



Full wwPDB EM Validation Report ⓘ

Jun 17, 2024 – 10:45 am BST

PDB ID : 8Q49
EMDB ID : EMD-18142
Title : Outward-facing, open2 proteoliposome complex I at 2.6 Å. Initially purified in LMNG.
Authors : Grba, D.N.; Hirst, J.
Deposited on : 2023-08-05
Resolution : 2.60 Å (reported)
Based on initial model : 7QSN

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:

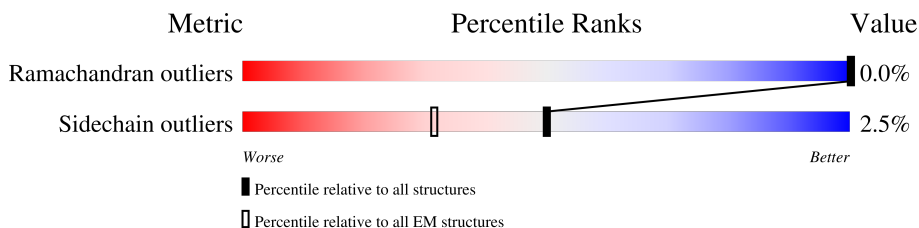
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

1 Overall quality at a glance

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

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	115	85% 12%
2	B	216	69% 28%
3	C	266	77% 22%
4	D	463	89% 10%
5	E	249	83% 14%
6	F	464	91% 7%
7	G	727	93% 5%
8	H	318	97%
9	I	212	82% 17%

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Mol	Chain	Length	Quality of chain
10	J	175	93%
11	K	98	95%
12	L	606	97%
13	M	459	97%
14	N	347	99%
15	O	343	92%
16	P	380	86%
17	Q	175	72%
18	R	124	77%
19	S	99	84%
20	T	156	54%
20	U	156	53%
21	V	116	97%
22	W	128	91%
23	X	172	98%
24	Y	141	96%
25	Z	144	97%
26	a	70	100%
27	b	84	98%
28	c	76	63%
29	d	120	99%
30	e	106	89%
31	f	57	91%
32	g	154	64%
33	h	189	73%

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Mol	Chain	Length	Quality of chain
34	i	128	 7% 95%
35	j	108	 6% 65% 34%
36	k	98	 5% 79% 17%
37	l	186	 81% 16%
38	m	129	 95%
39	n	179	 94%
40	o	137	 7% 82% 7% 11%
41	p	176	 97%
42	q	145	 97%
43	r	113	 82% 16%
44	s	109	 39% 60%

2 Entry composition i

There are 60 unique types of molecules in this entry. The entry contains 70056 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	101	815	555	116	139	5	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	207	1721	1111	296	311	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	417	3364	2151	577	611	25	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	129	ARG	GLN	variant	UNP P17694

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	214	1659	1059	278	312	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	432	3326	2096	594	616	20	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	691	5298	3318	925	1016	39	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	316	2496	1673	383	417	23	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	168	1281	861	183	225	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	98	745	486	112	131	16	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	606	4802	3195	737	827	43	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	459	3654	2436	570	609	39	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	347	2733	1817	416	457	43	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	320	2589	1662	429	488	10	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	255	LYS	ASN	variant	UNP P34942

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	335	2689	1739	476	469	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	129	1049	659	188	199	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	96	740	454	140	143	3	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	T	88	707	454	104	144	5	0	0
20	U	88	707	454	104	144	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	V	114	923	597	156	167	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	W	116	982	628	182	168	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	X	171	1402	887	253	252	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Y	140	1030	657	176	191	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Z	142	1157	743	202	203	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	a	70	569	365	104	95	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	b	83	654	427	109	116	2	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	c	49	414	273	70	71	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	d	120	999	650	172	172	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	e	98	825	521	157	141	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	f	57	492	322	86	82	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	g	101	846	544	140	158	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	h	138	1154	759	196	197	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	i	127	1097	722	191	183	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	j	71	597	390	99	107	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	k	81	653	427	110	114	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	l	156	1314	850	216	240	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	m	128	1070	686	188	196		0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	n	171	1487	952	272	256	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	o	122	1048	653	201	185	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	p	174	1458	913	269	268	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	q	145	1212	780	216	211	5	0	0

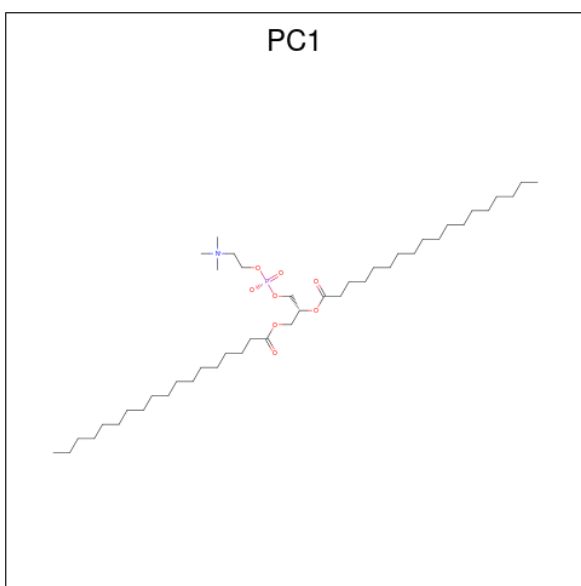
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	r	95	776	490	144	139	3	0	0

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

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

- Molecule 45 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



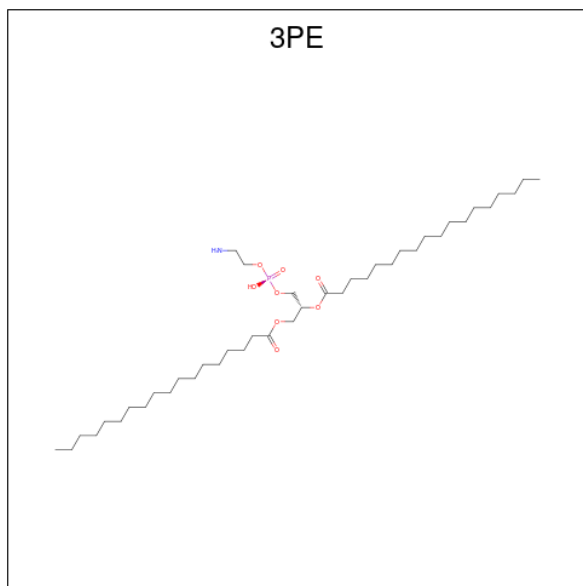
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
45	A	1	35	25	1	8	1	0
45	A	1	41	31	1	8	1	0
45	B	1	48	38	1	8	1	0
45	H	1	48	38	1	8	1	0
45	H	1	39	29	1	8	1	0
45	I	1	54	44	1	8	1	0
45	I	1	44	34	1	8	1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
45	L	1	Total 54	C 44	N 1	O 8	P 1	0
45	M	1	Total 35	C 25	N 1	O 8	P 1	0
45	d	1	Total 39	C 29	N 1	O 8	P 1	0
45	g	1	Total 44	C 34	N 1	O 8	P 1	0
45	h	1	Total 40	C 30	N 1	O 8	P 1	0
45	m	1	Total 40	C 30	N 1	O 8	P 1	0
45	q	1	Total 23	C 13	N 1	O 8	P 1	0

- Molecule 46 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	A	1	Total 43	C 33	N 1	O 8	P 1	0
46	A	1	Total 45	C 35	N 1	O 8	P 1	0
46	H	1	Total 36	C 26	N 1	O 8	P 1	0
46	J	1	Total 31	C 21	N 1	O 8	P 1	0

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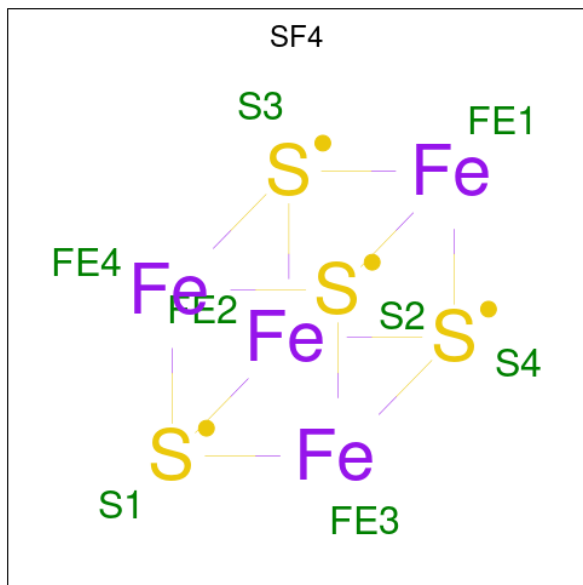
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	J	1	Total 36	C 26	N 1	O 8	P 1	0
46	K	1	Total 44	C 34	N 1	O 8	P 1	0
46	L	1	Total 45	C 35	N 1	O 8	P 1	0
46	L	1	Total 34	C 24	N 1	O 8	P 1	0
46	M	1	Total 50	C 40	N 1	O 8	P 1	0
46	M	1	Total 45	C 35	N 1	O 8	P 1	0
46	N	1	Total 49	C 39	N 1	O 8	P 1	0
46	N	1	Total 40	C 30	N 1	O 8	P 1	0
46	Y	1	Total 27	C 17	N 1	O 8	P 1	0
46	Y	1	Total 51	C 41	N 1	O 8	P 1	0
46	Y	1	Total 51	C 41	N 1	O 8	P 1	0
46	Y	1	Total 51	C 41	N 1	O 8	P 1	0
46	Y	1	Total 46	C 36	N 1	O 8	P 1	0
46	Y	1	Total 34	C 24	N 1	O 8	P 1	0
46	Y	1	Total 51	C 41	N 1	O 8	P 1	0
46	Z	1	Total 37	C 27	N 1	O 8	P 1	0
46	Z	1	Total 51	C 41	N 1	O 8	P 1	0
46	b	1	Total 47	C 37	N 1	O 8	P 1	0
46	b	1	Total 51	C 41	N 1	O 8	P 1	0
46	b	1	Total 37	C 27	N 1	O 8	P 1	0
46	d	1	Total 49	C 39	N 1	O 8	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
46	f	1	Total 30	C 20	N 1	O 8	P 1	0
46	f	1	Total 51	C 41	N 1	O 8	P 1	0
46	f	1	Total 32	C 22	N 1	O 8	P 1	0
46	m	1	Total 41	C 31	N 1	O 8	P 1	0
46	m	1	Total 30	C 20	N 1	O 8	P 1	0
46	q	1	Total 51	C 41	N 1	O 8	P 1	0
46	r	1	Total 28	C 18	N 1	O 8	P 1	0

- Molecule 47 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



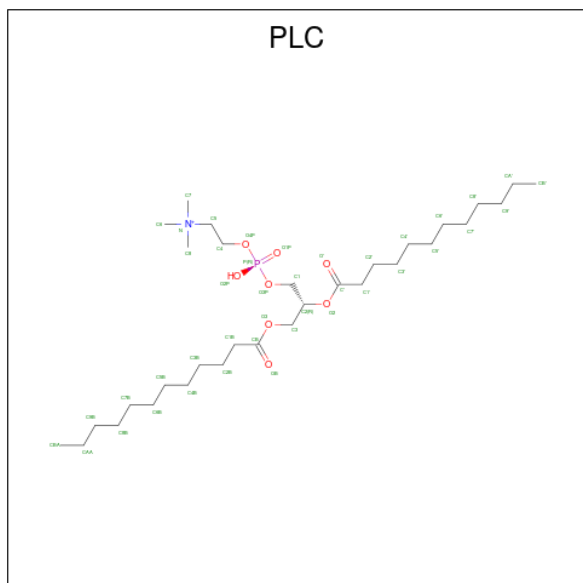
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
47	B	1	Total 8	Fe 4	S 4	0
47	F	1	Total 8	Fe 4	S 4	0
47	G	1	Total 8	Fe 4	S 4	0
47	G	1	Total 8	Fe 4	S 4	0

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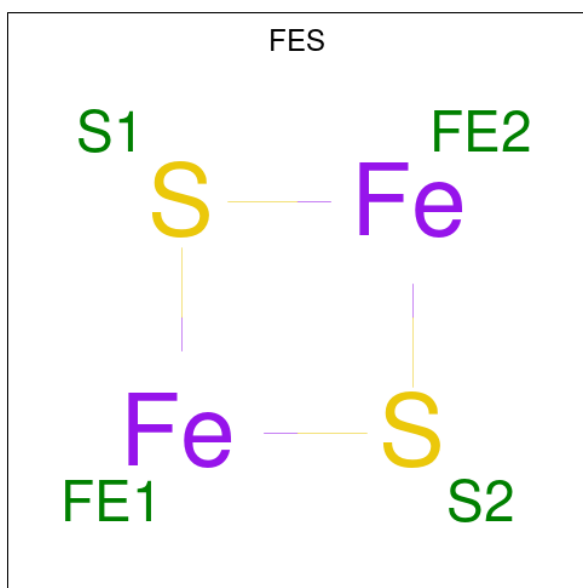
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
47	I	1	8	4	4	0
47	I	1	8	4	4	0

- Molecule 48 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula: $C_{32}H_{65}NO_8P$).



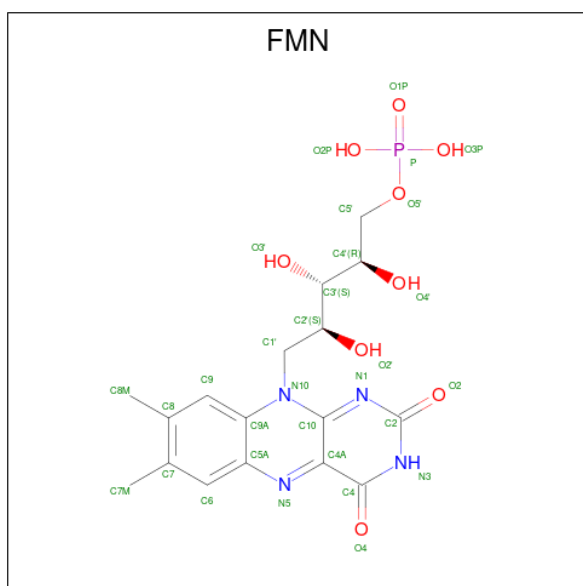
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
48	B	1	28	18	1	8	1	0
48	J	1	35	25	1	8	1	0
48	L	1	42	32	1	8	1	0
48	O	1	42	32	1	8	1	0
48	Y	1	37	27	1	8	1	0
48	Z	1	34	24	1	8	1	0
48	b	1	38	28	1	8	1	0
48	d	1	32	22	1	8	1	0
48	h	1	28	18	1	8	1	0

- Molecule 49 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



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

- Molecule 50 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).

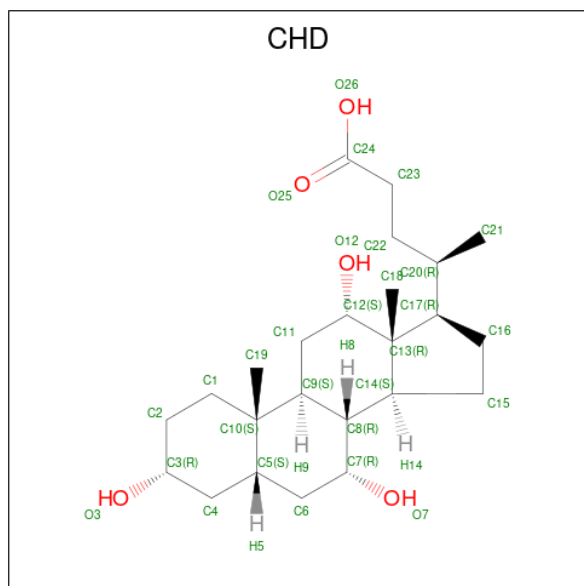


Mol	Chain	Residues	Atoms				AltConf	
50	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 51 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
51	G	1	Total K 1 1	0

- Molecule 52 is CHOLIC ACID (three-letter code: CHD) (formula: C₂₄H₄₀O₅).

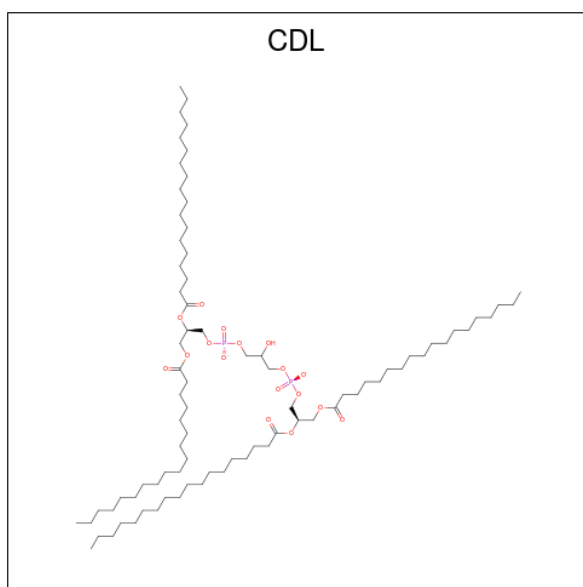


Mol	Chain	Residues	Atoms	AltConf
52	L	1	Total C O 29 24 5	0

- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

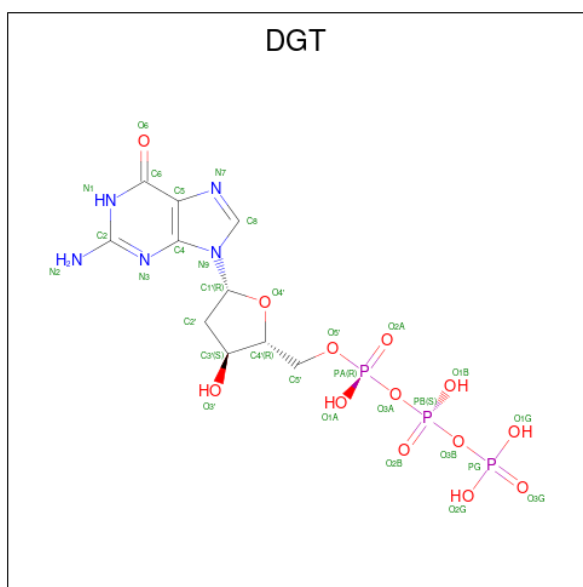
Mol	Chain	Residues	Atoms	AltConf
53	M	1	Total Zn 1 1	0
53	R	1	Total Zn 1 1	0

- Molecule 54 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
54	M	1	70	51	17	2	0
54	M	1	100	81	17	2	0
54	N	1	84	65	17	2	0
54	X	1	86	67	17	2	0
54	d	1	65	46	17	2	0
54	i	1	72	53	17	2	0
54	r	1	58	39	17	2	0

- Molecule 55 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

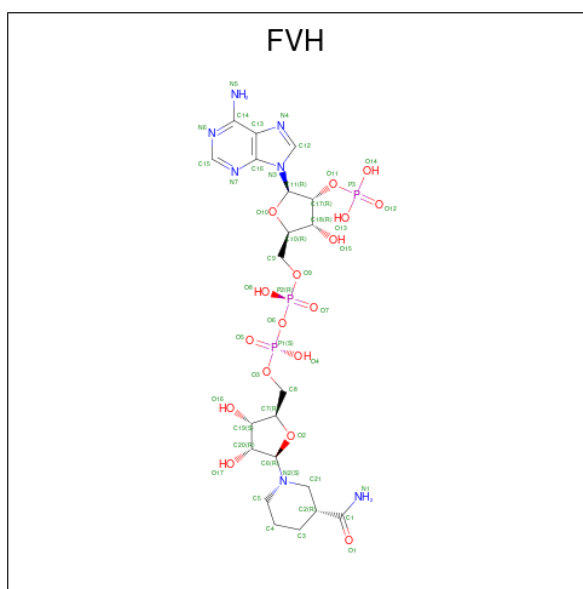


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
55	O	1	31	10	5	13	3	0

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

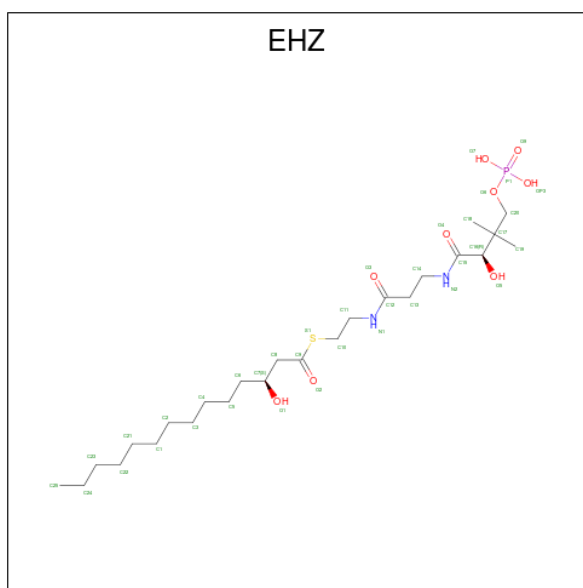
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
56	O	1	1	1	0

- Molecule 57 is [[(2 {R},3 {S},4 {R},5 {R})-5-[(3 {R})-3-aminocarbonylpiperidin-1-yl]-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] [(2 {R},3 {R},4 {R},5 {R})-5-(6-aminopurin-9-yl)-3-oxidanyl-4-phosphonoxy-oxolan-2-yl]methyl hydrogen phosphate (three-letter code: FVH) (formula: C₂₁H₃₄N₇O₁₇P₃).



