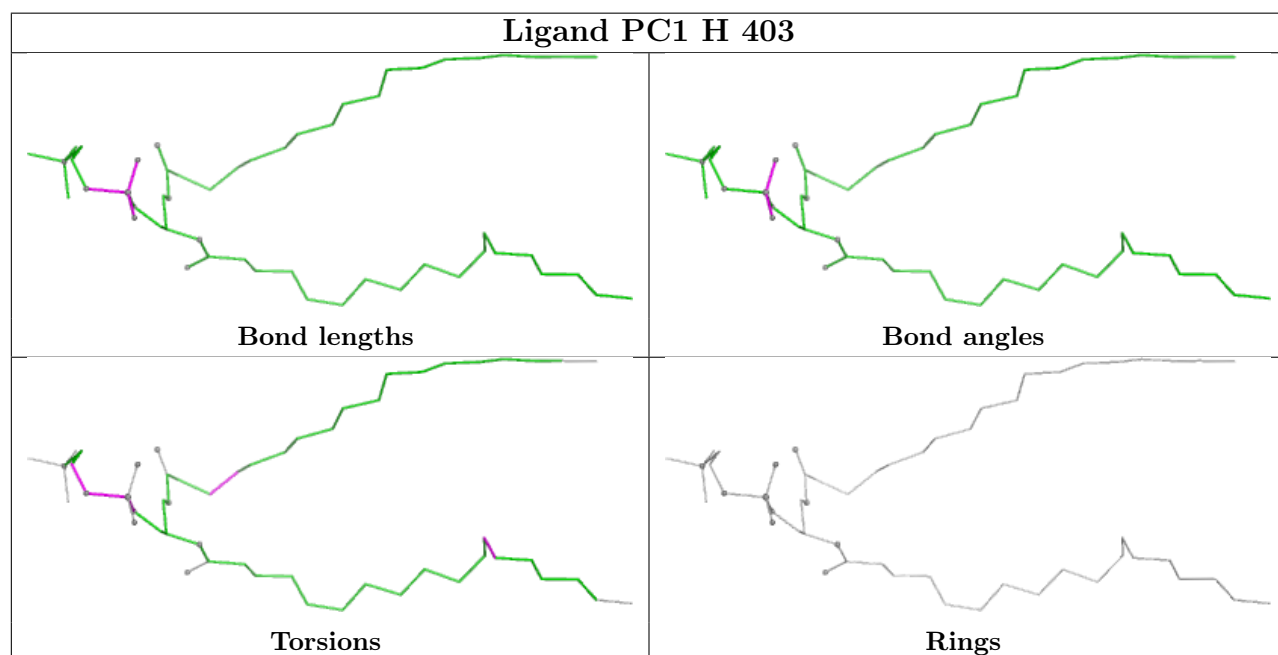
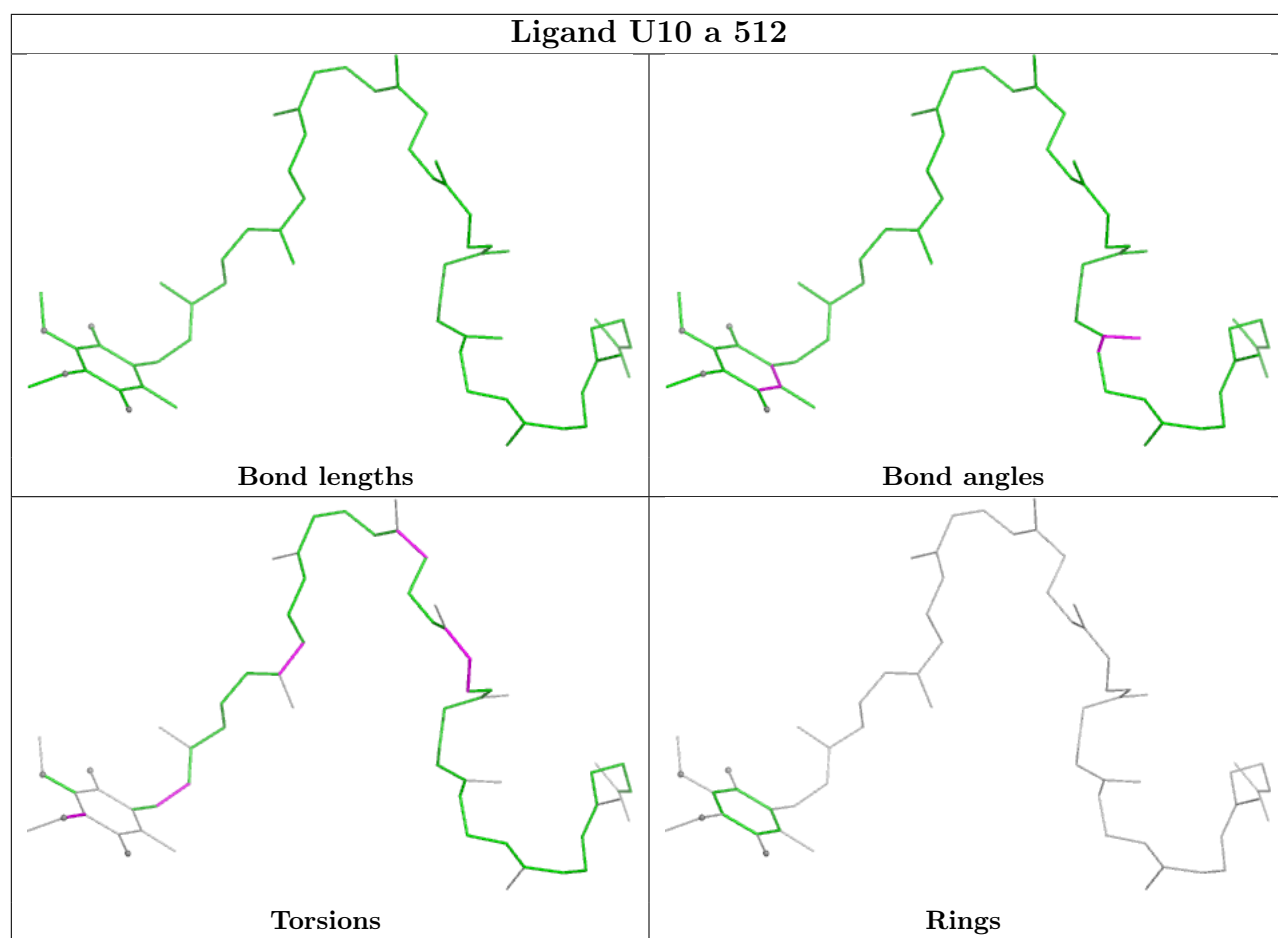


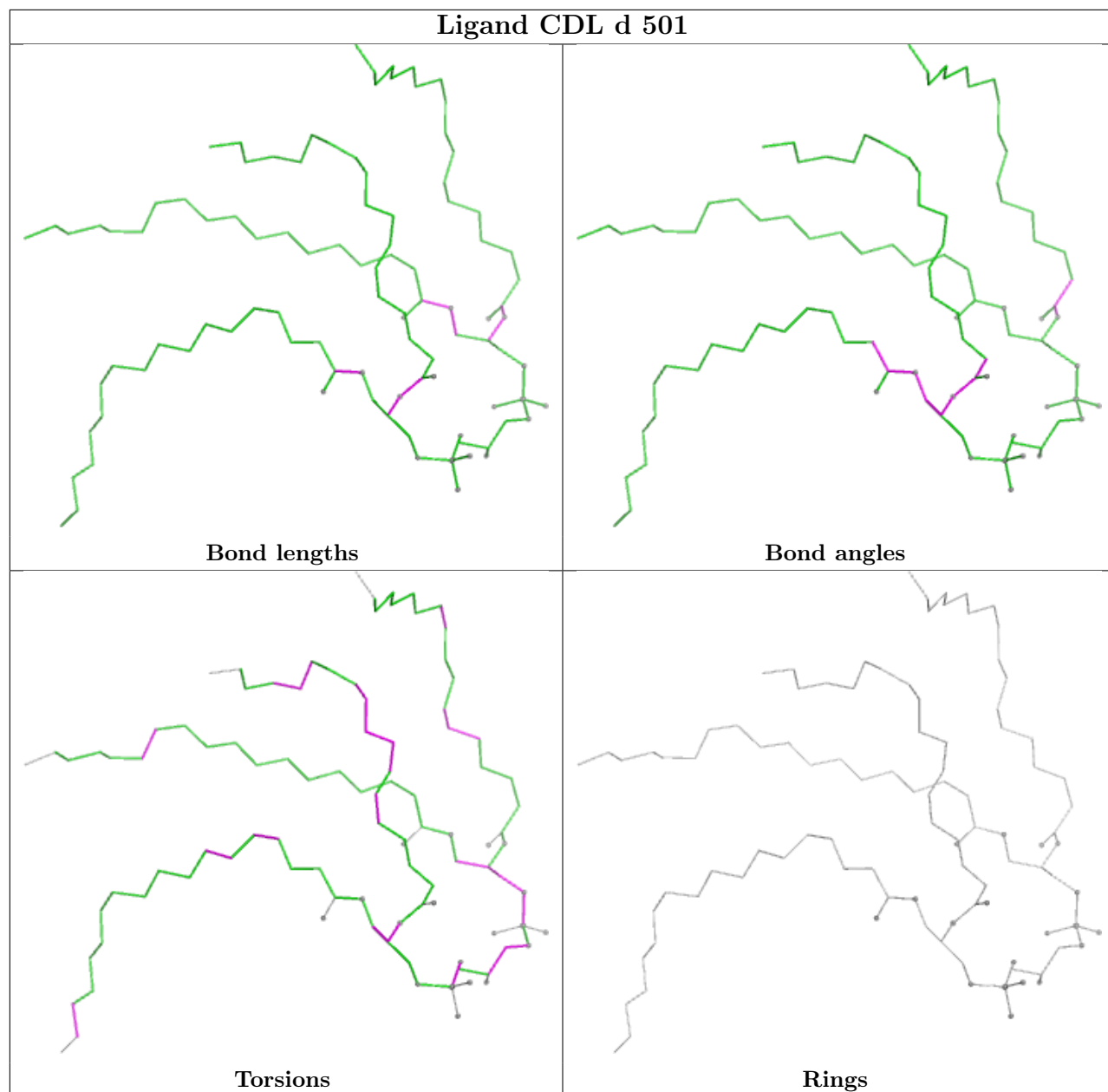


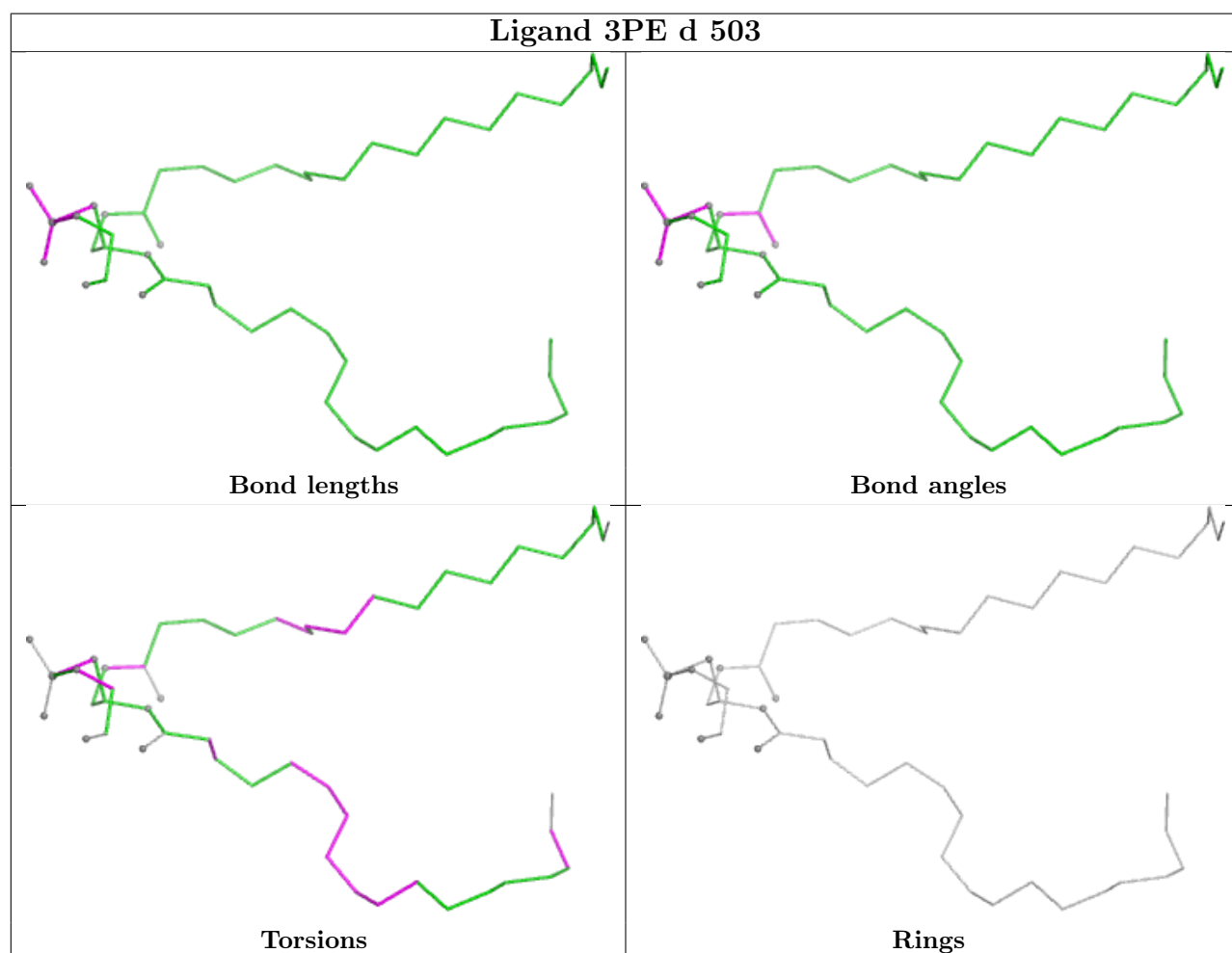
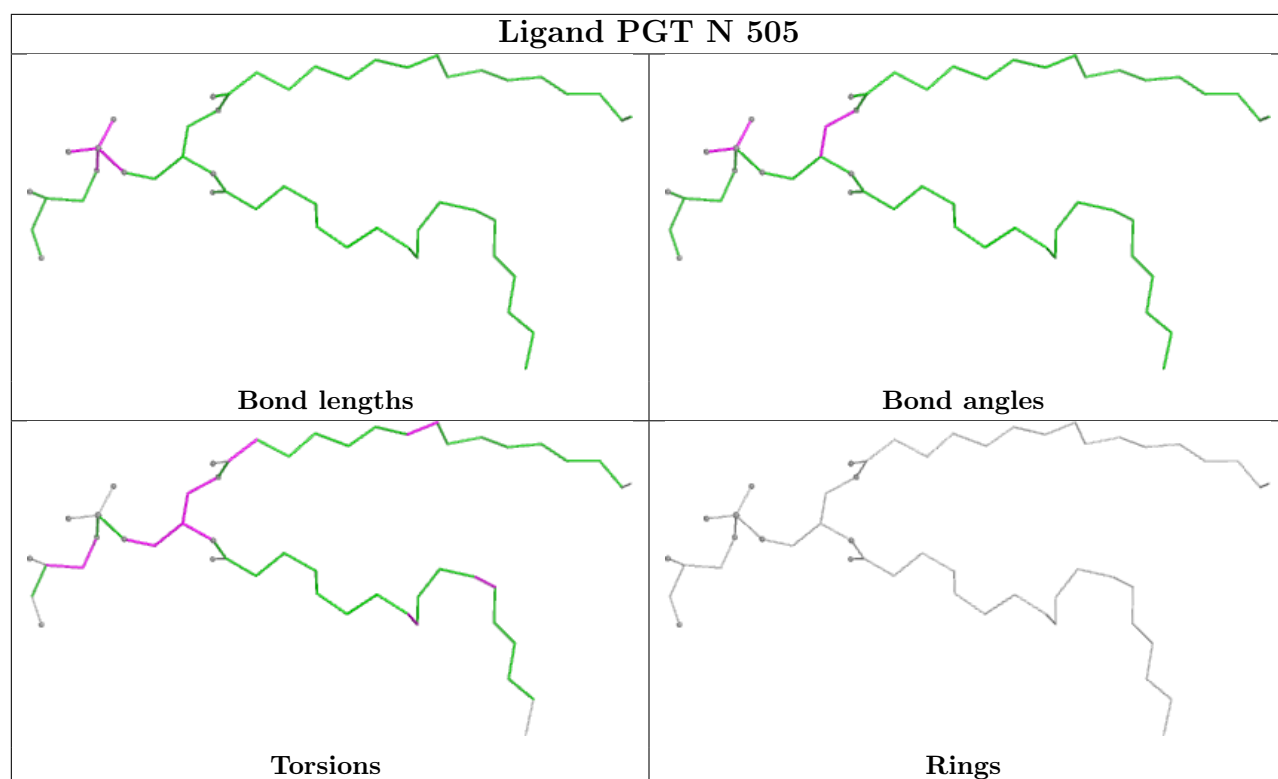


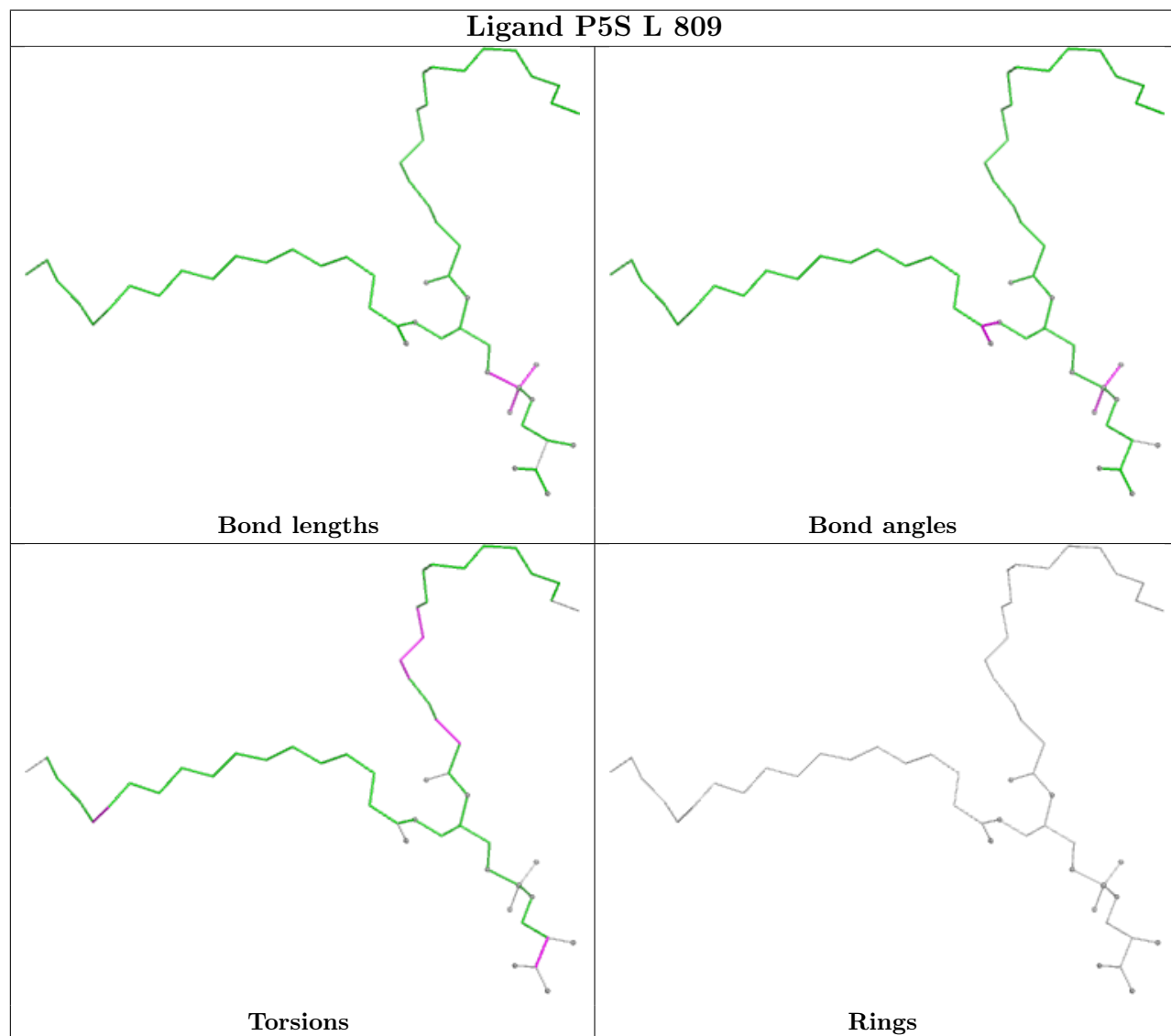
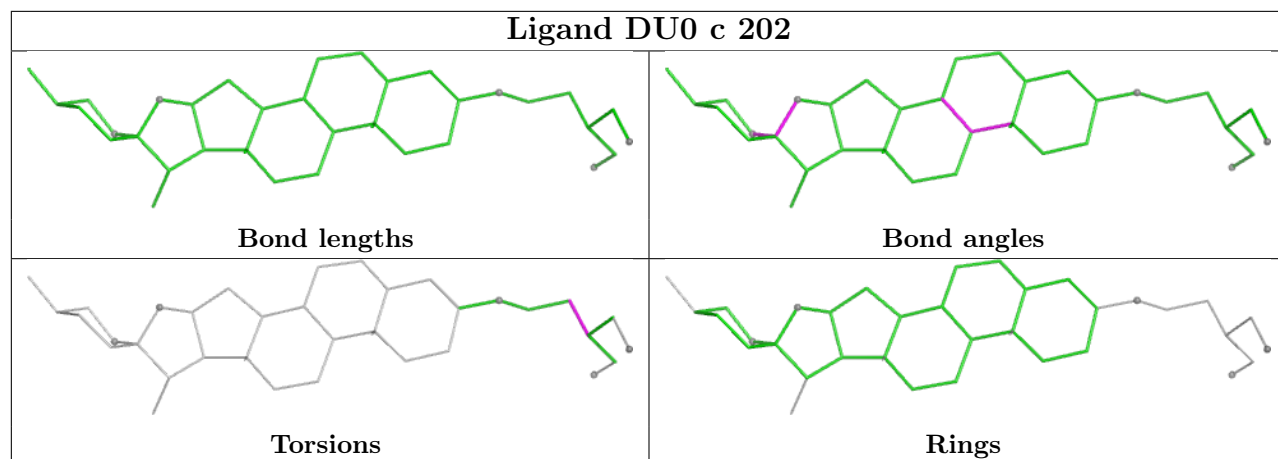


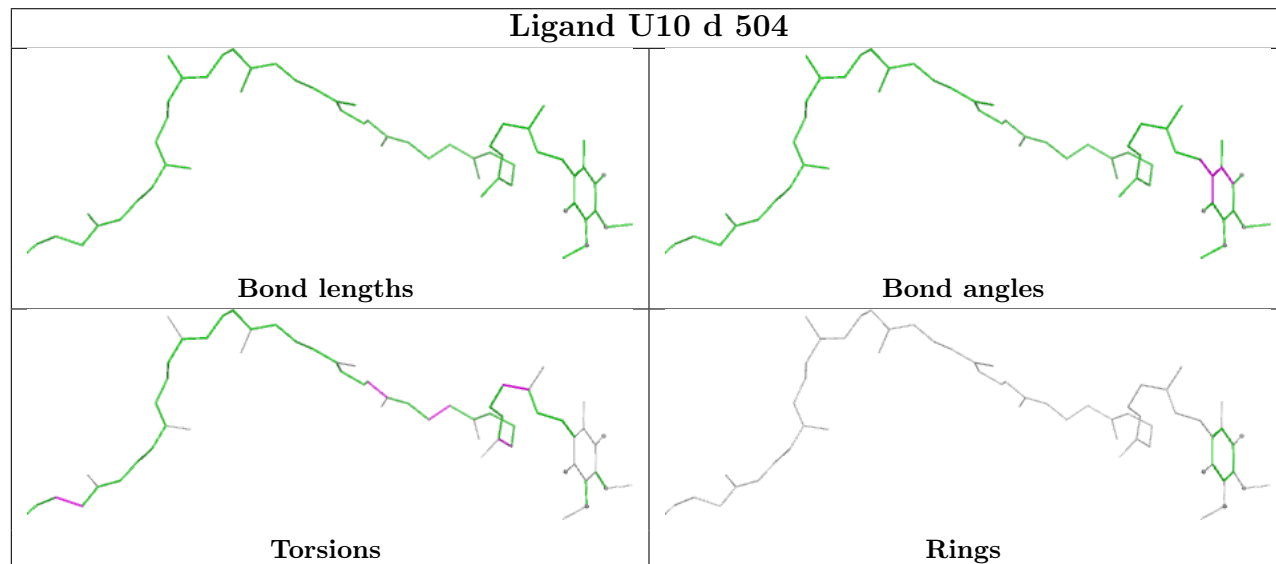
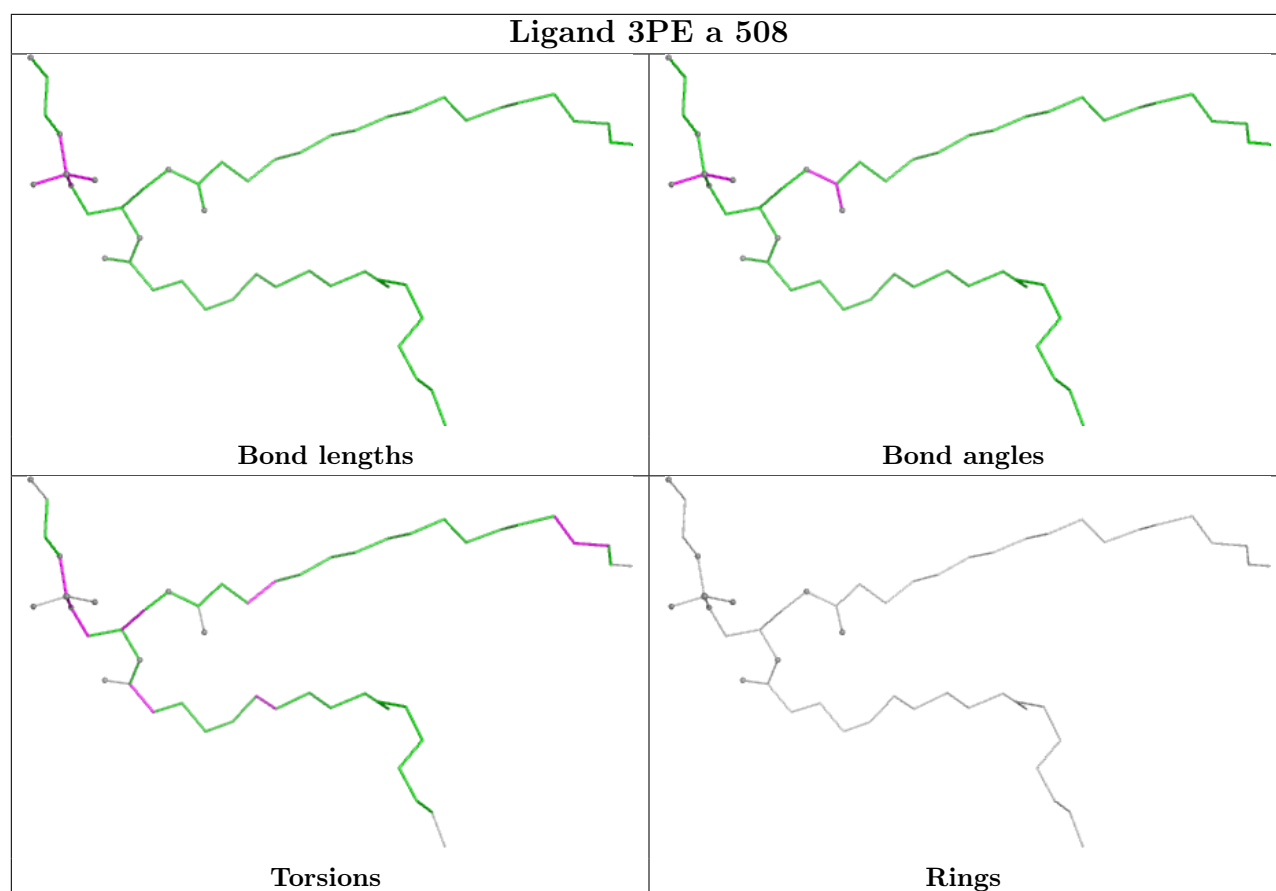