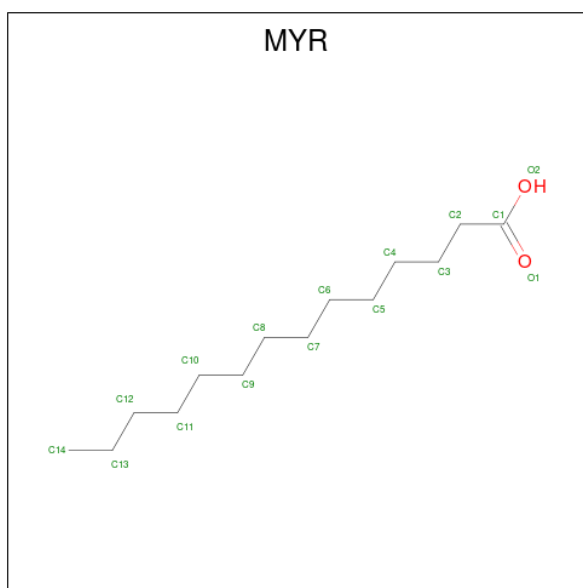
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
57	P	1	48	21	7	17	3	0

- Molecule 58 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
58	T	1	37	25	2	8	1	1	0
58	U	1	37	25	2	8	1	1	0

- Molecule 59 is MYRISTIC ACID (three-letter code: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms		AltConf
59	o	1	Total	C O	0
			15	14 1	

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		AltConf
60	A	5	Total	O	0
			5	5	
60	B	50	Total	O	0
			50	50	
60	C	59	Total	O	0
			59	59	
60	D	117	Total	O	0
			117	117	
60	E	3	Total	O	0
			3	3	
60	F	16	Total	O	0
			16	16	
60	G	120	Total	O	0
			120	120	
60	H	26	Total	O	0
			26	26	
60	I	78	Total	O	0
			78	78	
60	J	4	Total	O	0
			4	4	

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Mol	Chain	Residues	Atoms		AltConf
60	K	4	Total 4	O 4	0
60	L	4	Total 4	O 4	0
60	M	15	Total 15	O 15	0
60	N	16	Total 16	O 16	0
60	O	1	Total 1	O 1	0
60	P	16	Total 16	O 16	0
60	Q	50	Total 50	O 50	0
60	R	22	Total 22	O 22	0
60	T	1	Total 1	O 1	0
60	V	6	Total 6	O 6	0
60	W	8	Total 8	O 8	0
60	X	7	Total 7	O 7	0
60	Y	3	Total 3	O 3	0
60	Z	15	Total 15	O 15	0
60	a	6	Total 6	O 6	0
60	b	3	Total 3	O 3	0
60	d	5	Total 5	O 5	0
60	e	8	Total 8	O 8	0
60	f	2	Total 2	O 2	0
60	g	1	Total 1	O 1	0
60	h	6	Total 6	O 6	0

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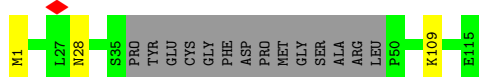
Mol	Chain	Residues	Atoms		AltConf
60	l	3	Total 3	O 3	0
60	m	3	Total 3	O 3	0
60	p	4	Total 4	O 4	0
60	q	23	Total 23	O 23	0
60	r	20	Total 20	O 20	0
60	s	2	Total 2	O 2	0

3 Residue-property plots [i](#)

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

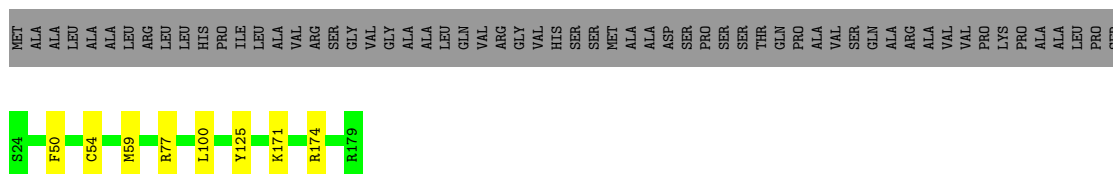
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A:  85% 12%




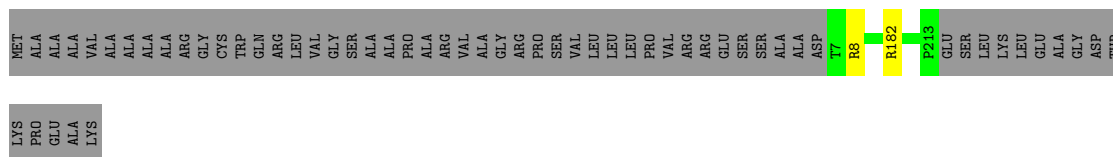
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B:  69% 28%




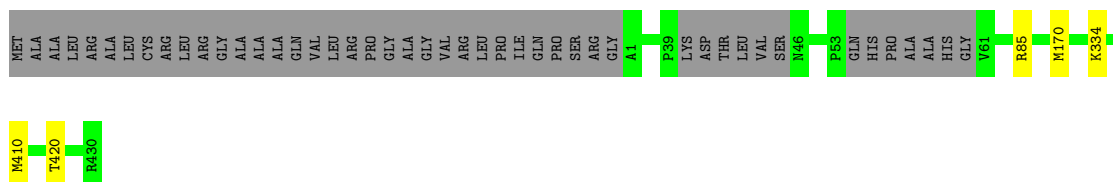
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C:  77% 22%




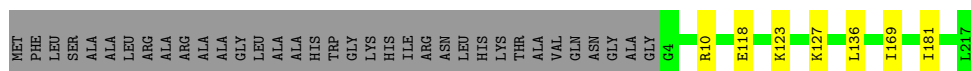
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D:  89% 10%



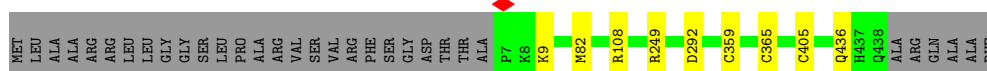
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:  83% 14%



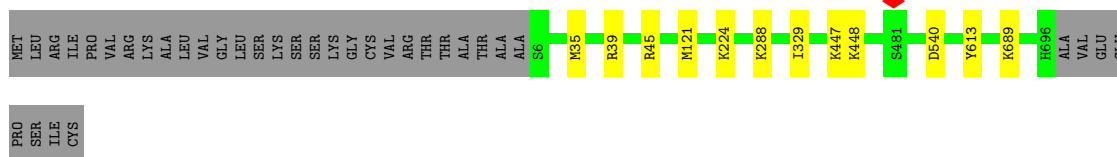
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F:  91% 7%



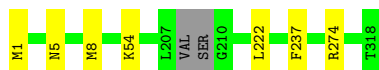
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G:  93% 5%




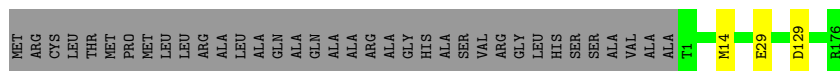
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H:  97%



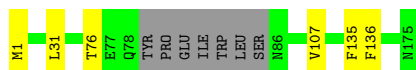
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:  82% 17%



- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:  93%



- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:  95% 5%



- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:  97%



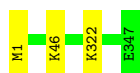
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:  97%



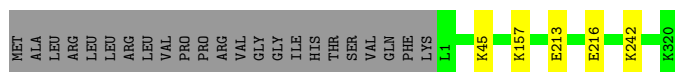
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:  99%



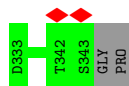
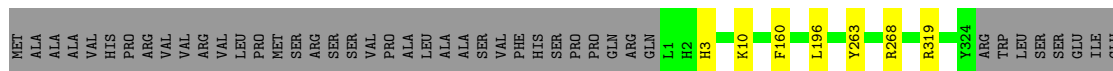
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:  92% 7%



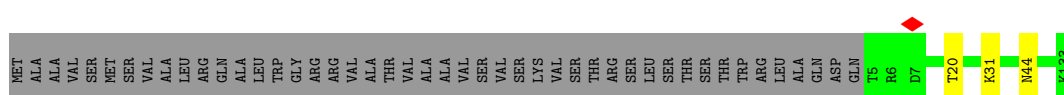
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:  86% 12%

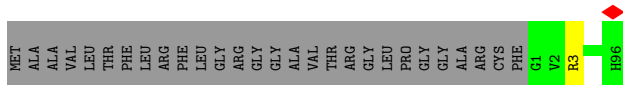
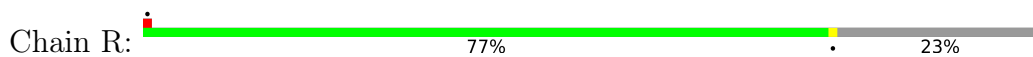


- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

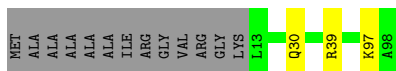
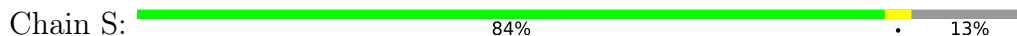
Chain Q:  72% 26%



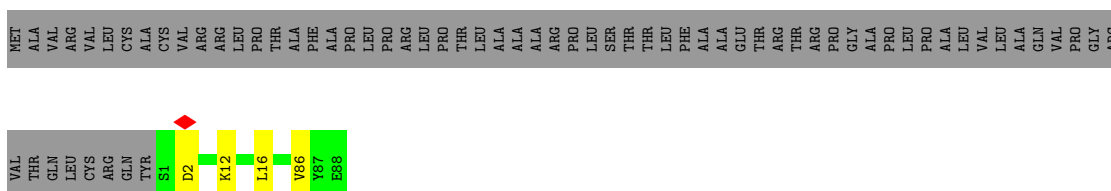
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



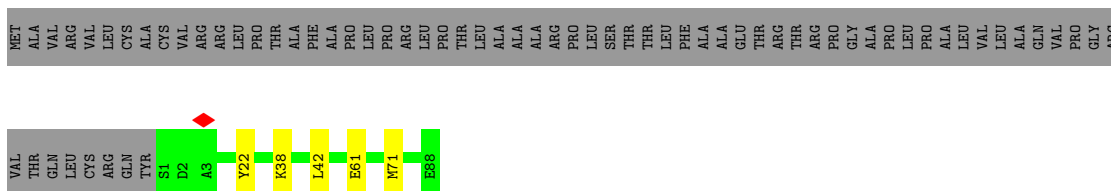
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



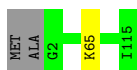
- Molecule 20: Acyl carrier protein, mitochondrial



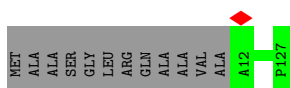
- Molecule 20: Acyl carrier protein, mitochondrial



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



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



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

Chain X:  98% ..



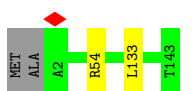
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y:  96% ..



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

Chain Z:  97% ..



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

Chain a:  100%

There are no outlier residues recorded for this chain.

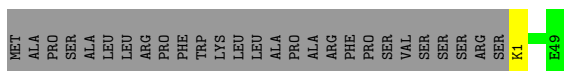
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b:  98% ..



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

Chain c:  63% . 36%




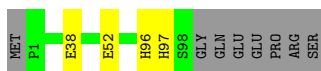
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d:  99% .

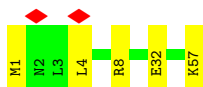


- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

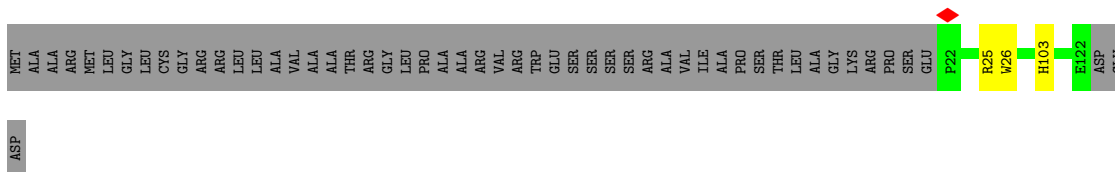
Chain e:  89% . 8%



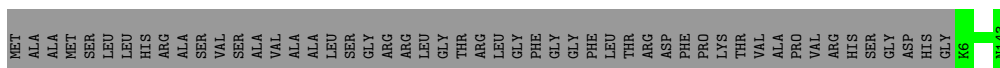
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



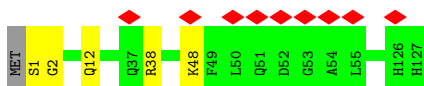
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



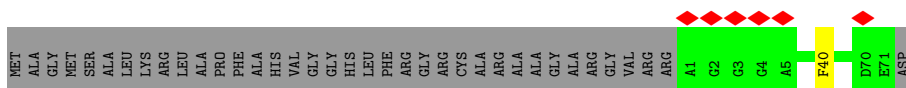
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



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

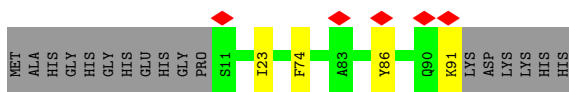


- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

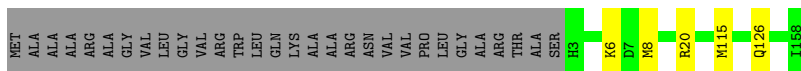
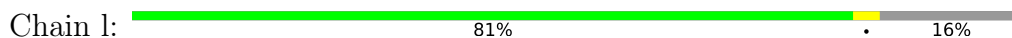


- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3





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



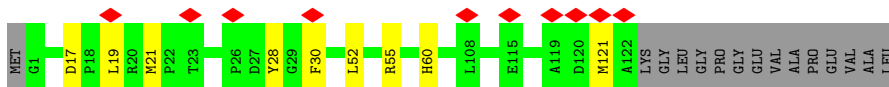
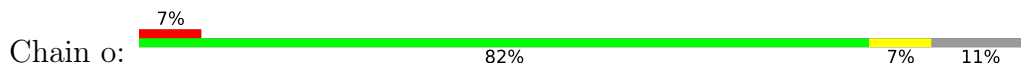
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



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



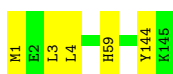
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



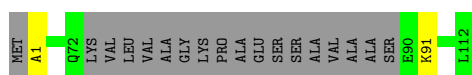
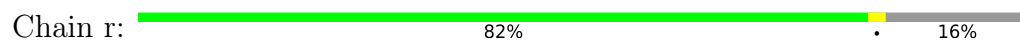
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



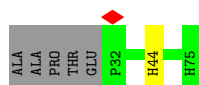
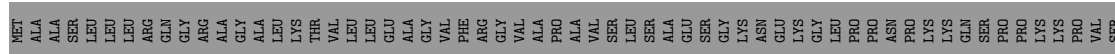
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	127085	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45.4	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.249	Depositor
Minimum map value	-0.004	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	479.69998, 479.69998, 479.69998	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.066, 1.066, 1.066	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, MYR, 2MR, FMN, K, 3PE, ZN, SAC, FME, EHZ, CHD, PC1, PLC, SF4, AME, FVH, FES, AYA, MG, DGT

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	0.24	0/825	0.37	0/1128
2	B	0.28	0/1278	0.52	0/1728
3	C	0.28	0/1772	0.51	0/2413
4	D	0.28	0/3437	0.49	0/4654
5	E	0.26	0/1699	0.46	0/2312
6	F	0.26	0/3401	0.49	0/4595
7	G	0.26	0/5387	0.50	0/7301
8	H	0.26	0/2557	0.43	0/3492
9	I	0.28	0/1445	0.52	0/1956
10	J	0.26	0/1301	0.40	0/1761
11	K	0.25	0/745	0.41	0/1008
12	L	0.24	0/4920	0.41	0/6694
13	M	0.24	0/3738	0.42	0/5097
14	N	0.24	0/2792	0.42	0/3800
15	O	0.25	0/2651	0.42	0/3587
16	P	0.26	0/2763	0.49	0/3747
17	Q	0.25	0/1072	0.51	0/1449
18	R	0.27	0/753	0.51	0/1014
19	S	0.24	0/702	0.51	0/945
20	T	0.24	0/719	0.39	0/971
20	U	0.25	0/719	0.42	0/971
21	V	0.24	0/943	0.40	0/1277
22	W	0.24	0/1006	0.50	0/1352
23	X	0.25	0/1439	0.48	0/1942
24	Y	0.23	0/1042	0.46	0/1414
25	Z	0.26	0/1186	0.49	0/1599
26	a	0.26	0/584	0.51	0/786
27	b	0.25	0/667	0.43	0/916
28	c	0.25	0/427	0.39	0/579
29	d	0.26	0/1018	0.48	0/1375
30	e	0.24	0/846	0.49	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.24	0/505	0.45	0/681
32	g	0.25	0/873	0.47	0/1186
33	h	0.25	0/1188	0.46	0/1607
34	i	0.24	0/1127	0.46	0/1534
35	j	0.25	0/624	0.44	0/855
36	k	0.24	0/672	0.45	0/906
37	l	0.25	0/1369	0.44	0/1873
38	m	0.25	0/1088	0.51	0/1472
39	n	0.24	0/1540	0.48	0/2085
40	o	0.25	0/1073	0.52	0/1437
41	p	0.24	0/1491	0.48	0/2011
42	q	0.27	0/1242	0.49	0/1688
43	r	0.27	0/789	0.50	0/1068
44	s	0.24	0/383	0.50	0/518
All	All	0.25	0/67798	0.46	0/91915

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	97/115 (84%)	92 (95%)	5 (5%)	0	100	100
2	B	154/216 (71%)	149 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	205/266 (77%)	202 (98%)	3 (2%)	0	100	100
4	D	410/463 (89%)	398 (97%)	12 (3%)	0	100	100
5	E	212/249 (85%)	202 (95%)	10 (5%)	0	100	100
6	F	430/464 (93%)	416 (97%)	14 (3%)	0	100	100
7	G	689/727 (95%)	662 (96%)	27 (4%)	0	100	100
8	H	312/318 (98%)	301 (96%)	11 (4%)	0	100	100
9	I	174/212 (82%)	169 (97%)	5 (3%)	0	100	100
10	J	164/175 (94%)	158 (96%)	6 (4%)	0	100	100
11	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
12	L	604/606 (100%)	574 (95%)	29 (5%)	1 (0%)	47	71
13	M	457/459 (100%)	451 (99%)	6 (1%)	0	100	100
14	N	345/347 (99%)	339 (98%)	6 (2%)	0	100	100
15	O	318/343 (93%)	311 (98%)	7 (2%)	0	100	100
16	P	331/380 (87%)	319 (96%)	12 (4%)	0	100	100
17	Q	127/175 (73%)	125 (98%)	2 (2%)	0	100	100
18	R	94/124 (76%)	91 (97%)	3 (3%)	0	100	100
19	S	84/99 (85%)	79 (94%)	5 (6%)	0	100	100
20	T	86/156 (55%)	84 (98%)	2 (2%)	0	100	100
20	U	86/156 (55%)	76 (88%)	10 (12%)	0	100	100
21	V	112/116 (97%)	111 (99%)	1 (1%)	0	100	100
22	W	114/128 (89%)	112 (98%)	2 (2%)	0	100	100
23	X	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
24	Y	138/141 (98%)	137 (99%)	1 (1%)	0	100	100
25	Z	140/144 (97%)	136 (97%)	4 (3%)	0	100	100
26	a	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
27	b	81/84 (96%)	76 (94%)	5 (6%)	0	100	100
28	c	47/76 (62%)	47 (100%)	0	0	100	100
29	d	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
30	e	96/106 (91%)	93 (97%)	3 (3%)	0	100	100
31	f	55/57 (96%)	52 (94%)	3 (6%)	0	100	100
32	g	99/154 (64%)	90 (91%)	9 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	h	136/189 (72%)	133 (98%)	3 (2%)	0	100	100
34	i	125/128 (98%)	118 (94%)	6 (5%)	1 (1%)	19	39
35	j	69/108 (64%)	65 (94%)	4 (6%)	0	100	100
36	k	79/98 (81%)	75 (95%)	4 (5%)	0	100	100
37	l	154/186 (83%)	141 (92%)	13 (8%)	0	100	100
38	m	126/129 (98%)	122 (97%)	4 (3%)	0	100	100
39	n	169/179 (94%)	157 (93%)	11 (6%)	1 (1%)	25	47
40	o	120/137 (88%)	104 (87%)	16 (13%)	0	100	100
41	p	172/176 (98%)	170 (99%)	2 (1%)	0	100	100
42	q	143/145 (99%)	143 (100%)	0	0	100	100
43	r	91/113 (80%)	89 (98%)	2 (2%)	0	100	100
44	s	42/109 (38%)	41 (98%)	1 (2%)	0	100	100
All	All	8138/9213 (88%)	7852 (96%)	283 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	562	LEU
34	i	2	GLY
39	n	152	ALA

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	89/100 (89%)	87 (98%)	2 (2%)	52	76
2	B	132/175 (75%)	124 (94%)	8 (6%)	18	38
3	C	188/228 (82%)	186 (99%)	2 (1%)	73	88
4	D	360/392 (92%)	356 (99%)	4 (1%)	73	88
5	E	183/205 (89%)	176 (96%)	7 (4%)	33	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	346/368 (94%)	337 (97%)	9 (3%)	46	72
7	G	579/608 (95%)	567 (98%)	12 (2%)	53	77
8	H	272/274 (99%)	266 (98%)	6 (2%)	52	76
9	I	151/175 (86%)	148 (98%)	3 (2%)	55	78
10	J	134/141 (95%)	129 (96%)	5 (4%)	34	60
11	K	85/85 (100%)	81 (95%)	4 (5%)	26	50
12	L	533/533 (100%)	519 (97%)	14 (3%)	46	72
13	M	412/412 (100%)	400 (97%)	12 (3%)	42	68
14	N	315/315 (100%)	313 (99%)	2 (1%)	86	95
15	O	283/303 (93%)	278 (98%)	5 (2%)	59	80
16	P	289/327 (88%)	282 (98%)	7 (2%)	49	74
17	Q	116/153 (76%)	113 (97%)	3 (3%)	46	72
18	R	79/97 (81%)	78 (99%)	1 (1%)	69	86
19	S	76/82 (93%)	73 (96%)	3 (4%)	32	58
20	T	81/135 (60%)	77 (95%)	4 (5%)	25	48
20	U	81/135 (60%)	76 (94%)	5 (6%)	18	37
21	V	101/102 (99%)	100 (99%)	1 (1%)	76	90
22	W	108/114 (95%)	108 (100%)	0	100	100
23	X	154/155 (99%)	151 (98%)	3 (2%)	57	79
24	Y	101/102 (99%)	98 (97%)	3 (3%)	41	67
25	Z	120/121 (99%)	118 (98%)	2 (2%)	60	81
26	a	59/59 (100%)	59 (100%)	0	100	100
27	b	71/72 (99%)	71 (100%)	0	100	100
28	c	45/68 (66%)	44 (98%)	1 (2%)	52	76
29	d	105/105 (100%)	105 (100%)	0	100	100
30	e	89/96 (93%)	85 (96%)	4 (4%)	27	52
31	f	54/54 (100%)	49 (91%)	5 (9%)	9	17
32	g	92/131 (70%)	89 (97%)	3 (3%)	38	64
33	h	121/158 (77%)	121 (100%)	0	100	100
34	i	120/121 (99%)	117 (98%)	3 (2%)	47	73
35	j	61/84 (73%)	60 (98%)	1 (2%)	62	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	k	63/76 (83%)	59 (94%)	4 (6%)	18	36
37	l	140/159 (88%)	135 (96%)	5 (4%)	35	61
38	m	113/114 (99%)	109 (96%)	4 (4%)	36	62
39	n	156/161 (97%)	154 (99%)	2 (1%)	69	86
40	o	110/120 (92%)	101 (92%)	9 (8%)	11	22
41	p	155/157 (99%)	151 (97%)	4 (3%)	46	72
42	q	130/130 (100%)	126 (97%)	4 (3%)	40	66
43	r	85/97 (88%)	84 (99%)	1 (1%)	71	87
44	s	43/92 (47%)	42 (98%)	1 (2%)	50	75
All	All	7180/7891 (91%)	7002 (98%)	178 (2%)	50	73

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	109	LYS
2	B	50	PHE
2	B	54	CYS
2	B	59	MET
2	B	77	ARG
2	B	100	LEU
2	B	125	TYR
2	B	171	LYS
2	B	174	ARG
3	C	8	ARG
3	C	182	ARG
4	D	170	MET
4	D	334	LYS
4	D	410	MET
4	D	420	THR
5	E	10	ARG
5	E	118	GLU
5	E	123	LYS
5	E	127	LYS
5	E	136	LEU
5	E	169	ILE
5	E	181	ILE
6	F	9	LYS
6	F	82	MET

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Mol	Chain	Res	Type
6	F	108	ARG
6	F	249	ARG
6	F	292	ASP
6	F	359	CYS
6	F	365	CYS
6	F	405	CYS
6	F	436	GLN
7	G	35	MET
7	G	39	ARG
7	G	45	ARG
7	G	121	MET
7	G	224	LYS
7	G	288	LYS
7	G	329	ILE
7	G	447	LYS
7	G	448	LYS
7	G	540	ASP
7	G	613	TYR
7	G	689	LYS
8	H	5	ASN
8	H	8	MET
8	H	54	LYS
8	H	222	LEU
8	H	237	PHE
8	H	274	ARG
9	I	14	MET
9	I	29	GLU
9	I	129	ASP
10	J	31	LEU
10	J	76	THR
10	J	107	VAL
10	J	135	PHE
10	J	136	PHE
11	K	34	GLU
11	K	37	MET
11	K	52	HIS
11	K	53	PHE
12	L	21	MET
12	L	84	TYR
12	L	295	GLN
12	L	336	LYS
12	L	397	GLU

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Mol	Chain	Res	Type
12	L	403	TYR
12	L	436	ARG
12	L	482	MET
12	L	498	PHE
12	L	514	HIS
12	L	530	PRO
12	L	554	ASP
12	L	580	GLN
12	L	581	LYS
13	M	3	LYS
13	M	57	PHE
13	M	72	LEU
13	M	114	GLU
13	M	207	MET
13	M	238	LEU
13	M	315	LEU
13	M	340	ARG
13	M	355	MET
13	M	413	MET
13	M	416	ARG
13	M	418	LYS
14	N	46	LYS
14	N	322	LYS
15	O	45	LYS
15	O	157	LYS
15	O	213	GLU
15	O	216	GLU
15	O	242	LYS
16	P	3	HIS
16	P	10	LYS
16	P	160	PHE
16	P	196	LEU
16	P	263	TYR
16	P	268	ARG
16	P	319	ARG
17	Q	20	THR
17	Q	31	LYS
17	Q	44	ASN
18	R	3	ARG
19	S	30	GLN
19	S	39	ARG
19	S	97	LYS

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Mol	Chain	Res	Type
20	T	2	ASP
20	T	12	LYS
20	T	16	LEU
20	T	86	VAL
20	U	22	TYR
20	U	38	LYS
20	U	42	LEU
20	U	61	GLU
20	U	71	MET
21	V	65	LYS
23	X	13	LYS
23	X	100	ARG
23	X	158	LYS
24	Y	49	LEU
24	Y	114	CYS
24	Y	119	LEU
25	Z	54	ARG
25	Z	133	LEU
28	c	1	LYS
30	e	38	GLU
30	e	52	GLU
30	e	96	HIS
30	e	97	HIS
31	f	1	MET
31	f	4	LEU
31	f	8	ARG
31	f	32	GLU
31	f	57	LYS
32	g	25	ARG
32	g	26	TRP
32	g	103	HIS
34	i	12	GLN
34	i	38	ARG
34	i	48	LYS
35	j	40	PHE
36	k	23	ILE
36	k	74	PHE
36	k	86	TYR
36	k	91	LYS
37	l	6	LYS
37	l	8	MET
37	l	20	ARG

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Mol	Chain	Res	Type
37	l	115	MET
37	l	126	GLN
38	m	30	LYS
38	m	79	PHE
38	m	91	LEU
38	m	110	ARG
39	n	84	SER
39	n	89	SER
40	o	17	ASP
40	o	19	LEU
40	o	21	MET
40	o	28	TYR
40	o	30	PHE
40	o	52	LEU
40	o	55	ARG
40	o	60	HIS
40	o	121	MET
41	p	69	ARG
41	p	126	LYS
41	p	133	GLN
41	p	166	ARG
42	q	3	LEU
42	q	4	LEU
42	q	59	HIS
42	q	144	TYR
43	r	91	LYS
44	s	44	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
8	H	287	HIS
13	M	338	HIS
37	l	104	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

15 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
8	FME	H	1	8	8,9,10	1.49	1 (12%)	7,9,11	1.75	3 (42%)
43	AYA	r	1	43	6,7,8	1.80	2 (33%)	5,8,10	1.39	1 (20%)
34	SAC	i	1	34	7,8,9	1.67	1 (14%)	8,9,11	1.49	1 (12%)
38	SAC	m	1	38	7,8,9	1.65	1 (14%)	8,9,11	1.25	1 (12%)
1	FME	A	1	1	8,9,10	1.52	1 (12%)	7,9,11	1.63	1 (14%)
4	2MR	D	85	4	10,12,13	2.42	2 (20%)	5,13,15	1.35	1 (20%)
10	FME	J	1	10	8,9,10	1.51	1 (12%)	7,9,11	1.64	2 (28%)
24	AYA	Y	1	24	6,7,8	1.80	2 (33%)	5,8,10	1.45	1 (20%)
13	FME	M	1	13	8,9,10	1.51	1 (12%)	7,9,11	1.67	1 (14%)
14	FME	N	1	14	8,9,10	1.50	1 (12%)	7,9,11	1.69	1 (14%)
27	AYA	b	1	27	6,7,8	1.81	1 (16%)	5,8,10	1.23	1 (20%)
29	AME	d	1	29	9,10,11	1.44	1 (11%)	9,11,13	1.48	2 (22%)
12	FME	L	1	12	8,9,10	1.51	1 (12%)	7,9,11	1.63	2 (28%)
42	AME	q	1	42	9,10,11	1.48	1 (11%)	9,11,13	1.95	2 (22%)
11	FME	K	1	11	8,9,10	1.50	1 (12%)	7,9,11	1.62	2 (28%)

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
8	FME	H	1	8	-	1/7/9/11	-
43	AYA	r	1	43	-	0/4/6/8	-
34	SAC	i	1	34	-	3/7/8/10	-
38	SAC	m	1	38	-	2/7/8/10	-
1	FME	A	1	1	-	3/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	2MR	D	85	4	-	0/10/13/15	-
10	FME	J	1	10	-	2/7/9/11	-
24	AYA	Y	1	24	-	0/4/6/8	-
13	FME	M	1	13	-	2/7/9/11	-
14	FME	N	1	14	-	3/7/9/11	-
27	AYA	b	1	27	-	0/4/6/8	-
29	AME	d	1	29	-	0/9/10/12	-
12	FME	L	1	12	-	2/7/9/11	-
42	AME	q	1	42	-	4/9/10/12	-
11	FME	K	1	11	-	3/7/9/11	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.34	1.45	1.33
4	D	85	2MR	CZ-NE	5.08	1.45	1.34
10	J	1	FME	CN-N	3.66	1.45	1.33
1	A	1	FME	CN-N	3.66	1.45	1.33
13	M	1	FME	CN-N	3.66	1.45	1.33
12	L	1	FME	CN-N	3.65	1.45	1.33
11	K	1	FME	CN-N	3.64	1.45	1.33
14	N	1	FME	CN-N	3.63	1.45	1.33
8	H	1	FME	CN-N	3.61	1.45	1.33
34	i	1	SAC	C1A-N	3.36	1.45	1.34
27	b	1	AYA	CT-N	3.29	1.45	1.34
42	q	1	AME	CT1-N	3.29	1.45	1.34
38	m	1	SAC	C1A-N	3.27	1.45	1.34
29	d	1	AME	CT1-N	3.22	1.45	1.34
24	Y	1	AYA	CT-N	3.18	1.45	1.34
43	r	1	AYA	CT-N	3.17	1.45	1.34
43	r	1	AYA	OT-CT	-2.04	1.18	1.23
24	Y	1	AYA	OT-CT	-2.02	1.18	1.23

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	q	1	AME	CE-SD-CG	4.09	114.45	100.40
34	i	1	SAC	C2A-C1A-N	3.05	121.26	116.10
8	H	1	FME	CE-SD-CG	2.78	109.93	100.40
1	A	1	FME	CE-SD-CG	2.73	109.78	100.40
14	N	1	FME	CE-SD-CG	2.70	109.68	100.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	1	FME	CE-SD-CG	2.69	109.66	100.40
29	d	1	AME	CE-SD-CG	2.66	109.54	100.40
12	L	1	FME	CE-SD-CG	2.65	109.49	100.40
13	M	1	FME	CE-SD-CG	2.59	109.31	100.40
11	K	1	FME	CE-SD-CG	2.53	109.10	100.40
42	q	1	AME	CT2-CT1-N	2.50	120.32	116.10
24	Y	1	AYA	CM-CT-N	2.44	120.23	116.10
43	r	1	AYA	CM-CT-N	2.44	120.23	116.10
4	D	85	2MR	CD-NE-CZ	-2.38	118.96	123.41
38	m	1	SAC	C2A-C1A-N	2.19	119.81	116.10
8	H	1	FME	CA-N-CN	-2.18	119.47	122.82
29	d	1	AME	CT2-CT1-N	2.12	119.69	116.10
27	b	1	AYA	CM-CT-N	2.11	119.67	116.10
8	H	1	FME	O1-CN-N	-2.10	119.74	125.27
11	K	1	FME	O1-CN-N	-2.05	119.88	125.27
12	L	1	FME	O1-CN-N	-2.02	119.94	125.27
10	J	1	FME	O1-CN-N	-2.02	119.96	125.27

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	C-CA-CB-CG
10	J	1	FME	O-C-CA-CB
11	K	1	FME	O1-CN-N-CA
12	L	1	FME	CB-CA-N-CN
13	M	1	FME	C-CA-CB-CG
14	N	1	FME	O1-CN-N-CA
34	i	1	SAC	O-C-CA-CB
42	q	1	AME	N-CA-CB-CG
42	q	1	AME	CB-CG-SD-CE
12	L	1	FME	CA-CB-CG-SD
34	i	1	SAC	C2A-C1A-N-CA
34	i	1	SAC	OAC-C1A-N-CA
1	A	1	FME	N-CA-CB-CG
10	J	1	FME	N-CA-CB-CG
14	N	1	FME	N-CA-CB-CG
38	m	1	SAC	N-CA-CB-OG
11	K	1	FME	CB-CG-SD-CE
42	q	1	AME	CA-CB-CG-SD
42	q	1	AME	C-CA-CB-CG
14	N	1	FME	CB-CG-SD-CE