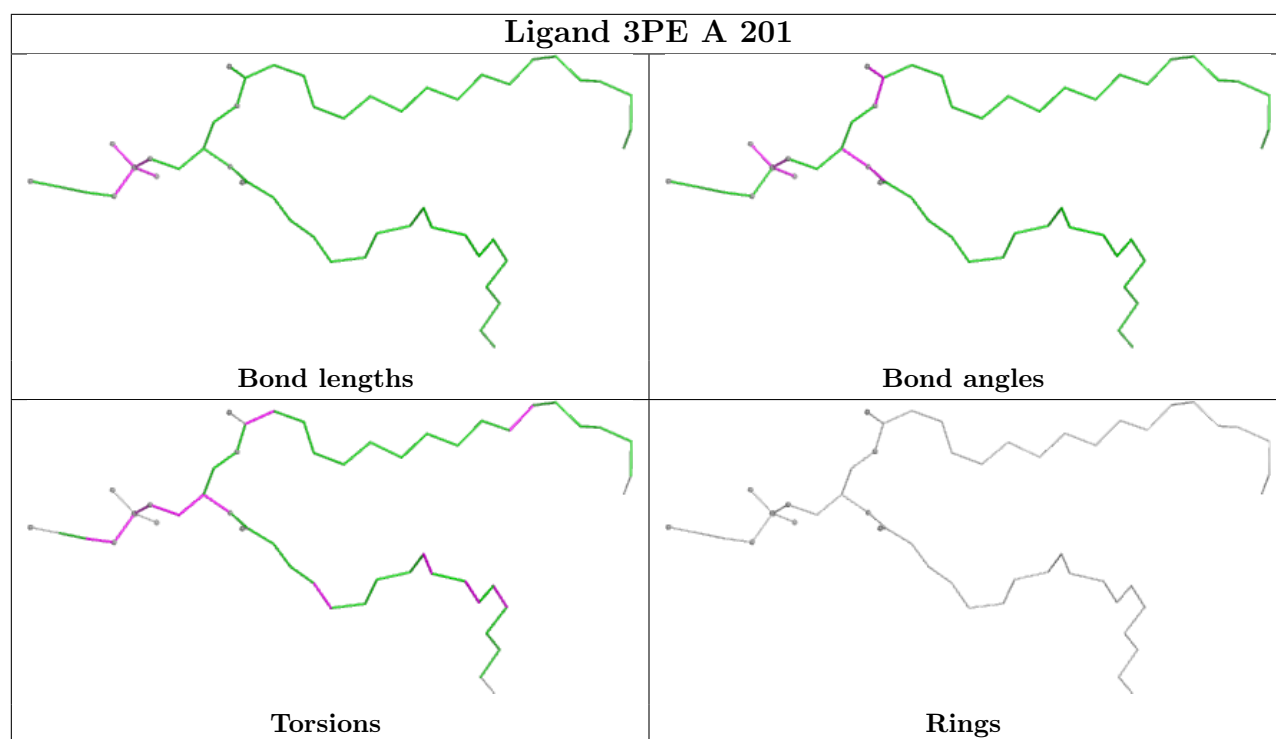


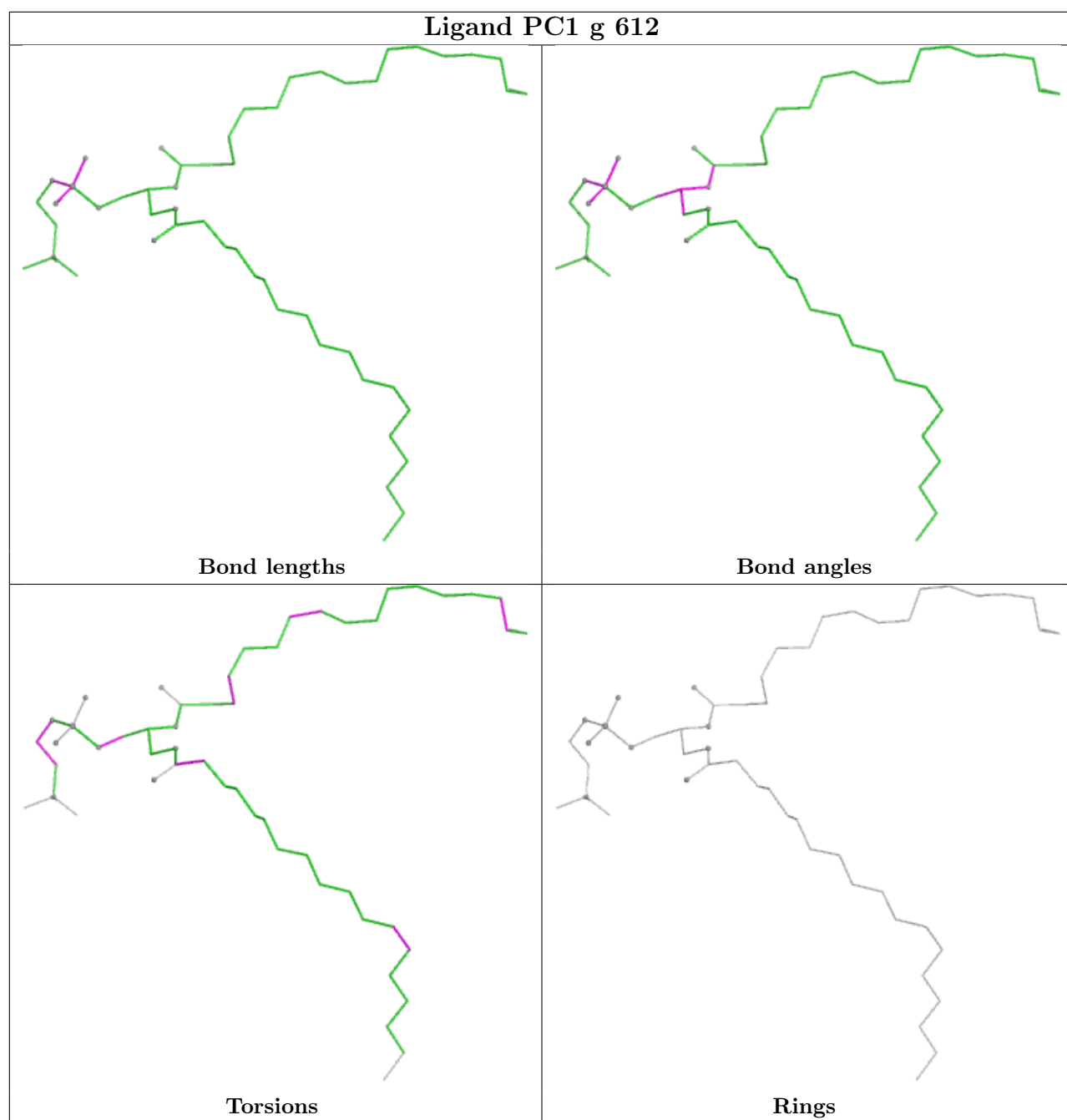


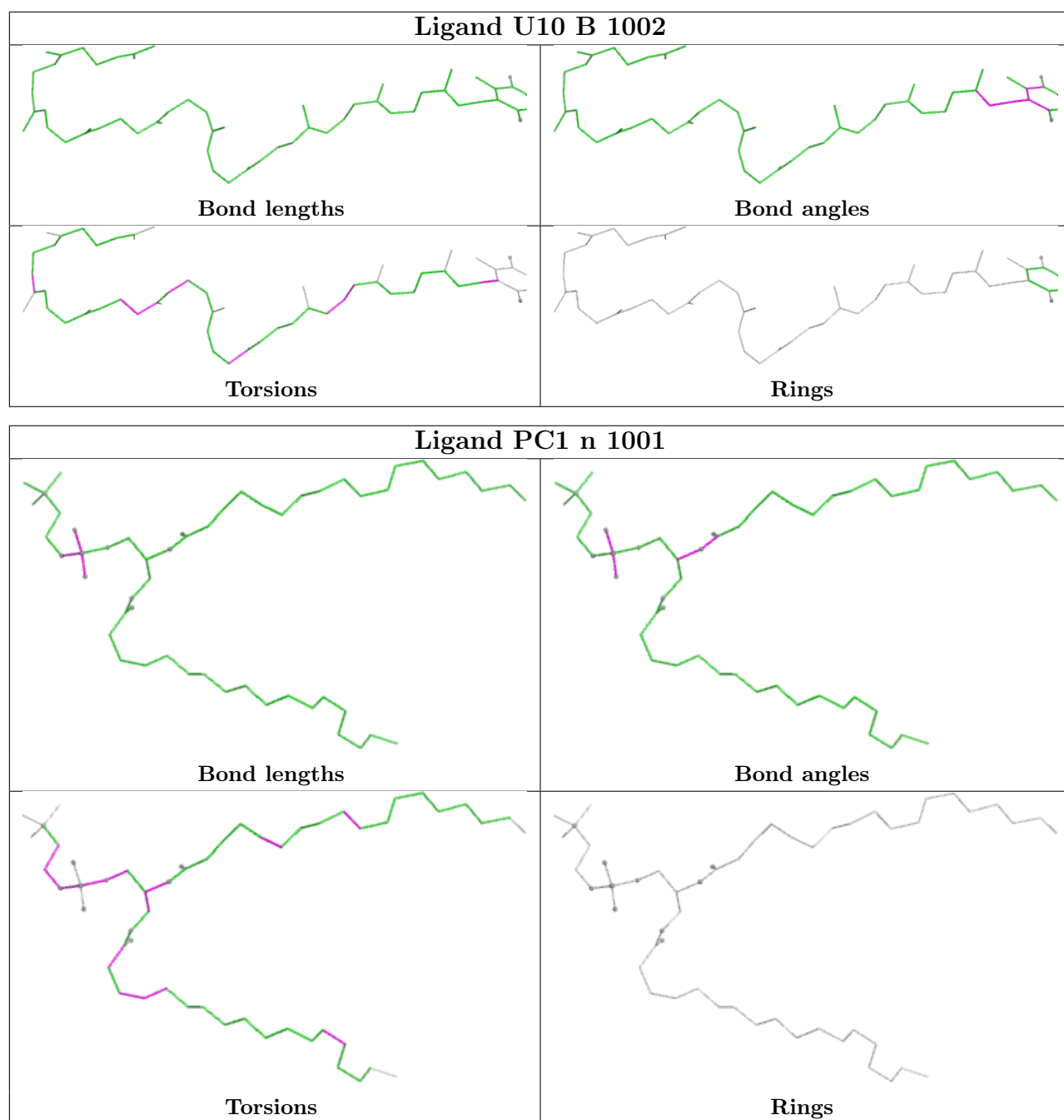


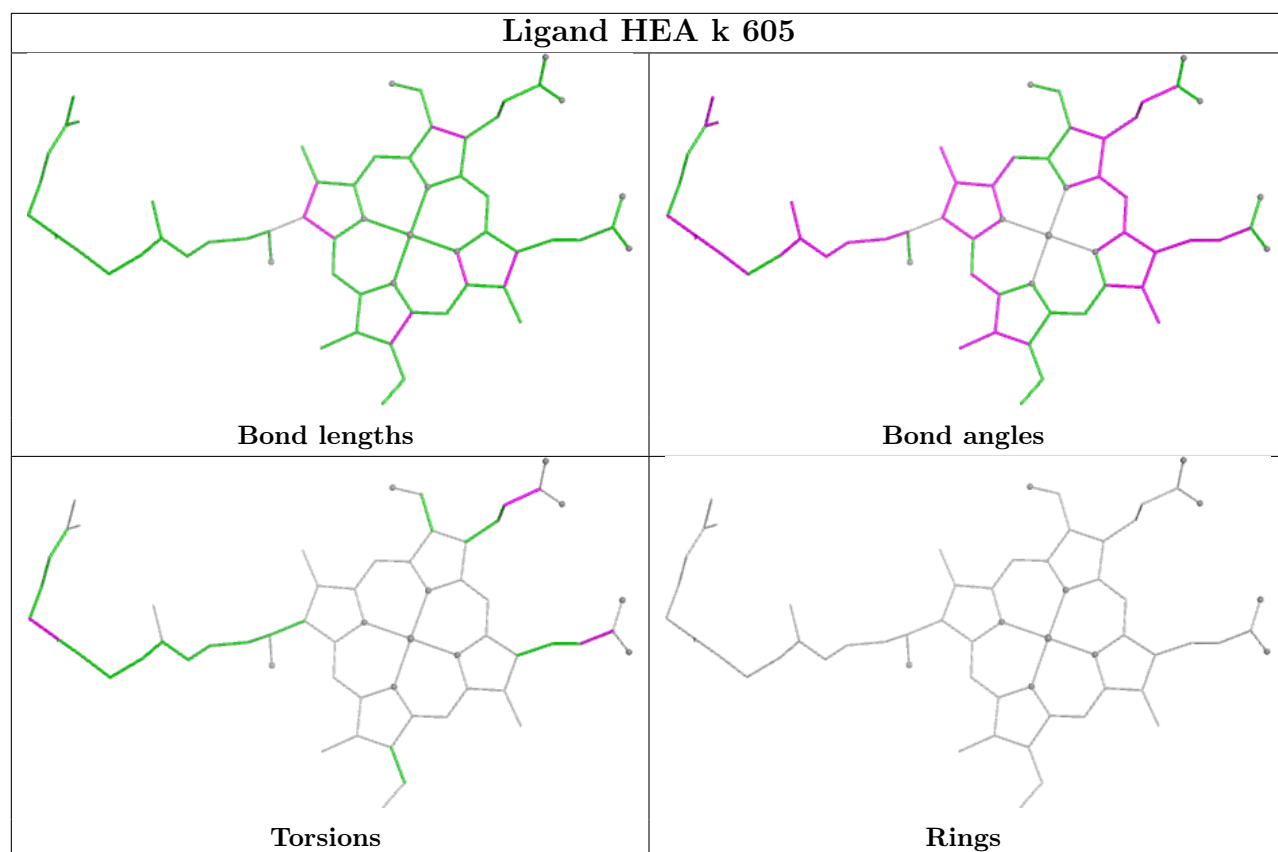
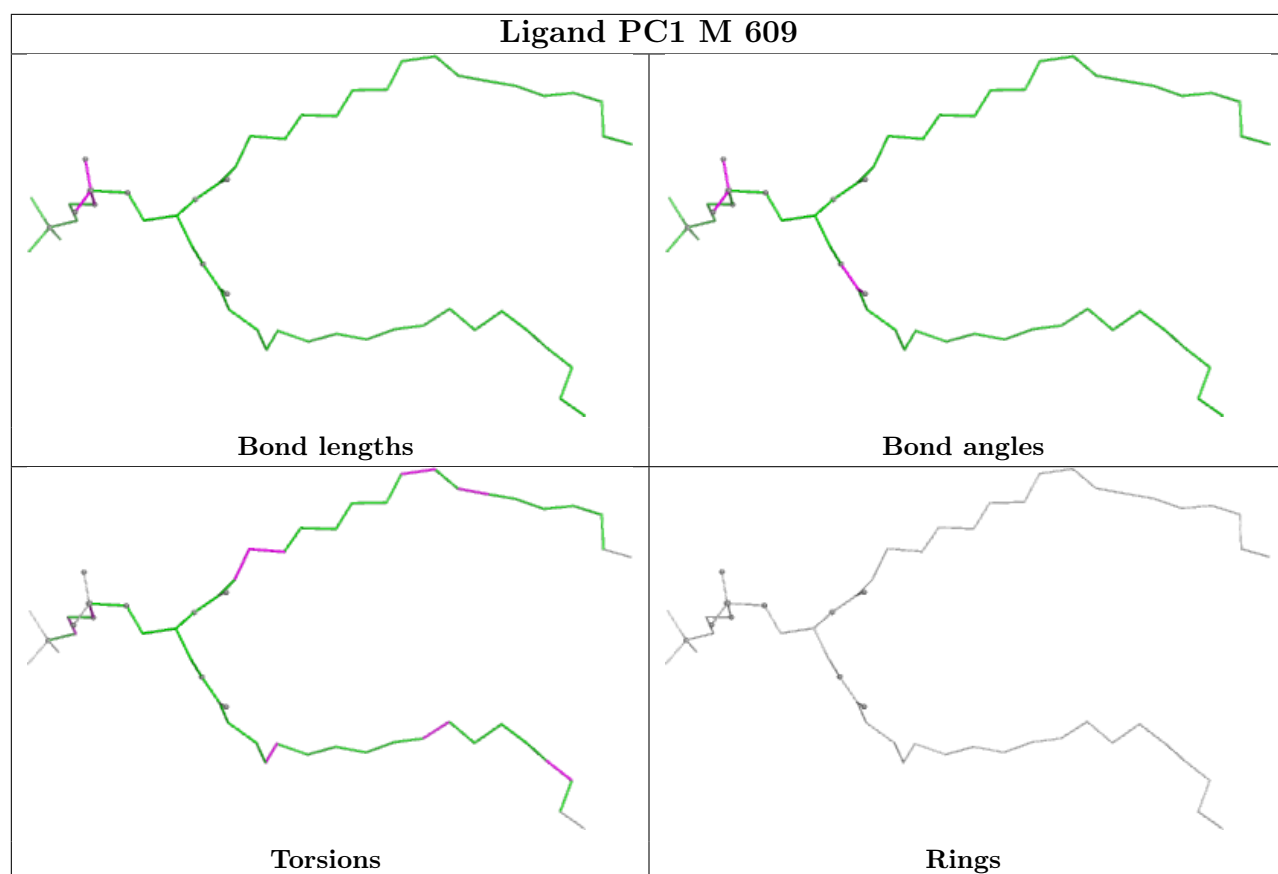


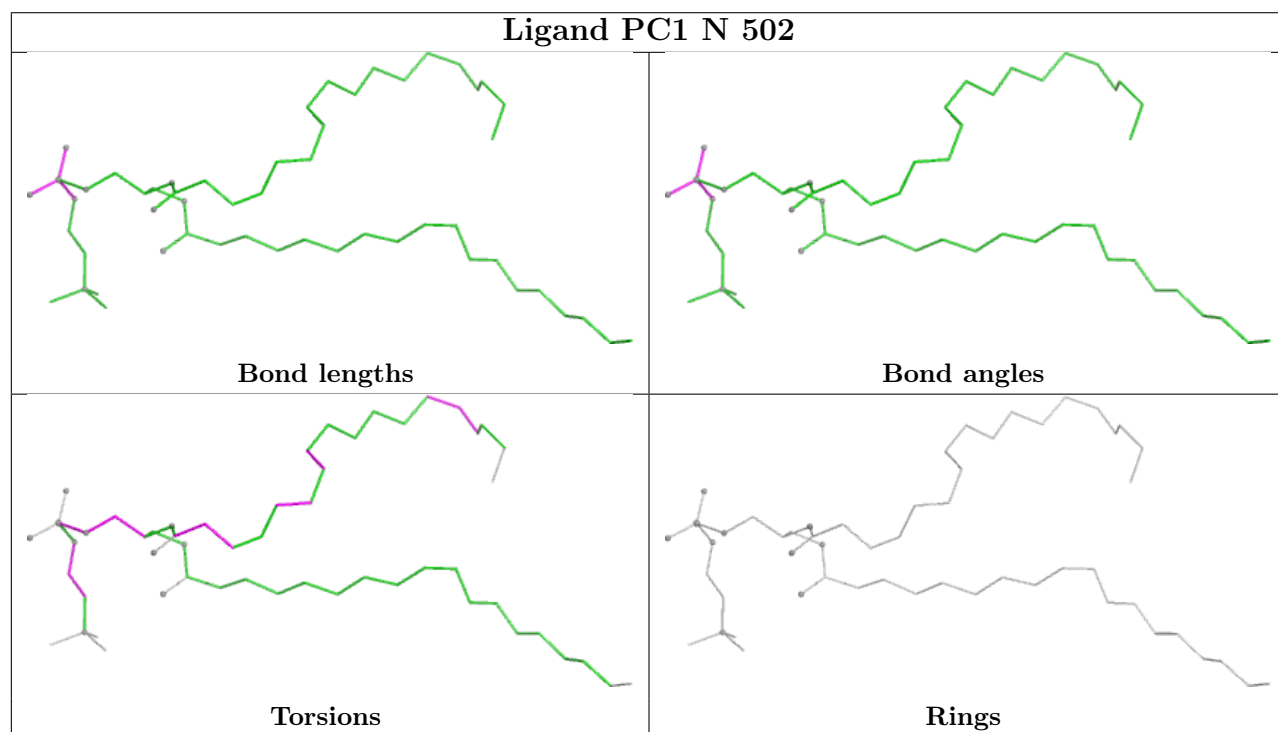
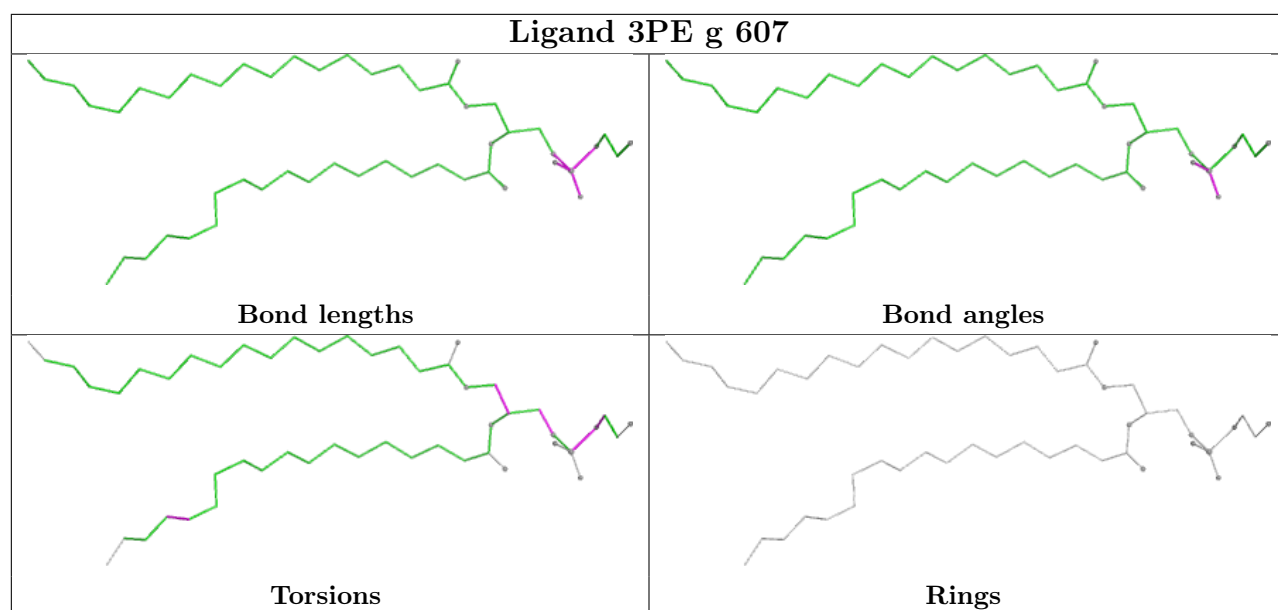


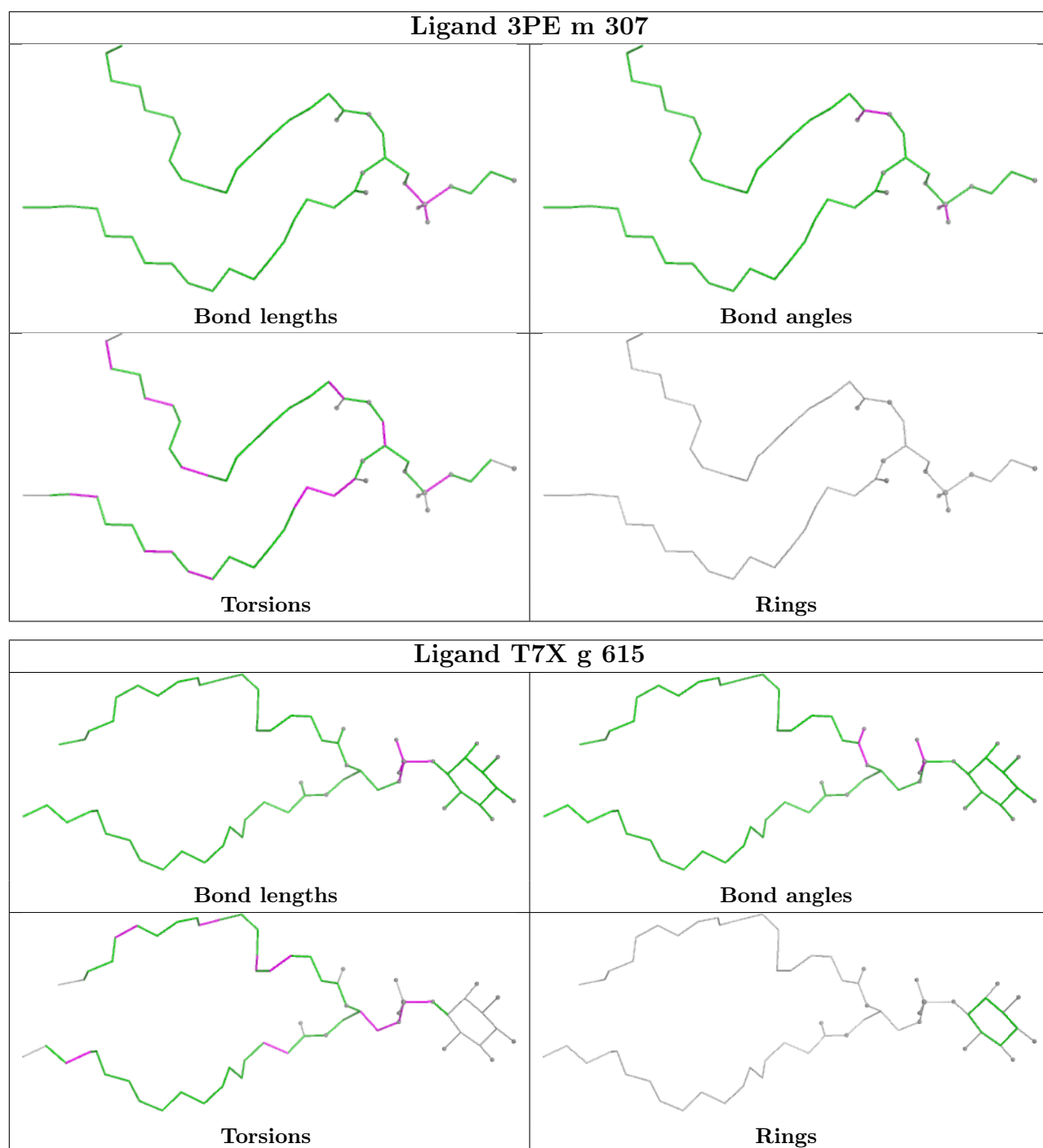


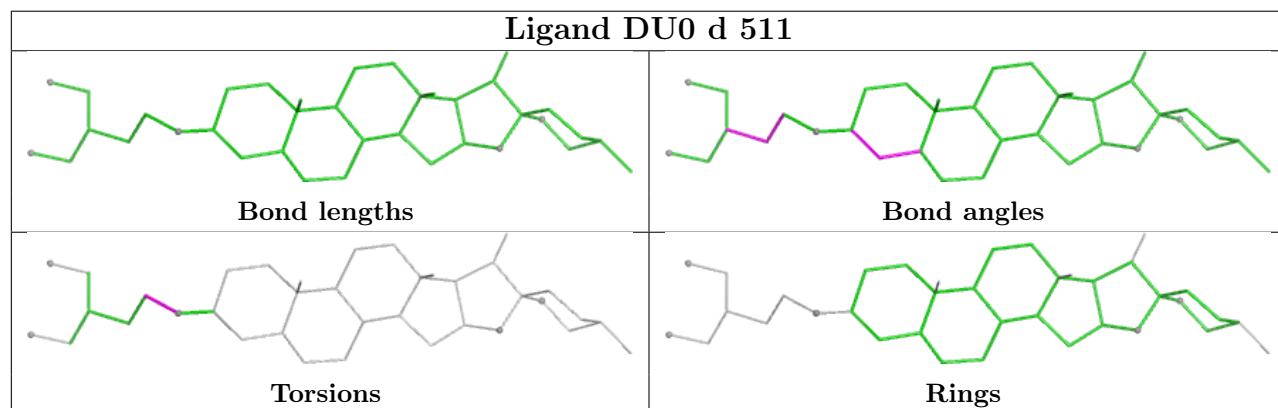
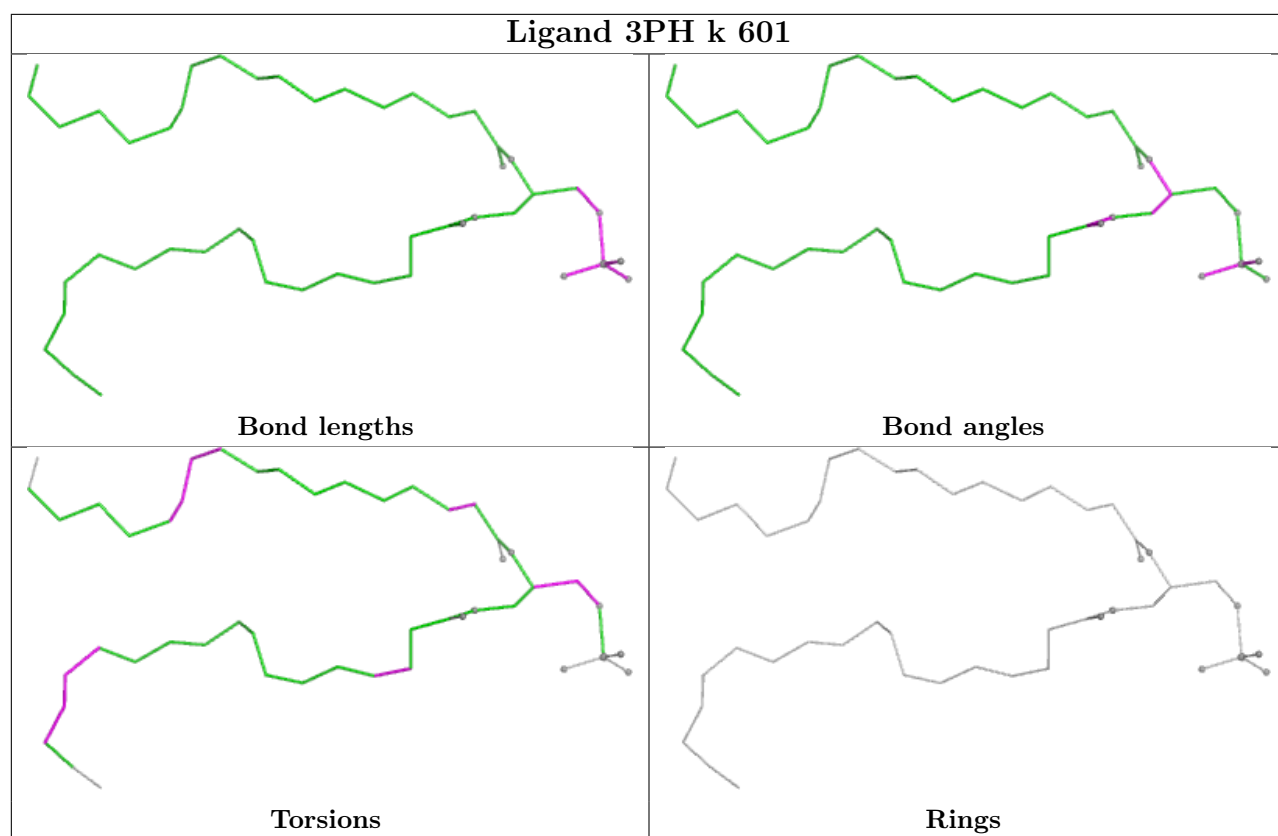


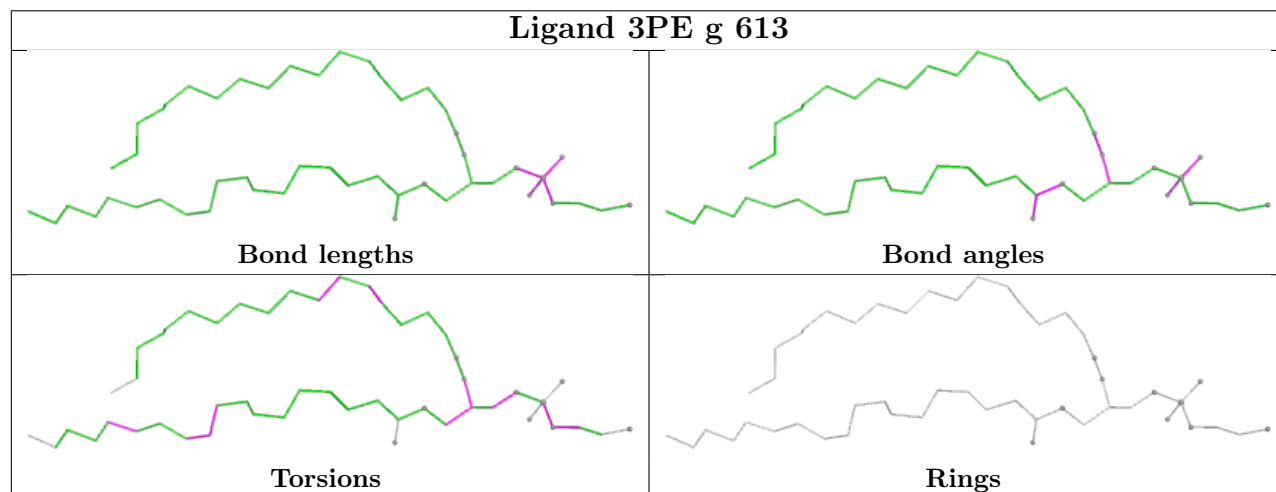
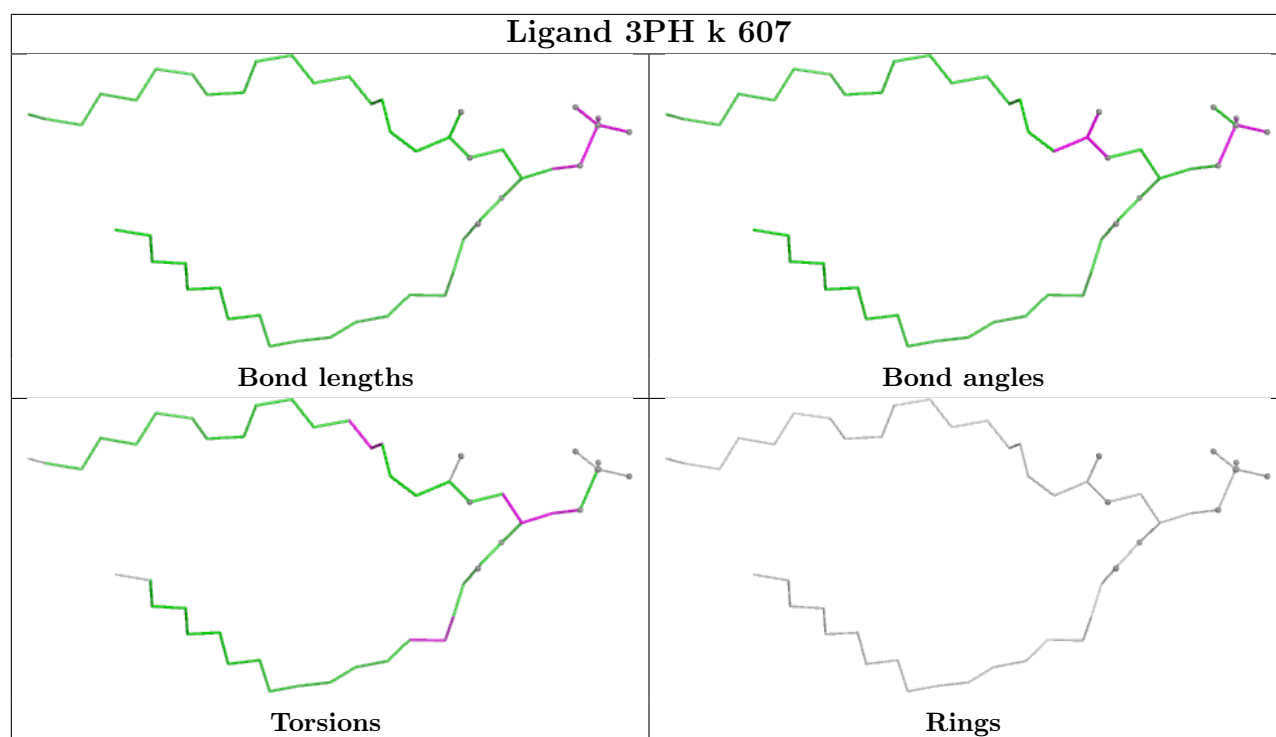


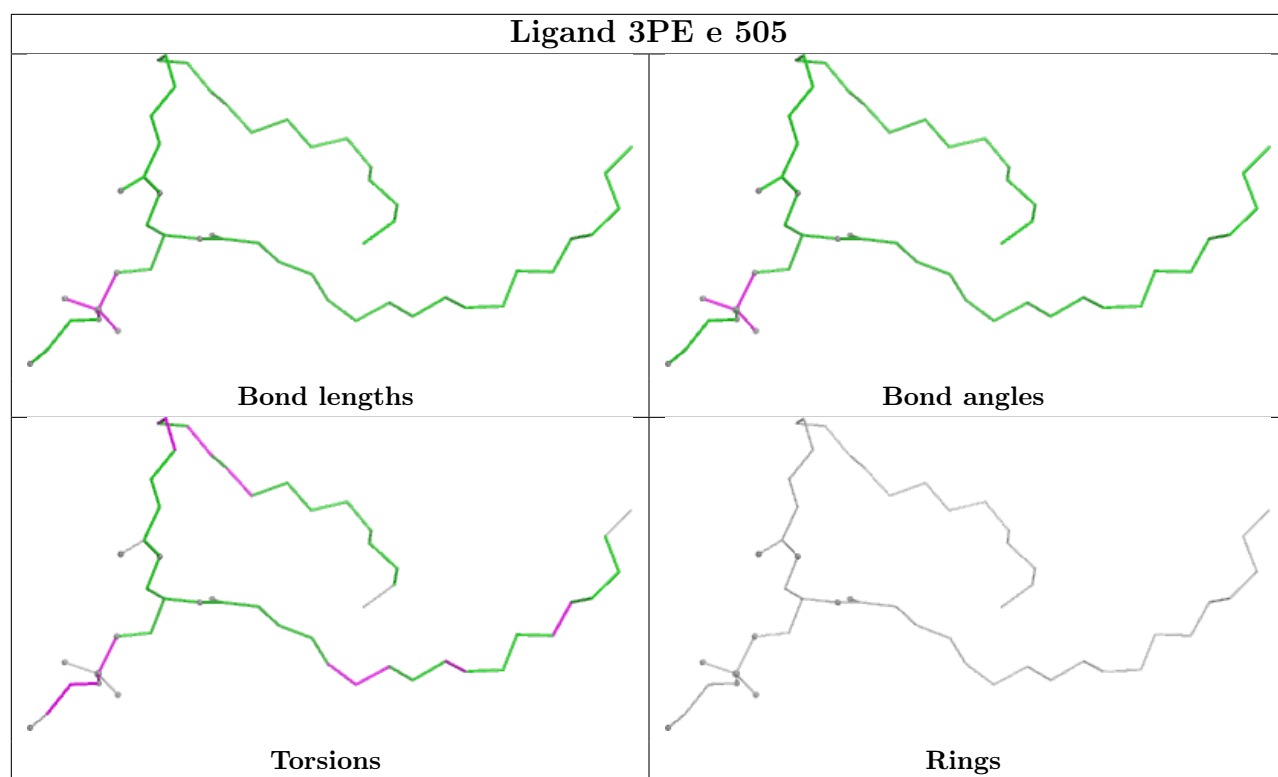


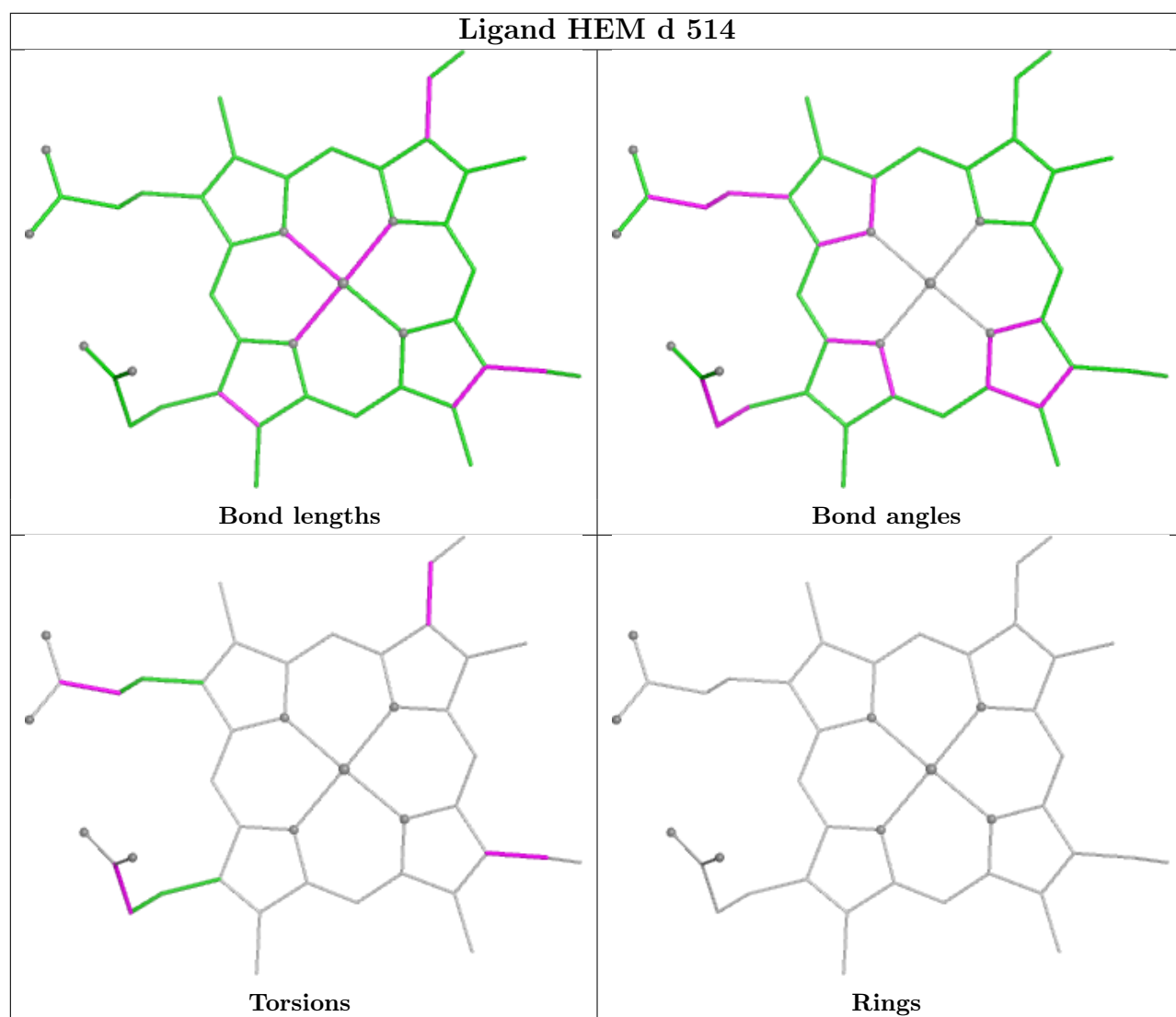


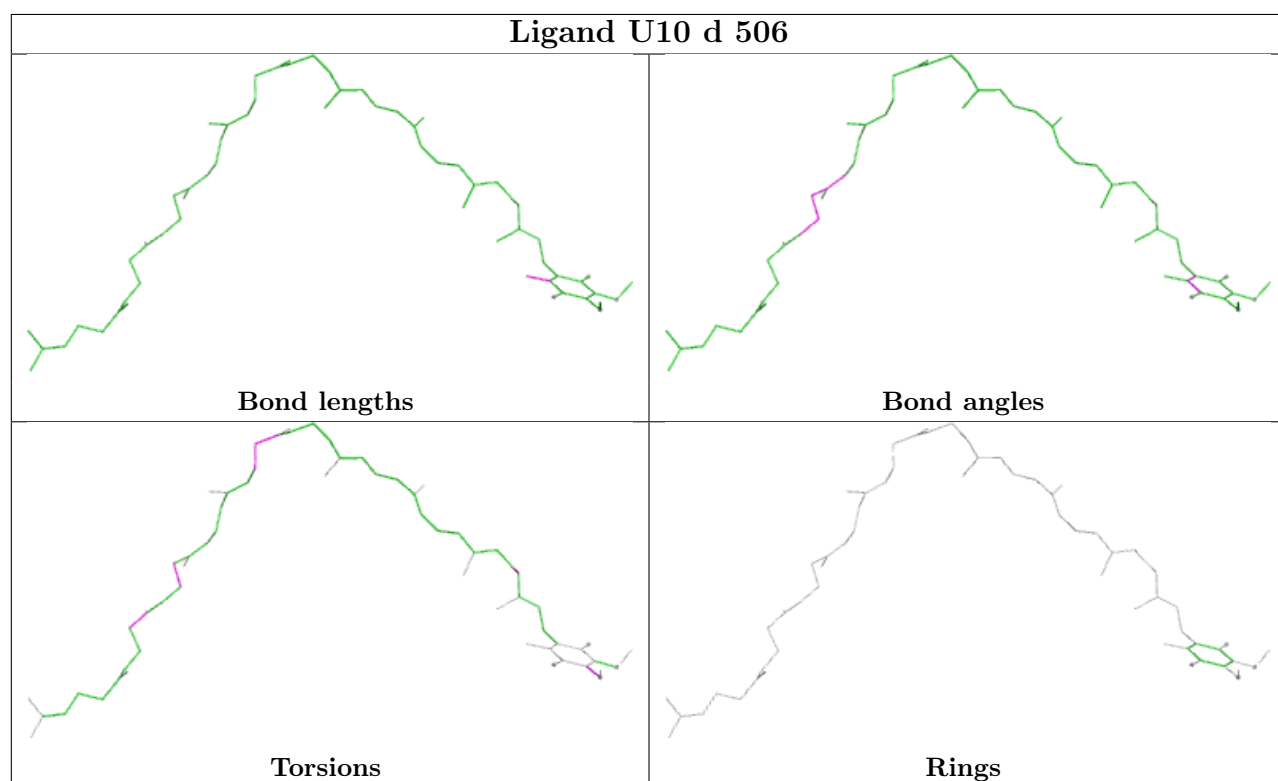
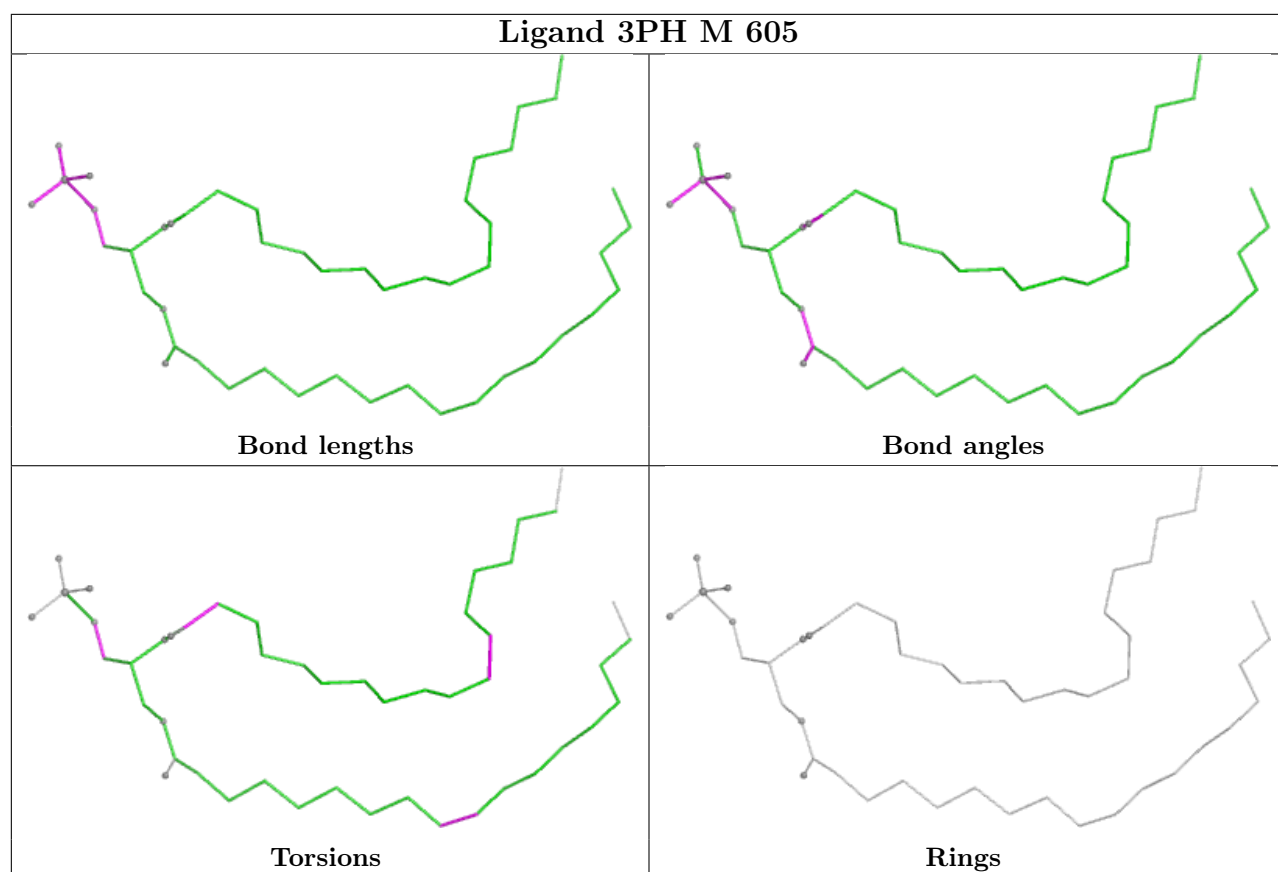