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Mol	Chain	Res	Type	Atoms
13	M	1	FME	N-CA-CB-CG
38	m	1	SAC	C-CA-CB-OG
8	H	1	FME	C-CA-CB-CG
1	A	1	FME	CB-CA-N-CN
11	K	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 81 ligands modelled in this entry, 4 are monoatomic - leaving 77 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
46	3PE	L	705	-	33,33,50	1.05	4 (12%)	36,38,55	1.15	2 (5%)
55	DGT	O	401	56	26,33,33	2.66	8 (30%)	32,52,52	1.66	10 (31%)
58	EHZ	T	101	20	29,36,37	1.70	5 (17%)	35,44,47	1.63	5 (14%)
46	3PE	b	101	-	46,46,50	0.90	4 (8%)	49,51,55	1.02	2 (4%)
59	MYR	o	201	40	14,14,15	0.45	0	13,13,15	0.95	0
54	CDL	r	202	-	57,57,99	1.13	8 (14%)	63,69,111	1.13	4 (6%)
46	3PE	N	402	-	39,39,50	0.96	4 (10%)	42,44,55	1.12	2 (4%)
46	3PE	b	104	-	36,36,50	1.00	4 (11%)	39,41,55	1.13	2 (5%)
47	SF4	G	802	7	0,12,12	-	-	-	-	-
46	3PE	H	401	-	35,35,50	1.02	4 (11%)	38,40,55	1.04	2 (5%)
46	3PE	M	603	-	44,44,50	0.91	4 (9%)	47,49,55	1.07	2 (4%)
54	CDL	M	606	-	99,99,99	0.88	8 (8%)	105,111,111	1.09	4 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	3PE	M	602	-	49,49,50	0.87	4 (8%)	52,54,55	1.03	2 (3%)
45	PC1	d	202	-	38,38,53	1.10	4 (10%)	44,46,61	1.01	2 (4%)
46	3PE	Z	202	-	36,36,50	1.00	4 (11%)	39,41,55	1.03	2 (5%)
46	3PE	m	201	-	40,40,50	0.95	3 (7%)	43,45,55	1.08	2 (4%)
46	3PE	J	201	-	30,30,50	1.09	4 (13%)	33,35,55	1.15	2 (6%)
49	FES	G	803	7	0,4,4	-	-	-	-	-
47	SF4	I	201	9	0,12,12	-	-	-	-	-
48	PLC	h	201	-	27,27,41	0.60	0	33,35,49	0.65	1 (3%)
54	CDL	d	204	-	64,64,99	1.06	8 (12%)	70,76,111	1.12	4 (5%)
48	PLC	J	203	-	34,34,41	0.55	0	40,42,49	0.53	0
46	3PE	q	202	-	50,50,50	0.86	4 (8%)	53,55,55	1.06	2 (3%)
45	PC1	q	201	-	22,22,53	1.33	3 (13%)	28,30,61	0.97	1 (3%)
46	3PE	Y	208	-	50,50,50	0.86	4 (8%)	53,55,55	1.05	2 (3%)
45	PC1	M	604	-	34,34,53	1.16	4 (11%)	40,42,61	1.07	2 (5%)
45	PC1	g	201	-	43,43,53	1.03	4 (9%)	49,51,61	1.00	2 (4%)
48	PLC	d	203	-	31,31,41	0.59	0	37,39,49	0.58	0
46	3PE	J	202	-	35,35,50	1.01	4 (11%)	38,40,55	1.18	2 (5%)
52	CHD	L	702	-	32,32,32	3.23	10 (31%)	51,51,51	2.28	17 (33%)
48	PLC	B	202	-	27,27,41	0.61	0	33,35,49	0.60	0
46	3PE	b	102	-	50,50,50	0.86	4 (8%)	53,55,55	1.07	2 (3%)
46	3PE	f	103	-	31,31,50	1.08	4 (12%)	34,36,55	1.16	2 (5%)
46	3PE	N	401	-	48,48,50	0.88	4 (8%)	51,53,55	1.03	2 (3%)
54	CDL	M	605	-	69,69,99	1.03	8 (11%)	75,81,111	1.11	4 (5%)
46	3PE	m	202	-	29,29,50	1.11	4 (13%)	32,34,55	1.18	2 (6%)
48	PLC	O	403	-	41,41,41	0.51	0	47,49,49	0.56	0
46	3PE	Y	202	-	50,50,50	0.86	4 (8%)	53,55,55	1.06	2 (3%)
45	PC1	I	204	-	43,43,53	1.04	4 (9%)	49,51,61	1.06	2 (4%)
54	CDL	X	201	-	85,85,99	0.94	8 (9%)	91,97,111	1.08	4 (4%)
45	PC1	H	403	-	38,38,53	1.09	4 (10%)	44,46,61	1.02	2 (4%)
48	PLC	Z	201	-	33,33,41	0.55	0	39,41,49	0.56	0
46	3PE	Y	205	-	45,45,50	0.91	4 (8%)	48,50,55	1.05	2 (4%)
47	SF4	G	801	7	0,12,12	-	-	-	-	-
50	FMN	F	502	-	33,33,33	2.75	10 (30%)	48,50,50	1.73	15 (31%)
45	PC1	A	201	-	34,34,53	1.15	4 (11%)	40,42,61	1.05	2 (5%)
48	PLC	b	103	-	37,37,41	0.53	0	43,45,49	0.54	0
45	PC1	A	204	-	40,40,53	1.07	4 (10%)	46,48,61	1.02	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	3PE	A	202	-	42,42,50	0.94	4 (9%)	45,47,55	1.03	2 (4%)
46	3PE	f	101	-	29,29,50	1.10	4 (13%)	32,34,55	1.06	2 (6%)
57	FVH	P	501	-	45,52,52	3.86	20 (44%)	58,80,80	3.08	13 (22%)
45	PC1	H	402	-	47,47,53	1.00	4 (8%)	53,55,61	1.01	2 (3%)
48	PLC	L	703	-	41,41,41	0.51	0	47,49,49	0.51	0
45	PC1	I	203	-	53,53,53	0.93	4 (7%)	59,61,61	0.99	2 (3%)
47	SF4	F	501	6	0,12,12	-	-	-	-	-
45	PC1	B	203	-	47,47,53	1.00	4 (8%)	53,55,61	1.09	2 (3%)
58	EHZ	U	101	20	29,36,37	1.69	5 (17%)	35,44,47	1.56	7 (20%)
54	CDL	i	201	-	71,71,99	1.02	8 (11%)	77,83,111	1.12	4 (5%)
46	3PE	Y	206	-	33,33,50	1.05	4 (12%)	36,38,55	1.13	2 (5%)
46	3PE	Y	201	-	26,26,50	1.17	4 (15%)	29,31,55	1.16	2 (6%)
45	PC1	h	202	-	39,39,53	1.07	4 (10%)	45,47,61	1.04	2 (4%)
47	SF4	B	201	2	0,12,12	-	-	-	-	-
48	PLC	Y	207	-	36,36,41	0.53	0	42,44,49	0.56	0
46	3PE	L	704	-	44,44,50	0.90	4 (9%)	47,49,55	1.08	2 (4%)
45	PC1	m	203	-	39,39,53	1.08	4 (10%)	45,47,61	1.08	2 (4%)
46	3PE	K	101	-	43,43,50	0.93	4 (9%)	46,48,55	1.04	2 (4%)
46	3PE	Y	204	-	50,50,50	0.86	4 (8%)	53,55,55	1.04	2 (3%)
46	3PE	r	201	-	27,27,50	1.16	4 (14%)	30,32,55	1.17	2 (6%)
49	FES	E	301	5	0,4,4	-	-	-	-	-
46	3PE	Y	203	-	50,50,50	0.87	4 (8%)	53,55,55	1.08	2 (3%)
54	CDL	N	403	-	83,83,99	0.95	8 (9%)	89,95,111	1.06	4 (4%)
46	3PE	d	201	-	48,48,50	0.88	4 (8%)	51,53,55	1.04	2 (3%)
46	3PE	A	203	-	44,44,50	0.91	4 (9%)	47,49,55	1.06	2 (4%)
46	3PE	Z	203	-	50,50,50	0.86	4 (8%)	53,55,55	1.03	2 (3%)
45	PC1	L	701	-	53,53,53	0.94	4 (7%)	59,61,61	0.97	2 (3%)
46	3PE	f	102	-	50,50,50	0.86	4 (8%)	53,55,55	1.04	2 (3%)
47	SF4	I	202	9	0,12,12	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	3PE	L	705	-	-	9/37/37/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	DGT	O	401	56	-	7/18/34/34	0/3/3/3
58	EHZ	T	101	20	-	14/42/44/45	-
46	3PE	b	101	-	-	23/50/50/54	-
59	MYR	o	201	40	-	3/11/12/13	-
54	CDL	r	202	-	-	28/68/68/110	-
46	3PE	N	402	-	-	20/43/43/54	-
46	3PE	b	104	-	-	16/40/40/54	-
47	SF4	G	802	7	-	-	0/6/5/5
46	3PE	H	401	-	-	18/39/39/54	-
46	3PE	M	603	-	-	11/48/48/54	-
54	CDL	M	606	-	-	47/110/110/110	-
46	3PE	M	602	-	-	18/53/53/54	-
45	PC1	d	202	-	-	23/42/42/57	-
46	3PE	Z	202	-	-	20/40/40/54	-
46	3PE	m	201	-	-	19/44/44/54	-
46	3PE	J	201	-	-	19/34/34/54	-
49	FES	G	803	7	-	-	0/1/1/1
48	PLC	h	201	-	-	11/30/30/45	-
47	SF4	I	201	9	-	-	0/6/5/5
54	CDL	d	204	-	-	26/75/75/110	-
48	PLC	J	203	-	-	15/38/38/45	-
46	3PE	q	202	-	-	25/54/54/54	-
45	PC1	q	201	-	-	10/25/25/57	-
46	3PE	Y	208	-	-	26/54/54/54	-
45	PC1	M	604	-	-	21/38/38/57	-
45	PC1	g	201	-	-	18/47/47/57	-
48	PLC	d	203	-	-	8/34/34/45	-
46	3PE	J	202	-	-	14/39/39/54	-
52	CHD	L	702	-	-	3/9/74/74	0/4/4/4
48	PLC	B	202	-	-	5/31/31/45	-
46	3PE	b	102	-	-	22/54/54/54	-
46	3PE	f	103	-	-	15/35/35/54	-
46	3PE	N	401	-	-	24/52/52/54	-
54	CDL	M	605	-	-	27/80/80/110	-
46	3PE	m	202	-	-	15/33/33/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	PLC	O	403	-	-	15/45/45/45	-
46	3PE	Y	202	-	-	18/54/54/54	-
45	PC1	I	204	-	-	17/47/47/57	-
54	CDL	X	201	-	-	49/96/96/110	-
45	PC1	H	403	-	-	17/42/42/57	-
48	PLC	Z	201	-	-	15/37/37/45	-
46	3PE	Y	205	-	-	21/49/49/54	-
50	FMN	F	502	-	-	9/18/18/18	0/3/3/3
47	SF4	G	801	7	-	-	0/6/5/5
45	PC1	A	201	-	-	19/38/38/57	-
48	PLC	b	103	-	-	15/41/41/45	-
45	PC1	A	204	-	-	14/44/44/57	-
46	3PE	A	202	-	-	25/46/46/54	-
46	3PE	f	101	-	-	17/33/33/54	-
57	FVH	P	501	-	-	14/31/77/77	0/5/5/5
45	PC1	H	402	-	-	16/51/51/57	-
48	PLC	L	703	-	-	20/45/45/45	-
45	PC1	I	203	-	-	20/57/57/57	-
47	SF4	F	501	6	-	-	0/6/5/5
45	PC1	B	203	-	-	21/51/51/57	-
58	EHZ	U	101	20	-	20/42/44/45	-
54	CDL	i	201	-	-	35/82/82/110	-
46	3PE	Y	206	-	-	16/37/37/54	-
46	3PE	Y	201	-	-	18/30/30/54	-
45	PC1	h	202	-	-	15/43/43/57	-
47	SF4	B	201	2	-	-	0/6/5/5
48	PLC	Y	207	-	-	15/40/40/45	-
46	3PE	L	704	-	-	28/48/48/54	-
45	PC1	m	203	-	-	11/43/43/57	-
46	3PE	K	101	-	-	21/47/47/54	-
46	3PE	Y	204	-	-	24/54/54/54	-
46	3PE	r	201	-	-	18/31/31/54	-
49	FES	E	301	5	-	-	0/1/1/1
46	3PE	Y	203	-	-	29/54/54/54	-
54	CDL	N	403	-	-	36/94/94/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	3PE	d	201	-	-	16/52/52/54	-
46	3PE	A	203	-	-	23/48/48/54	-
46	3PE	Z	203	-	-	25/54/54/54	-
45	PC1	L	701	-	-	23/57/57/57	-
46	3PE	f	102	-	-	22/54/54/54	-
47	SF4	I	202	9	-	-	0/6/5/5

All (296) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	P	501	FVH	O10-C11	14.87	1.61	1.41
57	P	501	FVH	C1-N1	8.98	1.55	1.32
52	L	702	CHD	C11-C12	8.74	1.68	1.53
55	O	401	DGT	O6-C6	8.32	1.40	1.23
57	P	501	FVH	O2-C6	8.18	1.61	1.42
50	F	502	FMN	C4A-N5	7.23	1.44	1.30
57	P	501	FVH	C20-C6	-7.19	1.30	1.53
52	L	702	CHD	C16-C15	7.15	1.73	1.54
50	F	502	FMN	C10-N1	6.50	1.46	1.33
57	P	501	FVH	O2-C7	-6.44	1.30	1.45
52	L	702	CHD	C20-C17	-6.15	1.43	1.54
58	U	101	EHZ	C15-N2	5.47	1.45	1.33
57	P	501	FVH	P3-O11	5.36	1.69	1.59
58	T	101	EHZ	C15-N2	5.35	1.45	1.33
58	U	101	EHZ	C12-N1	5.33	1.45	1.33
58	T	101	EHZ	C12-N1	5.31	1.45	1.33
52	L	702	CHD	C8-C9	5.27	1.64	1.53
52	L	702	CHD	O12-C12	-5.23	1.34	1.43
52	L	702	CHD	C13-C17	5.23	1.64	1.55
57	P	501	FVH	O10-C10	-5.20	1.33	1.45
50	F	502	FMN	C5A-N5	5.14	1.49	1.39
50	F	502	FMN	C9A-N10	4.78	1.49	1.41
55	O	401	DGT	C2-N2	4.76	1.45	1.34
57	P	501	FVH	O1-C1	-4.69	1.14	1.23
50	F	502	FMN	C2-N1	4.68	1.47	1.36
55	O	401	DGT	C2-N1	4.65	1.49	1.37
52	L	702	CHD	C6-C5	4.65	1.61	1.53
55	O	401	DGT	C2-N3	4.37	1.43	1.33
50	F	502	FMN	C2-N3	4.25	1.48	1.39
52	L	702	CHD	C15-C14	4.17	1.63	1.54
57	P	501	FVH	O17-C20	3.95	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	P	501	FVH	C14-N5	3.83	1.48	1.34
50	F	502	FMN	C4-N3	3.78	1.45	1.38
52	L	702	CHD	C6-C7	3.76	1.59	1.52
50	F	502	FMN	C10-N10	3.71	1.45	1.37
57	P	501	FVH	C13-C16	-3.53	1.31	1.40
57	P	501	FVH	C21-C2	-3.33	1.48	1.53
50	F	502	FMN	O2-C2	-3.09	1.18	1.24
57	P	501	FVH	C15-N7	2.84	1.36	1.32
57	P	501	FVH	C21-N2	-2.78	1.43	1.47
55	O	401	DGT	C5-C6	-2.76	1.41	1.47
50	F	502	FMN	O4-C4	-2.68	1.18	1.23
55	O	401	DGT	C1-N9	-2.67	1.41	1.49
54	X	201	CDL	OB6-CB4	-2.66	1.39	1.46
54	M	606	CDL	OB6-CB4	-2.66	1.39	1.46
45	L	701	PC1	O21-C2	-2.61	1.40	1.46
54	r	202	CDL	OA6-CA4	-2.61	1.40	1.46
54	i	201	CDL	OB6-CB4	-2.60	1.40	1.46
45	d	202	PC1	O21-C2	-2.60	1.40	1.46
54	r	202	CDL	OB6-CB4	-2.60	1.40	1.46
54	i	201	CDL	OA6-CA4	-2.60	1.40	1.46
54	d	204	CDL	OB6-CB4	-2.59	1.40	1.46
57	P	501	FVH	O16-C19	-2.59	1.36	1.43
46	q	202	3PE	O21-C2	-2.59	1.40	1.46
54	N	403	CDL	OB6-CB4	-2.59	1.40	1.46
54	d	204	CDL	OA6-CA4	-2.58	1.40	1.46
45	H	402	PC1	O21-C2	-2.57	1.40	1.46
45	m	203	PC1	O21-C2	-2.57	1.40	1.46
46	d	201	3PE	O21-C2	-2.56	1.40	1.46
46	f	102	3PE	O21-C2	-2.55	1.40	1.46
45	A	204	PC1	O21-C2	-2.55	1.40	1.46
46	m	201	3PE	O21-C2	-2.54	1.40	1.46
46	J	202	3PE	O21-C2	-2.54	1.40	1.46
46	M	603	3PE	O21-C2	-2.53	1.40	1.46
46	b	101	3PE	O21-C2	-2.53	1.40	1.46
45	M	604	PC1	O21-C2	-2.53	1.40	1.46
46	N	401	3PE	O21-C2	-2.52	1.40	1.46
54	M	605	CDL	OA6-CA4	-2.52	1.40	1.46
57	P	501	FVH	O15-C18	-2.52	1.37	1.43
45	g	201	PC1	O21-C2	-2.52	1.40	1.46
54	M	605	CDL	OB6-CB4	-2.52	1.40	1.46
54	M	606	CDL	OA6-CA4	-2.52	1.40	1.46
45	h	202	PC1	O21-C2	-2.51	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	H	401	3PE	O21-C2	-2.51	1.40	1.46
46	b	104	3PE	O21-C2	-2.51	1.40	1.46
46	Z	202	3PE	O21-C2	-2.51	1.40	1.46
46	A	202	3PE	O21-C2	-2.51	1.40	1.46
46	Y	206	3PE	O21-C2	-2.51	1.40	1.46
46	r	201	3PE	O21-C2	-2.50	1.40	1.46
46	Z	203	3PE	O21-C2	-2.50	1.40	1.46
46	K	101	3PE	O21-C2	-2.50	1.40	1.46
46	Y	205	3PE	O21-C2	-2.49	1.40	1.46
46	f	103	3PE	O21-C2	-2.49	1.40	1.46
54	M	606	CDL	OA8-CA7	2.49	1.40	1.33
45	q	201	PC1	O21-C2	-2.49	1.40	1.46
46	L	705	3PE	O21-C2	-2.49	1.40	1.46
46	Y	201	3PE	O21-C2	-2.48	1.40	1.46
46	N	402	3PE	O21-C2	-2.48	1.40	1.46
45	B	203	PC1	O21-C2	-2.48	1.40	1.46
46	M	602	3PE	O21-C2	-2.48	1.40	1.46
45	H	403	PC1	O21-C2	-2.48	1.40	1.46
54	r	202	CDL	OB8-CB7	2.47	1.40	1.33
46	Y	208	3PE	O21-C2	-2.46	1.40	1.46
46	m	202	3PE	O21-C2	-2.46	1.40	1.46
52	L	702	CHD	C13-C12	-2.46	1.50	1.54
45	I	203	PC1	O21-C2	-2.46	1.40	1.46
46	f	101	3PE	O21-C2	-2.46	1.40	1.46
46	Y	203	3PE	O21-C2	-2.46	1.40	1.46
46	J	201	3PE	O21-C2	-2.45	1.40	1.46
46	b	102	3PE	O21-C2	-2.45	1.40	1.46
45	A	201	PC1	O21-C2	-2.45	1.40	1.46
45	I	204	PC1	O21-C2	-2.45	1.40	1.46
54	N	403	CDL	OA6-CA4	-2.45	1.40	1.46
45	h	202	PC1	O31-C31	2.44	1.40	1.33
54	M	605	CDL	OA8-CA7	2.43	1.40	1.33
45	A	204	PC1	O31-C31	2.43	1.40	1.33
45	M	604	PC1	O31-C31	2.43	1.40	1.33
54	M	605	CDL	OB8-CB7	2.42	1.40	1.33
45	d	202	PC1	O31-C31	2.42	1.40	1.33
46	m	201	3PE	O31-C31	2.42	1.40	1.33
46	Y	202	3PE	O31-C31	2.42	1.40	1.33
46	d	201	3PE	O31-C31	2.42	1.40	1.33
54	M	606	CDL	OB8-CB7	2.41	1.40	1.33
46	Y	201	3PE	O31-C31	2.41	1.40	1.33
54	i	201	CDL	OB8-CB7	2.40	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	L	705	3PE	O31-C31	2.40	1.40	1.33
54	X	201	CDL	OA8-CA7	2.40	1.40	1.33
46	r	201	3PE	O31-C31	2.40	1.40	1.33
46	A	203	3PE	O31-C31	2.40	1.40	1.33
54	N	403	CDL	OB8-CB7	2.39	1.40	1.33
45	I	203	PC1	O31-C31	2.39	1.40	1.33
46	J	202	3PE	O31-C31	2.39	1.40	1.33
54	N	403	CDL	OA8-CA7	2.39	1.40	1.33
46	A	203	3PE	O21-C2	-2.38	1.40	1.46
45	m	203	PC1	O31-C31	2.38	1.40	1.33
46	Y	206	3PE	O31-C31	2.38	1.40	1.33
46	Y	204	3PE	O31-C31	2.37	1.40	1.33
46	Y	204	3PE	O21-C2	-2.37	1.40	1.46
54	r	202	CDL	OA8-CA7	2.37	1.40	1.33
46	M	603	3PE	O31-C31	2.37	1.40	1.33
46	Z	202	3PE	O31-C31	2.37	1.40	1.33
54	d	204	CDL	OB8-CB7	2.37	1.40	1.33
45	H	403	PC1	O31-C31	2.37	1.40	1.33
46	b	104	3PE	O31-C31	2.37	1.40	1.33
45	A	201	PC1	O31-C31	2.36	1.40	1.33
45	g	201	PC1	O31-C31	2.36	1.40	1.33
46	f	103	3PE	O31-C31	2.36	1.40	1.33
46	Y	208	3PE	O31-C31	2.36	1.40	1.33
46	Y	202	3PE	O21-C2	-2.36	1.40	1.46
45	L	701	PC1	O31-C31	2.36	1.40	1.33
46	N	402	3PE	O31-C31	2.36	1.40	1.33
58	T	101	EHZ	O3-C12	-2.36	1.18	1.23
46	M	602	3PE	O31-C31	2.35	1.40	1.33
46	J	201	3PE	O31-C31	2.35	1.40	1.33
46	H	401	3PE	O31-C31	2.35	1.40	1.33
46	L	704	3PE	O31-C31	2.35	1.40	1.33
54	X	201	CDL	OB8-CB7	2.35	1.40	1.33
46	Y	205	3PE	O31-C31	2.34	1.40	1.33
46	Z	203	3PE	O31-C31	2.34	1.40	1.33
46	A	202	3PE	O31-C31	2.34	1.40	1.33
46	f	102	3PE	O31-C31	2.34	1.40	1.33
46	b	101	3PE	O31-C31	2.33	1.40	1.33
54	i	201	CDL	OA8-CA7	2.33	1.40	1.33
45	H	402	PC1	O31-C31	2.33	1.40	1.33
46	m	202	3PE	O31-C31	2.33	1.40	1.33
46	Y	203	3PE	O31-C31	2.32	1.40	1.33
46	b	102	3PE	O31-C31	2.32	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	N	401	3PE	O31-C31	2.32	1.40	1.33
54	d	204	CDL	OA8-CA6	-2.32	1.39	1.45
46	K	101	3PE	O31-C31	2.31	1.40	1.33
45	I	204	PC1	O31-C31	2.31	1.40	1.33
46	L	704	3PE	O21-C2	-2.30	1.40	1.46
45	B	203	PC1	O31-C31	2.30	1.40	1.33
46	f	101	3PE	O31-C31	2.30	1.40	1.33
54	X	201	CDL	OA6-CA4	-2.29	1.40	1.46
46	q	202	3PE	O31-C31	2.28	1.40	1.33
45	B	203	PC1	O31-C3	-2.28	1.39	1.45
58	U	101	EHZ	O4-C15	-2.28	1.18	1.23
58	T	101	EHZ	C9-S1	2.28	1.81	1.76
58	U	101	EHZ	C9-S1	2.27	1.81	1.76
57	P	501	FVH	P2-O9	2.26	1.68	1.59
46	Y	203	3PE	O31-C3	-2.26	1.40	1.45
58	T	101	EHZ	O4-C15	-2.25	1.18	1.23
54	d	204	CDL	OA8-CA7	2.25	1.39	1.33
46	b	101	3PE	O31-C3	-2.24	1.40	1.45
54	X	201	CDL	OA6-CA5	2.24	1.40	1.34
46	A	202	3PE	O31-C3	-2.24	1.40	1.45
46	q	202	3PE	O31-C3	-2.24	1.40	1.45
54	X	201	CDL	OB8-CB6	-2.23	1.40	1.45
45	I	204	PC1	O21-C21	2.23	1.40	1.34
58	U	101	EHZ	O3-C12	-2.23	1.18	1.23
45	B	203	PC1	O21-C21	2.22	1.40	1.34
46	N	401	3PE	O31-C3	-2.22	1.40	1.45
46	K	101	3PE	O31-C3	-2.22	1.40	1.45
46	Y	205	3PE	O31-C3	-2.21	1.40	1.45
45	A	201	PC1	O21-C21	2.21	1.40	1.34
54	M	606	CDL	OA6-CA5	2.21	1.40	1.34
45	I	204	PC1	O31-C3	-2.20	1.40	1.45
46	L	704	3PE	O21-C21	2.20	1.40	1.34
46	m	202	3PE	O21-C21	2.20	1.40	1.34
57	P	501	FVH	P1-O5	2.20	1.58	1.50
45	g	201	PC1	O31-C3	-2.20	1.40	1.45
45	A	204	PC1	O31-C3	-2.20	1.40	1.45
46	H	401	3PE	O31-C3	-2.19	1.40	1.45
55	O	401	DGT	PG-O1G	-2.19	1.46	1.54
54	d	204	CDL	OB8-CB6	-2.19	1.40	1.45
57	P	501	FVH	P3-O12	2.19	1.57	1.50
46	f	101	3PE	O31-C3	-2.19	1.40	1.45
45	H	403	PC1	O31-C3	-2.19	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	Y	204	3PE	O21-C21	2.18	1.40	1.34
54	N	403	CDL	OA6-CA5	2.18	1.40	1.34
46	m	202	3PE	O31-C3	-2.18	1.40	1.45
45	H	402	PC1	O31-C3	-2.17	1.40	1.45
46	Y	203	3PE	O21-C21	2.17	1.40	1.34
46	Z	203	3PE	O31-C3	-2.17	1.40	1.45
46	f	102	3PE	O31-C3	-2.17	1.40	1.45
46	b	102	3PE	O31-C3	-2.17	1.40	1.45
54	N	403	CDL	OB8-CB6	-2.16	1.40	1.45
46	Y	208	3PE	O31-C3	-2.16	1.40	1.45
54	i	201	CDL	OA8-CA6	-2.16	1.40	1.45
46	Y	202	3PE	O21-C21	2.16	1.40	1.34
46	L	705	3PE	O31-C3	-2.16	1.40	1.45
46	r	201	3PE	O31-C3	-2.16	1.40	1.45
54	r	202	CDL	OA8-CA6	-2.16	1.40	1.45
46	Y	206	3PE	O31-C3	-2.16	1.40	1.45
54	d	204	CDL	OA6-CA5	2.15	1.40	1.34
45	m	203	PC1	O21-C21	2.15	1.40	1.34
45	g	201	PC1	O21-C21	2.15	1.40	1.34
46	N	402	3PE	O31-C3	-2.15	1.40	1.45
45	L	701	PC1	O31-C3	-2.15	1.40	1.45
46	M	602	3PE	O21-C21	2.15	1.40	1.34
45	M	604	PC1	O21-C21	2.15	1.40	1.34
46	A	203	3PE	O21-C21	2.15	1.40	1.34
55	O	401	DGT	PG-O2G	-2.15	1.46	1.54
46	L	705	3PE	O21-C21	2.14	1.40	1.34
54	M	605	CDL	OB8-CB6	-2.14	1.40	1.45
46	f	103	3PE	O31-C3	-2.14	1.40	1.45
46	b	102	3PE	O21-C21	2.14	1.40	1.34
46	Y	204	3PE	O31-C3	-2.14	1.40	1.45
46	K	101	3PE	O21-C21	2.14	1.40	1.34
46	f	101	3PE	O21-C21	2.14	1.40	1.34
54	M	605	CDL	OA6-CA5	2.14	1.40	1.34
45	A	201	PC1	O31-C3	-2.14	1.40	1.45
45	H	402	PC1	O21-C21	2.14	1.40	1.34
46	J	201	3PE	O21-C21	2.13	1.40	1.34
54	N	403	CDL	OB6-CB5	2.13	1.40	1.34
46	Z	202	3PE	O21-C21	2.13	1.40	1.34
46	r	201	3PE	O21-C21	2.13	1.40	1.34
45	M	604	PC1	O31-C3	-2.12	1.40	1.45
46	A	203	3PE	O31-C3	-2.12	1.40	1.45
46	b	101	3PE	O21-C21	2.12	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	m	203	PC1	O31-C3	-2.12	1.40	1.45
46	b	104	3PE	O31-C3	-2.12	1.40	1.45
45	h	202	PC1	O21-C21	2.12	1.40	1.34
46	Z	203	3PE	O21-C21	2.12	1.40	1.34
46	J	202	3PE	O31-C3	-2.12	1.40	1.45
46	Y	208	3PE	O21-C21	2.12	1.40	1.34
46	A	202	3PE	O21-C21	2.12	1.40	1.34
45	q	201	PC1	O21-C21	2.12	1.40	1.34
46	J	201	3PE	O31-C3	-2.11	1.40	1.45
45	d	202	PC1	O21-C21	2.11	1.40	1.34
46	N	401	3PE	O21-C21	2.11	1.40	1.34
54	M	606	CDL	OB8-CB6	-2.11	1.40	1.45
46	m	201	3PE	O31-C3	-2.11	1.40	1.45
54	i	201	CDL	OB8-CB6	-2.11	1.40	1.45
45	I	203	PC1	O21-C21	2.10	1.40	1.34
54	M	605	CDL	OB6-CB5	2.10	1.40	1.34
46	H	401	3PE	O21-C21	2.10	1.40	1.34
46	d	201	3PE	O31-C3	-2.10	1.40	1.45
45	H	403	PC1	O21-C21	2.10	1.40	1.34
54	X	201	CDL	OA8-CA6	-2.10	1.40	1.45
46	M	602	3PE	O31-C3	-2.10	1.40	1.45
54	r	202	CDL	OB6-CB5	2.10	1.40	1.34
46	f	103	3PE	O21-C21	2.10	1.40	1.34
45	d	202	PC1	O31-C3	-2.10	1.40	1.45
46	Y	206	3PE	O21-C21	2.09	1.40	1.34
45	L	701	PC1	O21-C21	2.09	1.40	1.34
54	d	204	CDL	OB6-CB5	2.09	1.40	1.34
45	A	204	PC1	O21-C21	2.09	1.40	1.34
46	Y	201	3PE	O31-C3	-2.08	1.40	1.45
54	M	606	CDL	OA8-CA6	-2.08	1.40	1.45
46	f	102	3PE	O21-C21	2.08	1.40	1.34
46	b	104	3PE	O21-C21	2.08	1.40	1.34
46	Y	205	3PE	O21-C21	2.08	1.40	1.34
45	h	202	PC1	O31-C3	-2.08	1.40	1.45
54	M	605	CDL	OA8-CA6	-2.08	1.40	1.45
46	M	603	3PE	O31-C3	-2.08	1.40	1.45
54	i	201	CDL	OB6-CB5	2.08	1.40	1.34
45	q	201	PC1	O31-C3	-2.08	1.40	1.45
54	N	403	CDL	OA8-CA6	-2.08	1.40	1.45
46	N	402	3PE	O21-C21	2.08	1.40	1.34
46	q	202	3PE	O21-C21	2.08	1.40	1.34
46	L	704	3PE	O31-C3	-2.08	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	I	203	PC1	O31-C3	-2.07	1.40	1.45
46	Z	202	3PE	O31-C3	-2.07	1.40	1.45
54	r	202	CDL	OB8-CB6	-2.07	1.40	1.45
46	Y	201	3PE	O21-C21	2.07	1.40	1.34
46	M	603	3PE	O21-C21	2.06	1.40	1.34
46	d	201	3PE	O21-C21	2.05	1.40	1.34
46	J	202	3PE	O21-C21	2.05	1.40	1.34
46	Y	202	3PE	O31-C3	-2.04	1.40	1.45
57	P	501	FVH	C9-C10	2.03	1.57	1.51
54	i	201	CDL	OA6-CA5	2.03	1.40	1.34
54	r	202	CDL	OA6-CA5	2.02	1.40	1.34
54	M	606	CDL	OB6-CB5	2.02	1.40	1.34
54	X	201	CDL	OB6-CB5	2.01	1.40	1.34