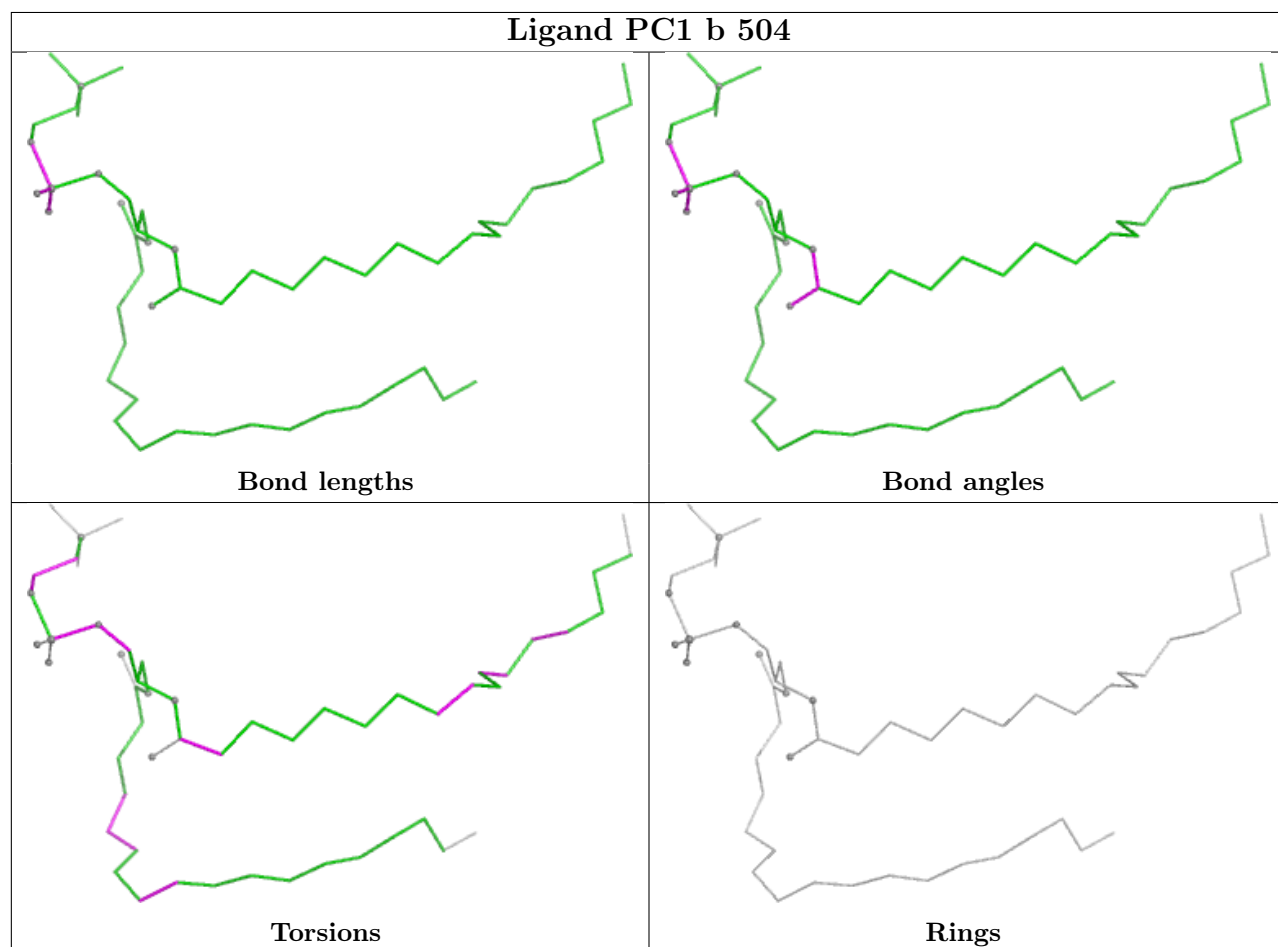
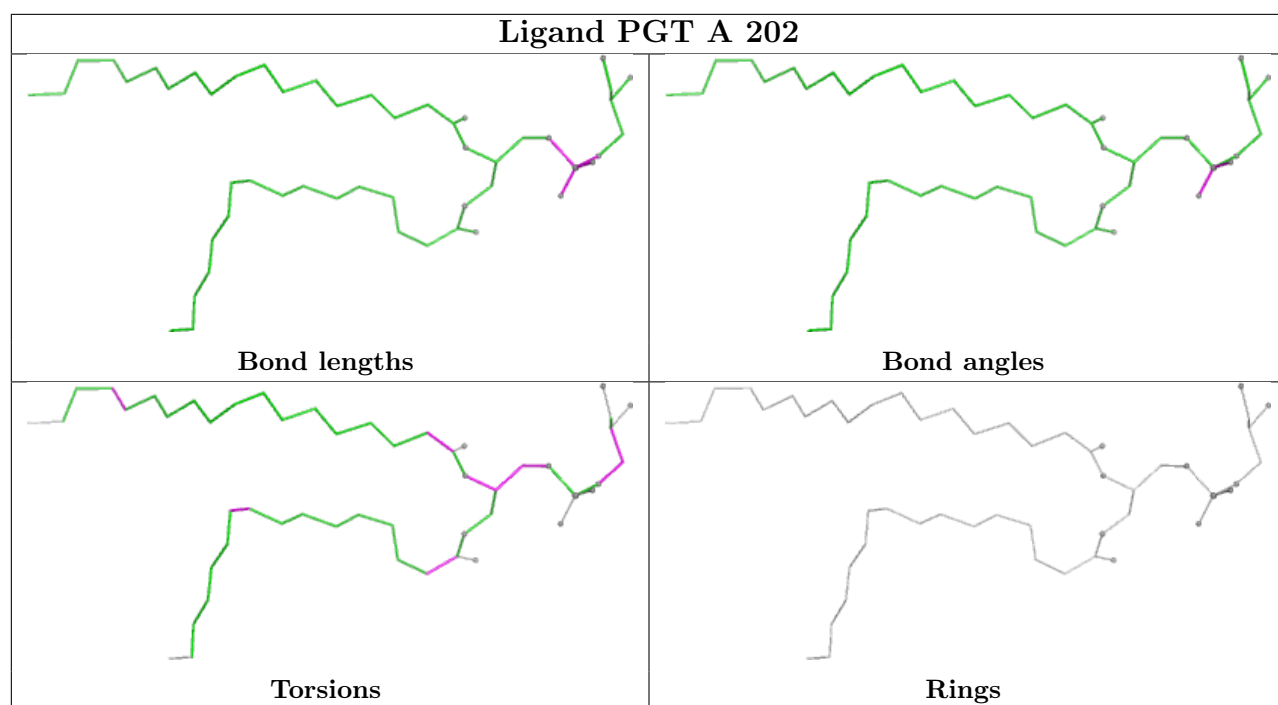


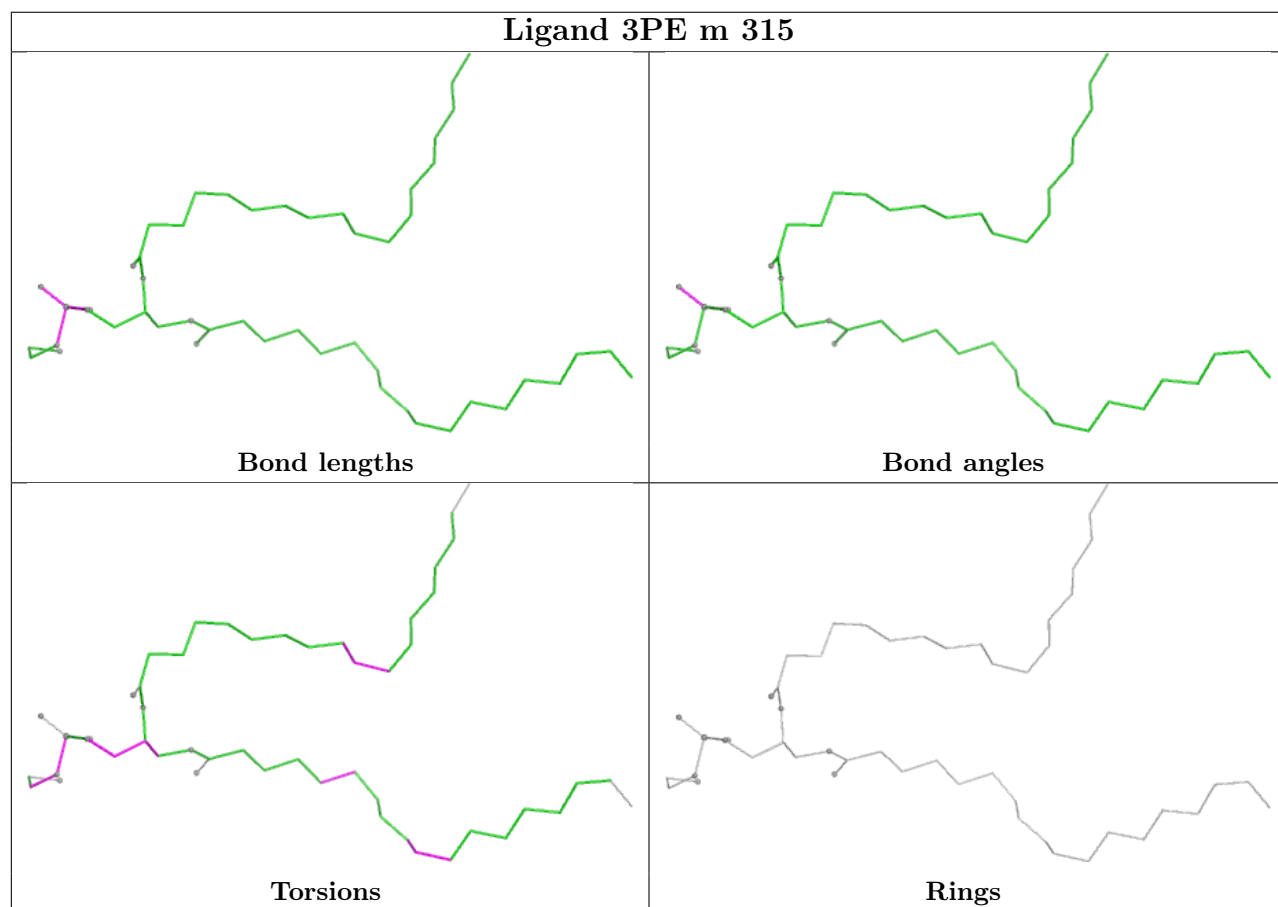
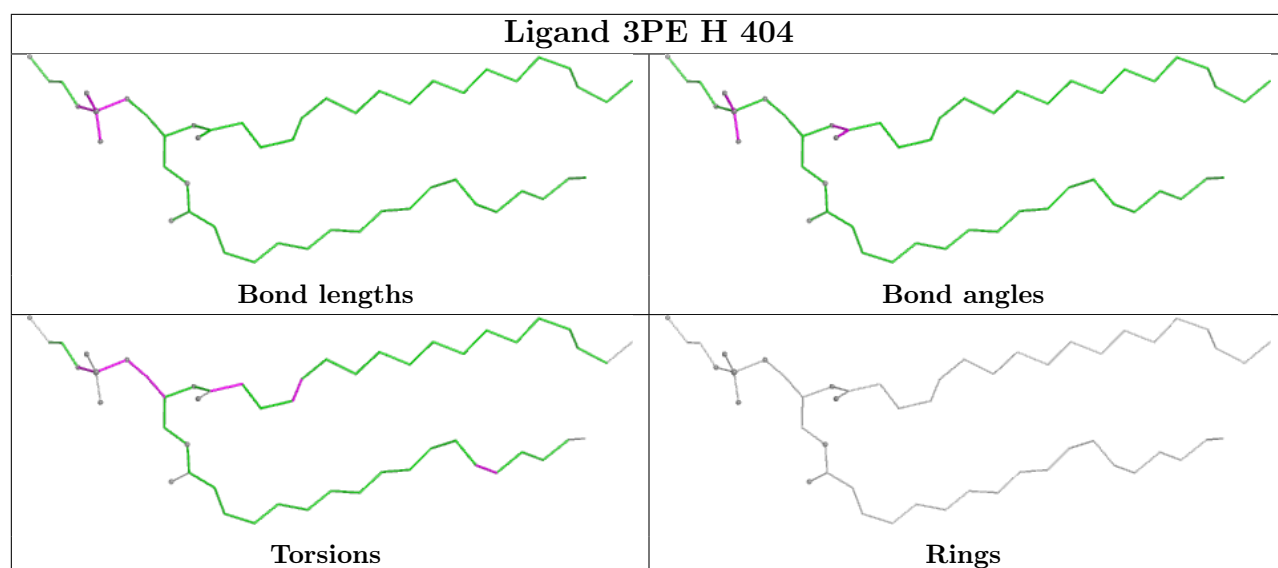


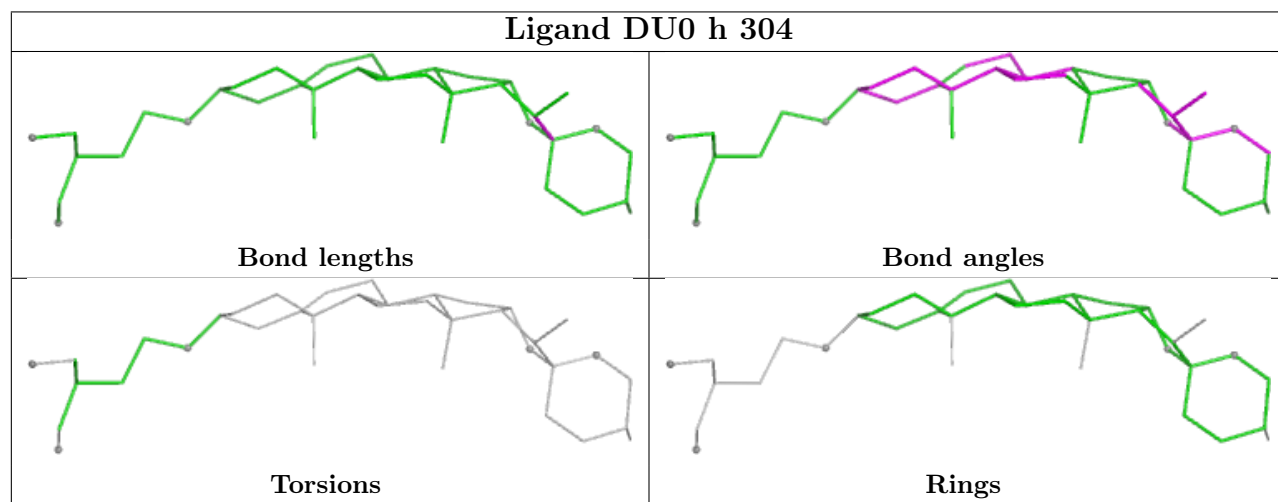
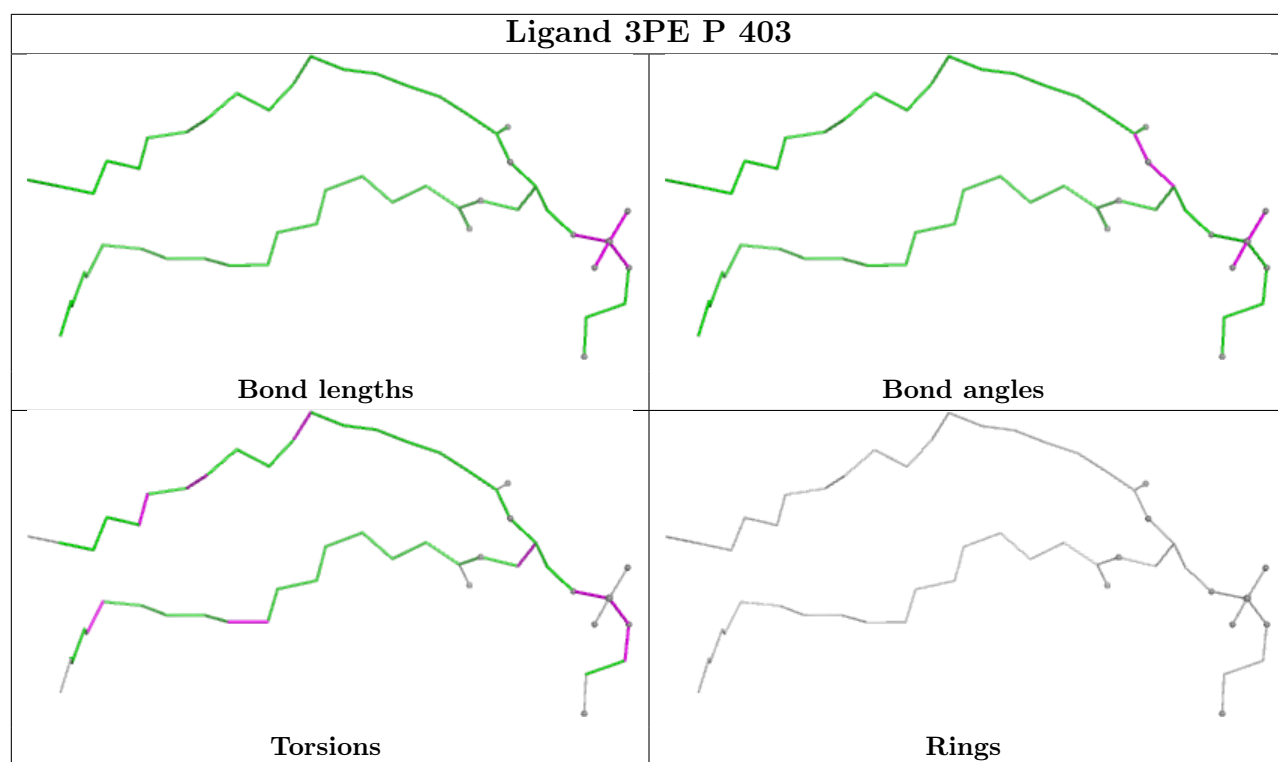


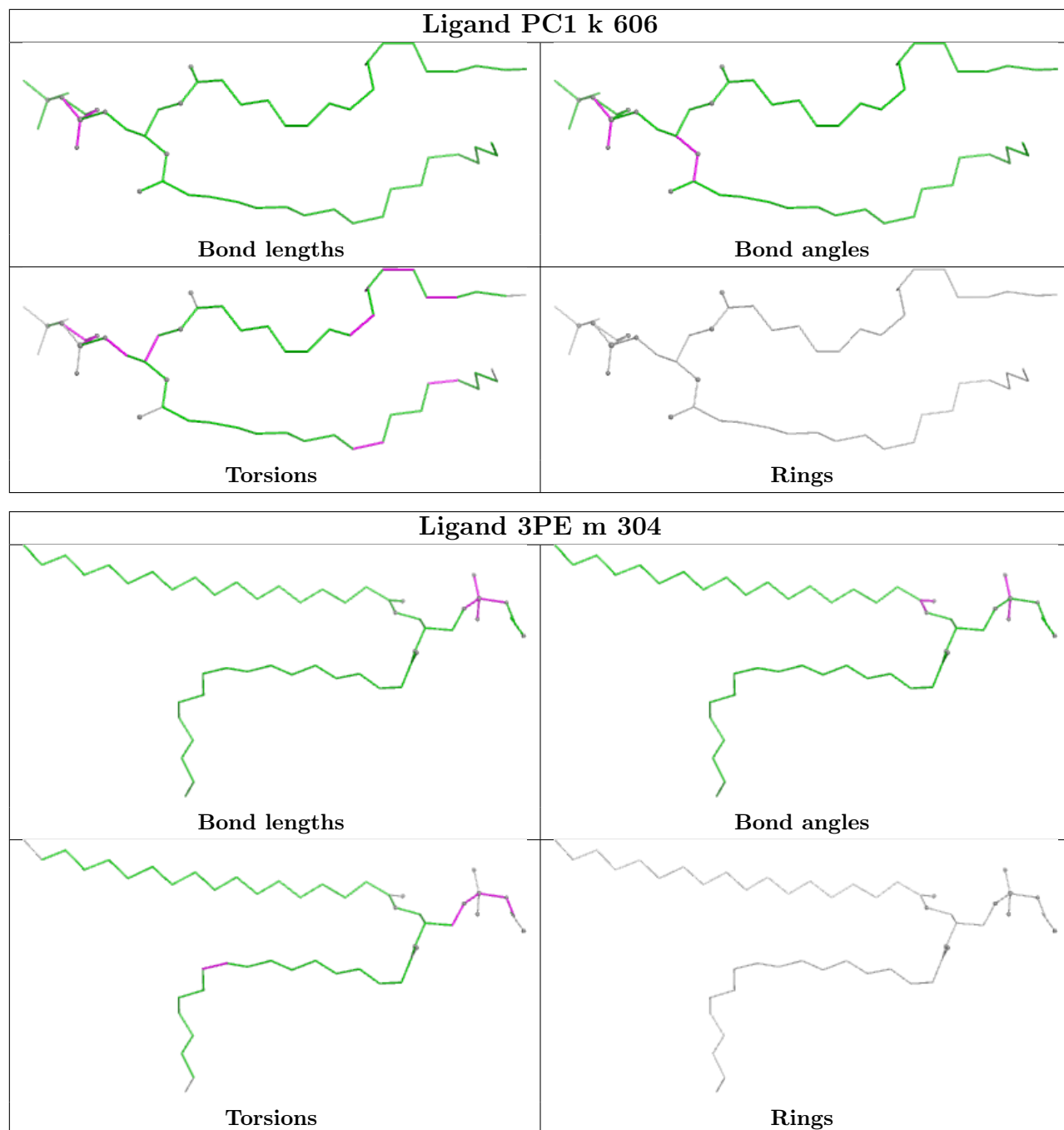


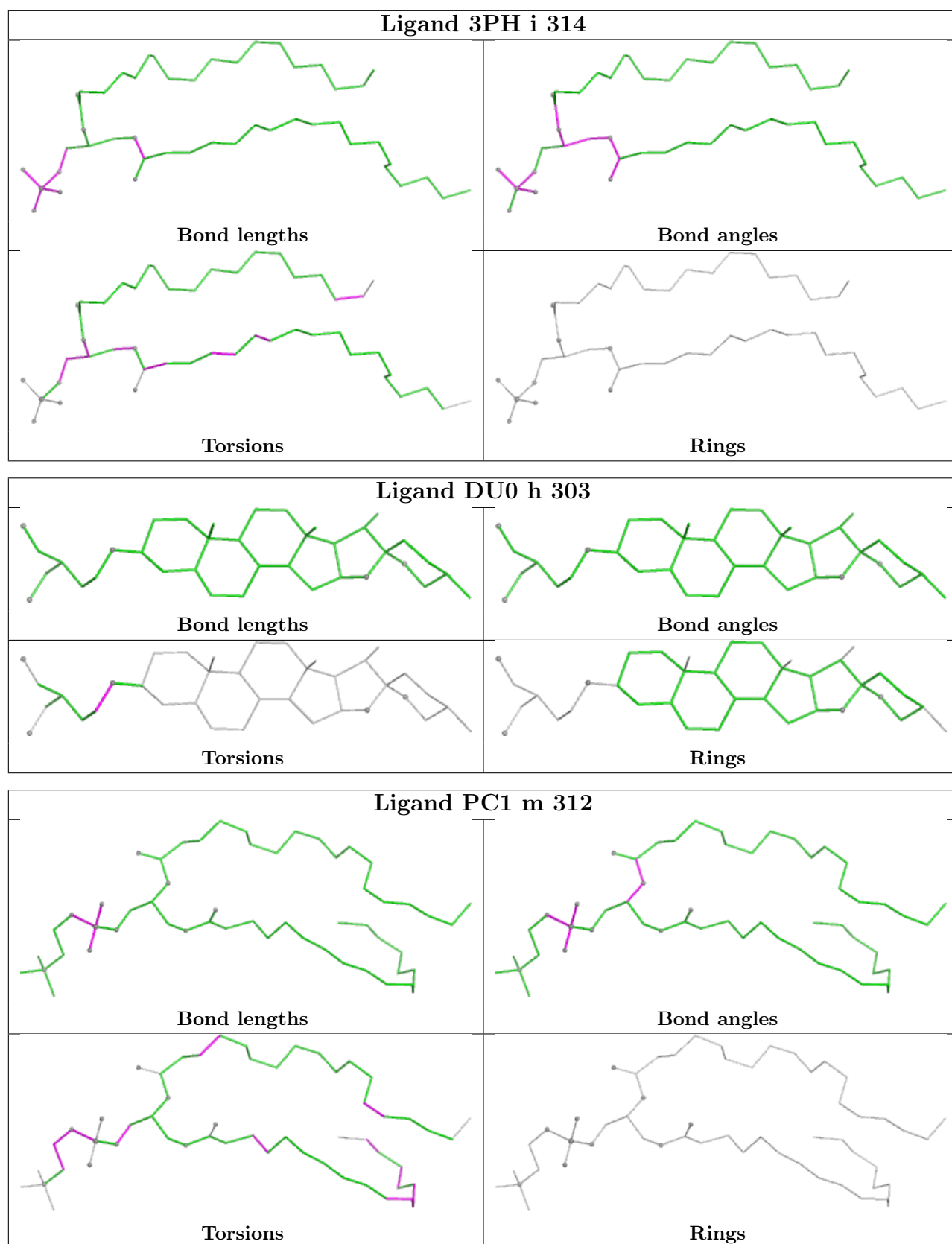


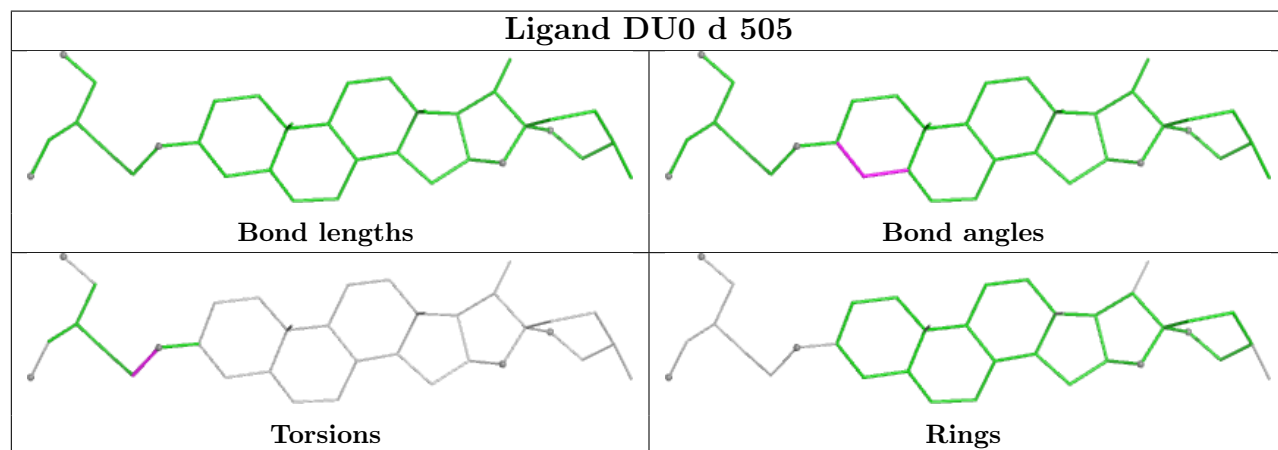
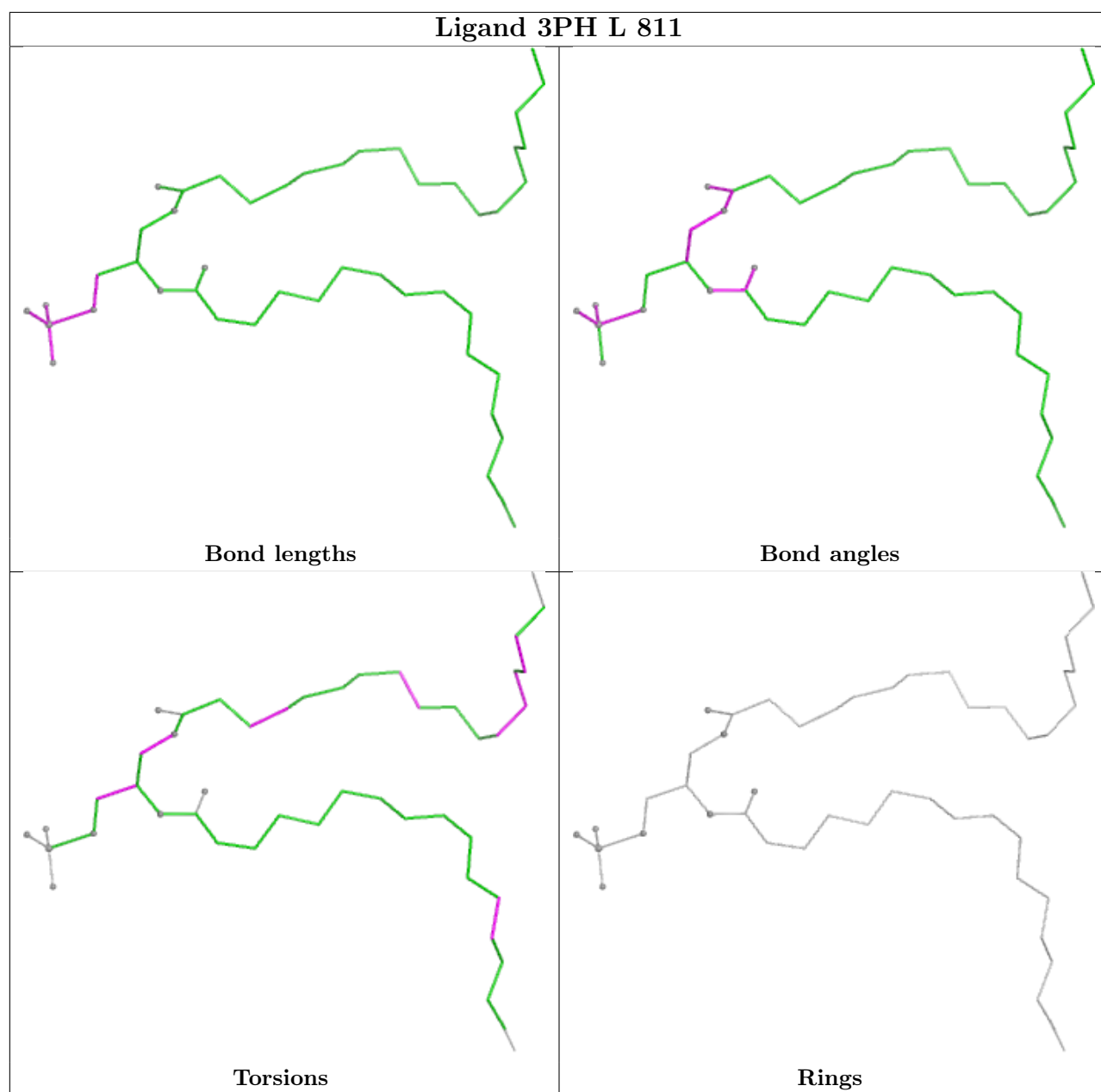


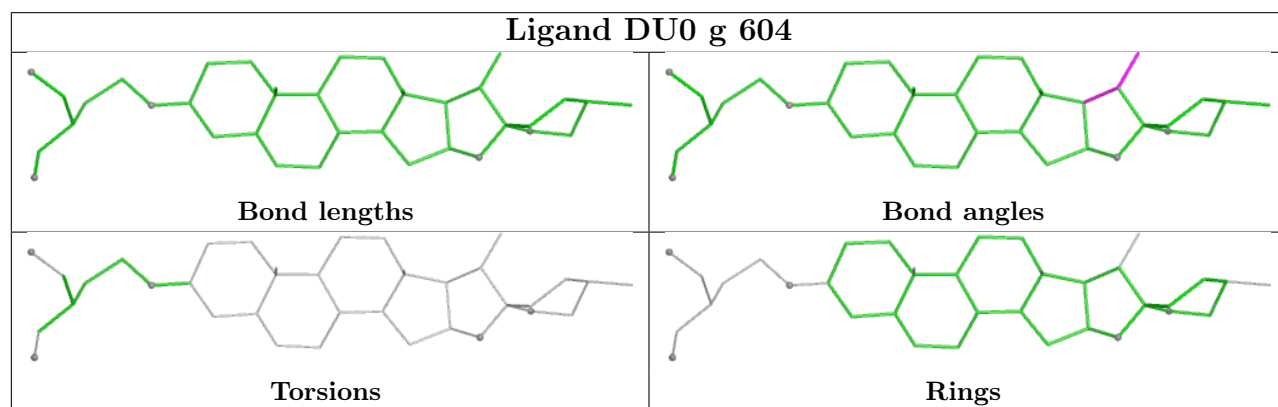
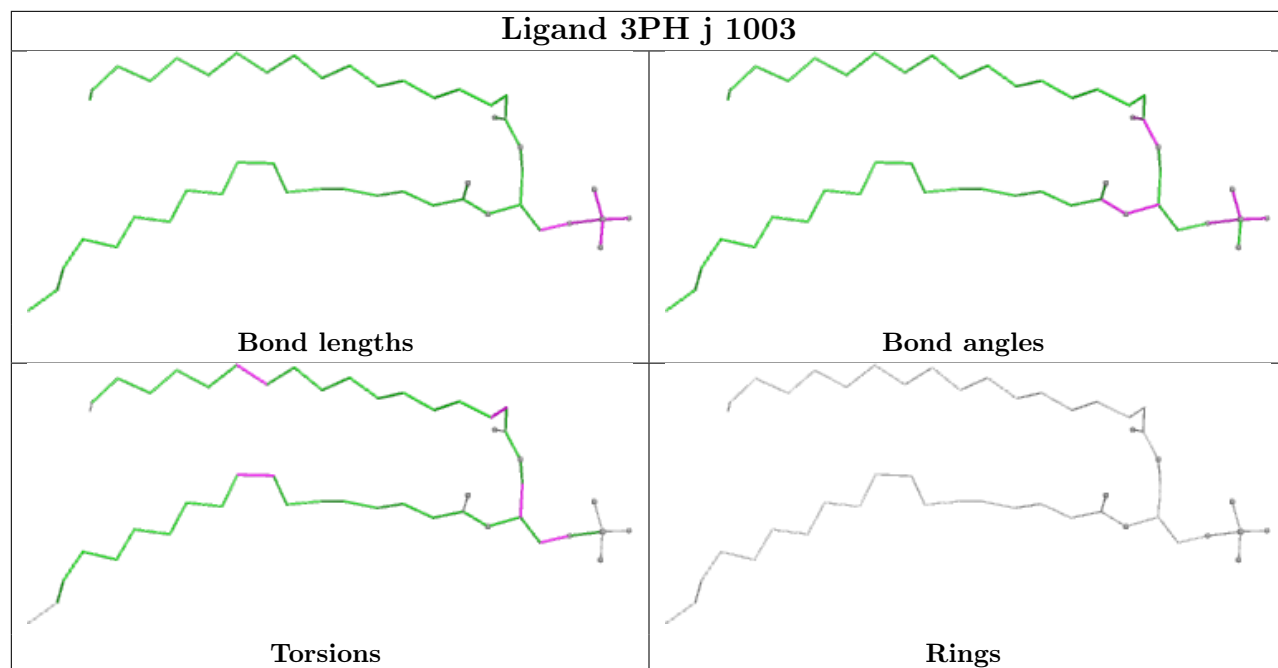


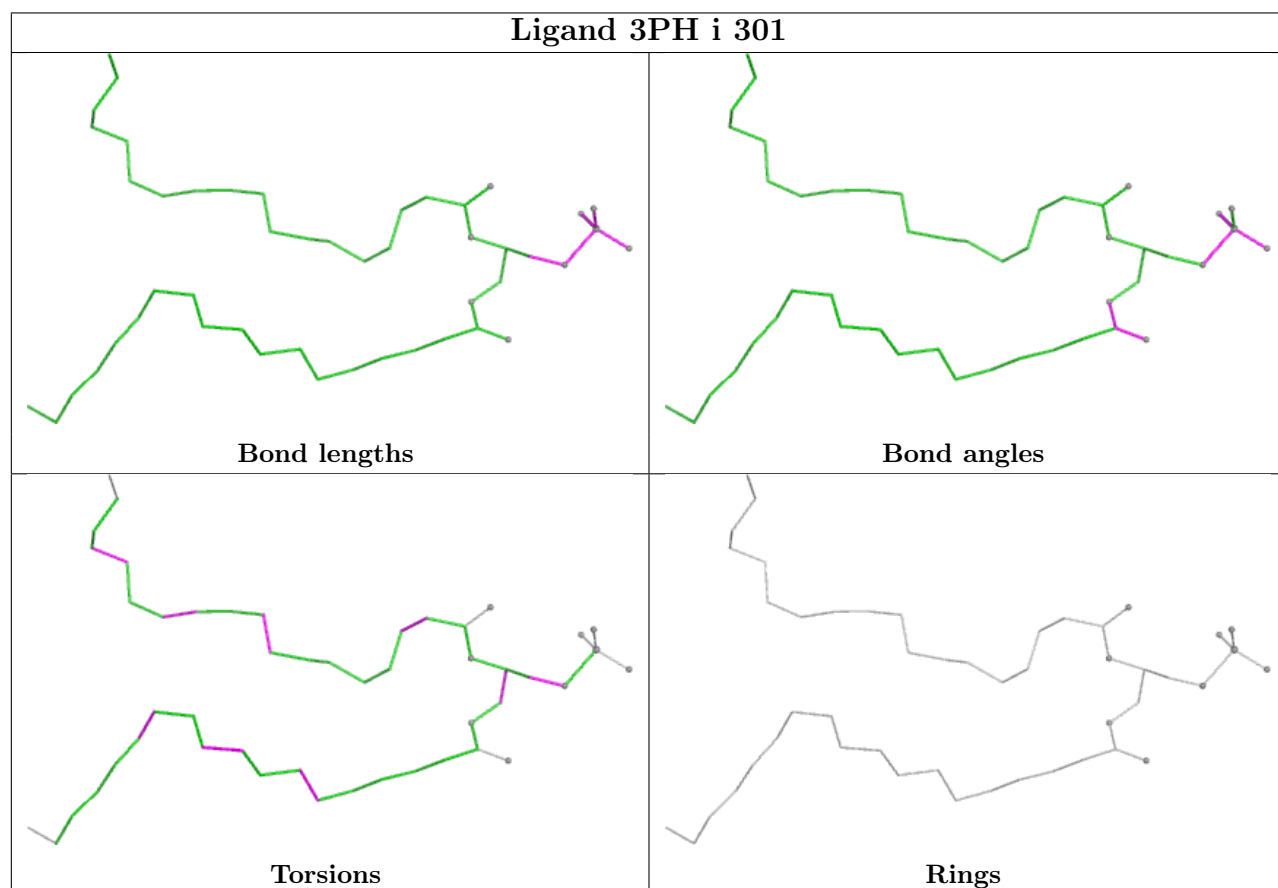
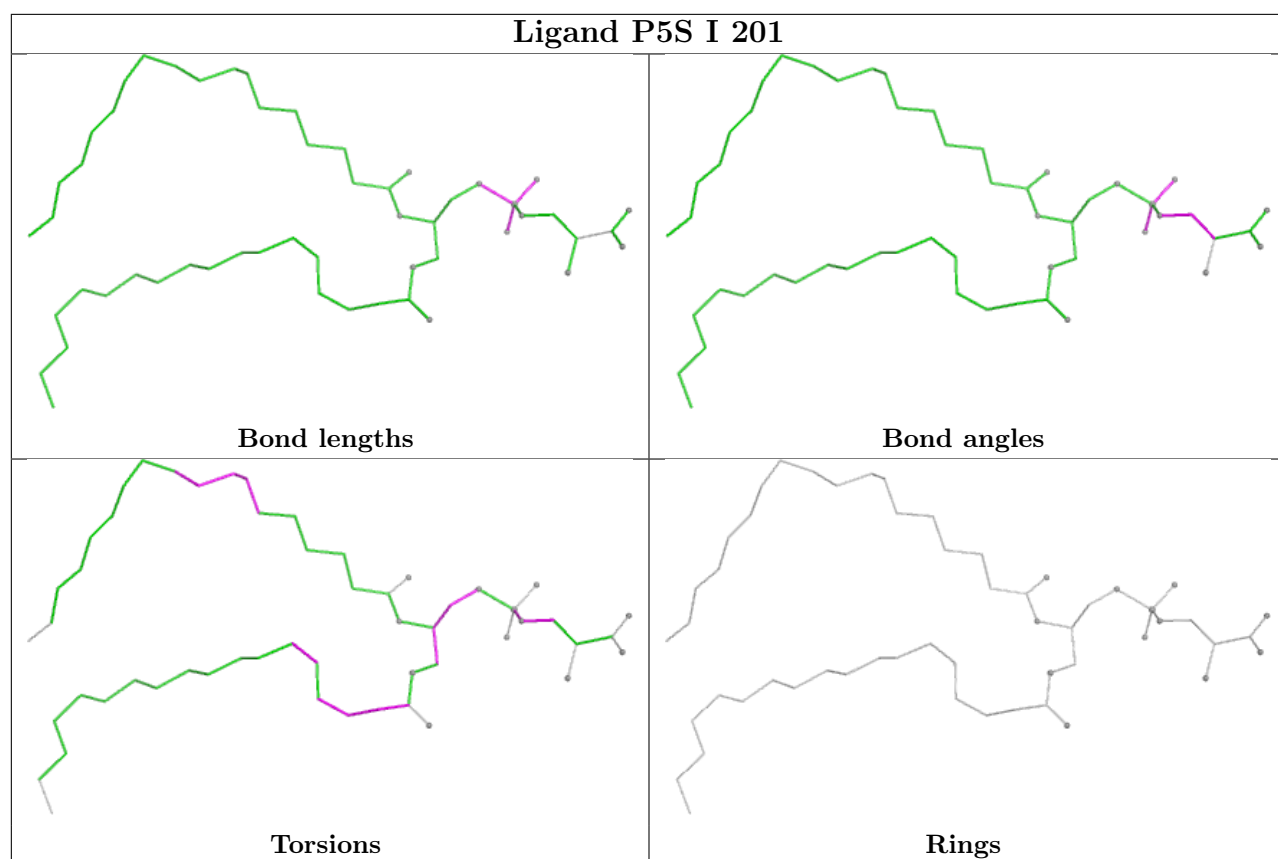


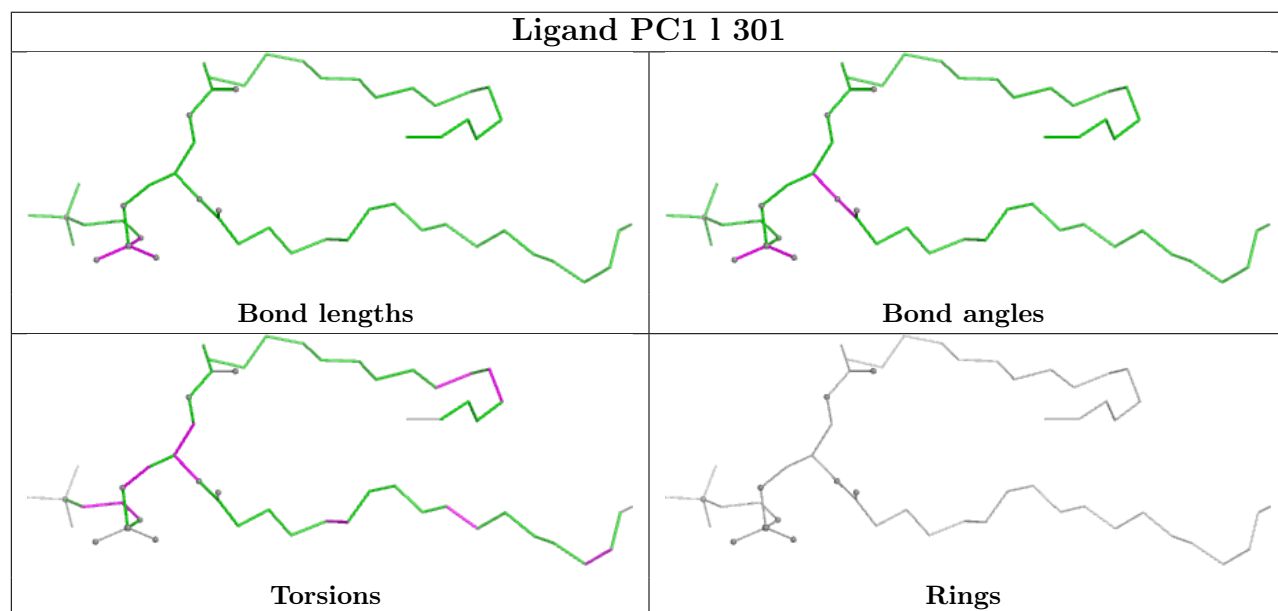
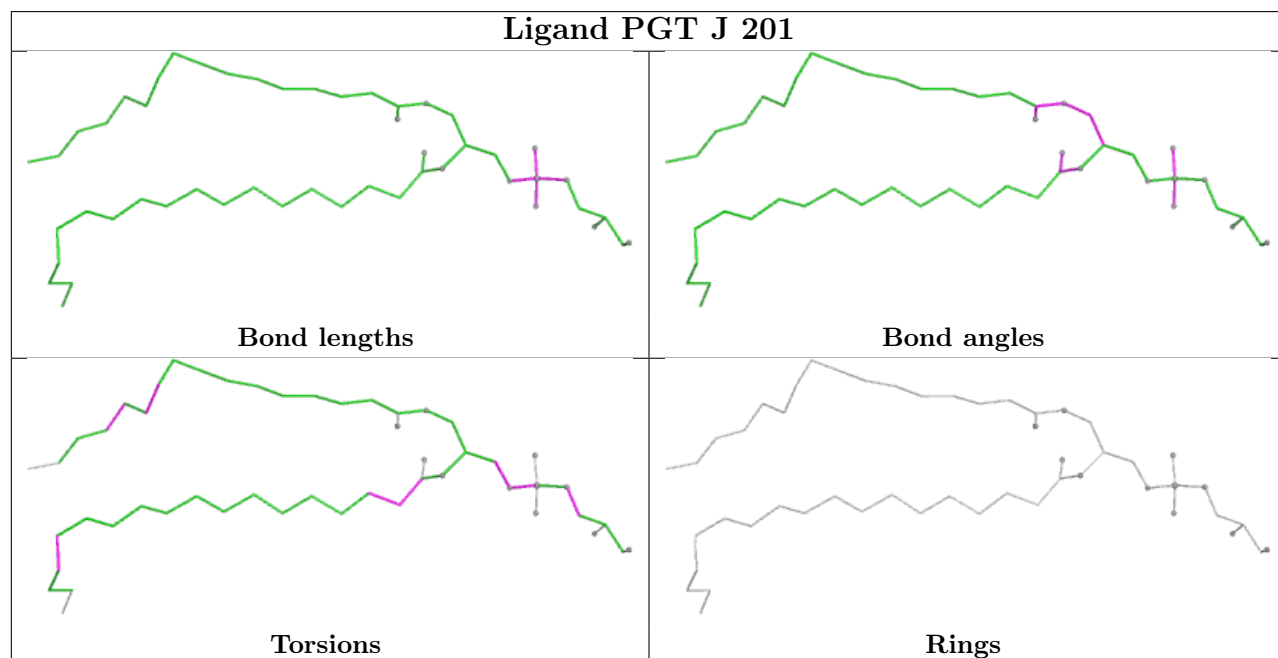
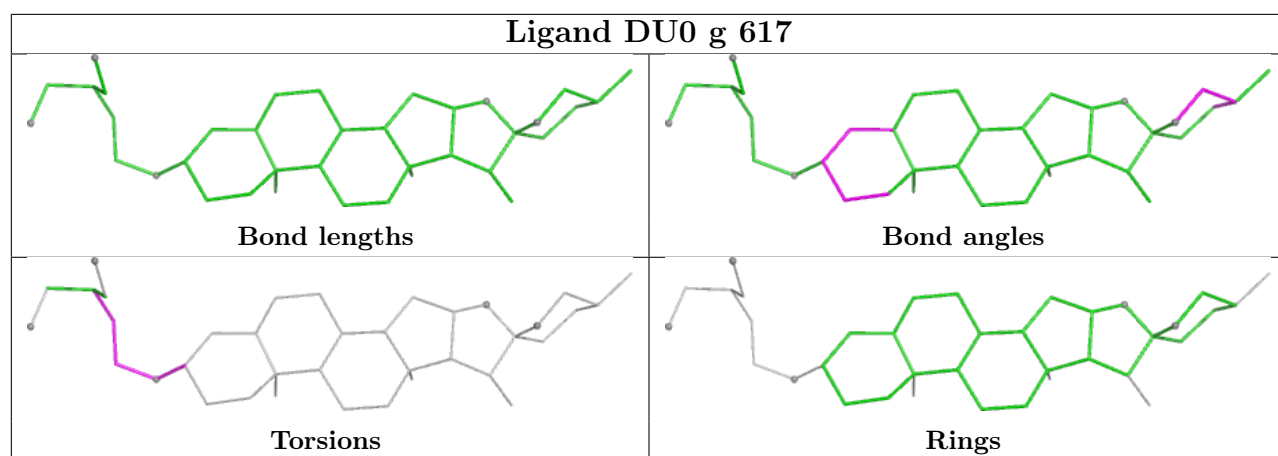


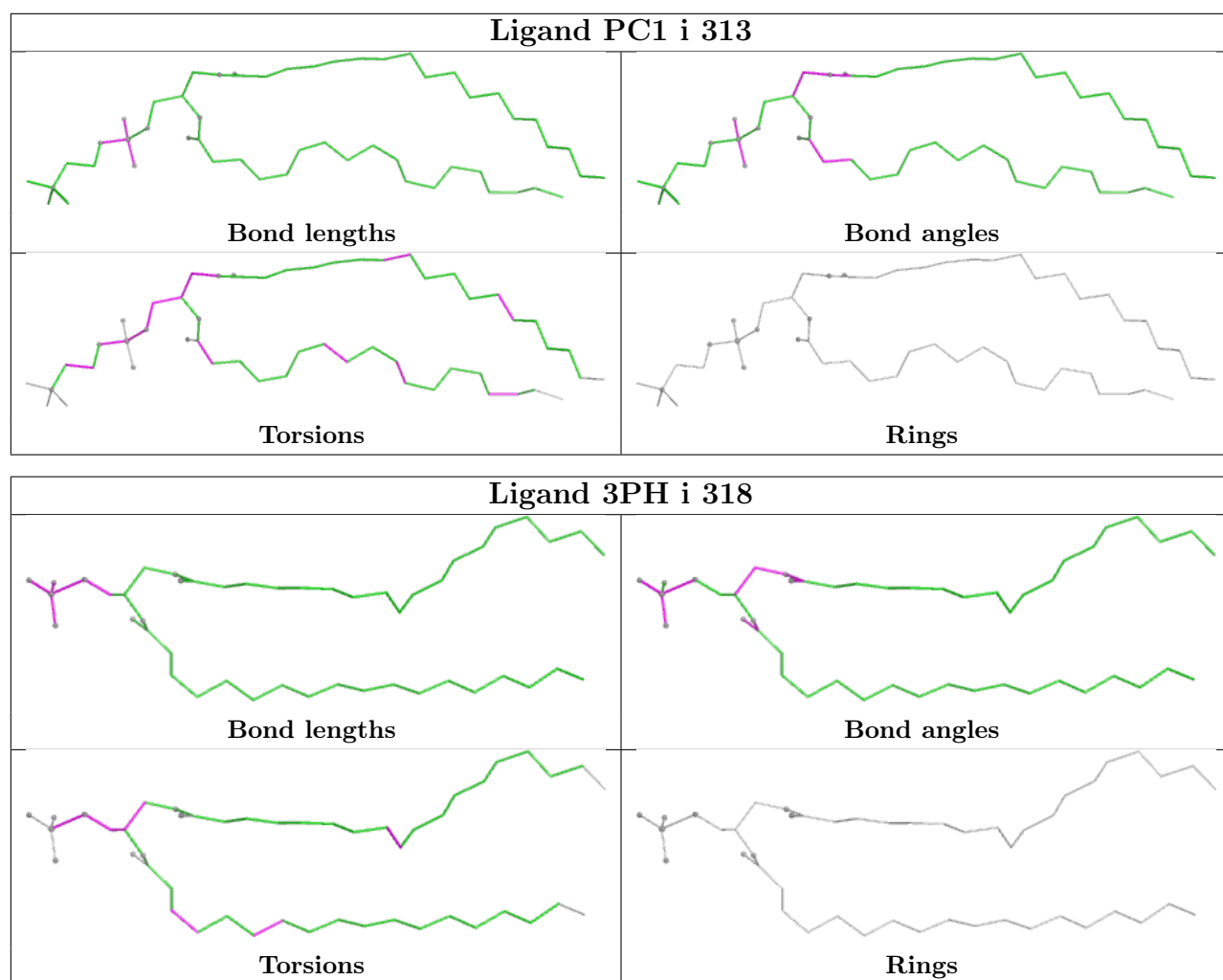


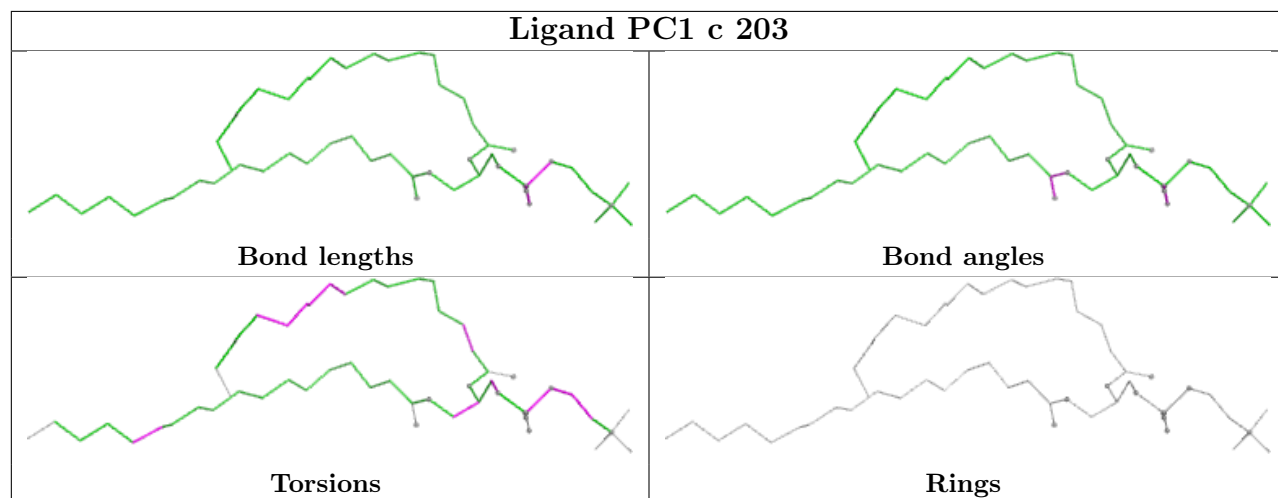
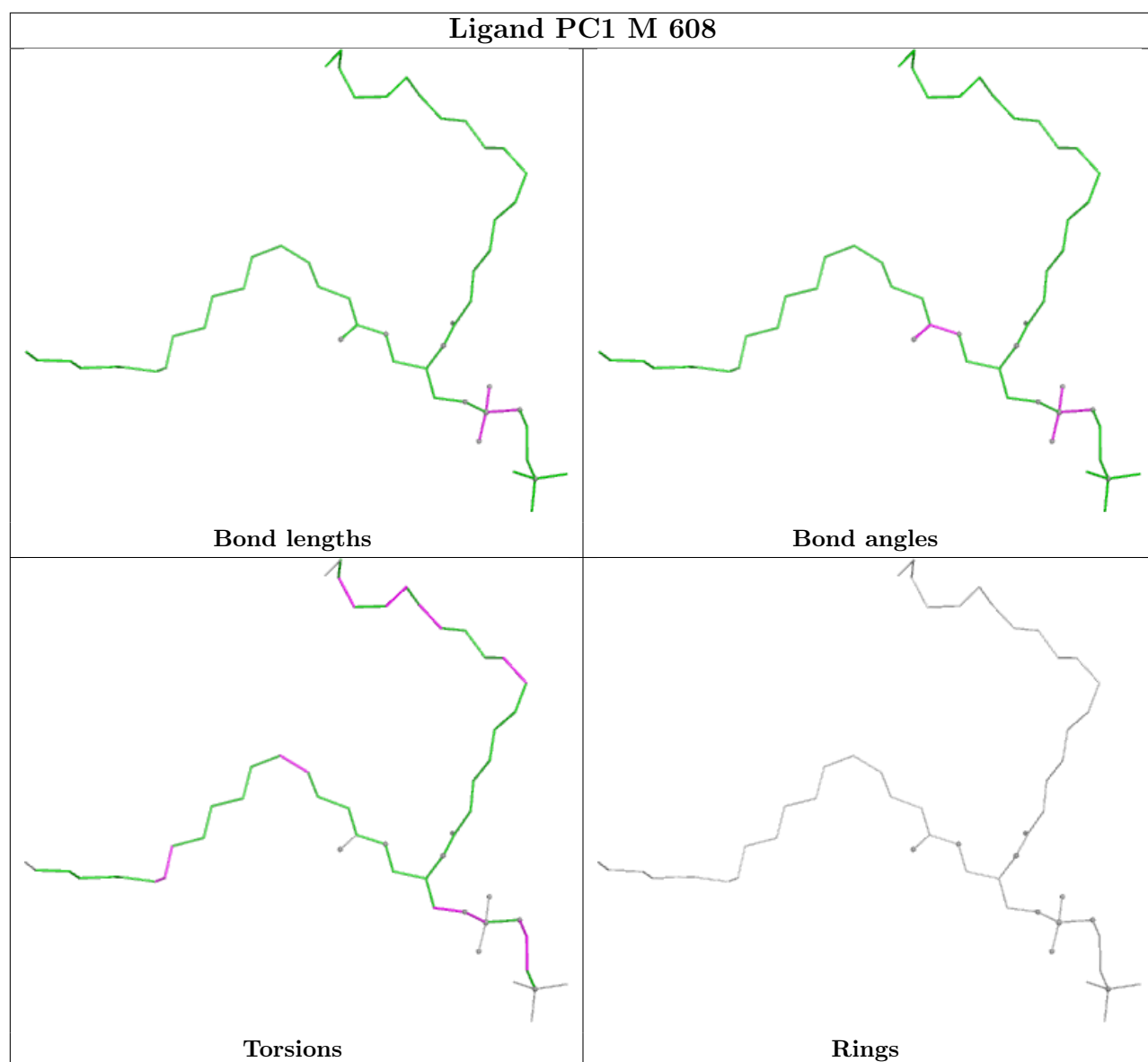