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	P	501	FVH	C5-N2-C21	11.31	119.35	108.19
57	P	501	FVH	C13-C14-N5	8.87	133.82	120.35
57	P	501	FVH	C11-N3-C16	-7.37	113.69	126.64
52	L	702	CHD	C13-C17-C20	-6.73	111.46	119.50
57	P	501	FVH	C2-C21-N2	6.58	120.28	111.14
57	P	501	FVH	C3-C4-C5	6.46	119.90	110.85
57	P	501	FVH	N5-C14-N6	-6.27	105.56	118.57
58	T	101	EHZ	C8-C9-S1	5.88	120.91	113.63
52	L	702	CHD	C14-C13-C12	5.53	112.55	107.40
57	P	501	FVH	N7-C15-N6	-5.41	120.22	128.68
57	P	501	FVH	C4-C5-N2	5.33	120.26	111.28
57	P	501	FVH	C3-C2-C21	5.31	119.43	109.92
57	P	501	FVH	C21-C2-C1	5.05	119.55	110.07
52	L	702	CHD	C17-C13-C12	5.04	122.27	117.67
52	L	702	CHD	C17-C13-C14	4.99	105.12	100.09
57	P	501	FVH	C3-C2-C1	4.81	118.93	110.76
58	U	101	EHZ	C8-C9-S1	4.78	119.55	113.63
50	F	502	FMN	C9-C8-C7	4.64	126.32	119.67
50	F	502	FMN	C7M-C7-C6	4.41	127.64	119.49
45	H	402	PC1	O21-C21-C22	4.35	120.89	111.50
45	I	204	PC1	O21-C21-C22	4.21	120.57	111.50
46	m	202	3PE	O21-C21-C22	4.20	120.56	111.50
54	M	606	CDL	OA6-CA5-C11	4.19	120.52	111.50
45	B	203	PC1	O21-C21-C22	4.17	120.48	111.50
46	q	202	3PE	O21-C21-C22	4.16	120.46	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	N	402	3PE	O21-C21-C22	4.15	120.44	111.50
46	b	102	3PE	O21-C21-C22	4.14	120.43	111.50
52	L	702	CHD	C18-C13-C12	-4.12	104.87	109.07
46	Y	203	3PE	O21-C21-C22	4.08	120.29	111.50
46	L	705	3PE	O21-C21-C22	4.08	120.29	111.50
45	h	202	PC1	O21-C21-C22	4.07	120.28	111.50
46	J	201	3PE	O21-C21-C22	4.07	120.27	111.50
46	f	103	3PE	O21-C21-C22	4.06	120.24	111.50
54	X	201	CDL	OB6-CB5-C51	4.05	120.22	111.50
54	i	201	CDL	OA6-CA5-C11	4.05	120.22	111.50
46	J	202	3PE	O21-C21-C22	4.04	120.21	111.50
46	m	201	3PE	O21-C21-C22	4.03	120.19	111.50
54	M	606	CDL	OB6-CB5-C51	4.03	120.18	111.50
46	M	603	3PE	O21-C21-C22	4.01	120.14	111.50
46	Y	206	3PE	O21-C21-C22	3.99	120.11	111.50
45	I	203	PC1	O21-C21-C22	3.99	120.10	111.50
45	m	203	PC1	O21-C21-C22	3.99	120.09	111.50
46	b	104	3PE	O21-C21-C22	3.98	120.08	111.50
46	Y	208	3PE	O21-C21-C22	3.98	120.08	111.50
54	M	605	CDL	OB6-CB5-C51	3.98	120.08	111.50
45	A	201	PC1	O21-C21-C22	3.98	120.08	111.50
46	L	704	3PE	O21-C21-C22	3.97	120.07	111.50
45	A	204	PC1	O21-C21-C22	3.96	120.03	111.50
46	Z	203	3PE	O21-C21-C22	3.95	120.02	111.50
45	M	604	PC1	O21-C21-C22	3.95	120.02	111.50
46	f	102	3PE	O21-C21-C22	3.95	120.01	111.50
46	Y	204	3PE	O21-C21-C22	3.93	119.97	111.50
54	r	202	CDL	OA6-CA5-C11	3.92	119.96	111.50
46	Y	201	3PE	O21-C21-C22	3.92	119.95	111.50
45	g	201	PC1	O21-C21-C22	3.90	119.90	111.50
54	N	403	CDL	OB6-CB5-C51	3.89	119.89	111.50
46	A	203	3PE	O21-C21-C22	3.88	119.86	111.50
46	Y	205	3PE	O21-C21-C22	3.87	119.85	111.50
52	L	702	CHD	C18-C13-C17	-3.85	105.18	111.21
46	N	401	3PE	O21-C21-C22	3.85	119.79	111.50
46	Y	202	3PE	O21-C21-C22	3.85	119.79	111.50
54	r	202	CDL	OB6-CB5-C51	3.83	119.76	111.50
46	r	201	3PE	O21-C21-C22	3.83	119.75	111.50
45	L	701	PC1	O21-C21-C22	3.82	119.73	111.50
54	M	605	CDL	OA6-CA5-C11	3.82	119.72	111.50
54	i	201	CDL	OB6-CB5-C51	3.81	119.71	111.50
46	d	201	3PE	O21-C21-C22	3.79	119.66	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	M	602	3PE	O21-C21-C22	3.75	119.59	111.50
45	d	202	PC1	O21-C21-C22	3.66	119.40	111.50
54	d	204	CDL	OA6-CA5-C11	3.66	119.39	111.50
52	L	702	CHD	C18-C13-C14	-3.65	105.50	111.21
46	A	202	3PE	O21-C21-C22	3.64	119.35	111.50
46	K	101	3PE	O21-C21-C22	3.61	119.27	111.50
58	T	101	EHZ	C13-C12-N1	3.55	122.40	116.42
46	Z	202	3PE	O21-C21-C22	3.54	119.14	111.50
54	N	403	CDL	OA6-CA5-C11	3.50	119.05	111.50
46	b	101	3PE	O21-C21-C22	3.48	119.01	111.50
46	H	401	3PE	O21-C21-C22	3.37	120.19	110.80
54	X	201	CDL	OA6-CA5-C11	3.36	118.73	111.50
54	d	204	CDL	OB6-CB5-C51	3.33	120.09	110.80
46	J	202	3PE	O31-C31-C32	3.32	120.09	111.38
46	f	101	3PE	O21-C21-C22	3.29	119.97	110.80
45	q	201	PC1	O21-C21-C22	3.28	119.95	110.80
50	F	502	FMN	C8M-C8-C7	-3.24	114.10	120.74
50	F	502	FMN	C4-N3-C2	-3.23	119.68	125.64
45	H	403	PC1	O21-C21-C22	3.21	119.74	110.80
55	O	401	DGT	C5-C6-N1	3.17	119.54	113.95
55	O	401	DGT	C2-N1-C6	-3.06	119.46	125.10
55	O	401	DGT	PB-O3B-PG	-3.01	122.50	132.83
54	M	606	CDL	OA8-CA7-C31	2.95	121.16	111.91
55	O	401	DGT	O2G-PG-O3B	2.94	114.50	104.64
52	L	702	CHD	C1-C10-C5	2.87	112.02	107.77
54	X	201	CDL	OB8-CB7-C71	2.87	120.91	111.91
46	r	201	3PE	O31-C31-C32	2.85	120.84	111.91
45	H	403	PC1	O31-C31-C32	2.79	120.67	111.91
45	B	203	PC1	O31-C31-C32	2.78	120.64	111.91
46	Y	204	3PE	O31-C31-C32	2.76	120.57	111.91
50	F	502	FMN	C4A-C10-N10	2.76	120.52	116.48
45	m	203	PC1	O31-C31-C32	2.75	120.53	111.91
54	M	605	CDL	OA8-CA7-C31	2.75	120.53	111.91
54	i	201	CDL	OA8-CA7-C31	2.74	120.51	111.91
55	O	401	DGT	O1G-PG-O3B	2.74	113.82	104.64
54	M	606	CDL	OB8-CB7-C71	2.73	120.48	111.91
46	Y	203	3PE	O31-C31-C32	2.73	120.47	111.91
52	L	702	CHD	C23-C22-C20	-2.72	109.55	114.52
46	Y	202	3PE	O31-C31-C32	2.70	120.38	111.91
46	m	201	3PE	O31-C31-C32	2.69	120.34	111.91
54	d	204	CDL	OA8-CA7-C31	2.68	120.33	111.91
54	N	403	CDL	OA8-CA7-C31	2.66	120.25	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	Y	205	3PE	O31-C31-C32	2.65	120.24	111.91
46	Z	202	3PE	O31-C31-C32	2.65	120.23	111.91
46	b	104	3PE	O31-C31-C32	2.65	120.23	111.91
46	L	704	3PE	O31-C31-C32	2.65	120.23	111.91
58	T	101	EHZ	O2-C9-S1	-2.65	119.17	122.61
45	M	604	PC1	O31-C31-C32	2.65	120.22	111.91
46	f	103	3PE	O31-C31-C32	2.64	120.20	111.91
46	Y	206	3PE	O31-C31-C32	2.64	120.19	111.91
46	H	401	3PE	O31-C31-C32	2.64	120.18	111.91
45	A	204	PC1	O31-C31-C32	2.63	120.17	111.91
46	b	102	3PE	O31-C31-C32	2.62	120.14	111.91
55	O	401	DGT	PA-O3A-PB	-2.62	123.83	132.83
46	Y	208	3PE	O31-C31-C32	2.62	120.13	111.91
46	f	102	3PE	O31-C31-C32	2.62	120.12	111.91
46	N	402	3PE	O31-C31-C32	2.61	120.10	111.91
46	m	202	3PE	O31-C31-C32	2.60	120.08	111.91
46	K	101	3PE	O31-C31-C32	2.60	120.08	111.91
45	A	201	PC1	O31-C31-C32	2.60	120.07	111.91
46	Y	201	3PE	O31-C31-C32	2.60	120.06	111.91
45	d	202	PC1	O31-C31-C32	2.60	120.06	111.91
45	h	202	PC1	O31-C31-C32	2.60	120.06	111.91
50	F	502	FMN	C6-C7-C8	-2.59	115.95	119.67
46	A	202	3PE	O31-C31-C32	2.59	120.04	111.91
46	L	705	3PE	O31-C31-C32	2.58	120.00	111.91
46	A	203	3PE	O31-C31-C32	2.58	120.00	111.91
45	I	204	PC1	O31-C31-C32	2.58	120.00	111.91
58	U	101	EHZ	C10-S1-C9	2.57	109.89	101.87
46	N	401	3PE	O31-C31-C32	2.57	119.97	111.91
46	M	603	3PE	O31-C31-C32	2.57	119.96	111.91
45	g	201	PC1	O31-C31-C32	2.56	119.96	111.91
54	X	201	CDL	OA8-CA7-C31	2.56	119.96	111.91
52	L	702	CHD	C15-C14-C8	2.56	121.91	118.33
45	L	701	PC1	O31-C31-C32	2.56	119.93	111.91
54	r	202	CDL	OA8-CA7-C31	2.55	119.92	111.91
54	d	204	CDL	OB8-CB7-C71	2.54	119.89	111.91
54	i	201	CDL	OB8-CB7-C71	2.54	119.89	111.91
54	N	403	CDL	OB8-CB7-C71	2.54	119.89	111.91
46	b	101	3PE	O31-C31-C32	2.54	119.88	111.91
54	M	605	CDL	OB8-CB7-C71	2.54	119.87	111.91
46	f	101	3PE	O31-C31-C32	2.54	119.87	111.91
46	J	201	3PE	O31-C31-C32	2.53	119.86	111.91
54	r	202	CDL	OB8-CB7-C71	2.53	119.83	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	M	602	3PE	O31-C31-C32	2.52	119.83	111.91
46	q	202	3PE	O31-C31-C32	2.51	119.79	111.91
50	F	502	FMN	C4A-C4-N3	2.47	119.45	113.19
45	I	203	PC1	O31-C31-C32	2.46	119.62	111.91
46	d	201	3PE	O31-C31-C32	2.46	119.62	111.91
57	P	501	FVH	P2-O6-P1	-2.43	124.48	132.83
46	Z	203	3PE	O31-C31-C32	2.42	119.52	111.91
52	L	702	CHD	C9-C10-C5	2.41	111.97	108.58
50	F	502	FMN	O4-C4-C4A	-2.40	120.24	126.60
45	H	402	PC1	O31-C31-C32	2.39	119.42	111.91
50	F	502	FMN	C5A-C9A-N10	2.34	120.37	117.95
52	L	702	CHD	C1-C2-C3	2.33	113.46	110.47
50	F	502	FMN	C9A-C5A-N5	-2.31	119.92	122.43
58	U	101	EHZ	C13-C12-N1	2.29	120.28	116.42
58	T	101	EHZ	C10-S1-C9	2.28	108.98	101.87
57	P	501	FVH	C2-C1-N1	2.27	120.19	116.54
52	L	702	CHD	C6-C5-C4	-2.24	108.61	111.19
55	O	401	DGT	O1A-PA-O2A	-2.22	101.26	112.24
50	F	502	FMN	C10-C4A-N5	-2.21	120.16	124.86
50	F	502	FMN	C4-C4A-C10	2.18	120.45	116.79
58	T	101	EHZ	O3-C12-N1	-2.18	118.91	123.01
55	O	401	DGT	O1B-PB-O2B	-2.17	101.51	112.24
58	U	101	EHZ	C5-C6-C7	-2.16	108.63	114.85
50	F	502	FMN	C6-C5A-C9A	2.15	121.98	118.94
58	U	101	EHZ	C16-C15-N2	2.14	120.84	116.58
48	h	201	PLC	C3-C2-C1	2.13	116.83	111.79
58	U	101	EHZ	C14-C13-C12	-2.13	108.81	112.36
50	F	502	FMN	C7M-C7-C8	-2.11	116.41	120.74
55	O	401	DGT	C2'-C3'-C4'	2.08	107.10	102.76
50	F	502	FMN	C4A-C10-N1	-2.08	119.90	124.73
58	U	101	EHZ	C11-N1-C12	-2.08	118.98	122.84
52	L	702	CHD	C19-C10-C9	-2.07	108.33	111.18
52	L	702	CHD	C11-C9-C10	-2.05	111.62	113.73
52	L	702	CHD	C5-C6-C7	-2.05	112.20	114.46
55	O	401	DGT	O6-C6-C5	-2.04	120.38	124.37
52	L	702	CHD	C4-C3-C2	2.02	112.97	110.55