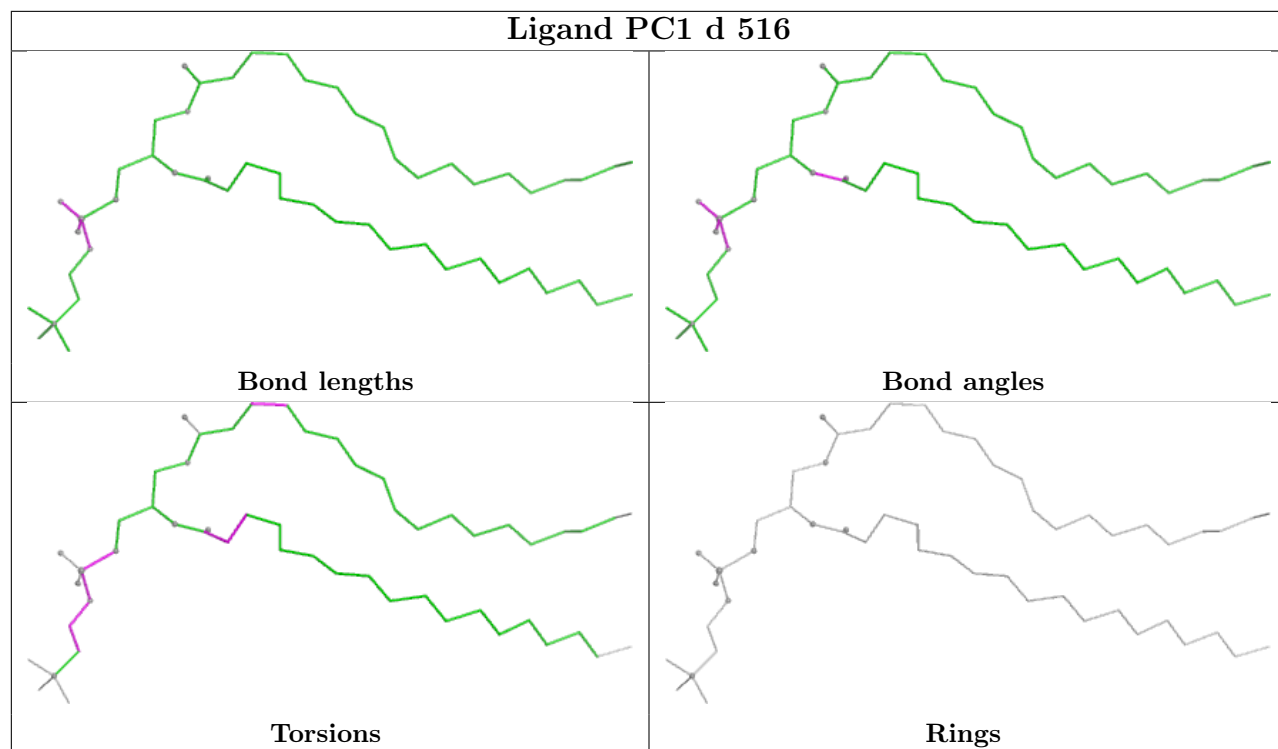


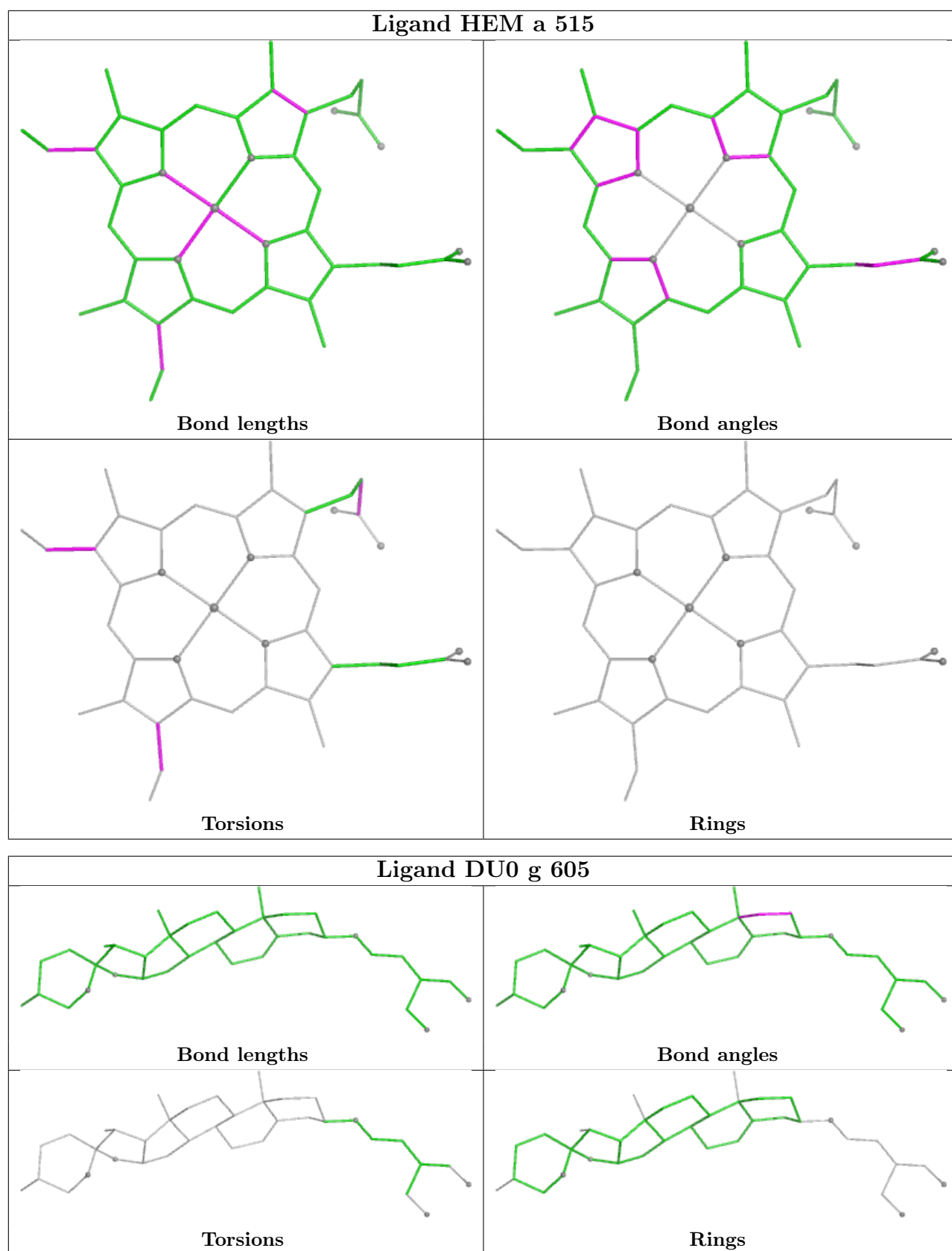


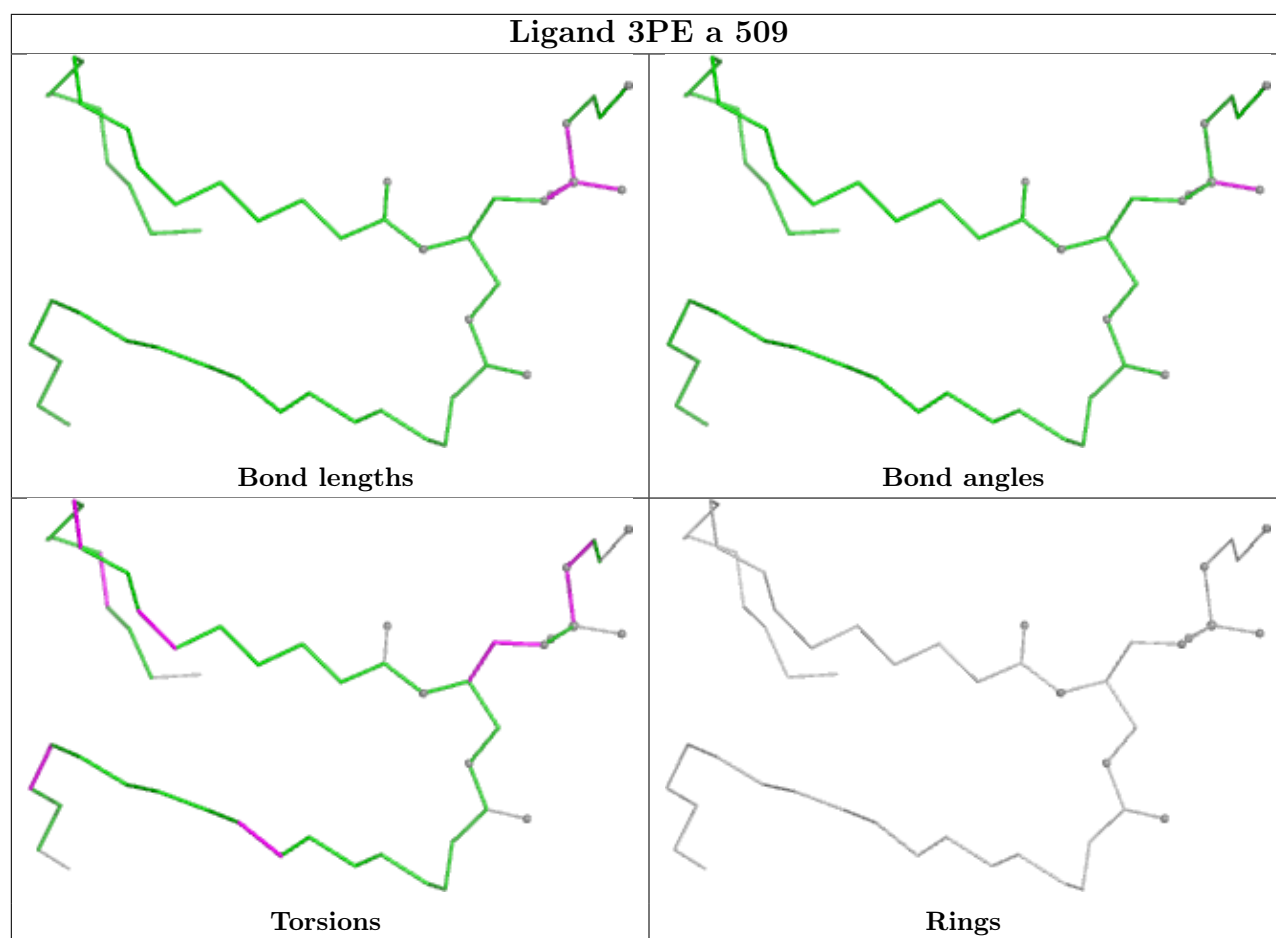


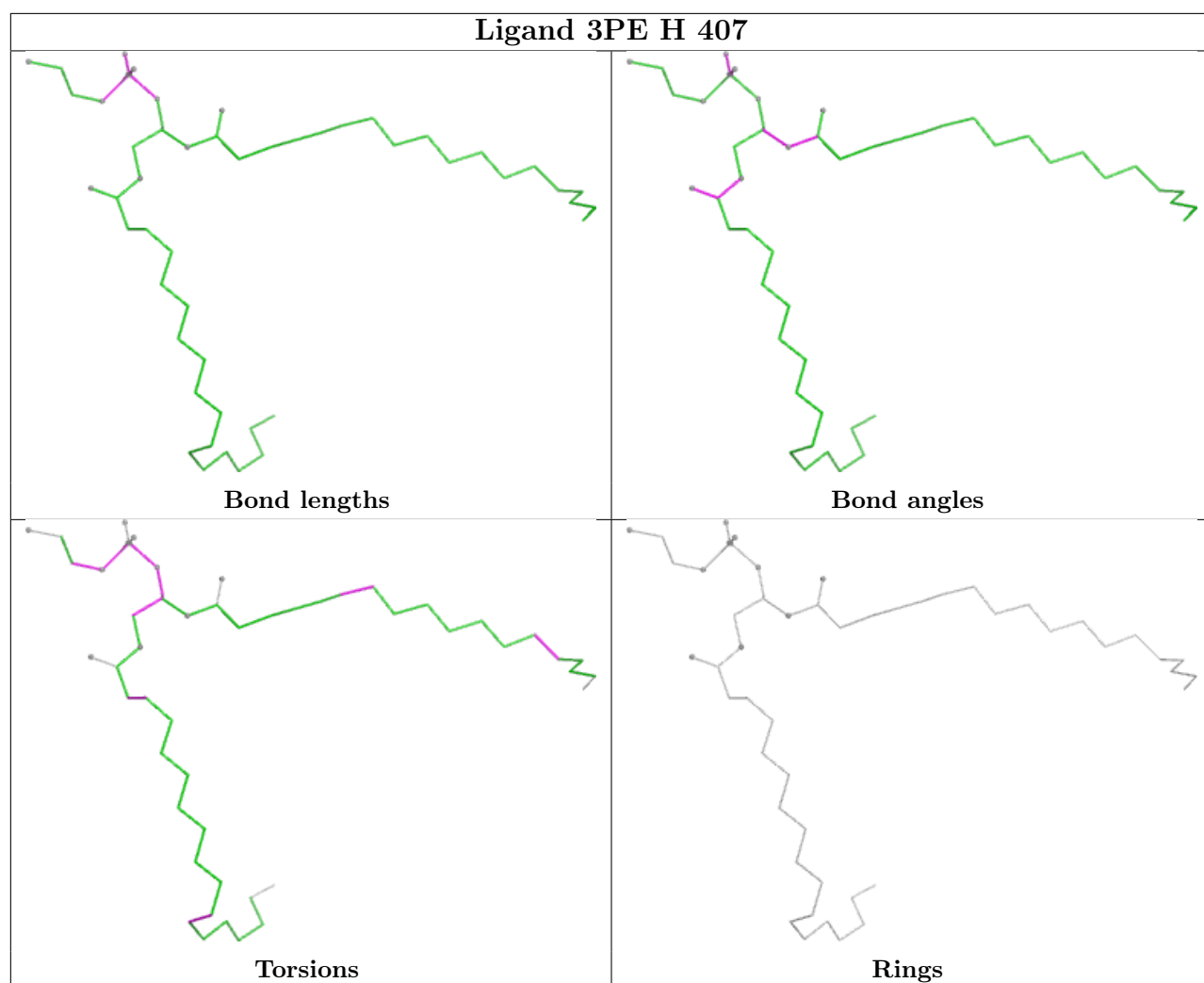


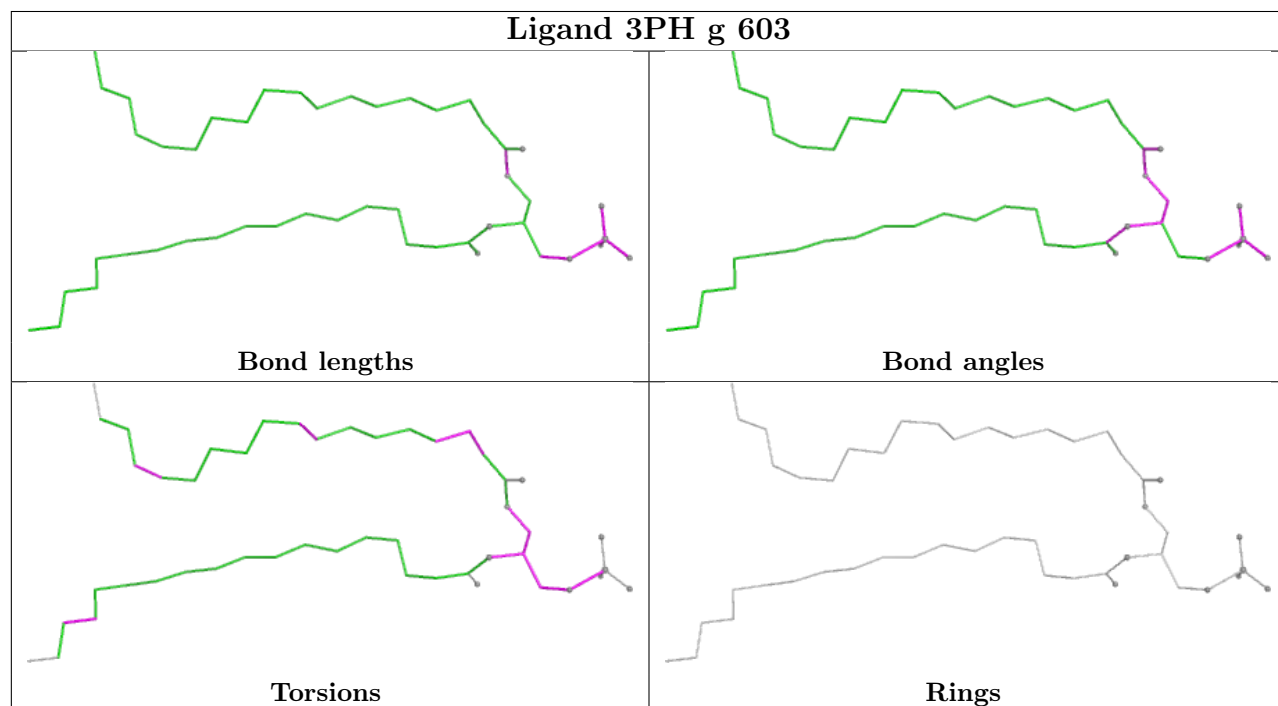
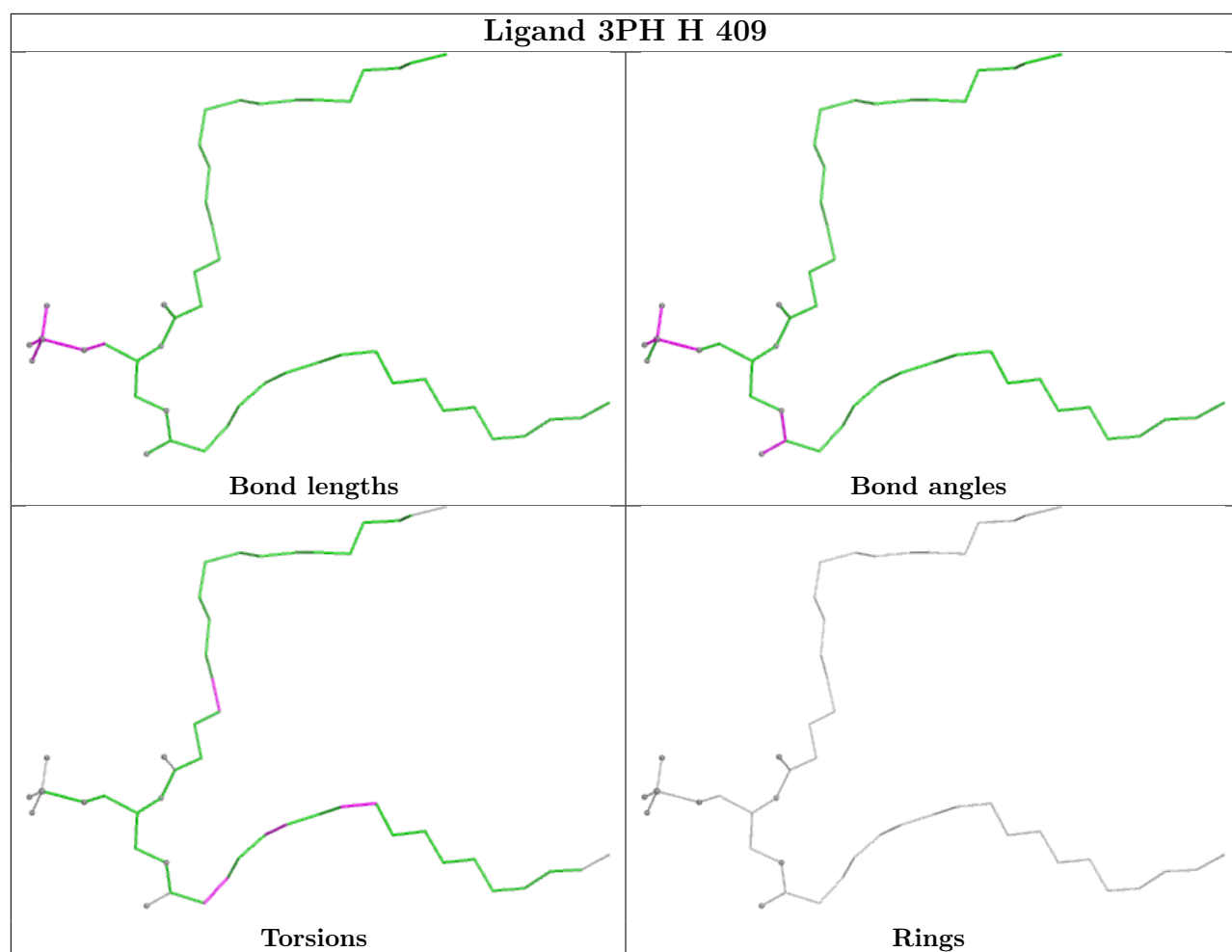


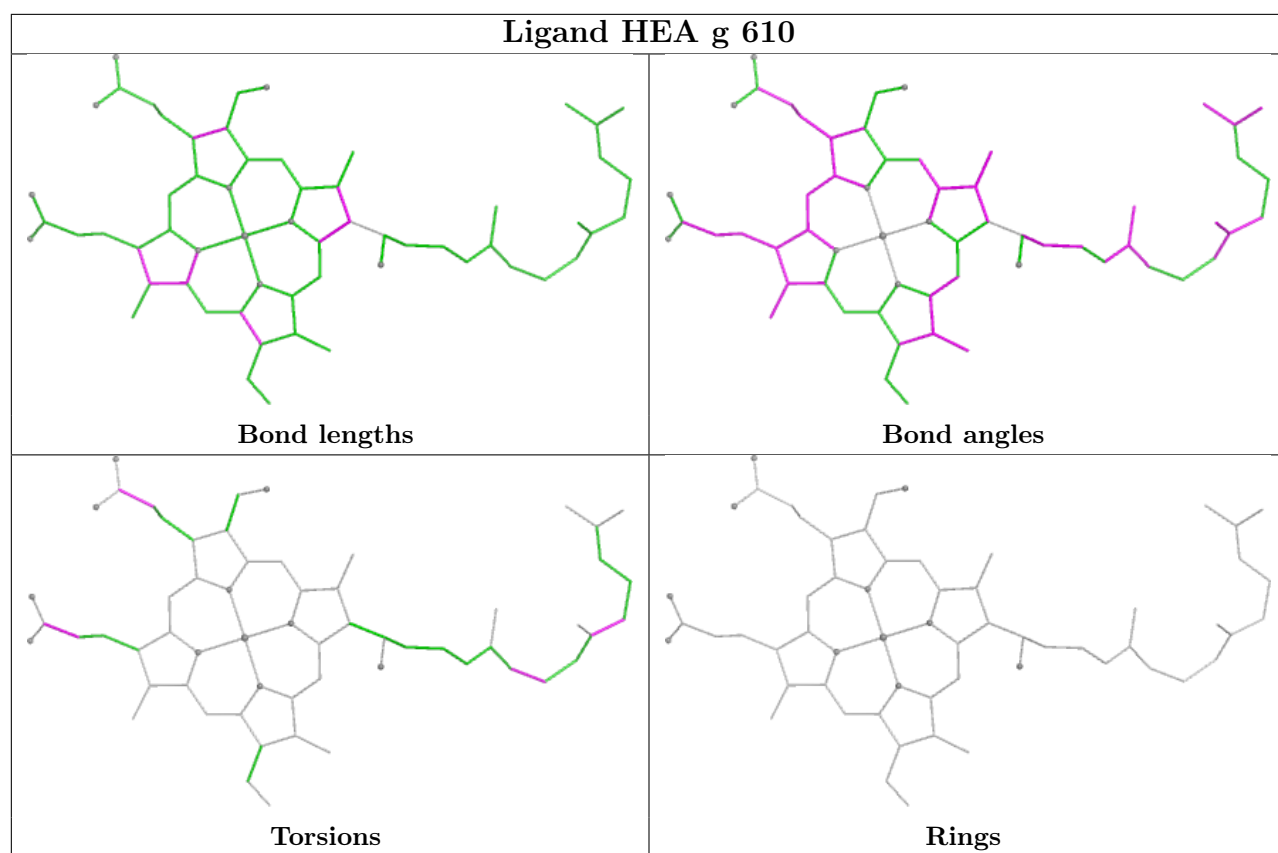


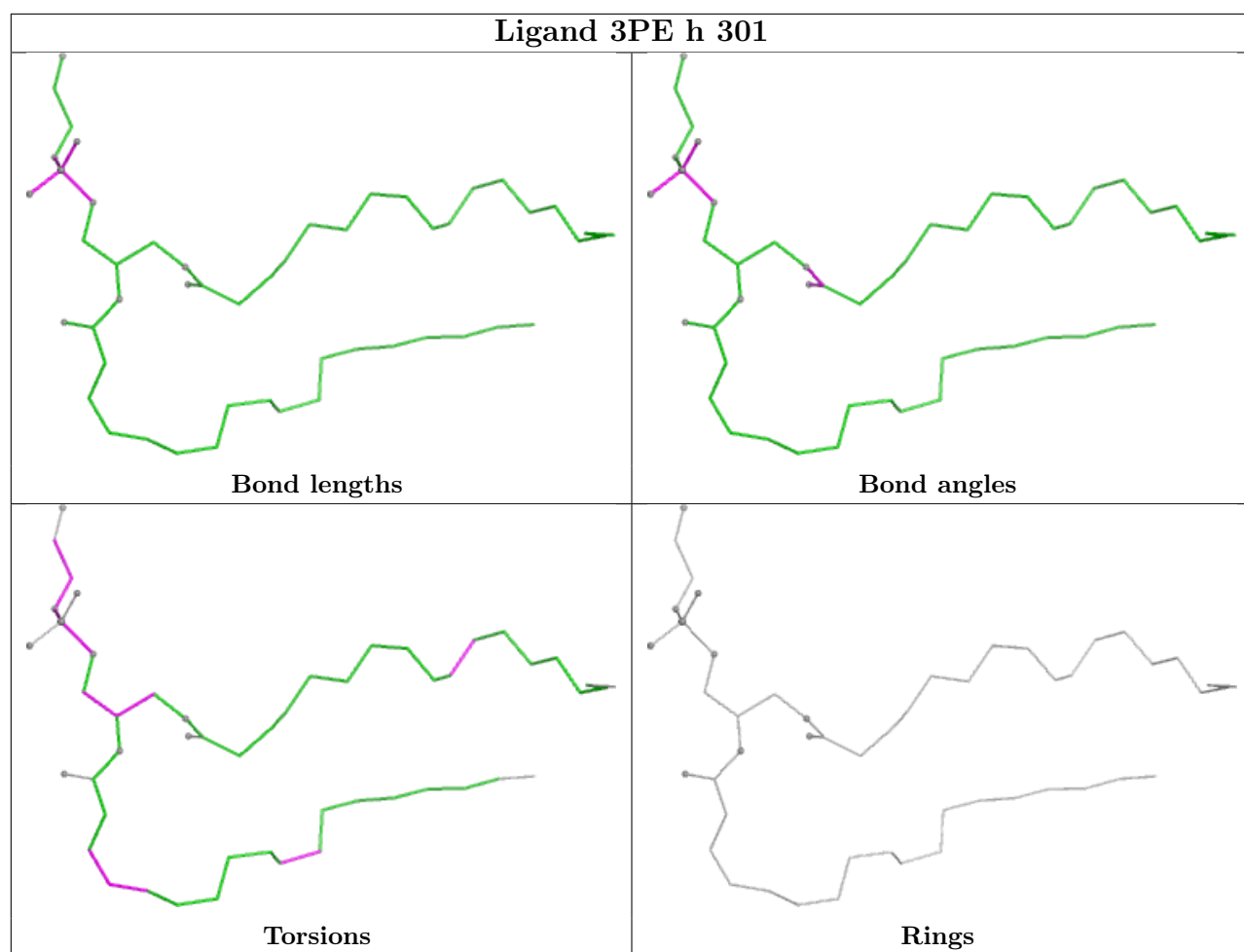


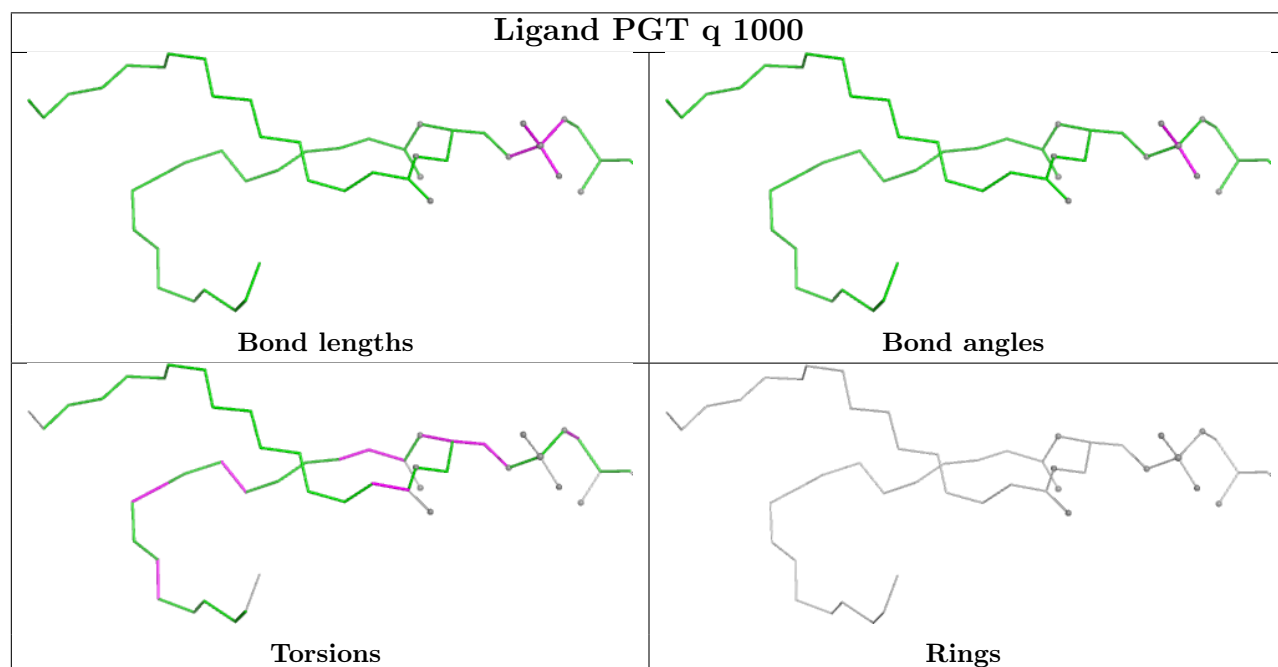
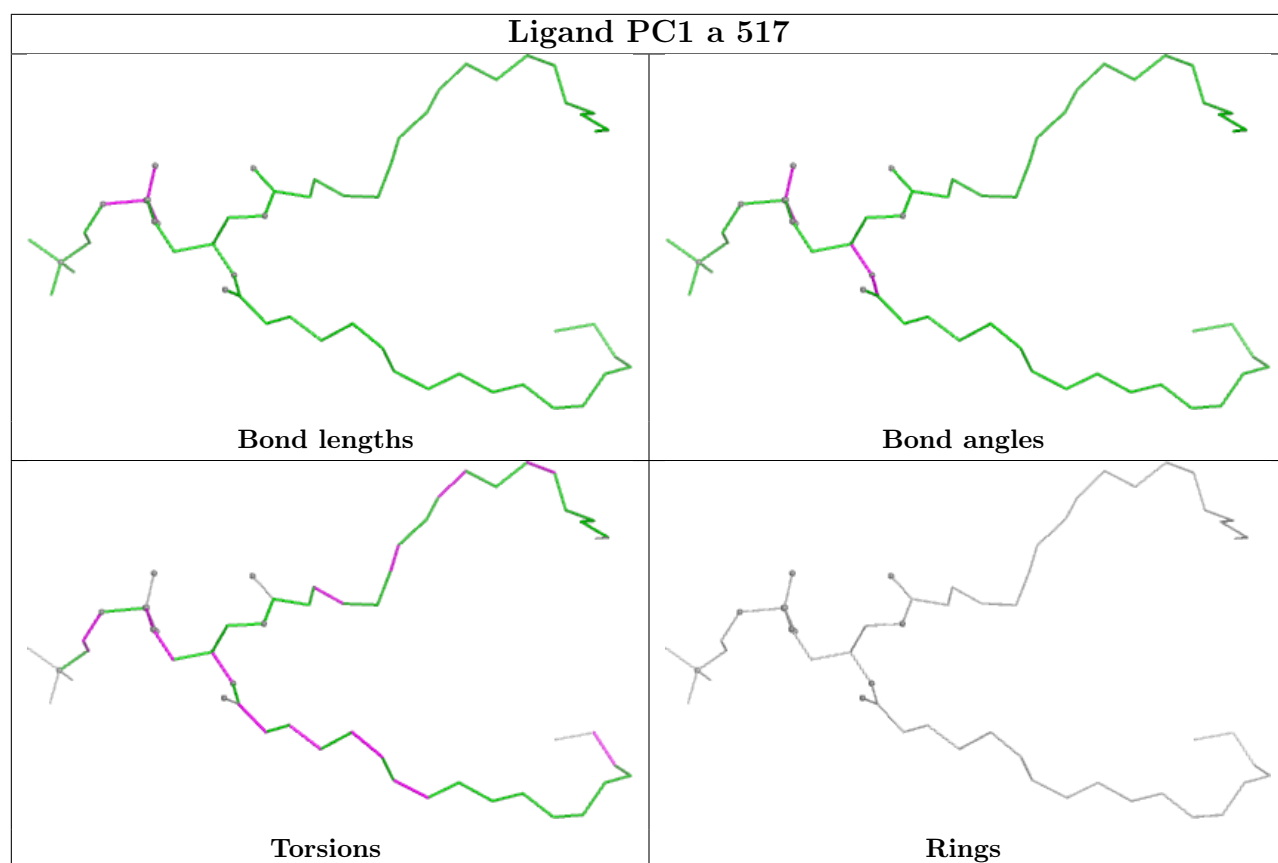


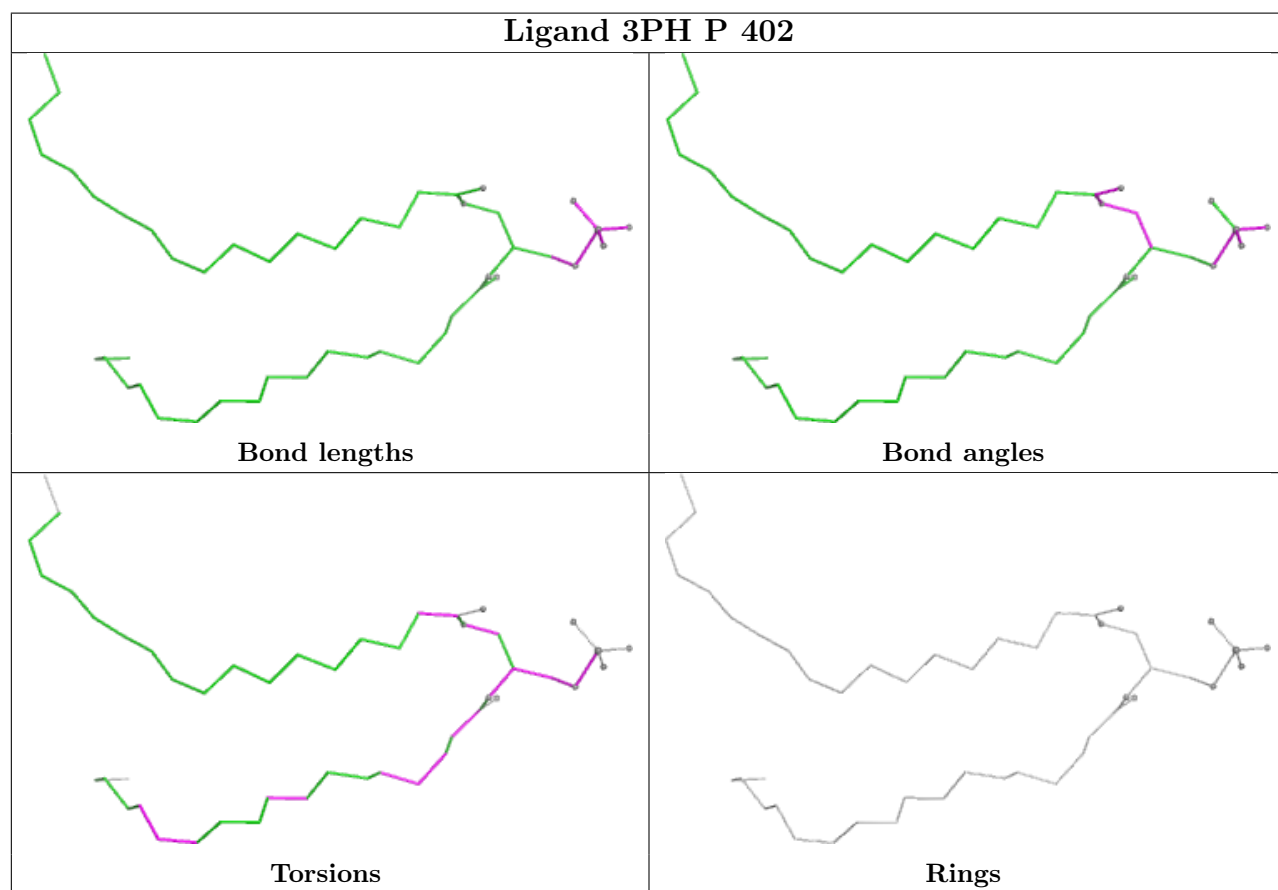
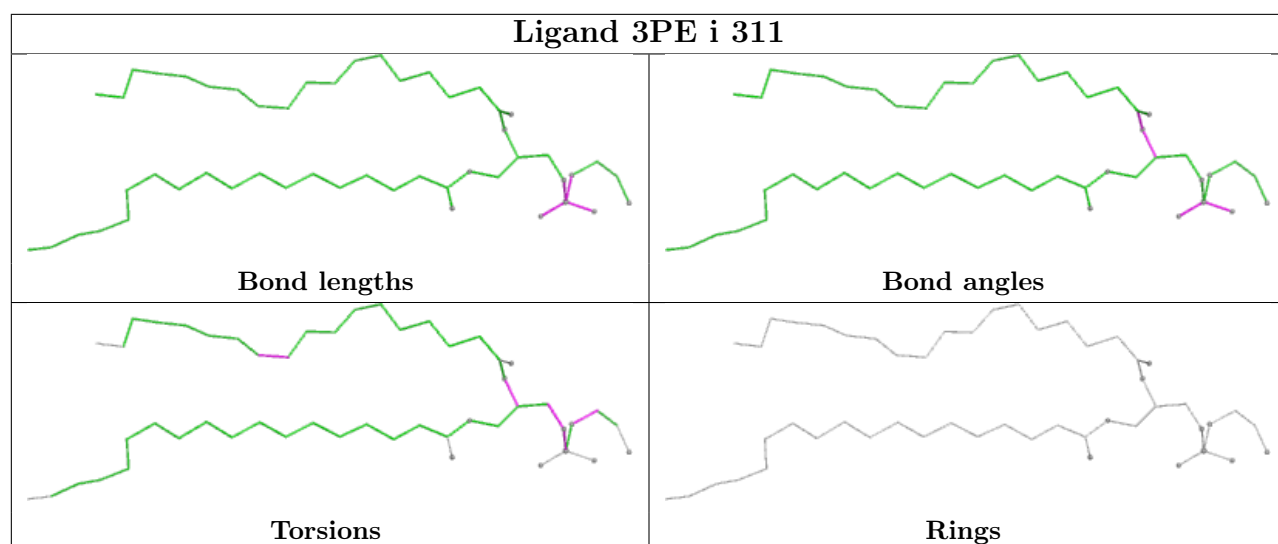


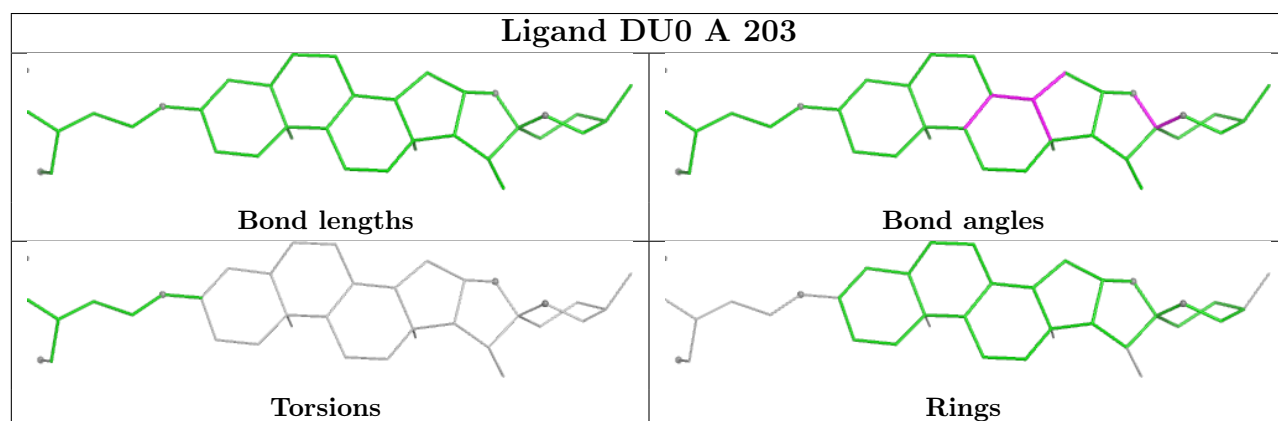
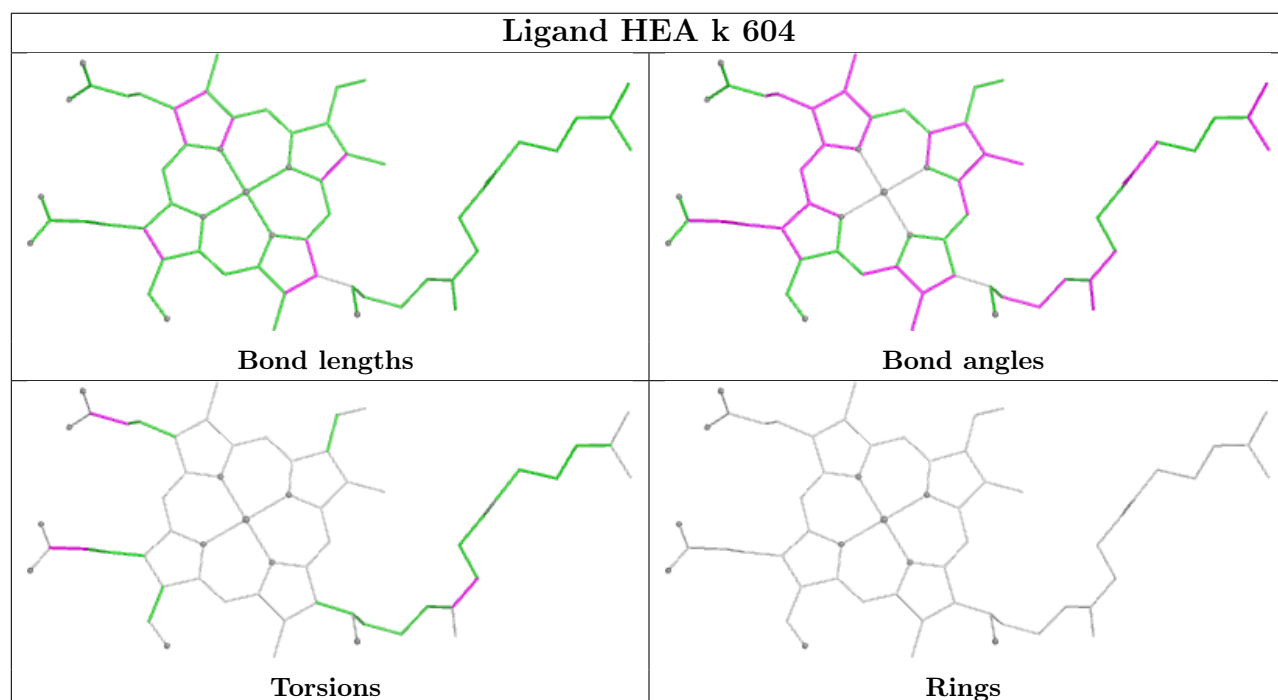
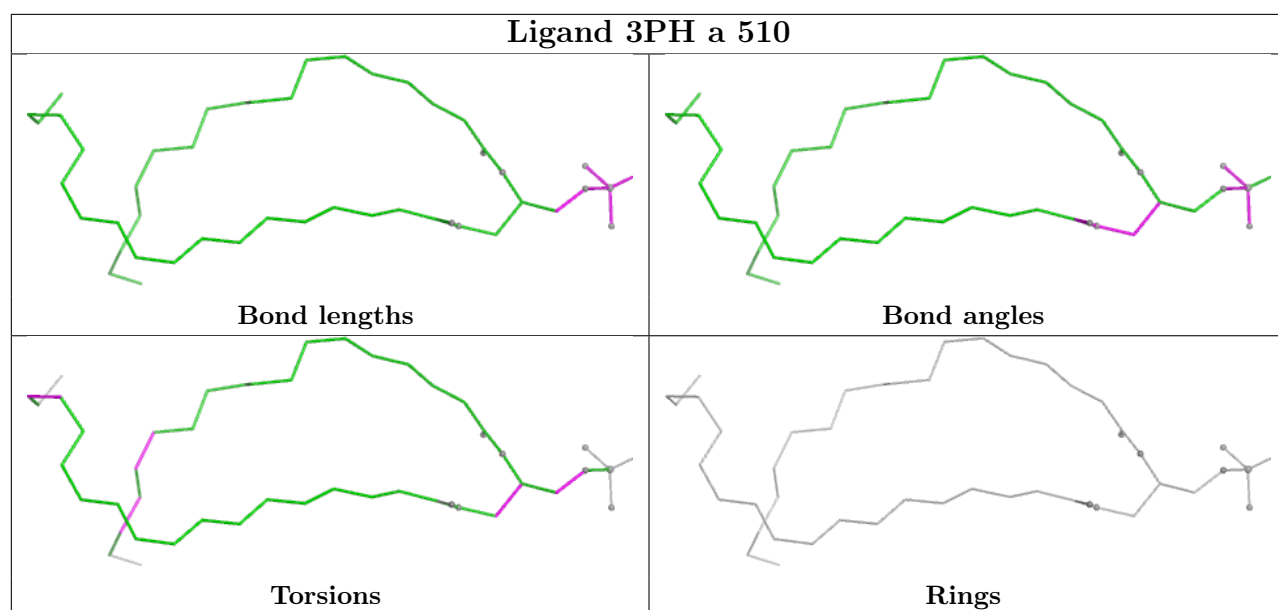


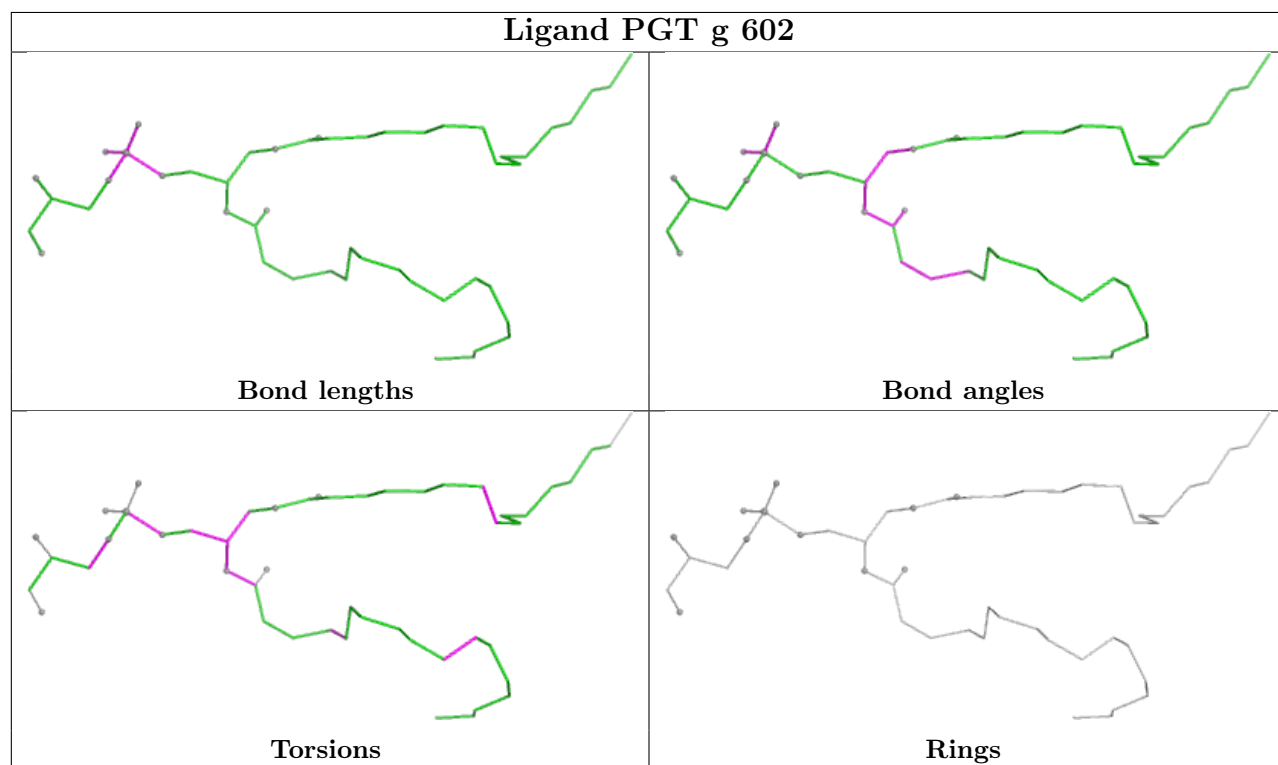
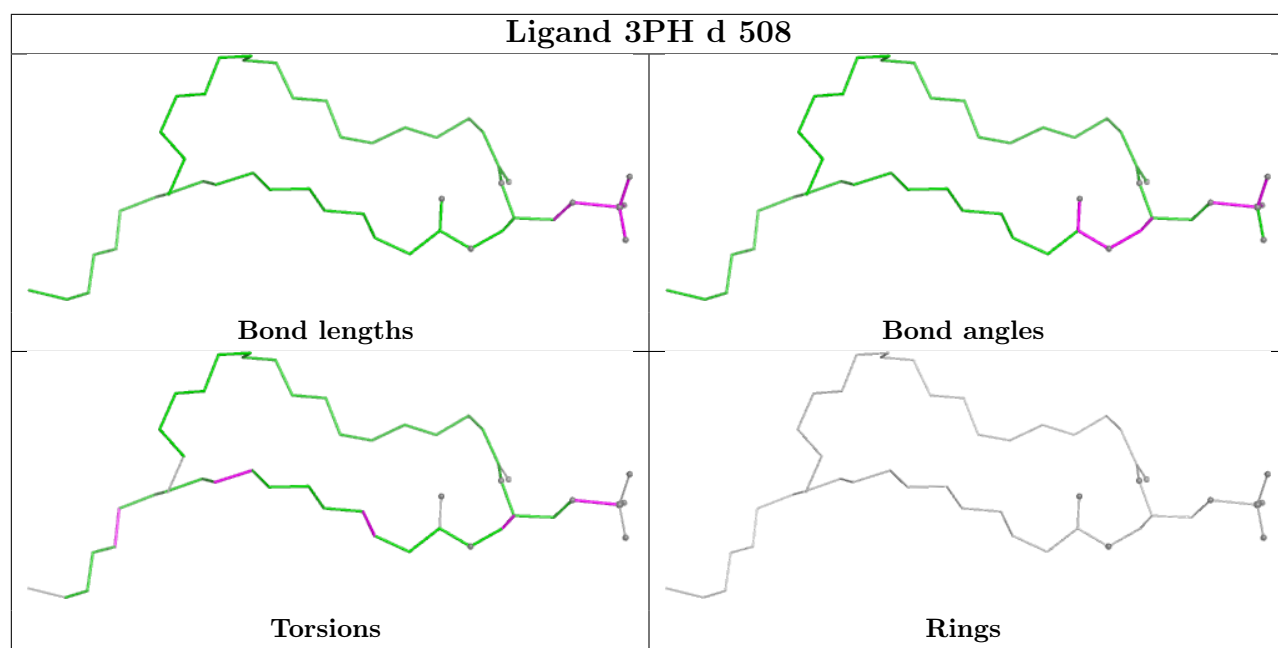


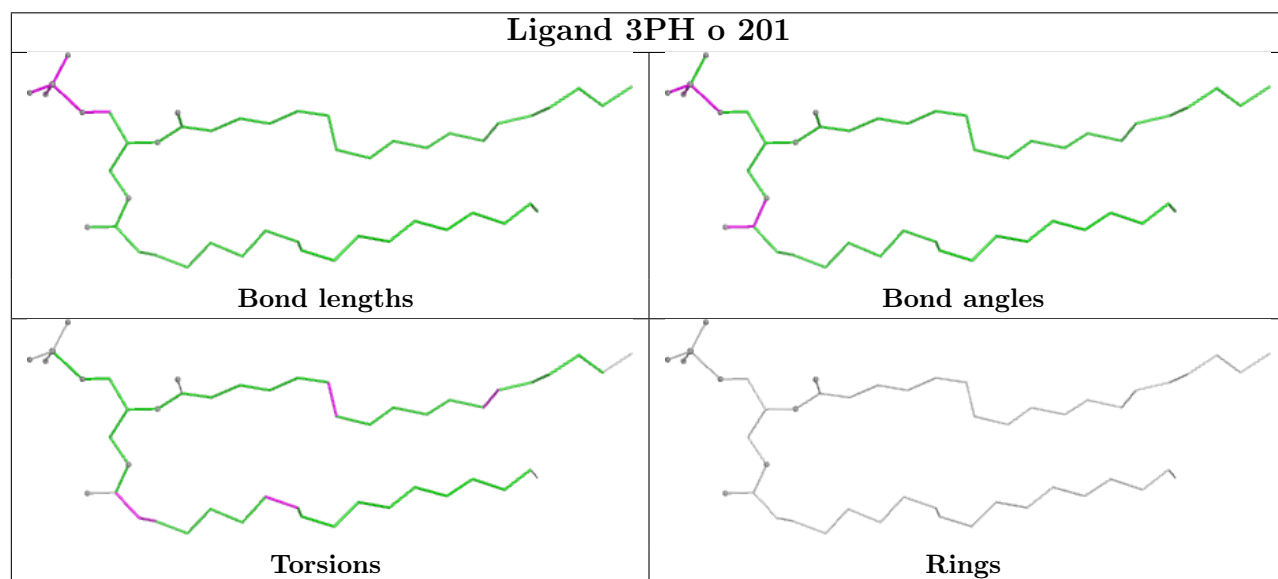
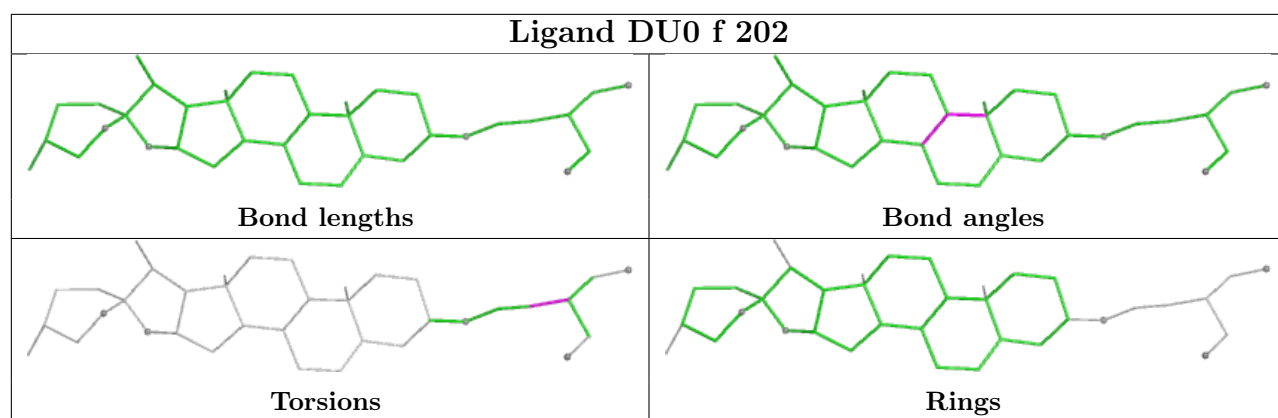


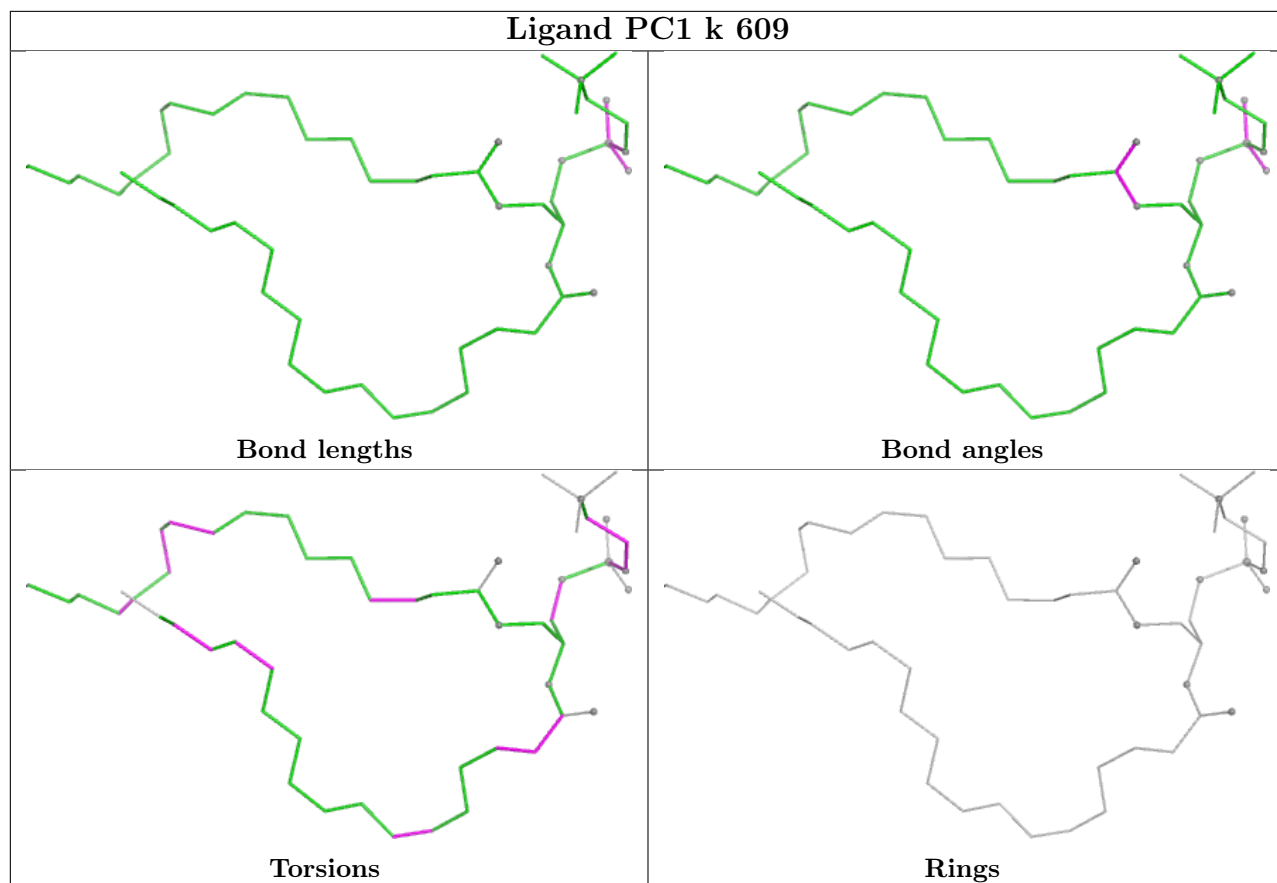
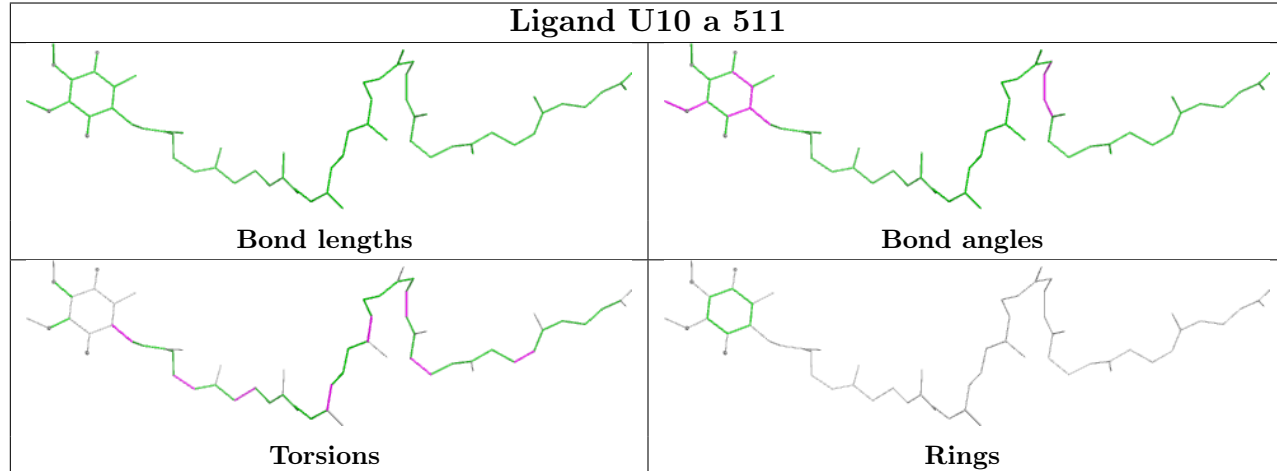


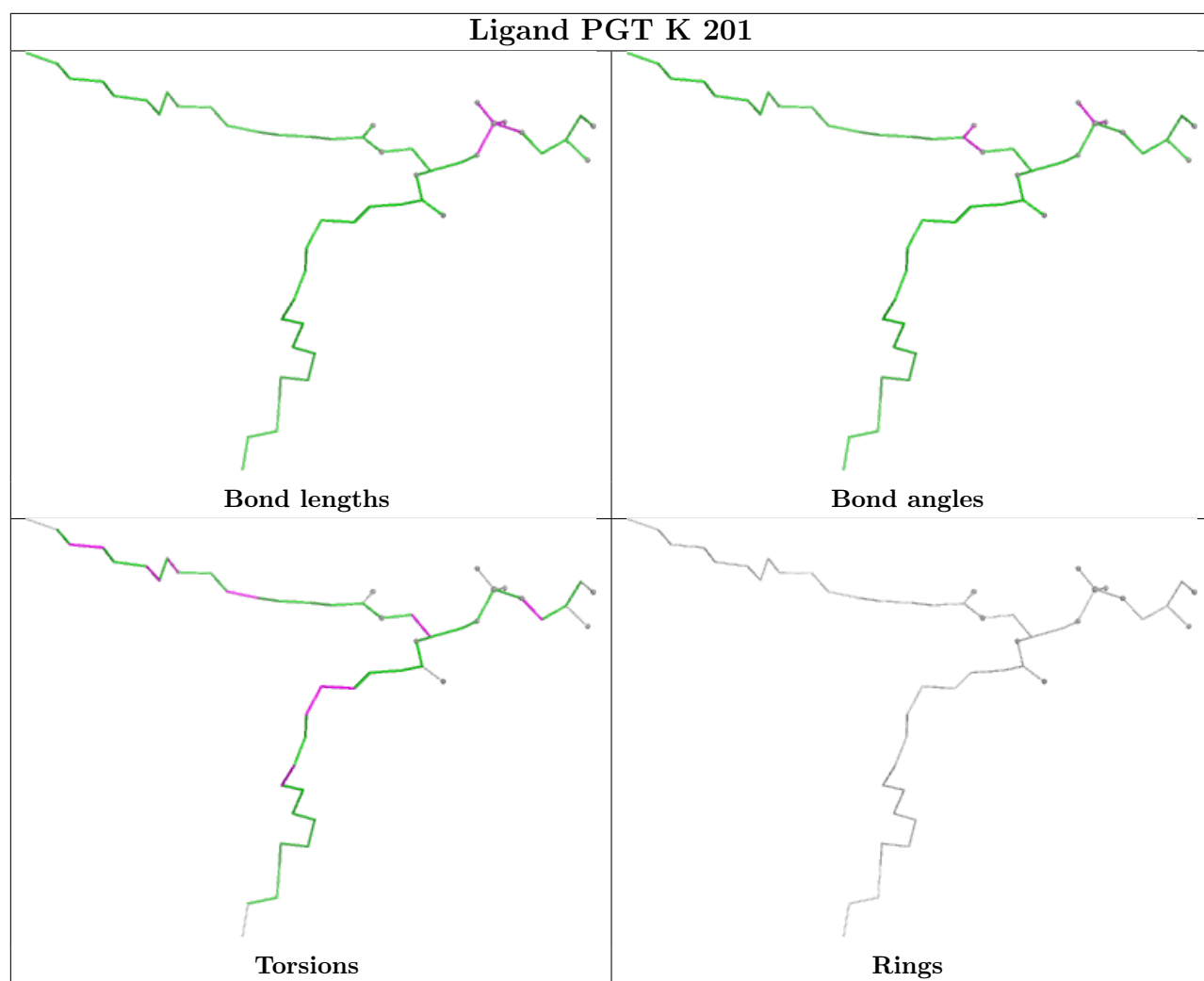


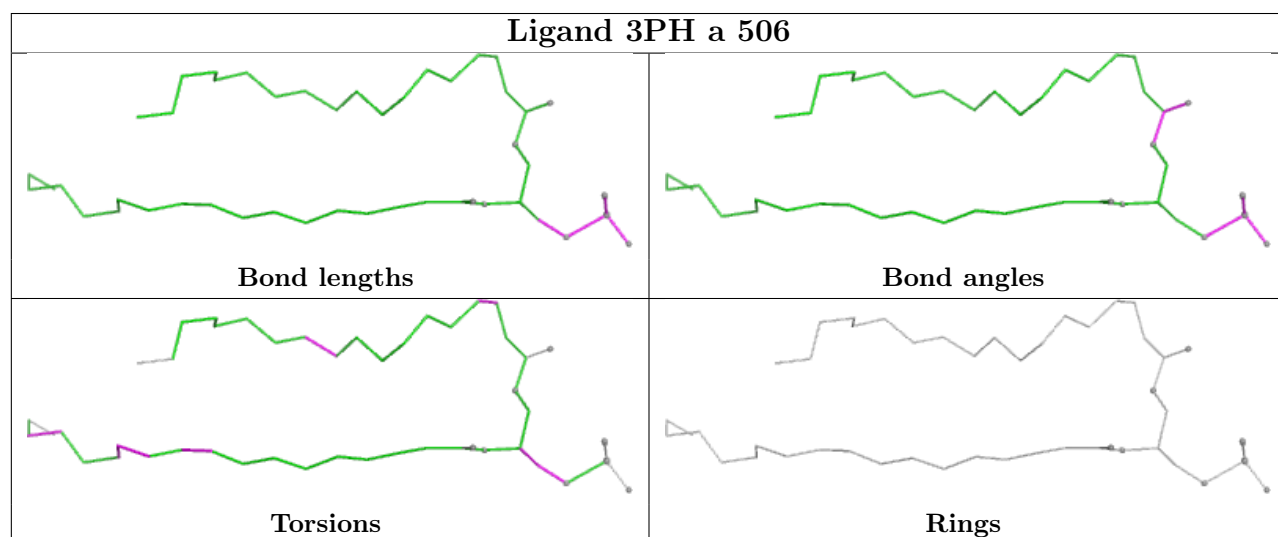
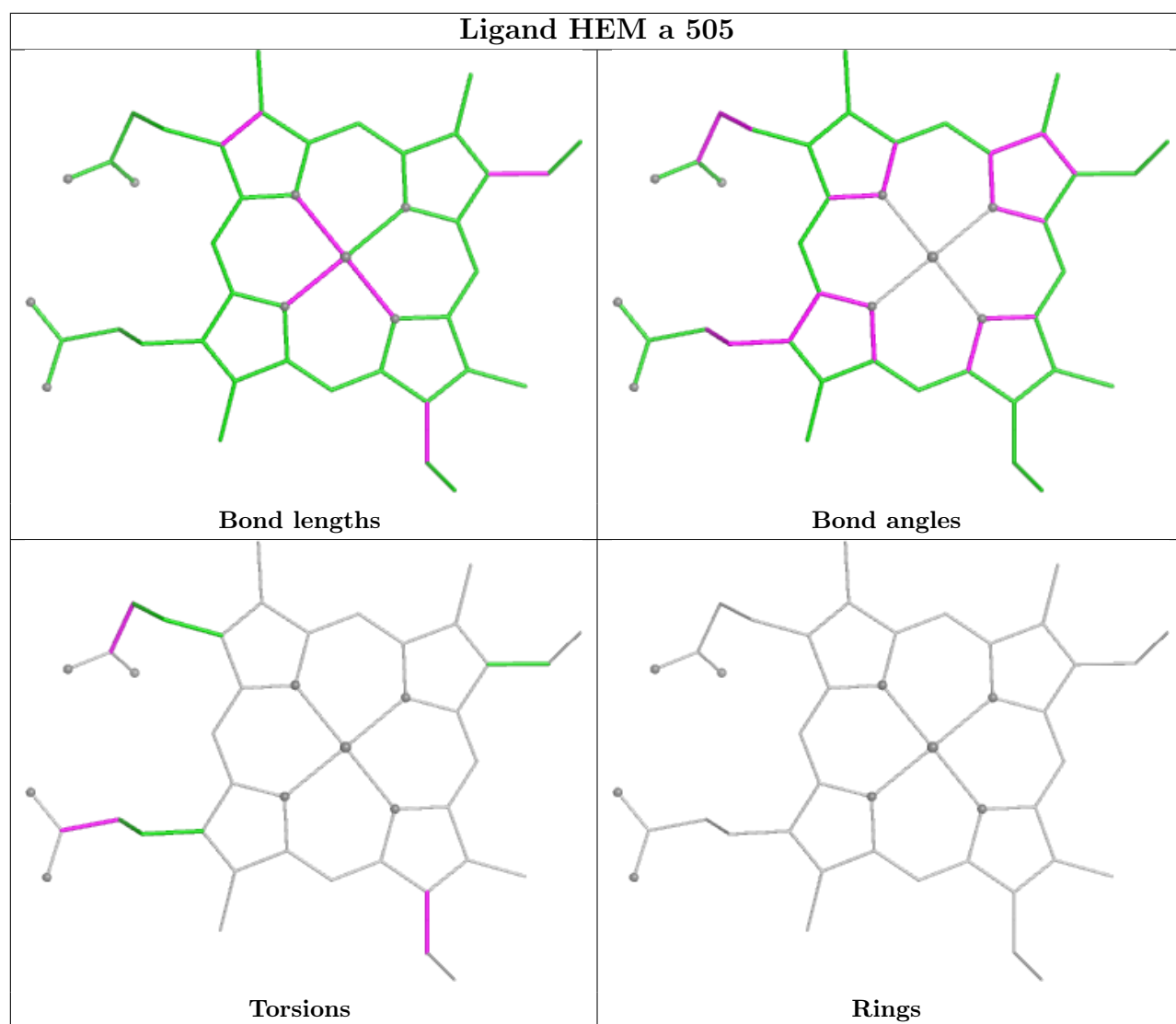


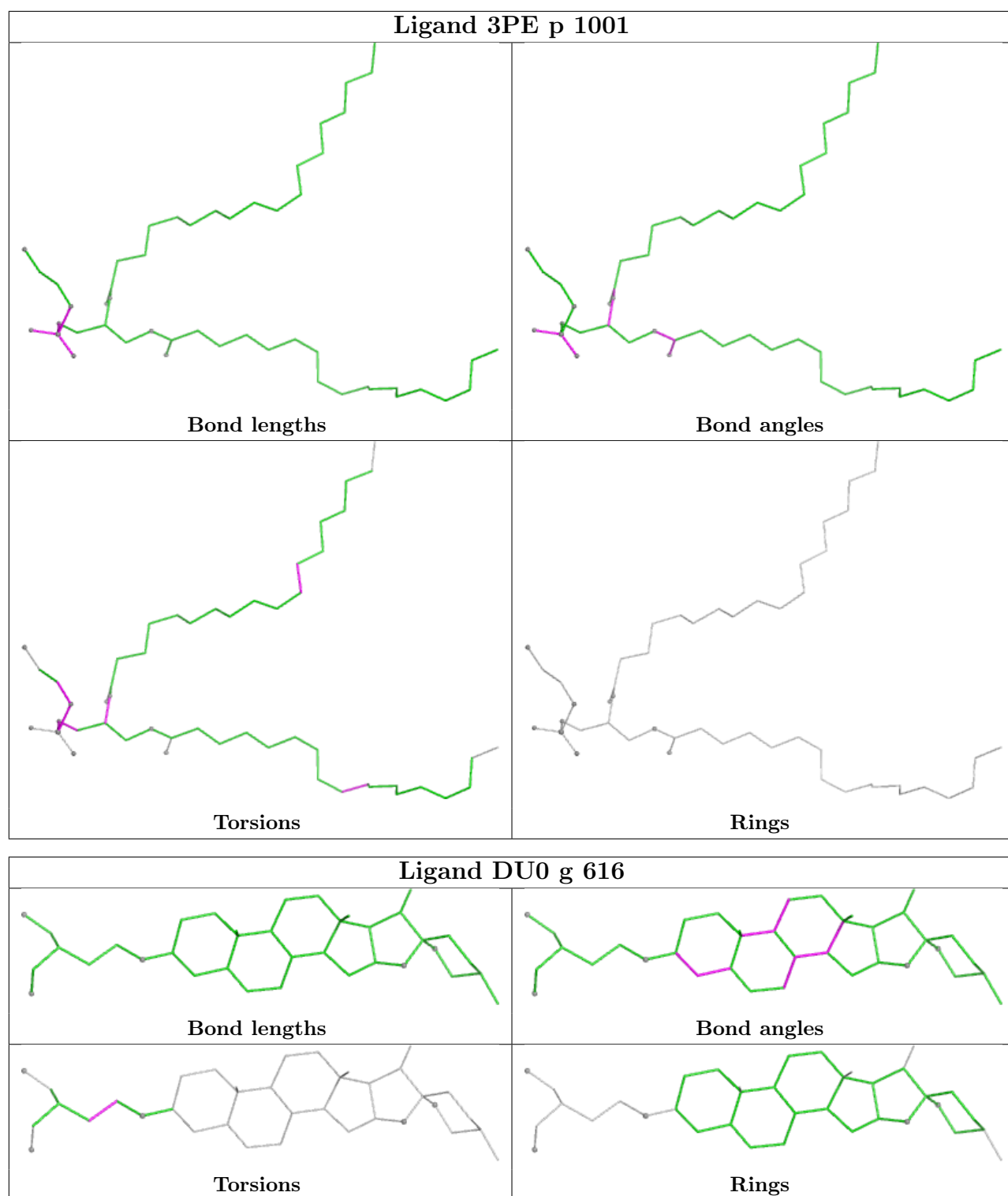


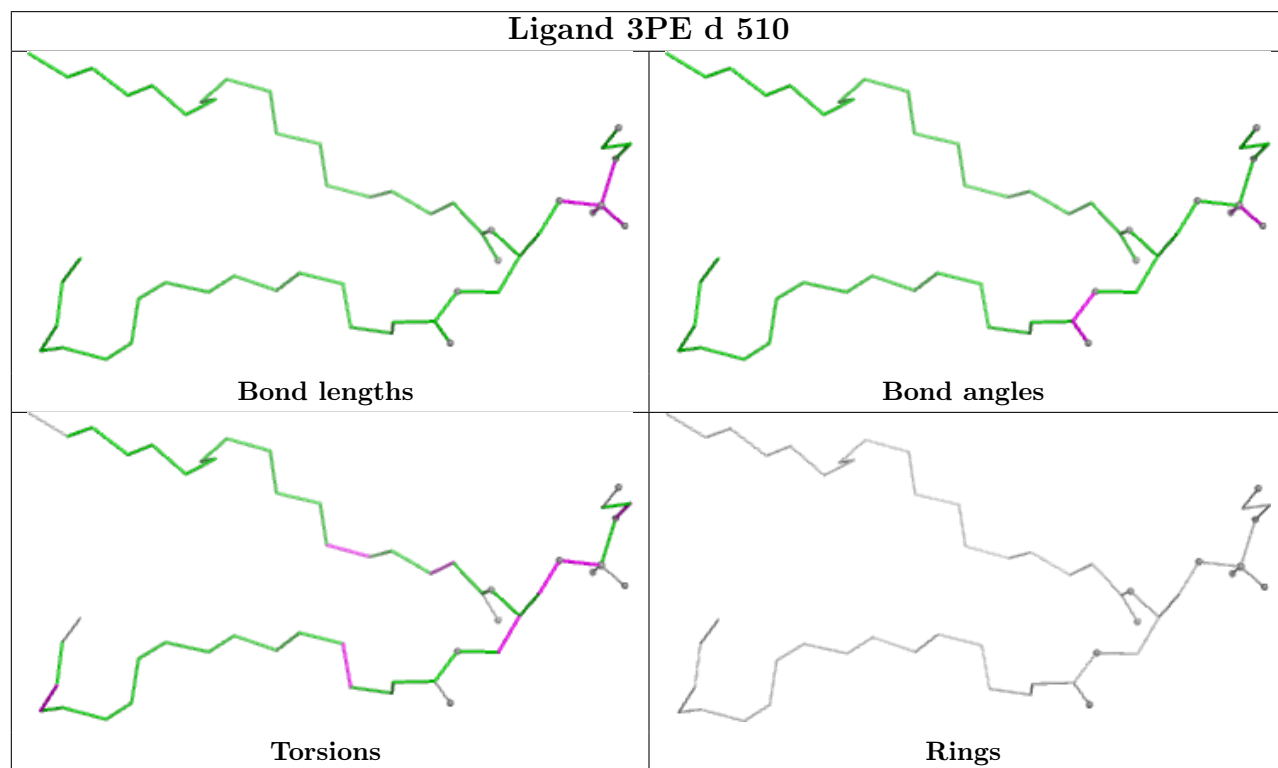
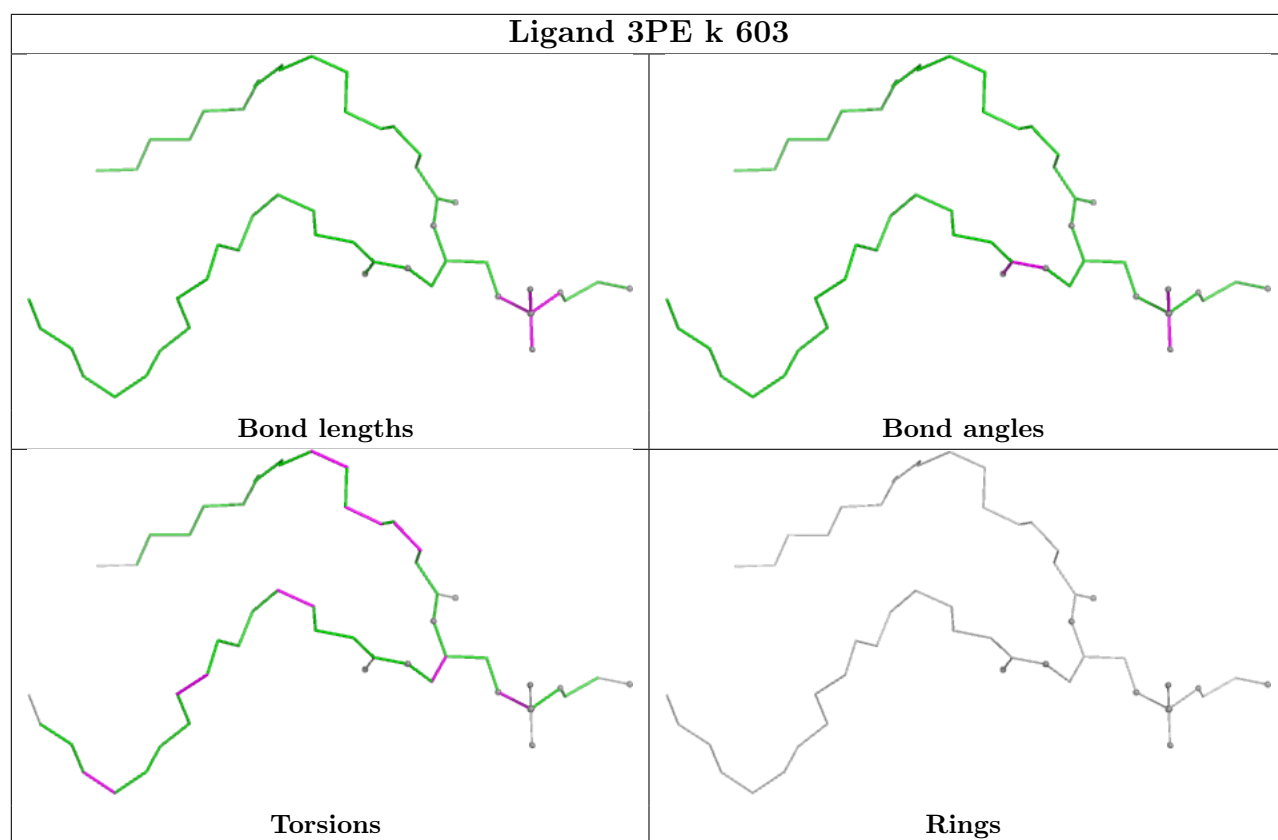


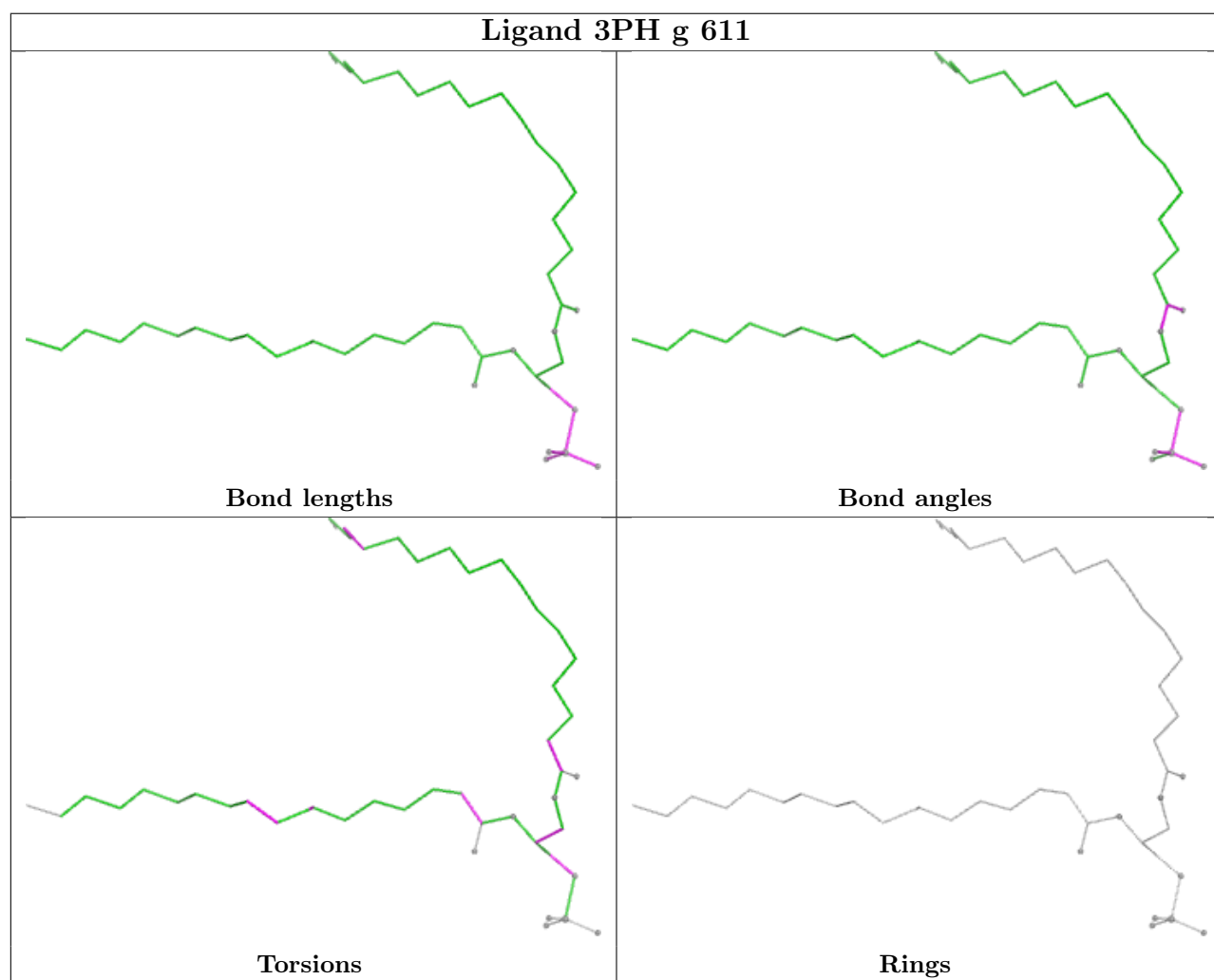
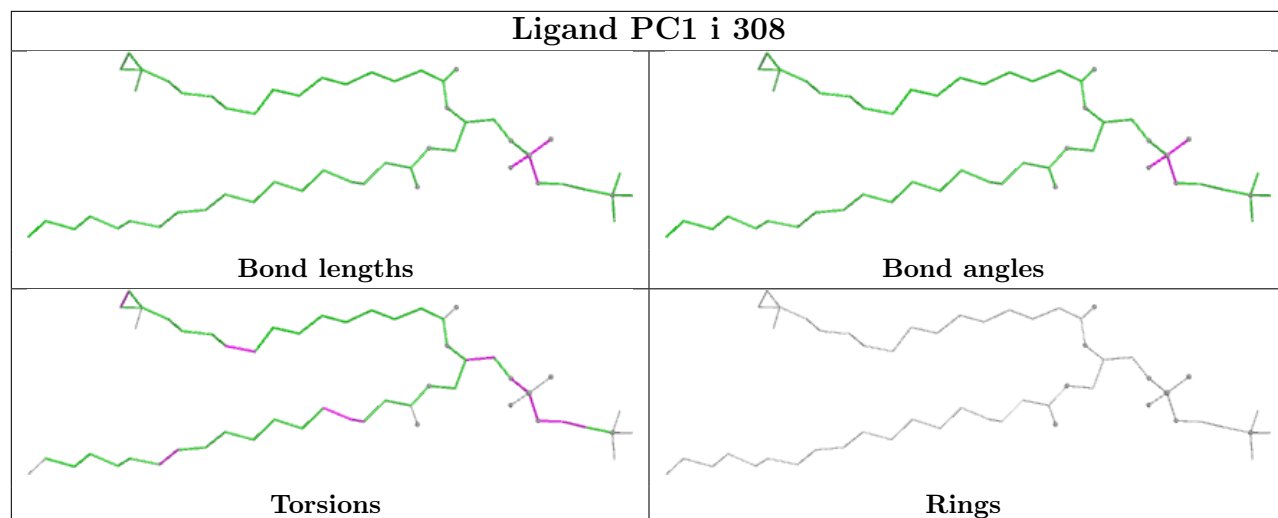
Ligand PC1 k 609**Ligand U10 a 511**