There are no chirality outliers.

All (1317) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	201	PC1	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
45	A	201	PC1	C11-O13-P-O14
45	A	201	PC1	C11-O13-P-O11
45	A	201	PC1	O13-C11-C12-N
45	A	204	PC1	C22-C21-O21-C2
45	B	203	PC1	C11-O13-P-O14
45	B	203	PC1	C1-O11-P-O12
45	B	203	PC1	C1-O11-P-O14
45	B	203	PC1	C2-C1-O11-P
45	B	203	PC1	O22-C21-O21-C2
45	H	402	PC1	C1-O11-P-O12
45	H	402	PC1	C1-O11-P-O14
45	H	402	PC1	O13-C11-C12-N
45	H	403	PC1	O13-C11-C12-N
45	I	203	PC1	C1-O11-P-O12
45	I	203	PC1	C1-O11-P-O14
45	I	203	PC1	C1-O11-P-O13
45	I	203	PC1	O13-C11-C12-N
45	I	204	PC1	C1-O11-P-O12
45	I	204	PC1	C1-O11-P-O14
45	L	701	PC1	C11-O13-P-O14
45	L	701	PC1	O21-C2-C3-O31
45	M	604	PC1	C11-O13-P-O12
45	M	604	PC1	C11-O13-P-O14
45	M	604	PC1	C1-O11-P-O12
45	M	604	PC1	C1-O11-P-O14
45	M	604	PC1	C22-C21-O21-C2
45	d	202	PC1	C11-O13-P-O12
45	d	202	PC1	C11-O13-P-O14
45	d	202	PC1	C11-O13-P-O11
45	d	202	PC1	C1-O11-P-O12
45	d	202	PC1	C1-O11-P-O14
45	d	202	PC1	C1-O11-P-O13
45	g	201	PC1	C1-O11-P-O12
45	g	201	PC1	C1-O11-P-O14
45	g	201	PC1	C1-O11-P-O13
45	g	201	PC1	O13-C11-C12-N
45	m	203	PC1	C11-O13-P-O12
45	m	203	PC1	C11-O13-P-O14
45	m	203	PC1	C11-O13-P-O11
45	m	203	PC1	C1-O11-P-O12
45	m	203	PC1	C1-O11-P-O14
45	m	203	PC1	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
45	m	203	PC1	C22-C21-O21-C2
45	m	203	PC1	O32-C31-O31-C3
45	q	201	PC1	C11-O13-P-O14
45	q	201	PC1	C1-O11-P-O13
46	A	202	3PE	C11-O13-P-O12
46	H	401	3PE	C1-O11-P-O13
46	H	401	3PE	C11-O13-P-O12
46	H	401	3PE	C11-O13-P-O14
46	H	401	3PE	O22-C21-O21-C2
46	H	401	3PE	C22-C21-O21-C2
46	J	201	3PE	C1-O11-P-O12
46	J	201	3PE	C1-O11-P-O14
46	J	201	3PE	C12-C11-O13-P
46	J	201	3PE	O22-C21-O21-C2
46	J	202	3PE	C11-O13-P-O14
46	J	202	3PE	C22-C21-O21-C2
46	K	101	3PE	C1-O11-P-O14
46	K	101	3PE	C11-O13-P-O11
46	K	101	3PE	C11-O13-P-O12
46	K	101	3PE	C11-O13-P-O14
46	L	704	3PE	C1-O11-P-O12
46	L	704	3PE	C11-O13-P-O12
46	L	704	3PE	C11-O13-P-O14
46	L	704	3PE	C22-C21-O21-C2
46	L	705	3PE	C22-C21-O21-C2
46	M	602	3PE	O13-C11-C12-N
46	M	603	3PE	C11-O13-P-O11
46	M	603	3PE	C11-O13-P-O14
46	N	402	3PE	C11-O13-P-O11
46	N	402	3PE	C11-O13-P-O12
46	N	402	3PE	O13-C11-C12-N
46	N	402	3PE	O22-C21-O21-C2
46	N	402	3PE	C22-C21-O21-C2
46	Y	201	3PE	C1-O11-P-O12
46	Y	201	3PE	C1-O11-P-O14
46	Y	201	3PE	C11-O13-P-O11
46	Y	201	3PE	C11-O13-P-O14
46	Y	202	3PE	C11-O13-P-O14
46	Y	202	3PE	C22-C21-O21-C2
46	Y	203	3PE	C1-O11-P-O12
46	Y	203	3PE	C1-O11-P-O13
46	Y	203	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
46	Y	203	3PE	C22-C21-O21-C2
46	Y	204	3PE	C22-C21-O21-C2
46	Y	206	3PE	C11-O13-P-O11
46	Y	206	3PE	C11-O13-P-O14
46	Y	206	3PE	O22-C21-O21-C2
46	Y	208	3PE	C1-O11-P-O12
46	Y	208	3PE	C1-O11-P-O14
46	Y	208	3PE	C11-O13-P-O11
46	Y	208	3PE	C11-O13-P-O12
46	Y	208	3PE	C11-O13-P-O14
46	Y	208	3PE	O22-C21-O21-C2
46	Y	208	3PE	C22-C21-O21-C2
46	Z	202	3PE	O21-C2-C3-O31
46	Z	203	3PE	C1-O11-P-O12
46	Z	203	3PE	C1-O11-P-O14
46	b	101	3PE	C1-O11-P-O14
46	b	101	3PE	C11-O13-P-O11
46	b	102	3PE	C1-O11-P-O13
46	b	102	3PE	O21-C2-C3-O31
46	b	102	3PE	O22-C21-O21-C2
46	b	104	3PE	C11-O13-P-O12
46	b	104	3PE	C11-O13-P-O14
46	b	104	3PE	O13-C11-C12-N
46	b	104	3PE	C22-C21-O21-C2
46	d	201	3PE	C1-O11-P-O12
46	d	201	3PE	C22-C21-O21-C2
46	f	101	3PE	C1-O11-P-O12
46	f	101	3PE	C1-O11-P-O14
46	f	101	3PE	C12-C11-O13-P
46	f	101	3PE	O21-C2-C3-O31
46	f	102	3PE	C1-O11-P-O13
46	f	102	3PE	C1-O11-P-O14
46	f	102	3PE	C11-O13-P-O11
46	f	102	3PE	C22-C21-O21-C2
46	f	103	3PE	C11-O13-P-O12
46	f	103	3PE	O11-C1-C2-O21
46	f	103	3PE	C22-C21-O21-C2
46	m	201	3PE	C11-O13-P-O11
46	m	201	3PE	C11-O13-P-O12
46	m	201	3PE	C11-O13-P-O14
46	m	201	3PE	O32-C31-O31-C3
46	m	201	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
46	m	201	3PE	O22-C21-O21-C2
46	m	201	3PE	C22-C21-O21-C2
46	m	202	3PE	C11-O13-P-O12
46	m	202	3PE	C11-O13-P-O14
46	m	202	3PE	O22-C21-O21-C2
46	q	202	3PE	C11-O13-P-O12
46	q	202	3PE	C11-O13-P-O14
46	q	202	3PE	O21-C2-C3-O31
46	q	202	3PE	O22-C21-O21-C2
46	r	201	3PE	C1-O11-P-O12
46	r	201	3PE	C11-O13-P-O12
46	r	201	3PE	C11-O13-P-O14
46	r	201	3PE	C22-C21-O21-C2
48	B	202	PLC	C4-O4P-P-O1P
48	L	703	PLC	C1-O3P-P-O1P
48	L	703	PLC	C1-O3P-P-O2P
48	L	703	PLC	C1-O3P-P-O4P
48	O	403	PLC	C1-O3P-P-O2P
48	Y	207	PLC	C1-O3P-P-O4P
48	Z	201	PLC	C1'-C'-O2-C2
48	Z	201	PLC	C4-O4P-P-O1P
48	b	103	PLC	C1-O3P-P-O4P
48	d	203	PLC	C1-O3P-P-O2P
48	d	203	PLC	C4-O4P-P-O1P
48	d	203	PLC	C4-O4P-P-O2P
50	F	502	FMN	C5'-O5'-P-O1P
50	F	502	FMN	C5'-O5'-P-O2P
50	F	502	FMN	C5'-O5'-P-O3P
54	M	606	CDL	O1-C1-CA2-OA2
54	M	606	CDL	CA2-OA2-PA1-OA3
54	M	606	CDL	CA2-OA2-PA1-OA4
54	M	606	CDL	CA3-OA5-PA1-OA3
54	M	606	CDL	CA3-OA5-PA1-OA4
54	M	606	CDL	OB5-CB3-CB4-OB6
54	M	606	CDL	OB7-CB5-OB6-CB4
54	M	606	CDL	C51-CB5-OB6-CB4
54	N	403	CDL	CB3-OB5-PB2-OB3
54	N	403	CDL	CB3-OB5-PB2-OB4
54	N	403	CDL	C51-CB5-OB6-CB4
54	X	201	CDL	C1-CA2-OA2-PA1
54	X	201	CDL	CA2-OA2-PA1-OA4
54	X	201	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
54	X	201	CDL	C51-CB5-OB6-CB4
54	d	204	CDL	O1-C1-CA2-OA2
54	d	204	CDL	OB5-CB3-CB4-OB6
54	d	204	CDL	OB7-CB5-OB6-CB4
54	i	201	CDL	C11-CA5-OA6-CA4
54	i	201	CDL	CB2-OB2-PB2-OB3
54	i	201	CDL	CB2-OB2-PB2-OB4
54	r	202	CDL	CA3-OA5-PA1-OA4
54	r	202	CDL	CB2-OB2-PB2-OB3
54	r	202	CDL	OB5-CB3-CB4-OB6
55	O	401	DGT	C5'-O5'-PA-O1A
55	O	401	DGT	C5'-O5'-PA-O2A
57	P	501	FVH	N1-C1-C2-C21
57	P	501	FVH	O1-C1-C2-C21
57	P	501	FVH	O2-C6-N2-C5
57	P	501	FVH	C20-C6-N2-C5
57	P	501	FVH	C8-O3-P1-O5
57	P	501	FVH	C8-O3-P1-O6
57	P	501	FVH	C9-O9-P2-O7
57	P	501	FVH	C9-O9-P2-O8
58	T	101	EHZ	C6-C7-C8-C9
58	T	101	EHZ	S1-C10-C11-N1
58	U	101	EHZ	O1-C7-C8-C9
58	U	101	EHZ	C6-C7-C8-C9
58	U	101	EHZ	S1-C10-C11-N1
58	U	101	EHZ	C11-C10-S1-C9
58	U	101	EHZ	C15-C16-C17-C18
58	U	101	EHZ	C15-C16-C17-C19
58	U	101	EHZ	C15-C16-C17-C20
58	U	101	EHZ	O2-C9-S1-C10
58	U	101	EHZ	C8-C9-S1-C10
45	A	204	PC1	O32-C31-O31-C3
46	A	202	3PE	O32-C31-O31-C3
46	J	202	3PE	O32-C31-O31-C3
46	L	705	3PE	O32-C31-O31-C3
46	f	102	3PE	O32-C31-O31-C3
54	M	605	CDL	OA9-CA7-OA8-CA6
54	X	201	CDL	OA9-CA7-OA8-CA6
54	X	201	CDL	OB9-CB7-OB8-CB6
45	A	204	PC1	C32-C31-O31-C3
54	M	605	CDL	C31-CA7-OA8-CA6
54	X	201	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
45	B	203	PC1	O32-C31-O31-C3
45	H	403	PC1	O32-C31-O31-C3
45	L	701	PC1	O32-C31-O31-C3
45	d	202	PC1	O32-C31-O31-C3
45	h	202	PC1	O32-C31-O31-C3
46	A	203	3PE	O32-C31-O31-C3
46	H	401	3PE	O32-C31-O31-C3
46	J	201	3PE	O32-C31-O31-C3
46	N	401	3PE	O32-C31-O31-C3
46	Y	203	3PE	O32-C31-O31-C3
46	Y	204	3PE	O32-C31-O31-C3
46	Y	205	3PE	O32-C31-O31-C3
46	Y	206	3PE	O32-C31-O31-C3
46	b	102	3PE	O32-C31-O31-C3
46	b	104	3PE	O32-C31-O31-C3
46	r	201	3PE	O32-C31-O31-C3
54	M	606	CDL	OA9-CA7-OA8-CA6
54	M	606	CDL	OB9-CB7-OB8-CB6
54	i	201	CDL	OA9-CA7-OA8-CA6
45	A	204	PC1	O22-C21-O21-C2
45	M	604	PC1	O22-C21-O21-C2
45	h	202	PC1	O22-C21-O21-C2
46	J	202	3PE	O22-C21-O21-C2
46	L	704	3PE	O22-C21-O21-C2
46	L	705	3PE	O22-C21-O21-C2
46	Y	202	3PE	O22-C21-O21-C2
46	Y	203	3PE	O22-C21-O21-C2
46	Y	204	3PE	O22-C21-O21-C2
46	f	102	3PE	O22-C21-O21-C2
46	f	103	3PE	O22-C21-O21-C2
46	r	201	3PE	O22-C21-O21-C2
48	Z	201	PLC	O'-C'-O2-C2
54	N	403	CDL	OB7-CB5-OB6-CB4
54	X	201	CDL	OA7-CA5-OA6-CA4
54	X	201	CDL	OB7-CB5-OB6-CB4
54	i	201	CDL	OA7-CA5-OA6-CA4
54	i	201	CDL	OB9-CB7-OB8-CB6
45	B	203	PC1	C32-C31-O31-C3
45	H	403	PC1	C32-C31-O31-C3
45	d	202	PC1	C32-C31-O31-C3
45	h	202	PC1	C32-C31-O31-C3
45	m	203	PC1	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
46	A	202	3PE	C32-C31-O31-C3
46	A	203	3PE	C32-C31-O31-C3
46	H	401	3PE	C32-C31-O31-C3
46	J	201	3PE	C32-C31-O31-C3
46	J	202	3PE	C32-C31-O31-C3
46	L	705	3PE	C32-C31-O31-C3
46	Y	203	3PE	C32-C31-O31-C3
46	Y	204	3PE	C32-C31-O31-C3
46	Y	205	3PE	C32-C31-O31-C3
46	Y	206	3PE	C32-C31-O31-C3
46	f	102	3PE	C32-C31-O31-C3
46	r	201	3PE	C32-C31-O31-C3
54	M	605	CDL	C71-CB7-OB8-CB6
54	M	606	CDL	C31-CA7-OA8-CA6
54	M	606	CDL	C71-CB7-OB8-CB6
54	N	403	CDL	C31-CA7-OA8-CA6
54	X	201	CDL	C71-CB7-OB8-CB6
45	q	201	PC1	O32-C31-O31-C3
45	B	203	PC1	C22-C21-O21-C2
45	h	202	PC1	C22-C21-O21-C2
46	J	201	3PE	C22-C21-O21-C2
46	Y	206	3PE	C22-C21-O21-C2
46	b	102	3PE	C22-C21-O21-C2
46	m	202	3PE	C22-C21-O21-C2
46	q	202	3PE	C22-C21-O21-C2
54	d	204	CDL	C51-CB5-OB6-CB4
52	L	702	CHD	C20-C22-C23-C24
54	d	204	CDL	OA9-CA7-OA8-CA6
45	L	701	PC1	C32-C31-O31-C3
46	N	401	3PE	C32-C31-O31-C3
46	b	102	3PE	C32-C31-O31-C3
46	b	104	3PE	C32-C31-O31-C3
46	d	201	3PE	C32-C31-O31-C3
46	f	101	3PE	C32-C31-O31-C3
54	i	201	CDL	C31-CA7-OA8-CA6
54	i	201	CDL	C71-CB7-OB8-CB6
45	q	201	PC1	C32-C31-O31-C3
45	m	203	PC1	O22-C21-O21-C2
46	b	104	3PE	O22-C21-O21-C2
46	d	201	3PE	O22-C21-O21-C2
45	M	604	PC1	O32-C31-O31-C3
46	f	101	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
46	f	103	3PE	O32-C31-O31-C3
54	M	605	CDL	OB9-CB7-OB8-CB6
54	N	403	CDL	OB9-CB7-OB8-CB6
54	N	403	CDL	O1-C1-CA2-OA2
45	M	604	PC1	C32-C31-O31-C3
54	N	403	CDL	C71-CB7-OB8-CB6
54	d	204	CDL	C31-CA7-OA8-CA6
46	d	201	3PE	O32-C31-O31-C3
54	N	403	CDL	OA9-CA7-OA8-CA6
54	r	202	CDL	C11-CA5-OA6-CA4
46	Y	208	3PE	C32-C31-O31-C3
46	f	103	3PE	C32-C31-O31-C3
46	Y	208	3PE	O32-C31-O31-C3
45	A	201	PC1	C32-C31-O31-C3
54	d	204	CDL	C71-CB7-OB8-CB6
54	d	204	CDL	OB9-CB7-OB8-CB6
54	M	606	CDL	CB2-C1-CA2-OA2
54	d	204	CDL	CB2-C1-CA2-OA2
45	A	201	PC1	O32-C31-O31-C3
48	O	403	PLC	C4-C5-N-C8
45	I	204	PC1	C32-C31-O31-C3
46	Y	201	3PE	C32-C31-O31-C3
46	m	202	3PE	C32-C31-O31-C3
48	O	403	PLC	C1B-CB-O3-C3
48	b	103	PLC	C1B-CB-O3-C3
46	N	402	3PE	C32-C31-O31-C3
46	A	203	3PE	C22-C21-O21-C2
54	M	606	CDL	C11-CA5-OA6-CA4
54	M	606	CDL	CA5-C11-C12-C13
54	r	202	CDL	CB7-C71-C72-C73
46	m	202	3PE	O32-C31-O31-C3
45	g	201	PC1	C32-C31-O31-C3
46	Z	203	3PE	C32-C31-O31-C3
45	B	203	PC1	C21-C22-C23-C24
46	q	202	3PE	C31-C32-C33-C34
45	H	402	PC1	C21-C22-C23-C24
45	h	202	PC1	C31-C32-C33-C34
46	L	704	3PE	C21-C22-C23-C24
46	r	201	3PE	C31-C32-C33-C34
54	N	403	CDL	CB7-C71-C72-C73
54	r	202	CDL	CA5-C11-C12-C13
58	U	101	EHZ	C5-C6-C7-O1