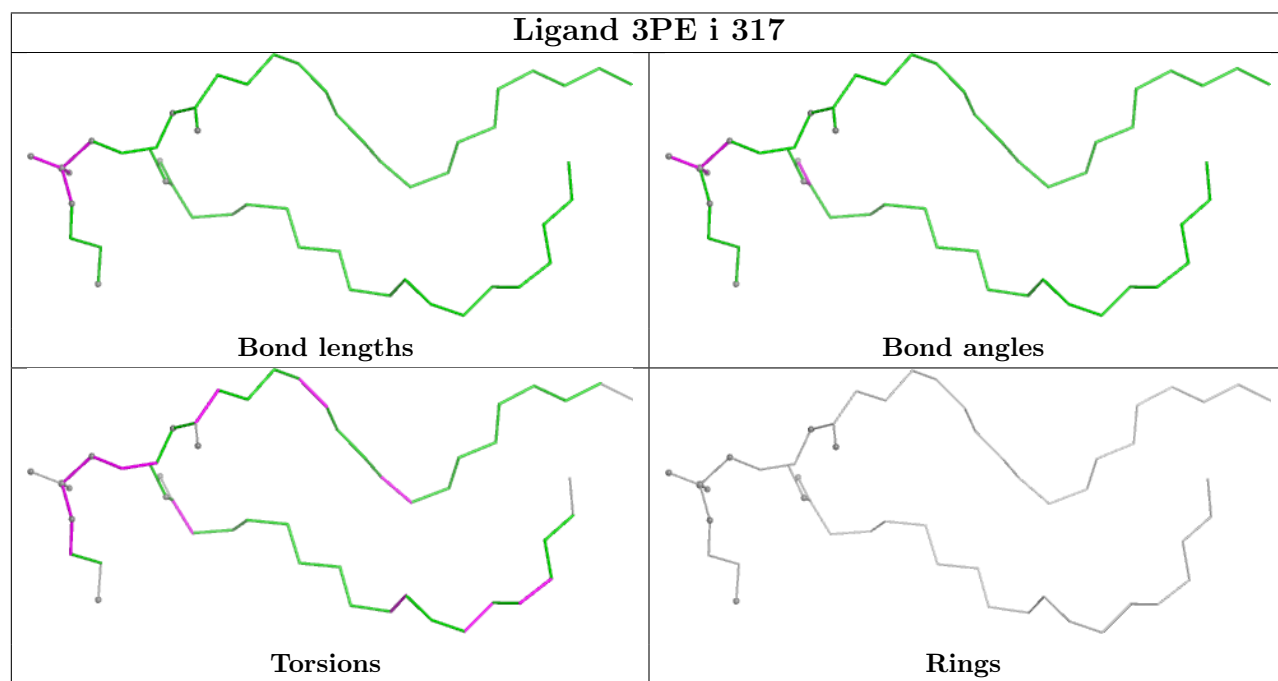
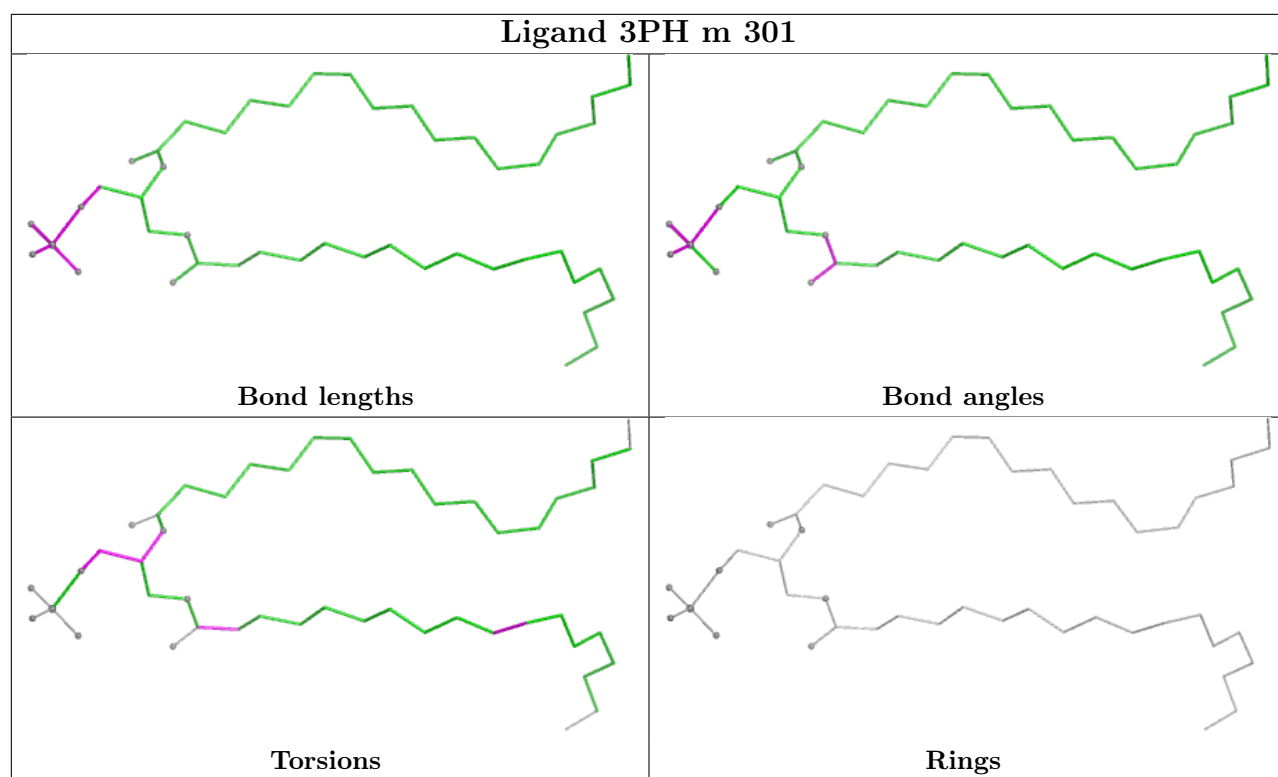


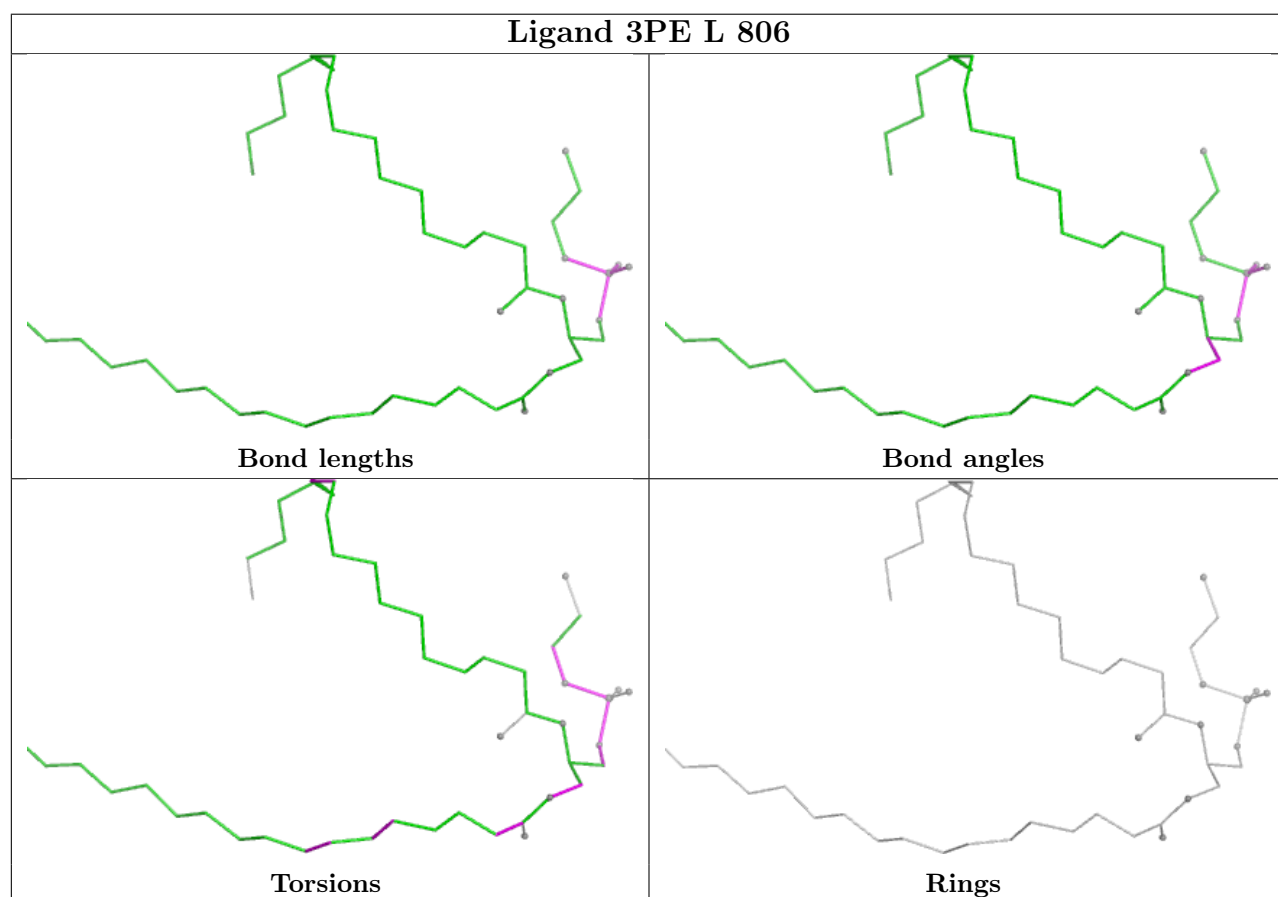
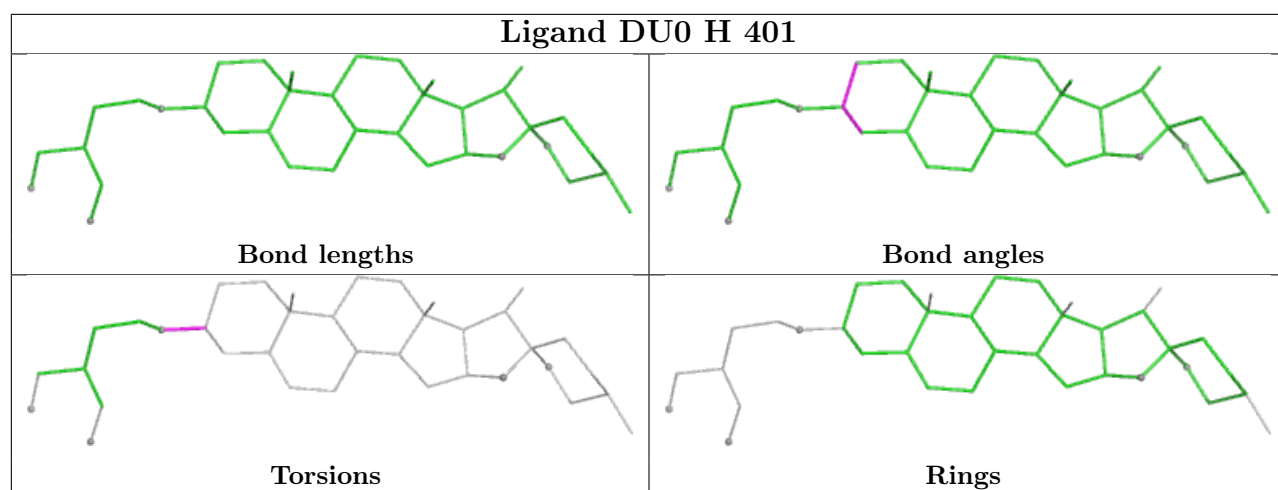


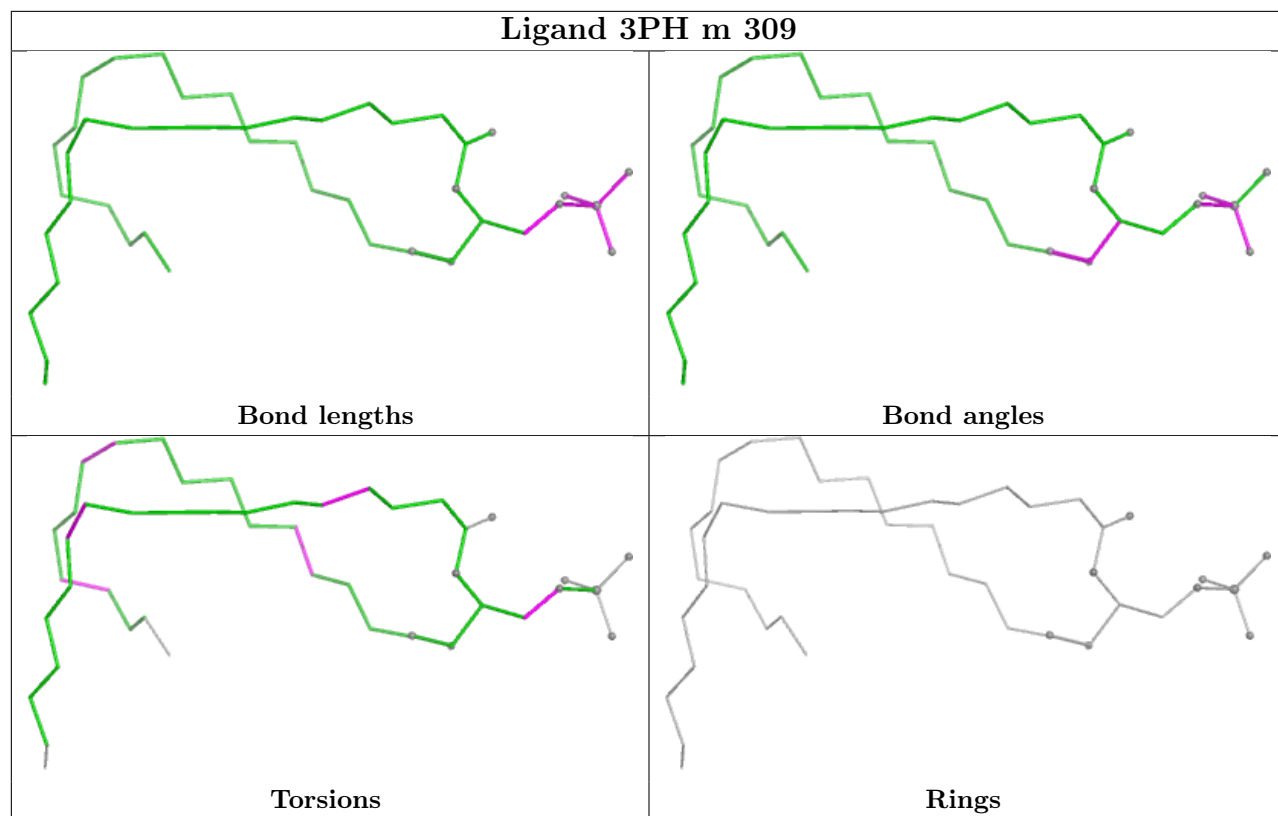


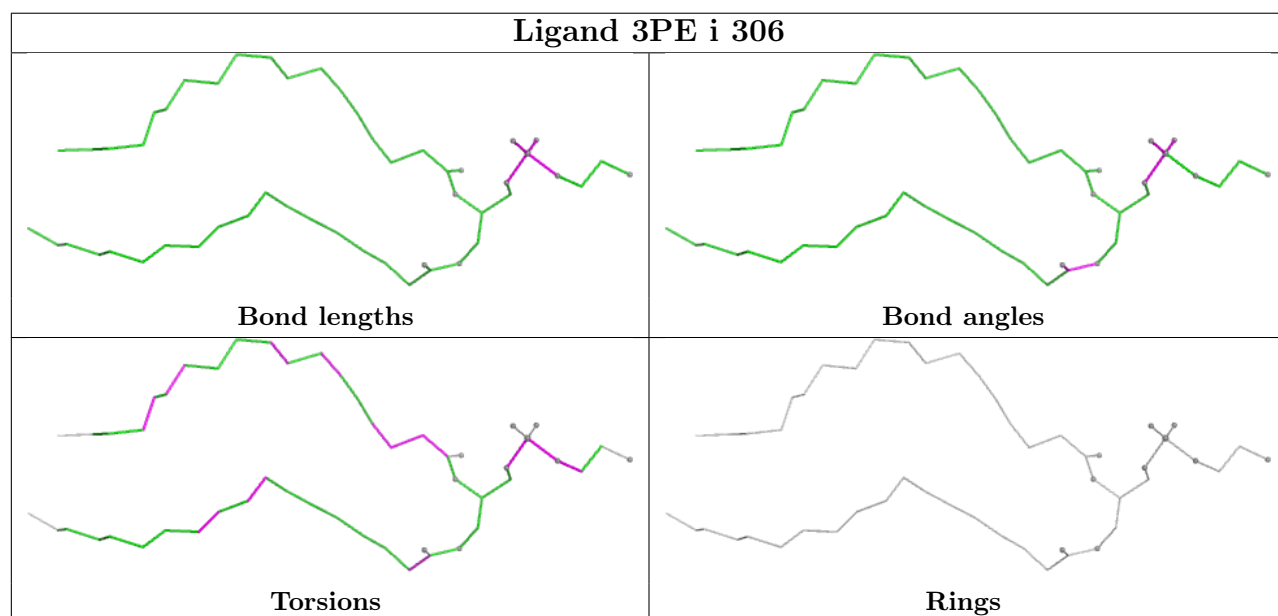
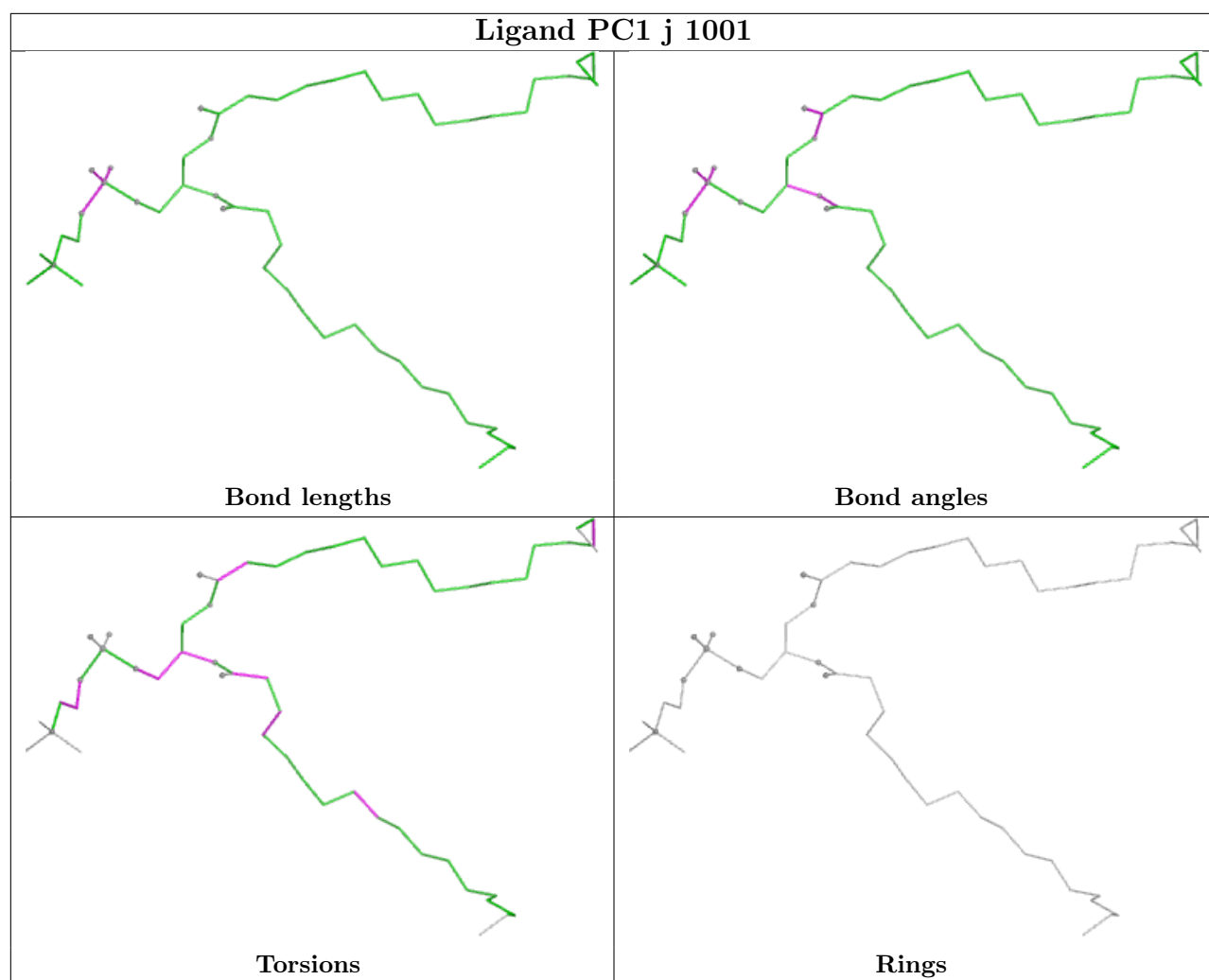


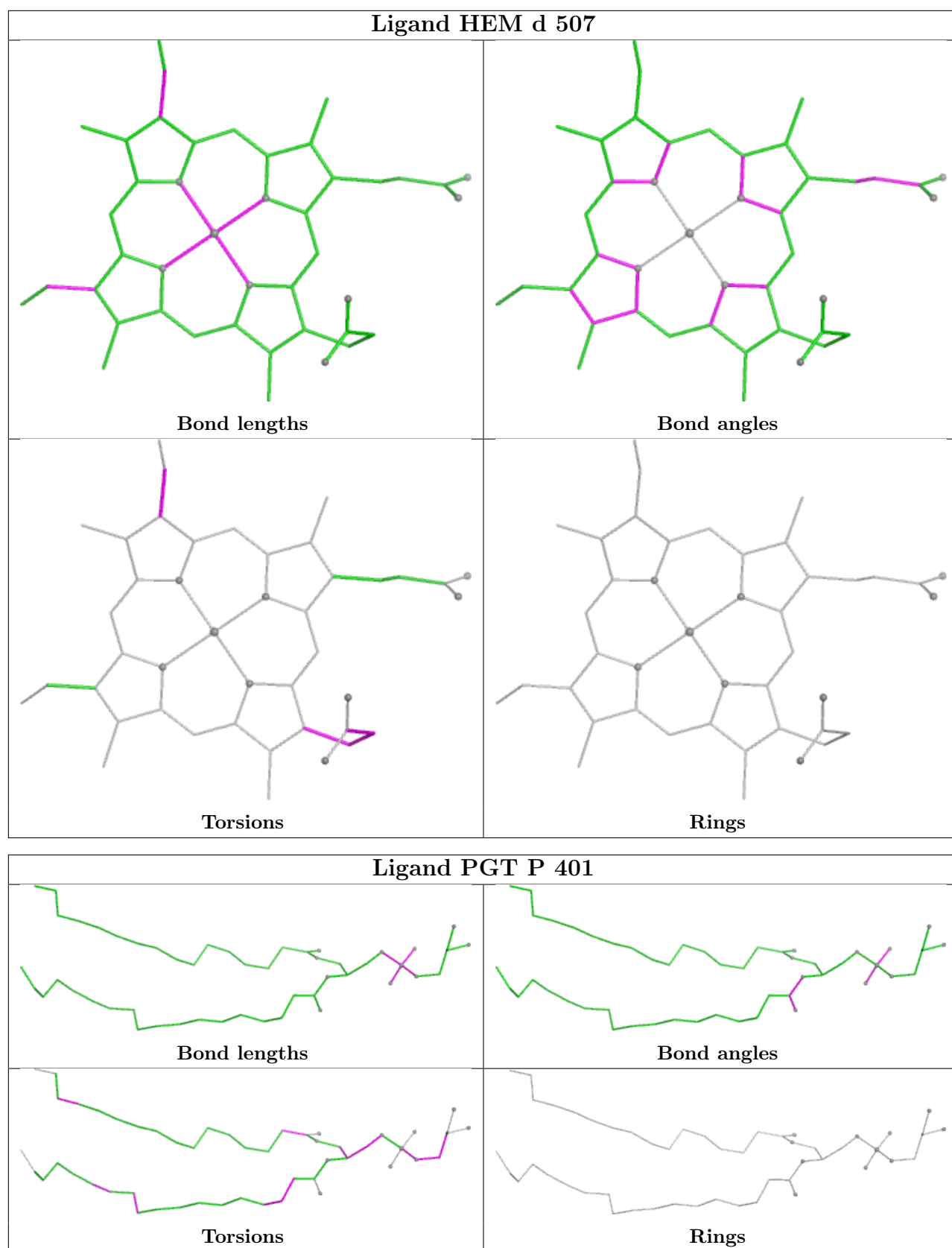




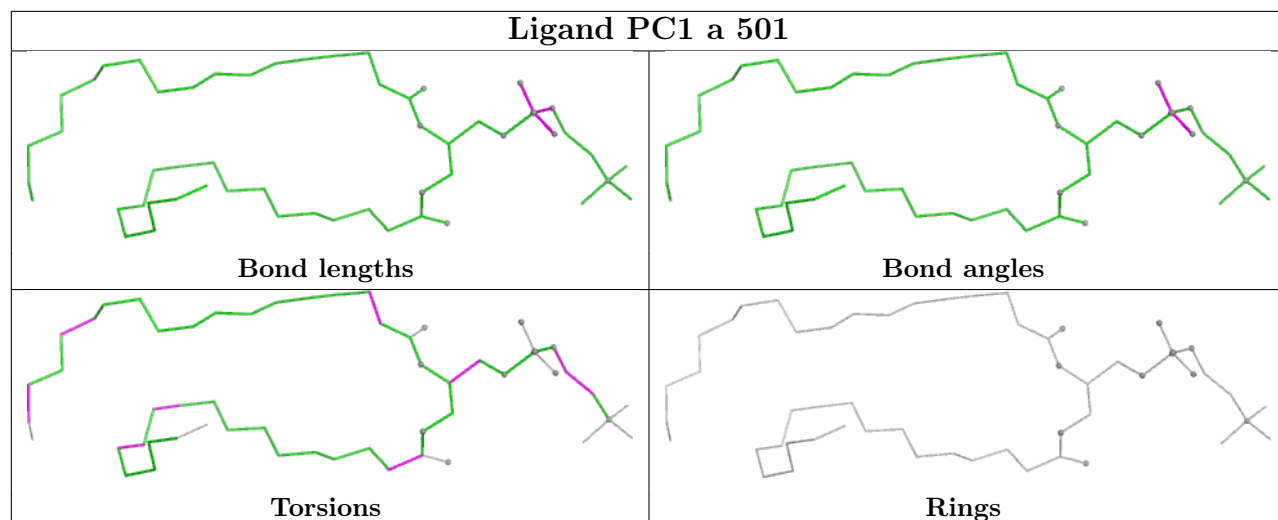




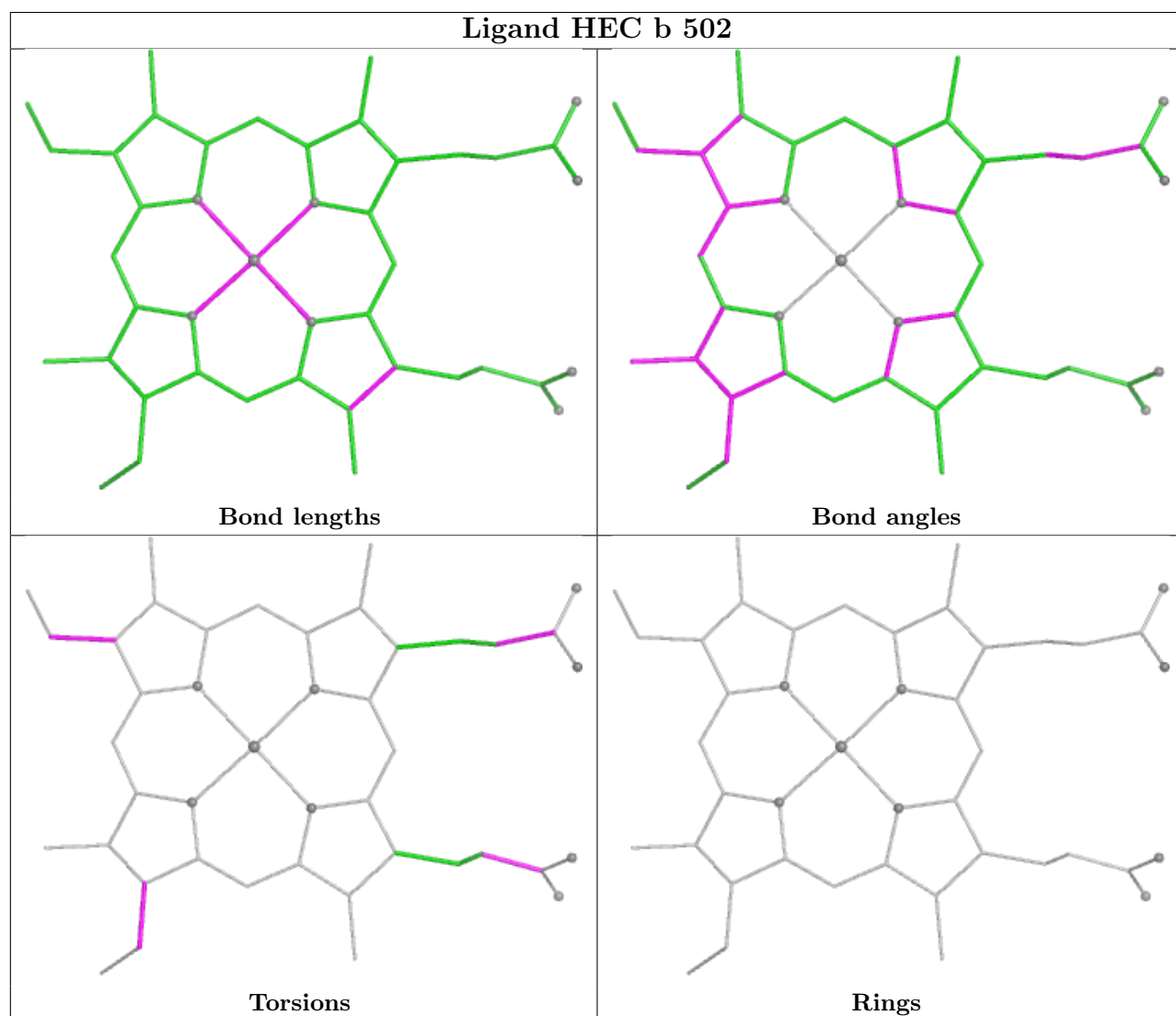


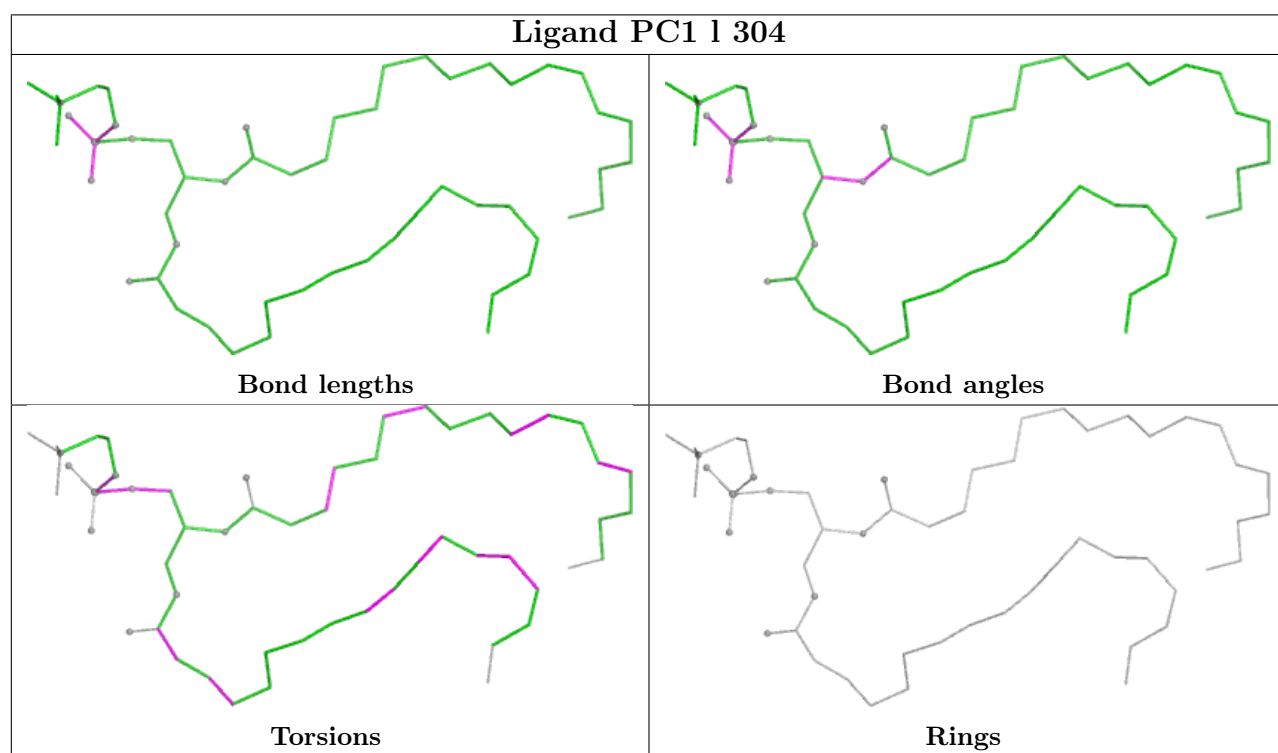
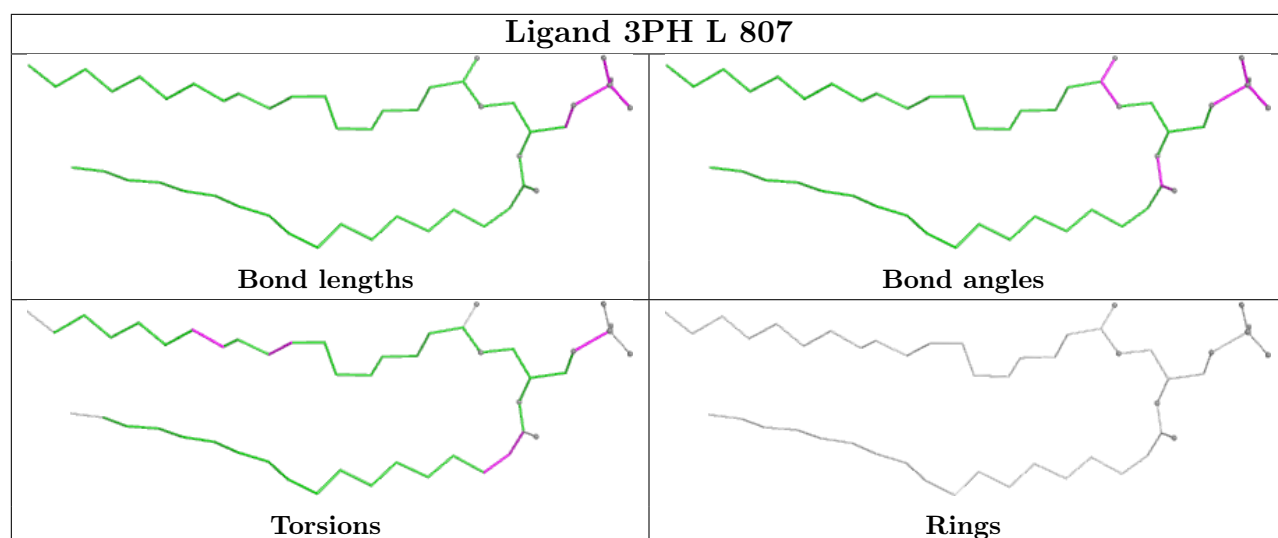