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Mol	Chain	Res	Type	Atoms
46	Z	202	3PE	C32-C31-O31-C3
54	r	202	CDL	OA7-CA5-OA6-CA4
48	L	703	PLC	C2-C1-O3P-P
50	F	502	FMN	C4'-C5'-O5'-P
46	Y	204	3PE	C21-C22-C23-C24
46	d	201	3PE	C31-C32-C33-C34
54	r	202	CDL	CA7-C31-C32-C33
45	I	204	PC1	O32-C31-O31-C3
48	b	103	PLC	OB-CB-O3-C3
46	Y	201	3PE	O32-C31-O31-C3
46	Z	203	3PE	O32-C31-O31-C3
48	O	403	PLC	OB-CB-O3-C3
46	Z	203	3PE	C31-C32-C33-C34
45	g	201	PC1	O32-C31-O31-C3
46	N	402	3PE	O32-C31-O31-C3
45	I	203	PC1	C22-C21-O21-C2
45	A	201	PC1	C1-O11-P-O13
45	B	203	PC1	C1-O11-P-O13
45	H	402	PC1	C1-O11-P-O13
45	H	403	PC1	C11-O13-P-O11
45	I	203	PC1	C11-O13-P-O11
45	I	204	PC1	C1-O11-P-O13
45	L	701	PC1	C11-O13-P-O11
45	M	604	PC1	C11-O13-P-O11
45	M	604	PC1	C1-O11-P-O13
45	g	201	PC1	C11-O13-P-O11
46	A	202	3PE	C11-O13-P-O11
46	A	203	3PE	C11-O13-P-O11
46	H	401	3PE	C11-O13-P-O11
46	J	201	3PE	C1-O11-P-O13
46	J	201	3PE	C11-O13-P-O11
46	K	101	3PE	C1-O11-P-O13
46	L	704	3PE	C1-O11-P-O13
46	L	704	3PE	C11-O13-P-O11
46	N	402	3PE	C1-O11-P-O13
46	Y	201	3PE	C1-O11-P-O13
46	Y	204	3PE	C1-O11-P-O13
46	Y	204	3PE	C11-O13-P-O11
46	Y	208	3PE	C1-O11-P-O13
46	Z	202	3PE	C11-O13-P-O11
46	Z	203	3PE	C1-O11-P-O13
46	b	101	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
46	b	104	3PE	C11-O13-P-O11
46	d	201	3PE	C1-O11-P-O13
46	f	101	3PE	C1-O11-P-O13
46	f	101	3PE	C11-O13-P-O11
46	f	103	3PE	C11-O13-P-O11
46	m	202	3PE	C11-O13-P-O11
46	q	202	3PE	C11-O13-P-O11
46	r	201	3PE	C1-O11-P-O13
46	r	201	3PE	C11-O13-P-O11
48	B	202	PLC	C4-O4P-P-O3P
48	J	203	PLC	C4-O4P-P-O3P
48	Z	201	PLC	C1-O3P-P-O4P
48	Z	201	PLC	C4-O4P-P-O3P
48	b	103	PLC	C4-O4P-P-O3P
48	d	203	PLC	C4-O4P-P-O3P
54	M	606	CDL	CA2-OA2-PA1-OA5
54	M	606	CDL	CA3-OA5-PA1-OA2
54	M	606	CDL	CB3-OB5-PB2-OB2
54	N	403	CDL	CB3-OB5-PB2-OB2
54	X	201	CDL	CA2-OA2-PA1-OA5
54	X	201	CDL	CB3-OB5-PB2-OB2
54	i	201	CDL	CB2-OB2-PB2-OB5
54	r	202	CDL	CA3-OA5-PA1-OA2
46	Z	202	3PE	O32-C31-O31-C3
54	N	403	CDL	CB2-C1-CA2-OA2
46	A	203	3PE	O22-C21-O21-C2
54	M	606	CDL	OA7-CA5-OA6-CA4
48	O	403	PLC	C4-C5-N-C7
45	I	204	PC1	C31-C32-C33-C34
46	Y	208	3PE	C21-C22-C23-C24
46	A	202	3PE	C3A-C3B-C3C-C3D
46	Y	206	3PE	C36-C37-C38-C39
45	L	701	PC1	C32-C33-C34-C35
46	M	602	3PE	C3A-C3B-C3C-C3D
54	M	606	CDL	C34-C35-C36-C37
58	T	101	EHZ	C1-C2-C3-C4
46	M	602	3PE	C35-C36-C37-C38
46	M	603	3PE	C33-C34-C35-C36
46	Y	205	3PE	C28-C29-C2A-C2B
46	Y	206	3PE	C33-C34-C35-C36
46	Z	203	3PE	C27-C28-C29-C2A
54	X	201	CDL	C58-C59-C60-C61

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Mol	Chain	Res	Type	Atoms
54	d	204	CDL	C35-C36-C37-C38
54	d	204	CDL	C74-C75-C76-C77
58	T	101	EHZ	C2-C3-C4-C5
45	I	203	PC1	O22-C21-O21-C2
45	A	201	PC1	C21-C22-C23-C24
46	N	402	3PE	C33-C34-C35-C36
46	b	101	3PE	C36-C37-C38-C39
46	b	101	3PE	C24-C25-C26-C27
46	b	102	3PE	C28-C29-C2A-C2B
46	f	102	3PE	C2E-C2F-C2G-C2H
46	q	202	3PE	C25-C26-C27-C28
48	b	103	PLC	C4'-C5'-C6'-C7'
54	i	201	CDL	C39-C40-C41-C42
46	J	202	3PE	C29-C2A-C2B-C2C
46	Z	203	3PE	C38-C39-C3A-C3B
48	O	403	PLC	C6B-C7B-C8B-C9B
45	H	402	PC1	C24-C25-C26-C27
46	Y	208	3PE	C39-C3A-C3B-C3C
46	b	102	3PE	C35-C36-C37-C38
48	h	201	PLC	C'-C1'-C2'-C3'
45	A	201	PC1	C23-C24-C25-C26
45	I	203	PC1	C2B-C2C-C2D-C2E
46	A	203	3PE	C2B-C2C-C2D-C2E
46	J	202	3PE	C27-C28-C29-C2A
46	M	603	3PE	C27-C28-C29-C2A
48	L	703	PLC	C5'-C6'-C7'-C8'
54	X	201	CDL	C37-C38-C39-C40
45	I	203	PC1	C36-C37-C38-C39
45	d	202	PC1	C36-C37-C38-C39
48	L	703	PLC	C5B-C6B-C7B-C8B
54	M	606	CDL	C83-C84-C85-C86
54	N	403	CDL	C78-C79-C80-C81
45	L	701	PC1	C26-C27-C28-C29
46	A	202	3PE	C34-C35-C36-C37
46	A	202	3PE	C36-C37-C38-C39
46	M	602	3PE	C23-C24-C25-C26
46	Y	202	3PE	C33-C34-C35-C36
46	Y	203	3PE	C28-C29-C2A-C2B
46	f	102	3PE	C32-C33-C34-C35
45	H	402	PC1	C2B-C2C-C2D-C2E
46	Y	202	3PE	C3E-C3F-C3G-C3H
46	Y	208	3PE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
48	b	103	PLC	C2B-C3B-C4B-C5B
54	X	201	CDL	C77-C78-C79-C80
45	q	201	PC1	C22-C21-O21-C2
45	H	403	PC1	C36-C37-C38-C39
46	H	401	3PE	C3E-C3F-C3G-C3H
54	M	605	CDL	C60-C61-C62-C63
54	X	201	CDL	C51-C52-C53-C54
54	i	201	CDL	C32-C33-C34-C35
45	d	202	PC1	C21-C22-C23-C24
46	q	202	3PE	C21-C22-C23-C24
48	Y	207	PLC	C'-C1'-C2'-C3'
45	I	203	PC1	C22-C23-C24-C25
45	L	701	PC1	C35-C36-C37-C38
45	L	701	PC1	C3B-C3C-C3D-C3E
45	L	701	PC1	C3E-C3F-C3G-C3H
45	d	202	PC1	C34-C35-C36-C37
46	K	101	3PE	C23-C24-C25-C26
46	L	704	3PE	C3A-C3B-C3C-C3D
46	Y	208	3PE	C33-C34-C35-C36
46	b	104	3PE	C22-C23-C24-C25
46	q	202	3PE	C3B-C3C-C3D-C3E
54	M	606	CDL	C37-C38-C39-C40
54	N	403	CDL	C22-C23-C24-C25
54	X	201	CDL	C82-C83-C84-C85
48	O	403	PLC	C4-C5-N-C6
45	H	402	PC1	C34-C35-C36-C37
46	N	401	3PE	C24-C25-C26-C27
46	Y	208	3PE	C3B-C3C-C3D-C3E
54	N	403	CDL	C72-C73-C74-C75
46	H	401	3PE	O13-C11-C12-N
46	J	201	3PE	O13-C11-C12-N
46	b	102	3PE	O13-C11-C12-N
45	B	203	PC1	C39-C3A-C3B-C3C
46	K	101	3PE	C37-C38-C39-C3A
46	L	704	3PE	C38-C39-C3A-C3B
46	N	402	3PE	C26-C27-C28-C29
46	Y	203	3PE	C2D-C2E-C2F-C2G
46	Z	203	3PE	C3B-C3C-C3D-C3E
54	M	606	CDL	C23-C24-C25-C26
46	f	102	3PE	C21-C22-C23-C24
46	m	201	3PE	C21-C22-C23-C24
54	M	605	CDL	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
54	M	605	CDL	C72-C73-C74-C75
45	L	701	PC1	C39-C3A-C3B-C3C
45	d	202	PC1	C38-C39-C3A-C3B
48	O	403	PLC	C4'-C5'-C6'-C7'
54	X	201	CDL	C71-C72-C73-C74
54	i	201	CDL	C36-C37-C38-C39
45	I	204	PC1	C27-C28-C29-C2A
46	A	203	3PE	C32-C33-C34-C35
46	N	401	3PE	C2B-C2C-C2D-C2E
46	Y	205	3PE	C33-C34-C35-C36
46	b	101	3PE	C27-C28-C29-C2A
45	H	403	PC1	C3B-C3C-C3D-C3E
46	A	202	3PE	C3E-C3F-C3G-C3H
46	Y	202	3PE	C2C-C2D-C2E-C2F
46	Y	208	3PE	C2C-C2D-C2E-C2F
46	Z	203	3PE	C2B-C2C-C2D-C2E
46	Y	201	3PE	C22-C23-C24-C25
54	M	606	CDL	CB5-C51-C52-C53
45	I	203	PC1	C25-C26-C27-C28
46	M	603	3PE	C22-C21-O21-C2
46	L	704	3PE	C2-C3-O31-C31
45	H	403	PC1	C3A-C3B-C3C-C3D
46	K	101	3PE	C35-C36-C37-C38
46	K	101	3PE	C22-C23-C24-C25
45	H	402	PC1	C28-C29-C2A-C2B
46	A	203	3PE	C27-C28-C29-C2A
46	Z	203	3PE	C35-C36-C37-C38
55	O	401	DGT	C3'-C4'-C5'-O5'
46	M	602	3PE	C2A-C2B-C2C-C2D
46	f	103	3PE	C33-C34-C35-C36
58	T	101	EHZ	C5-C6-C7-O1
45	A	204	PC1	C34-C35-C36-C37
46	Y	204	3PE	C36-C37-C38-C39
46	f	103	3PE	C23-C24-C25-C26
45	q	201	PC1	O22-C21-O21-C2
46	A	202	3PE	C3C-C3D-C3E-C3F
54	M	606	CDL	C18-C19-C20-C21
45	M	604	PC1	C25-C26-C27-C28
46	Z	203	3PE	C29-C2A-C2B-C2C
54	X	201	CDL	C35-C36-C37-C38
46	M	602	3PE	C31-C32-C33-C34
54	N	403	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
45	H	403	PC1	C32-C33-C34-C35
45	m	203	PC1	C24-C25-C26-C27
46	Y	204	3PE	C33-C34-C35-C36
46	b	101	3PE	C39-C3A-C3B-C3C
54	N	403	CDL	C20-C21-C22-C23
48	J	203	PLC	C1B-C2B-C3B-C4B
46	M	603	3PE	C35-C36-C37-C38
46	M	603	3PE	O22-C21-O21-C2
54	N	403	CDL	OA7-CA5-OA6-CA4
45	I	203	PC1	C21-C22-C23-C24
54	M	605	CDL	CA5-C11-C12-C13
54	N	403	CDL	CA7-C31-C32-C33
46	b	101	3PE	C32-C31-O31-C3
46	Y	203	3PE	C32-C33-C34-C35
46	Y	204	3PE	C3C-C3D-C3E-C3F
54	d	204	CDL	C76-C77-C78-C79
48	J	203	PLC	C6B-C7B-C8B-C9B
54	M	606	CDL	C14-C15-C16-C17
46	Y	203	3PE	C21-C22-C23-C24
46	Y	205	3PE	C21-C22-C23-C24
46	A	202	3PE	C24-C25-C26-C27
46	A	203	3PE	C24-C25-C26-C27
48	L	703	PLC	C7'-C8'-C9'-CA'
46	Y	204	3PE	C26-C27-C28-C29
46	b	101	3PE	C29-C2A-C2B-C2C
46	d	201	3PE	C28-C29-C2A-C2B
58	T	101	EHZ	C12-C13-C14-N2
46	H	401	3PE	C33-C34-C35-C36
46	m	201	3PE	C22-C23-C24-C25
45	H	403	PC1	C22-C21-O21-C2
46	K	101	3PE	C22-C21-O21-C2
46	Z	202	3PE	C22-C21-O21-C2
54	N	403	CDL	C11-CA5-OA6-CA4
54	d	204	CDL	C11-CA5-OA6-CA4
54	r	202	CDL	C51-CB5-OB6-CB4
46	H	401	3PE	O11-C1-C2-O21
46	N	401	3PE	O11-C1-C2-O21
46	b	104	3PE	O11-C1-C2-O21
45	M	604	PC1	C32-C33-C34-C35
46	f	102	3PE	C2A-C2B-C2C-C2D
46	Y	202	3PE	C3A-C3B-C3C-C3D
45	H	403	PC1	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
54	d	204	CDL	OA7-CA5-OA6-CA4
48	O	403	PLC	O2-C2-C3-O3
45	H	402	PC1	C32-C33-C34-C35
46	J	201	3PE	C32-C33-C34-C35
54	M	605	CDL	C35-C36-C37-C38
54	i	201	CDL	C12-C13-C14-C15
48	b	103	PLC	C ¹ -C1 ¹ -C2 ¹ -C3 ¹
55	O	401	DGT	O4 ¹ -C4 ¹ -C5 ¹ -O5 ¹
57	P	501	FVH	O2-C7-C8-O3
57	P	501	FVH	C19-C7-C8-O3
45	g	201	PC1	C25-C26-C27-C28
46	A	202	3PE	C23-C24-C25-C26
46	Y	204	3PE	C34-C35-C36-C37
46	N	402	3PE	C2C-C2D-C2E-C2F
48	L	703	PLC	C1B-C2B-C3B-C4B
46	K	101	3PE	O22-C21-O21-C2
46	Z	202	3PE	O22-C21-O21-C2
54	r	202	CDL	OB7-CB5-OB6-CB4
45	B	203	PC1	C33-C34-C35-C36
45	B	203	PC1	C11-O13-P-O11
46	Y	202	3PE	C11-O13-P-O11
48	h	201	PLC	C1-O3P-P-O4P
54	M	606	CDL	C13-C14-C15-C16
54	i	201	CDL	C54-C55-C56-C57
58	U	101	EHZ	C22-C23-C24-C25
46	N	401	3PE	C31-C32-C33-C34
46	Z	203	3PE	C21-C22-C23-C24
46	Y	202	3PE	O11-C1-C2-C3
46	f	103	3PE	O11-C1-C2-C3
48	J	203	PLC	O3P-C1-C2-C3
54	M	606	CDL	OB5-CB3-CB4-CB6
54	d	204	CDL	OA5-CA3-CA4-CA6
46	Z	202	3PE	C21-C22-C23-C24
54	M	606	CDL	C73-C74-C75-C76
48	h	201	PLC	C1 ¹ -C2 ¹ -C3 ¹ -C4 ¹
46	b	104	3PE	C28-C29-C2A-C2B
54	X	201	CDL	C31-C32-C33-C34
46	f	101	3PE	C35-C36-C37-C38
54	M	606	CDL	C63-C64-C65-C66
46	L	704	3PE	C24-C25-C26-C27
59	o	201	MYR	C2-C3-C4-C5
45	g	201	PC1	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
54	N	403	CDL	C74-C75-C76-C77
46	L	704	3PE	C1-C2-C3-O31
46	M	602	3PE	C1-C2-C3-O31
46	N	402	3PE	C1-C2-C3-O31
46	Y	201	3PE	C1-C2-C3-O31
46	Z	202	3PE	C1-C2-C3-O31
46	q	202	3PE	C1-C2-C3-O31
48	L	703	PLC	C1-C2-C3-O3
54	M	605	CDL	CB3-CB4-CB6-OB8
54	r	202	CDL	CA3-CA4-CA6-OA8
46	Y	203	3PE	C22-C23-C24-C25
48	b	103	PLC	C2-C3-O3-CB
46	H	401	3PE	C36-C37-C38-C39
46	J	201	3PE	C33-C34-C35-C36
46	m	202	3PE	C33-C34-C35-C36
46	q	202	3PE	C2F-C2G-C2H-C2I
46	q	202	3PE	C2B-C2C-C2D-C2E
46	J	202	3PE	C2F-C2G-C2H-C2I
46	b	101	3PE	O32-C31-O31-C3
46	Y	206	3PE	C39-C3A-C3B-C3C
54	r	202	CDL	C12-C13-C14-C15
45	h	202	PC1	C2B-C2C-C2D-C2E
54	X	201	CDL	C44-C45-C46-C47
46	A	203	3PE	C3-C2-O21-C21
50	F	502	FMN	O3'-C3'-C4'-C5'
45	H	402	PC1	C2F-C2G-C2H-C2I
45	A	204	PC1	C3C-C3D-C3E-C3F
46	q	202	3PE	C27-C28-C29-C2A
46	r	201	3PE	C36-C37-C38-C39
48	J	203	PLC	C2B-C3B-C4B-C5B
54	M	605	CDL	C38-C39-C40-C41
54	N	403	CDL	C76-C77-C78-C79
45	H	403	PC1	C2-C1-O11-P
46	J	202	3PE	O11-C1-C2-O21
46	Z	202	3PE	O11-C1-C2-O21
54	N	403	CDL	OA5-CA3-CA4-OA6
45	A	204	PC1	C32-C33-C34-C35
46	Y	203	3PE	C36-C37-C38-C39
54	N	403	CDL	C31-C32-C33-C34
54	i	201	CDL	C56-C57-C58-C59
45	M	604	PC1	C23-C24-C25-C26
46	Y	203	3PE	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
46	Y	205	3PE	C38-C39-C3A-C3B
46	A	202	3PE	O21-C2-C3-O31
58	U	101	EHZ	O5-C16-C17-C18
58	U	101	EHZ	O5-C16-C17-C19
46	N	401	3PE	C28-C29-C2A-C2B
46	N	401	3PE	C23-C24-C25-C26
46	L	704	3PE	C31-C32-C33-C34
46	M	603	3PE	C2E-C2F-C2G-C2H
54	N	403	CDL	C51-C52-C53-C54
54	N	403	CDL	C56-C57-C58-C59
46	Y	204	3PE	C39-C3A-C3B-C3C
58	T	101	EHZ	C5-C6-C7-C8
46	f	102	3PE	C24-C25-C26-C27
45	d	202	PC1	C22-C21-O21-C2
46	Y	208	3PE	C3C-C3D-C3E-C3F
54	N	403	CDL	C12-C13-C14-C15
54	N	403	CDL	C60-C61-C62-C63
48	L	703	PLC	C1B-CB-O3-C3
54	M	606	CDL	C74-C75-C76-C77
48	L	703	PLC	C3B-C4B-C5B-C6B
45	I	204	PC1	C3B-C3C-C3D-C3E
46	b	102	3PE	C23-C24-C25-C26
45	B	203	PC1	O11-C1-C2-C3
46	H	401	3PE	O11-C1-C2-C3
46	N	401	3PE	O11-C1-C2-C3
46	b	104	3PE	O11-C1-C2-C3
54	N	403	CDL	OA5-CA3-CA4-CA6
54	X	201	CDL	OA5-CA3-CA4-CA6
54	i	201	CDL	OB5-CB3-CB4-CB6
46	A	203	3PE	C22-C23-C24-C25
45	h	202	PC1	C29-C2A-C2B-C2C
46	d	201	3PE	C21-C22-C23-C24
46	K	101	3PE	C3A-C3B-C3C-C3D
54	i	201	CDL	C16-C17-C18-C19
46	N	402	3PE	C23-C24-C25-C26
46	d	201	3PE	C39-C3A-C3B-C3C
46	K	101	3PE	C31-C32-C33-C34
45	M	604	PC1	C24-C25-C26-C27
46	M	602	3PE	C2-C1-O11-P
45	L	701	PC1	C23-C24-C25-C26
46	Y	204	3PE	C29-C2A-C2B-C2C
46	Z	202	3PE	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
46	f	102	3PE	C35-C36-C37-C38
45	I	203	PC1	C35-C36-C37-C38
46	q	202	3PE	C3D-C3E-C3F-C3G
54	M	606	CDL	C40-C41-C42-C43
54	i	201	CDL	C41-C42-C43-C44
54	M	605	CDL	C31-C32-C33-C34
48	J	203	PLC	C1B-CB-O3-C3
46	L	704	3PE	C35-C36-C37-C38
45	L	701	PC1	C1-C2-C3-O31
45	d	202	PC1	C1-C2-C3-O31
45	h	202	PC1	C1-C2-C3-O31
46	H	401	3PE	C1-C2-C3-O31
46	f	103	3PE	C1-C2-C3-O31
48	O	403	PLC	C1-C2-C3-O3
48	Z	201	PLC	C1-C2-C3-O3
48	b	103	PLC	C1-C2-C3-O3
54	i	201	CDL	CA3-CA4-CA6-OA8
46	J	201	3PE	C36-C37-C38-C39
46	b	101	3PE	C34-C35-C36-C37
46	N	401	3PE	C34-C35-C36-C37
54	M	606	CDL	CB7-C71-C72-C73
45	I	204	PC1	C23-C24-C25-C26
45	g	201	PC1	C22-C23-C24-C25
46	Y	205	3PE	C36-C37-C38-C39
54	r	202	CDL	CB2-OB2-PB2-OB5
46	A	203	3PE	C38-C39-C3A-C3B
46	Y	203	3PE	C25-C26-C27-C28
54	M	605	CDL	C37-C38-C39-C40
45	A	201	PC1	O11-C1-C2-O21
45	q	201	PC1	O11-C1-C2-O21
46	Y	202	3PE	O11-C1-C2-O21
48	L	703	PLC	O3P-C1-C2-O2
54	M	605	CDL	OA5-CA3-CA4-OA6
54	X	201	CDL	C84-C85-C86-C87
45	A	204	PC1	C31-C32-C33-C34
46	f	101	3PE	C37-C38-C39-C3A
54	X	201	CDL	C64-C65-C66-C67
54	i	201	CDL	C35-C36-C37-C38
45	B	203	PC1	O21-C2-C3-O31
45	M	604	PC1	O21-C2-C3-O31
46	M	602	3PE	O21-C2-C3-O31
46	N	401	3PE	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
48	L	703	PLC	O2-C2-C3-O3
54	M	605	CDL	OB6-CB4-CB6-OB8
54	M	606	CDL	OA6-CA4-CA6-OA8
45	g	201	PC1	C2F-C2G-C2H-C2I
46	K	101	3PE	C36-C37-C38-C39
46	b	102	3PE	C32-C33-C34-C35
46	Y	202	3PE	C3B-C3C-C3D-C3E
46	M	603	3PE	C29-C2A-C2B-C2C
54	N	403	CDL	C55-C56-C57-C58
46	J	201	3PE	C2-C1-O11-P
54	X	201	CDL	CA4-CA3-OA5-PA1
46	A	202	3PE	C38-C39-C3A-C3B
46	b	102	3PE	C33-C34-C35-C36
46	b	102	3PE	C22-C23-C24-C25
48	O	403	PLC	C5B-C6B-C7B-C8B
58	T	101	EHZ	O2-C9-S1-C10
45	d	202	PC1	O22-C21-O21-C2
54	i	201	CDL	C51-CB5-OB6-CB4
45	M	604	PC1	C22-C23-C24-C25
46	Z	202	3PE	C2F-C2G-C2H-C2I
58	T	101	EHZ	C22-C23-C24-C25
46	Y	202	3PE	C21-C22-C23-C24
57	P	501	FVH	P1-O6-P2-O9
54	N	403	CDL	C36-C37-C38-C39
45	A	201	PC1	O11-C1-C2-C3
45	L	701	PC1	O11-C1-C2-C3
48	O	403	PLC	O3P-C1-C2-C3
54	M	605	CDL	OA5-CA3-CA4-CA6
54	d	204	CDL	OB5-CB3-CB4-CB6
54	r	202	CDL	OB5-CB3-CB4-CB6
45	H	403	PC1	C3E-C3F-C3G-C3H
45	g	201	PC1	C2B-C2C-C2D-C2E
59	o	201	MYR	C9-C10-C11-C12
54	M	606	CDL	C75-C76-C77-C78
45	H	402	PC1	O21-C21-C22-C23
46	b	102	3PE	C3C-C3D-C3E-C3F
46	M	602	3PE	C22-C21-O21-C2
46	q	202	3PE	C35-C36-C37-C38
46	L	705	3PE	C35-C36-C37-C38
46	L	704	3PE	C1-C2-O21-C21
58	T	101	EHZ	C8-C9-S1-C10
54	M	606	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
46	Y	205	3PE	C2A-C2B-C2C-C2D
50	F	502	FMN	C2'-C3'-C4'-O4'
46	Y	205	3PE	C29-C2A-C2B-C2C
46	Z	203	3PE	C2-C1-O11-P
46	Z	203	3PE	C1-C2-C3-O31
46	b	102	3PE	C1-C2-C3-O31
46	m	202	3PE	C1-C2-C3-O31
48	h	201	PLC	C1-C2-C3-O3
54	M	606	CDL	CA3-CA4-CA6-OA8
54	r	202	CDL	C1-CB2-OB2-PB2
46	Z	202	3PE	C2B-C2C-C2D-C2E
54	i	201	CDL	C11-C12-C13-C14
45	B	203	PC1	O11-C1-C2-O21
45	L	701	PC1	O11-C1-C2-O21
46	m	201	3PE	O11-C1-C2-O21
48	J	203	PLC	O3P-C1-C2-O2
48	h	201	PLC	O3P-C1-C2-O2
54	X	201	CDL	OA5-CA3-CA4-OA6
45	L	701	PC1	O21-C21-C22-C23
46	b	101	3PE	O21-C21-C22-C23
46	M	602	3PE	O22-C21-O21-C2
54	i	201	CDL	OB7-CB5-OB6-CB4
58	T	101	EHZ	O1-C7-C8-C9
48	J	203	PLC	OB-CB-O3-C3
45	L	701	PC1	C29-C2A-C2B-C2C
54	X	201	CDL	C60-C61-C62-C63
45	d	202	PC1	O21-C2-C3-O31
45	h	202	PC1	O21-C2-C3-O31
46	L	704	3PE	O21-C2-C3-O31
46	N	402	3PE	O21-C2-C3-O31
46	Y	201	3PE	O21-C2-C3-O31
46	Y	208	3PE	O21-C2-C3-O31
46	f	103	3PE	O21-C2-C3-O31
46	m	202	3PE	O21-C2-C3-O31
54	X	201	CDL	OA6-CA4-CA6-OA8
46	m	201	3PE	C29-C2A-C2B-C2C
48	L	703	PLC	OB-CB-O3-C3
46	Y	202	3PE	C2A-C2B-C2C-C2D
46	q	202	3PE	C39-C3A-C3B-C3C
55	O	401	DGT	C5'-O5'-PA-O3A
46	Z	202	3PE	C2E-C2F-C2G-C2H
48	L	703	PLC	C3'-C4'-C5'-C6'