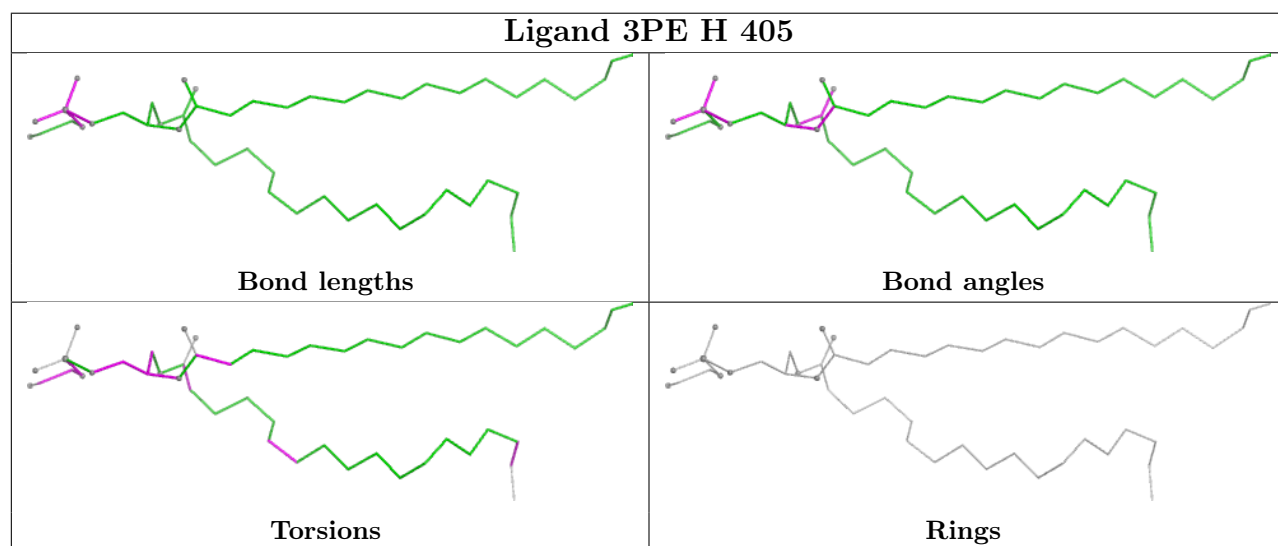
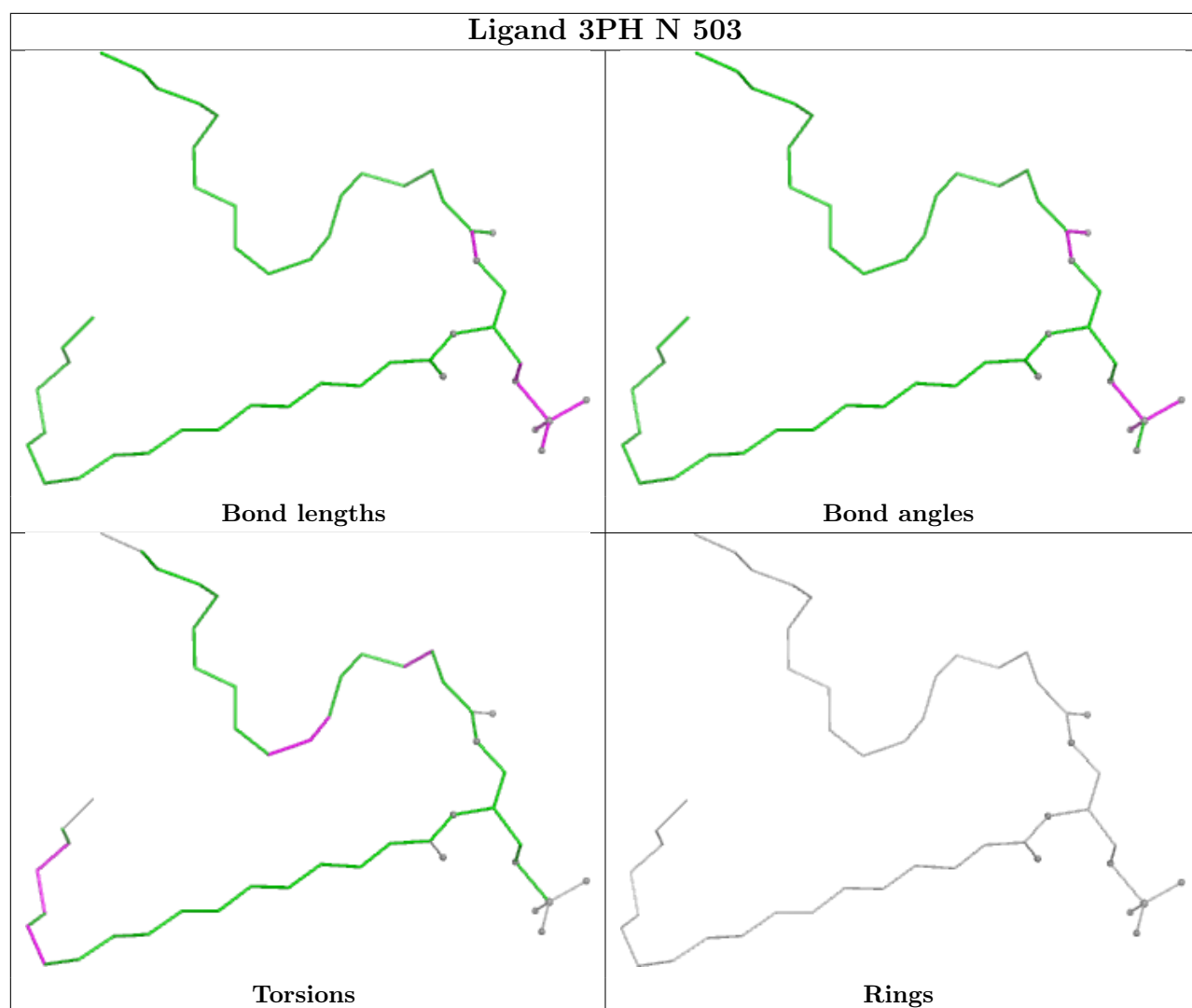
Ligand PC1 a 501

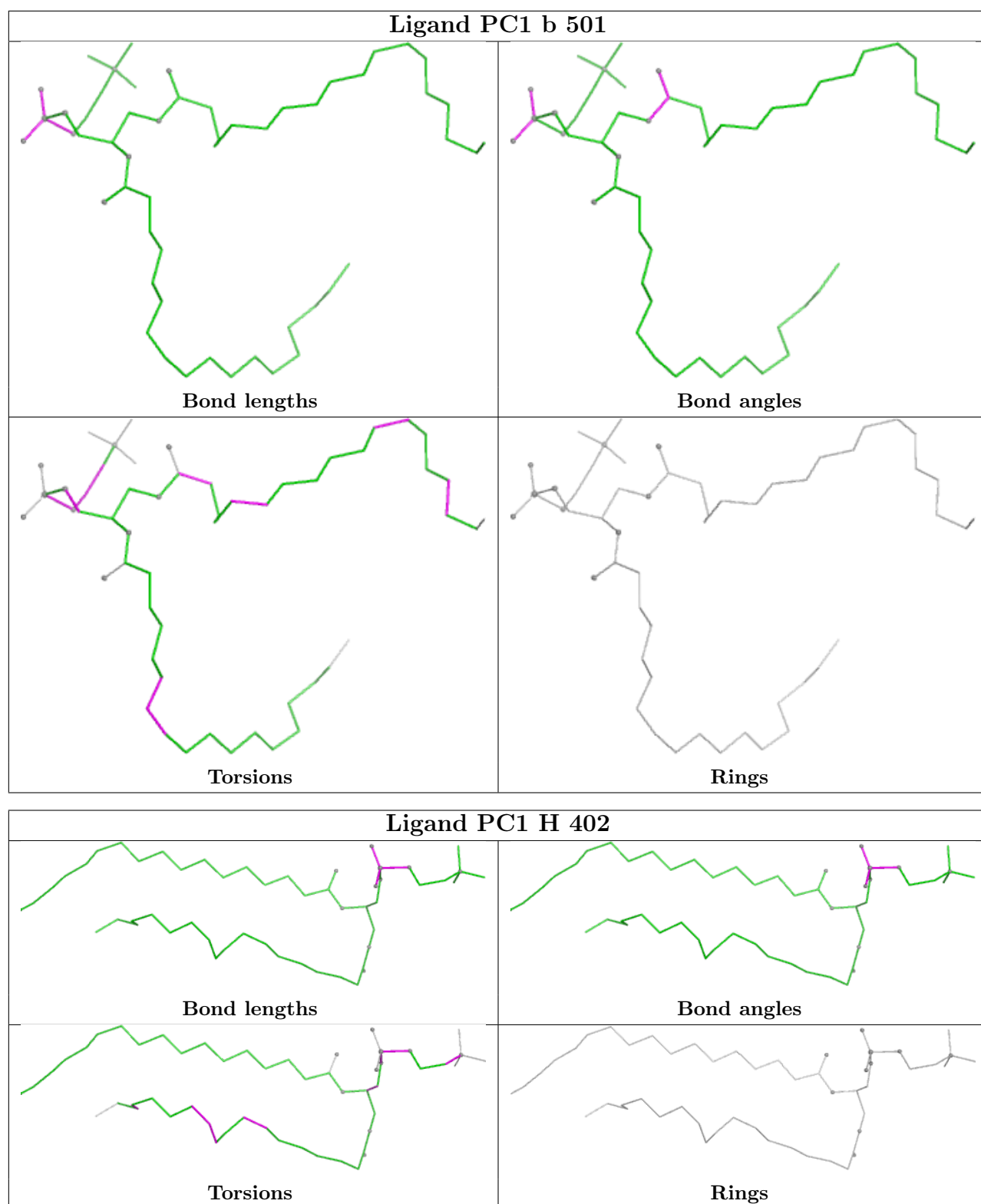


Ligand HEC b 502









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

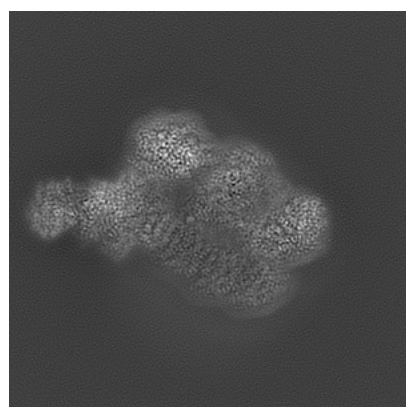
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51181. These allow visual inspection of the internal detail of the map and identification of artifacts.

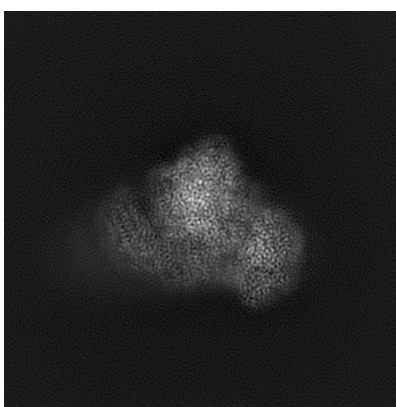
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

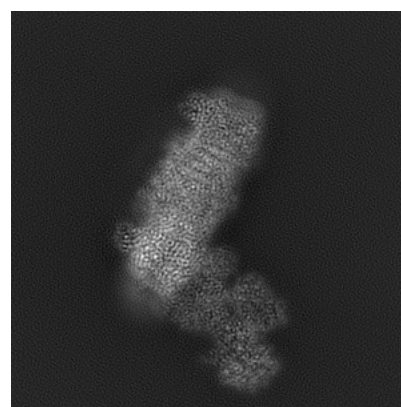
6.1.1 Primary map



X



Y

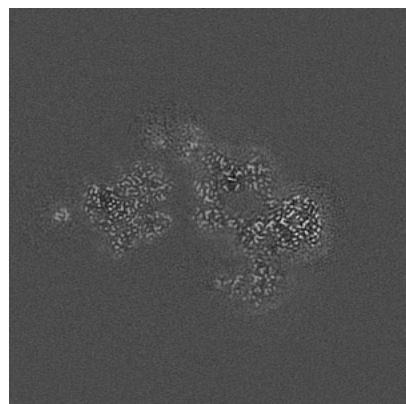


Z

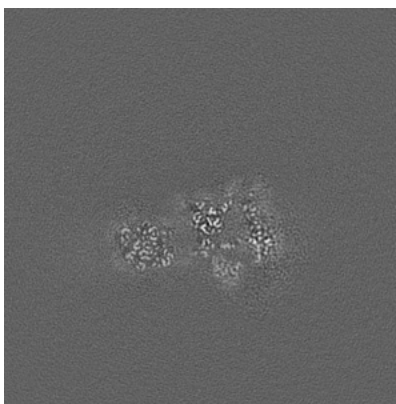
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

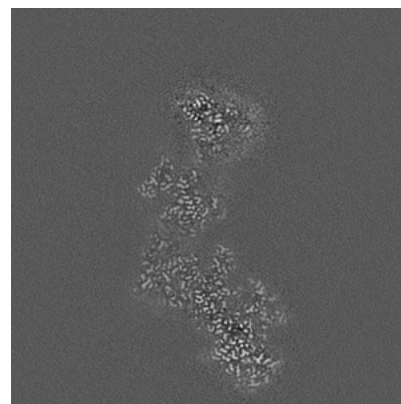
6.2.1 Primary map



X Index: 187



Y Index: 187

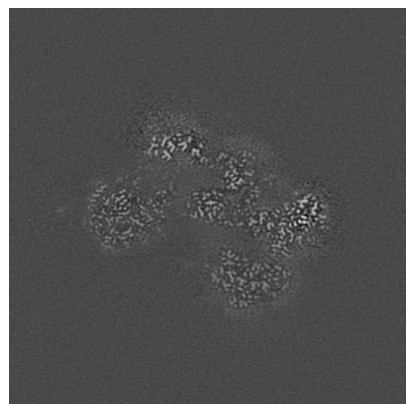


Z Index: 187

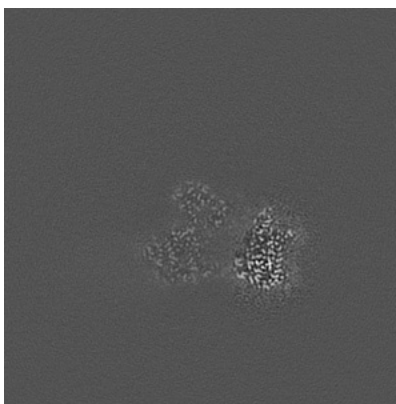
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

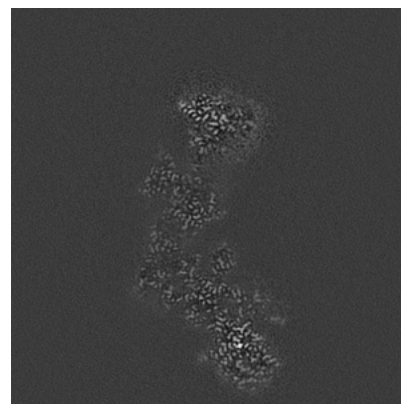
6.3.1 Primary map



X Index: 175



Y Index: 144



Z Index: 184

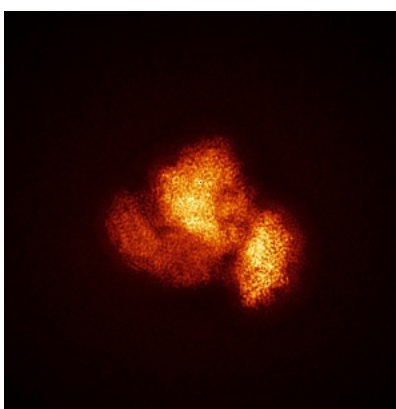
The images above show the largest variance slices of the map in three orthogonal directions.

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

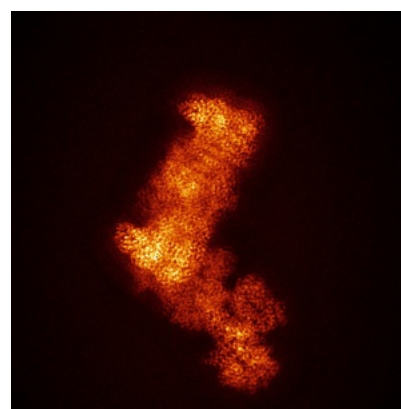
6.4.1 Primary map



X



Y

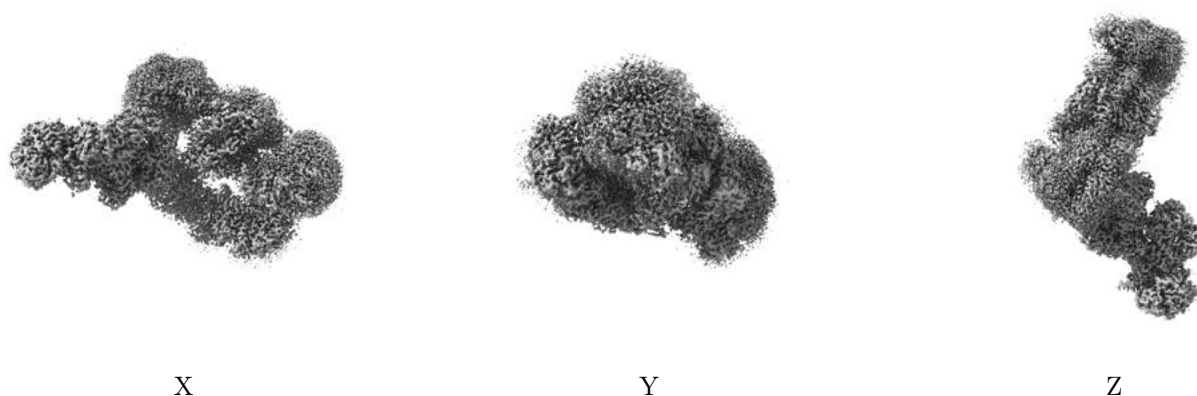


Z

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



The images above show the 3D surface view of the map at the recommended contour level 5.34. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

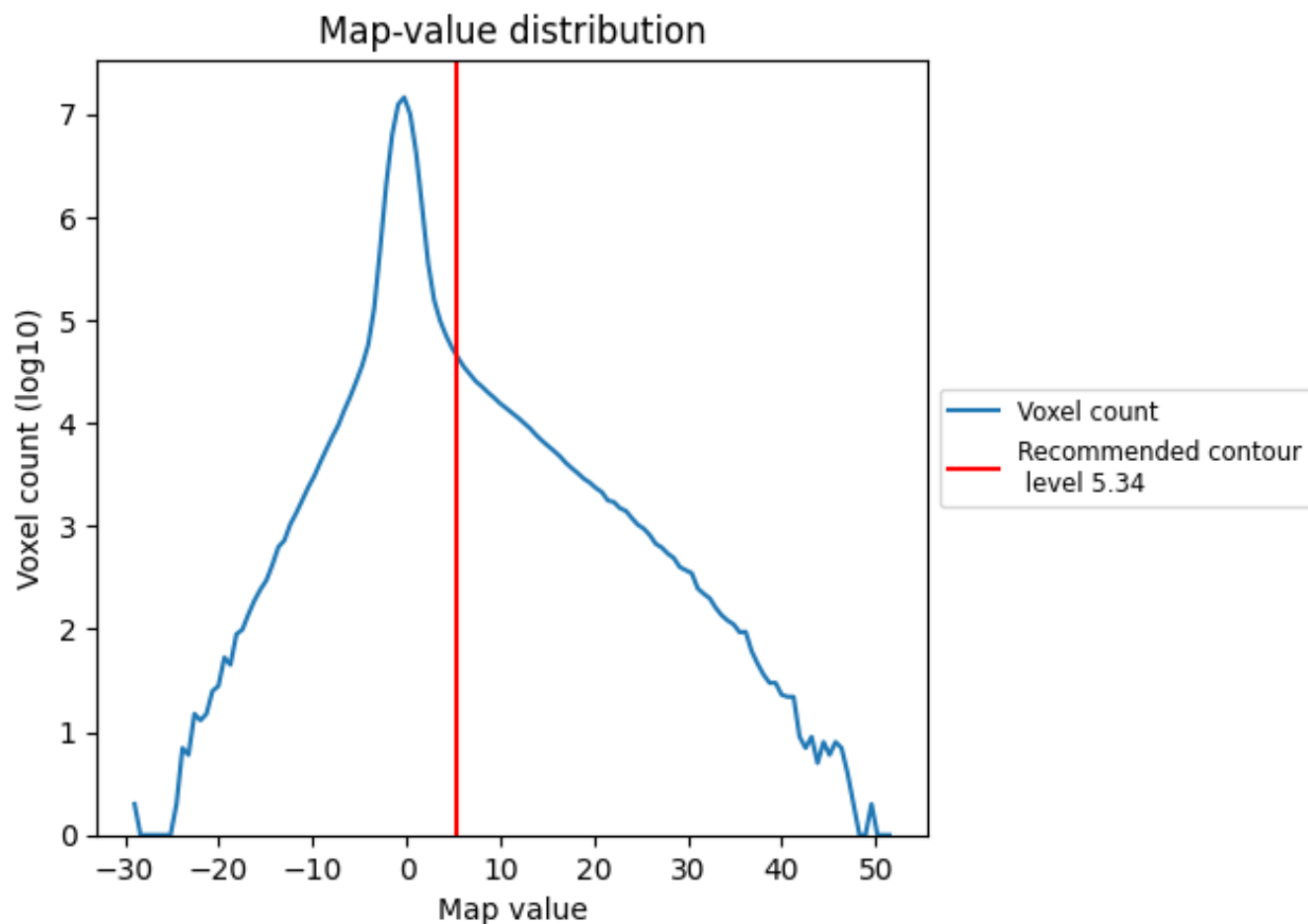
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

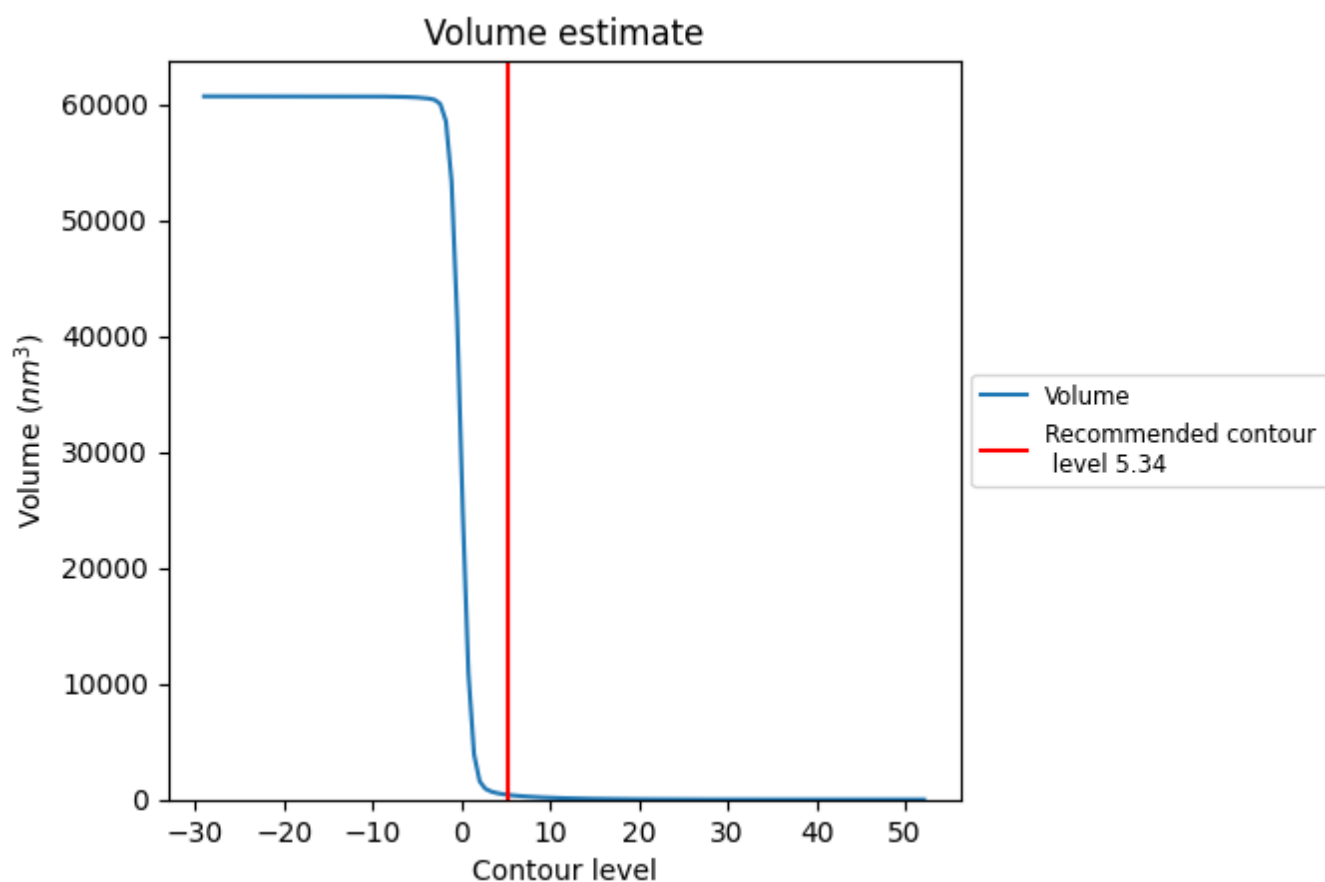
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

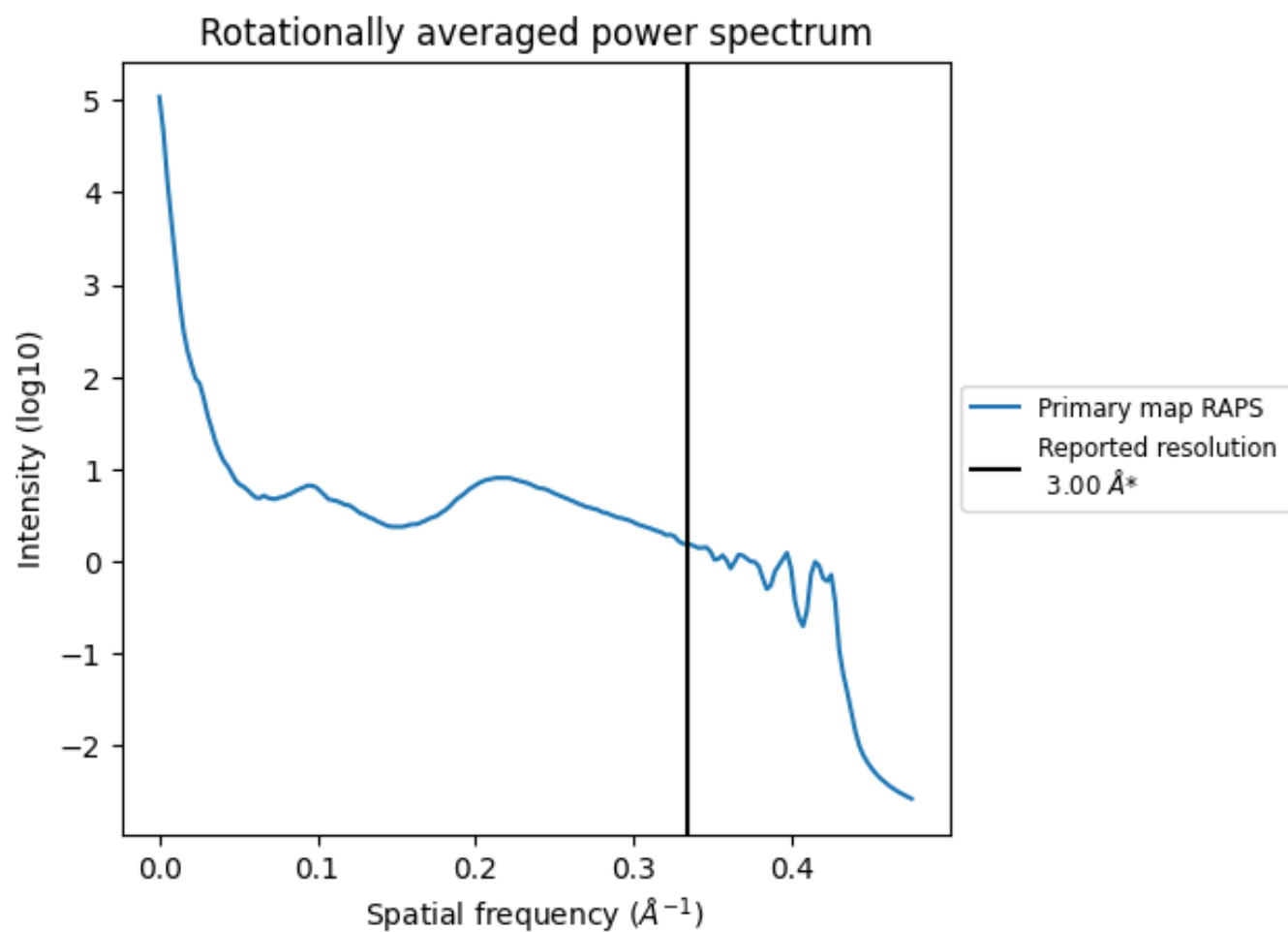
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 399 nm^3 ; this corresponds to an approximate mass of 360 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 0.333 Å⁻¹

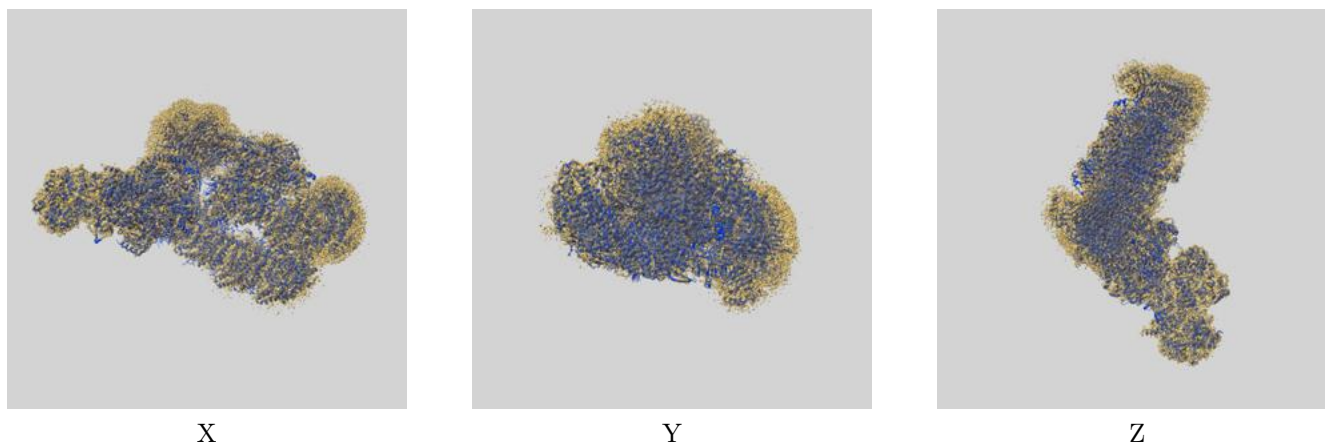
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

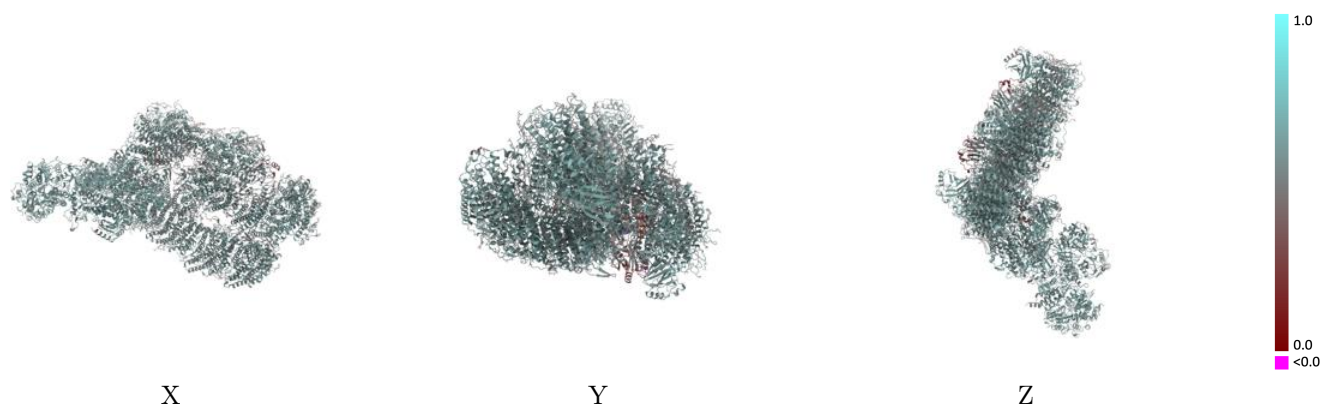
This section contains information regarding the fit between EMDB map EMD-51181 and PDB model 9GAE. Per-residue inclusion information can be found in [section 3](#) on [page 28](#).

9.1 Map-model overlay [i](#)



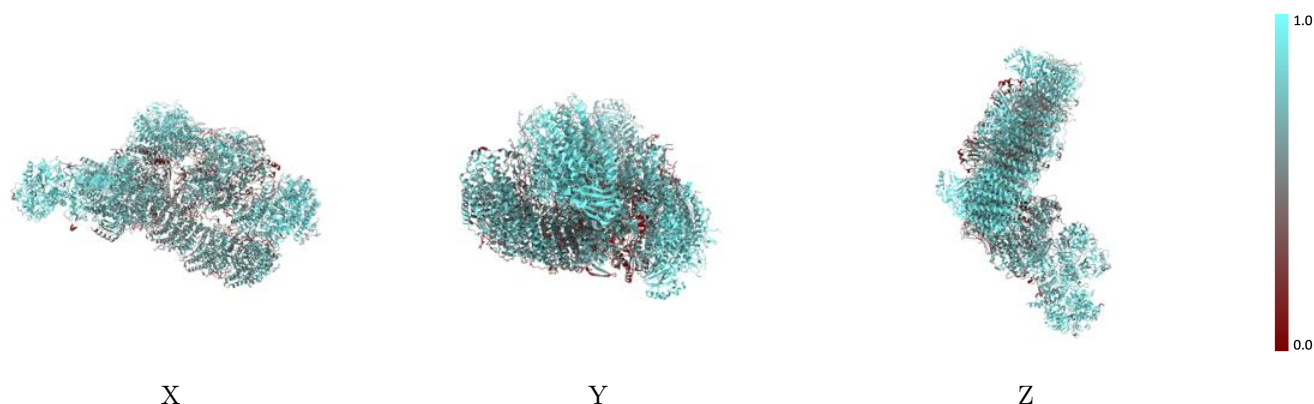
The images above show the 3D surface view of the map at the recommended contour level 5.34 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



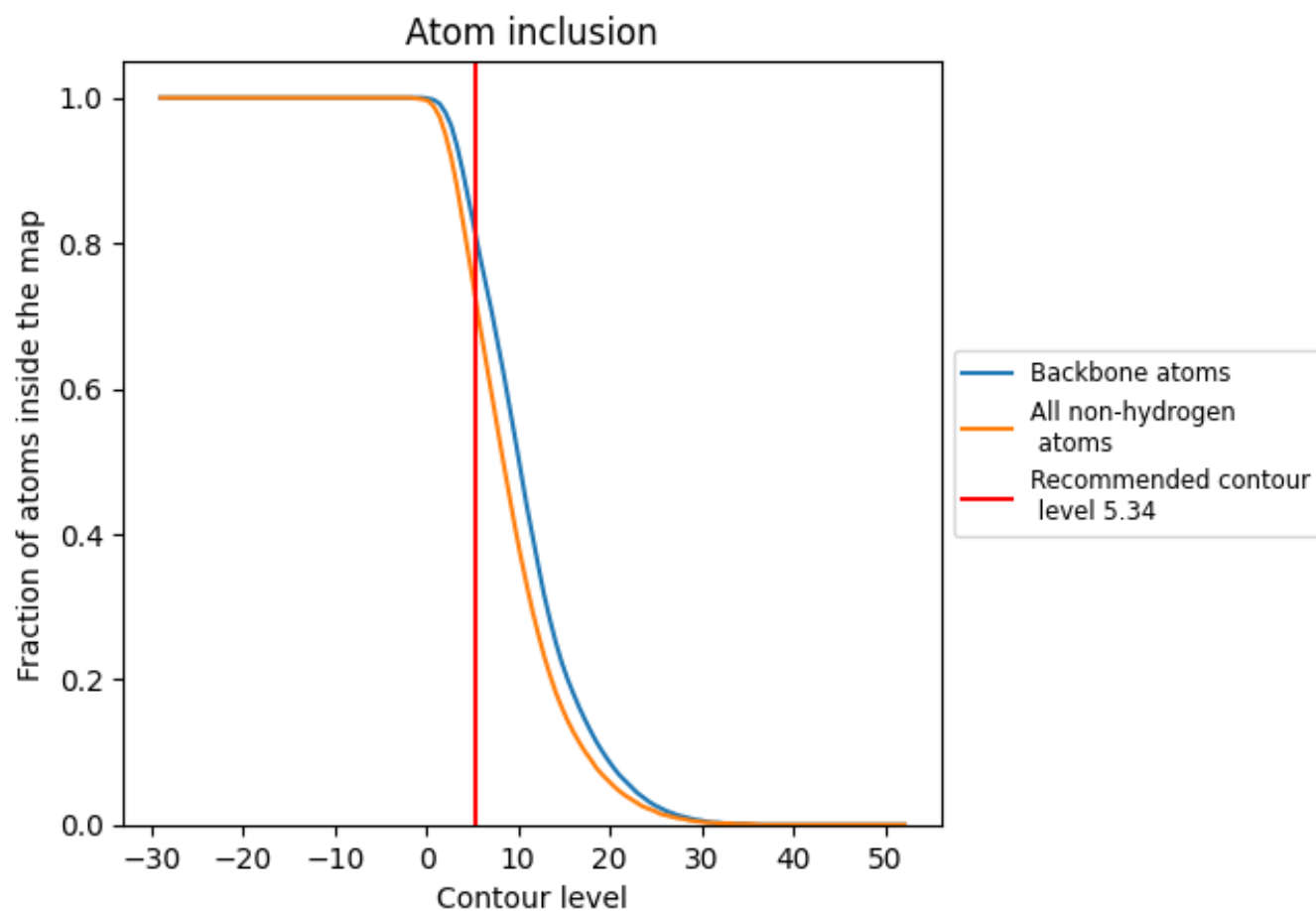
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5.34).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 73% 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 (5.34) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7260	 0.5710
A	 0.5860	 0.5730
B	 0.7190	 0.5970
C	 0.7180	 0.5980
D	 0.7180	 0.6000
E	 0.8500	 0.5760
F	 0.8560	 0.5780
G	 0.8120	 0.5790
H	 0.6170	 0.5810
I	 0.7650	 0.6040
J	 0.5410	 0.5670
K	 0.6090	 0.5870
L	 0.6790	 0.5710
M	 0.6820	 0.5790
N	 0.6640	 0.5850
P	 0.5080	 0.5420
Q	 0.7720	 0.5830
R	 0.4400	 0.5440
Z	 0.6430	 0.5830
a	 0.6740	 0.5770
b	 0.5890	 0.5600
c	 0.4400	 0.4490
d	 0.7490	 0.5740
e	 0.7720	 0.5730
f	 0.4810	 0.4310
g	 0.8830	 0.5860
h	 0.8580	 0.5630
i	 0.7250	 0.5550
j	 0.7030	 0.5230
k	 0.9260	 0.5870
l	 0.8850	 0.5690
m	 0.8300	 0.5570
n	 0.7510	 0.5280
o	 0.6790	 0.5460
p	 0.5380	 0.5610
q	 0.6180	 0.5750