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Mol	Chain	Res	Type	Atoms
54	M	606	CDL	C44-C45-C46-C47
46	L	704	3PE	C27-C28-C29-C2A
46	b	101	3PE	C2A-C2B-C2C-C2D
54	X	201	CDL	C80-C81-C82-C83
45	A	201	PC1	C24-C25-C26-C27
54	N	403	CDL	C18-C19-C20-C21
54	d	204	CDL	C71-C72-C73-C74
55	O	401	DGT	PA-O3A-PB-O1B
45	h	202	PC1	C23-C24-C25-C26
54	d	204	CDL	C72-C73-C74-C75
46	Y	203	3PE	C31-C32-C33-C34
46	K	101	3PE	C32-C33-C34-C35
46	Y	203	3PE	C3B-C3C-C3D-C3E
54	X	201	CDL	C56-C57-C58-C59
46	b	102	3PE	C34-C35-C36-C37
46	N	401	3PE	C38-C39-C3A-C3B
46	b	101	3PE	C2C-C2D-C2E-C2F
45	H	403	PC1	C1-O11-P-O13
46	J	202	3PE	C11-O13-P-O11
46	M	602	3PE	C11-O13-P-O11
46	Y	205	3PE	C11-O13-P-O11
46	Z	203	3PE	C11-O13-P-O11
46	m	202	3PE	C1-O11-P-O13
54	d	204	CDL	CB2-OB2-PB2-OB5
46	M	602	3PE	C36-C37-C38-C39
46	Y	203	3PE	C38-C39-C3A-C3B
46	A	203	3PE	C2-C1-O11-P
46	b	104	3PE	C2-C1-O11-P
48	O	403	PLC	C2-C1-O3P-P
48	d	203	PLC	C2-C1-O3P-P
48	h	201	PLC	C2-C1-O3P-P
54	d	204	CDL	C1-CB2-OB2-PB2
45	A	201	PC1	C1-O11-P-O14
45	B	203	PC1	C11-O13-P-O12
45	H	403	PC1	C11-O13-P-O12
45	I	203	PC1	C11-O13-P-O14
45	g	201	PC1	C11-O13-P-O12
46	A	203	3PE	C11-O13-P-O12
46	A	203	3PE	C11-O13-P-O14
46	J	201	3PE	C11-O13-P-O14
46	K	101	3PE	C1-O11-P-O12
46	N	401	3PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
46	N	402	3PE	C1-O11-P-O12
46	N	402	3PE	C1-O11-P-O14
46	N	402	3PE	C11-O13-P-O14
46	Y	202	3PE	C11-O13-P-O12
46	Y	204	3PE	C1-O11-P-O12
46	Y	204	3PE	C11-O13-P-O14
46	Y	205	3PE	C11-O13-P-O12
46	Y	205	3PE	C11-O13-P-O14
46	Z	202	3PE	C11-O13-P-O12
46	Z	202	3PE	C11-O13-P-O14
46	b	101	3PE	C1-O11-P-O12
46	f	101	3PE	C11-O13-P-O14
48	B	202	PLC	C4-O4P-P-O2P
48	J	203	PLC	C4-O4P-P-O1P
48	Y	207	PLC	C1-O3P-P-O2P
48	Z	201	PLC	C1-O3P-P-O1P
48	Z	201	PLC	C4-O4P-P-O2P
48	b	103	PLC	C1-O3P-P-O2P
48	b	103	PLC	C4-O4P-P-O1P
48	h	201	PLC	C1-O3P-P-O2P
54	M	606	CDL	CB3-OB5-PB2-OB4
54	X	201	CDL	CA2-OA2-PA1-OA3
54	X	201	CDL	CB3-OB5-PB2-OB3
54	r	202	CDL	CA3-OA5-PA1-OA3
45	I	203	PC1	O11-C1-C2-C3
45	q	201	PC1	O11-C1-C2-C3
46	J	201	3PE	O11-C1-C2-C3
46	Y	205	3PE	O11-C1-C2-C3
46	Z	202	3PE	O11-C1-C2-C3
46	m	201	3PE	O11-C1-C2-C3
45	q	201	PC1	C12-C11-O13-P
46	A	203	3PE	C12-C11-O13-P
46	M	602	3PE	C12-C11-O13-P
46	N	401	3PE	C12-C11-O13-P
46	N	402	3PE	C12-C11-O13-P
46	Y	204	3PE	C12-C11-O13-P
46	Y	205	3PE	C12-C11-O13-P
46	b	102	3PE	C12-C11-O13-P
46	f	103	3PE	C12-C11-O13-P
46	m	201	3PE	C12-C11-O13-P
46	m	202	3PE	C12-C11-O13-P
48	Y	207	PLC	C5-C4-O4P-P

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Mol	Chain	Res	Type	Atoms
46	Y	203	3PE	C34-C35-C36-C37
46	b	101	3PE	C37-C38-C39-C3A
45	I	203	PC1	O11-C1-C2-O21
46	J	201	3PE	O11-C1-C2-O21
46	Y	206	3PE	O11-C1-C2-O21
46	r	201	3PE	O11-C1-C2-O21
54	i	201	CDL	OB5-CB3-CB4-OB6
46	Y	203	3PE	C39-C3A-C3B-C3C
46	r	201	3PE	C33-C34-C35-C36
45	B	203	PC1	C2B-C2C-C2D-C2E
46	Y	203	3PE	C24-C25-C26-C27
46	N	401	3PE	O21-C21-C22-C23
48	d	203	PLC	C2B-C1B-CB-O3
48	B	202	PLC	C1'-C'-O2-C2
54	M	606	CDL	C52-C53-C54-C55
46	A	203	3PE	C37-C38-C39-C3A
45	H	402	PC1	C11-C12-N-C13
45	d	202	PC1	C11-C12-N-C15
45	d	202	PC1	C3B-C3C-C3D-C3E
46	f	101	3PE	C33-C34-C35-C36
59	o	201	MYR	C4-C5-C6-C7
46	M	603	3PE	O21-C21-C22-C23
46	Y	208	3PE	C1-C2-C3-O31
46	f	101	3PE	C1-C2-C3-O31
46	q	202	3PE	C29-C2A-C2B-C2C
48	Y	207	PLC	O4P-C4-C5-N
48	b	103	PLC	O4P-C4-C5-N
54	X	201	CDL	C33-C34-C35-C36
58	T	101	EHZ	C16-C17-C20-O6
58	U	101	EHZ	O5-C16-C17-C20
58	U	101	EHZ	C16-C17-C20-O6
45	I	204	PC1	O21-C2-C3-O31
46	Z	203	3PE	O21-C2-C3-O31
48	Z	201	PLC	O2-C2-C3-O3
48	b	103	PLC	O2-C2-C3-O3
54	i	201	CDL	OA6-CA4-CA6-OA8
54	r	202	CDL	OA6-CA4-CA6-OA8
46	Y	208	3PE	C28-C29-C2A-C2B
46	M	603	3PE	C23-C24-C25-C26
54	r	202	CDL	C16-C17-C18-C19
46	b	101	3PE	C38-C39-C3A-C3B
46	N	401	3PE	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
46	Y	203	3PE	C35-C36-C37-C38
46	Y	201	3PE	C22-C21-O21-C2
46	M	602	3PE	C2D-C2E-C2F-C2G
54	r	202	CDL	C72-C73-C74-C75
46	Z	202	3PE	C2A-C2B-C2C-C2D
46	q	202	3PE	C3F-C3G-C3H-C3I
48	Y	207	PLC	C7'-C8'-C9'-CA'
54	M	605	CDL	C56-C57-C58-C59
46	d	201	3PE	C22-C23-C24-C25
46	f	103	3PE	C32-C33-C34-C35
54	X	201	CDL	CA5-C11-C12-C13
46	A	202	3PE	C33-C34-C35-C36
46	Z	203	3PE	C37-C38-C39-C3A
45	I	204	PC1	C21-C22-C23-C24
45	A	204	PC1	C11-C12-N-C15
54	M	605	CDL	C33-C34-C35-C36
46	Y	208	3PE	C2F-C2G-C2H-C2I
46	A	202	3PE	C31-C32-C33-C34
58	T	101	EHZ	C18-C17-C20-O6
58	U	101	EHZ	C18-C17-C20-O6
46	Y	204	3PE	C23-C24-C25-C26
46	Y	204	3PE	C28-C29-C2A-C2B
46	q	202	3PE	C33-C34-C35-C36
54	i	201	CDL	C72-C73-C74-C75
45	M	604	PC1	C34-C35-C36-C37
46	b	101	3PE	C32-C33-C34-C35
46	m	201	3PE	C2A-C2B-C2C-C2D
46	Y	202	3PE	C3-C2-O21-C21
48	J	203	PLC	C1-C2-O2-C'
48	J	203	PLC	C3-C2-O2-C'
48	Y	207	PLC	C1-C2-O2-C'
54	N	403	CDL	CA6-CA4-OA6-CA5
46	J	202	3PE	O11-C1-C2-C3
46	Y	206	3PE	O11-C1-C2-C3
46	Y	201	3PE	O22-C21-O21-C2
48	B	202	PLC	O'-C'-O2-C2
54	M	605	CDL	CA7-C31-C32-C33
46	N	401	3PE	C2D-C2E-C2F-C2G
46	L	704	3PE	C3C-C3D-C3E-C3F
45	M	604	PC1	O11-C1-C2-O21
46	Y	205	3PE	O11-C1-C2-O21
54	d	204	CDL	OA5-CA3-CA4-OA6

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Mol	Chain	Res	Type	Atoms
45	h	202	PC1	C27-C28-C29-C2A
45	H	402	PC1	C11-C12-N-C14
45	I	204	PC1	C22-C23-C24-C25
50	F	502	FMN	C2'-C3'-C4'-C5'
46	N	402	3PE	C29-C2A-C2B-C2C
48	h	201	PLC	O2-C2-C3-O3
45	I	204	PC1	C11-O13-P-O11
45	h	202	PC1	C11-O13-P-O11
46	f	103	3PE	C1-O11-P-O13
48	Y	207	PLC	C4-O4P-P-O3P
48	d	203	PLC	C1-O3P-P-O4P
54	M	605	CDL	CA2-OA2-PA1-OA5
54	X	201	CDL	CB2-OB2-PB2-OB5
54	i	201	CDL	CA7-C31-C32-C33
54	r	202	CDL	CB5-C51-C52-C53
45	L	701	PC1	C27-C28-C29-C2A
45	d	202	PC1	C32-C33-C34-C35
46	H	401	3PE	C39-C3A-C3B-C3C
46	Y	203	3PE	C2C-C2D-C2E-C2F
48	O	403	PLC	C2-C3-O3-CB
46	A	203	3PE	C21-C22-C23-C24
46	A	202	3PE	C1-C2-C3-O31
54	X	201	CDL	CA3-CA4-CA6-OA8
46	J	202	3PE	O31-C31-C32-C33
46	A	203	3PE	C28-C29-C2A-C2B
46	Z	202	3PE	C27-C28-C29-C2A
45	g	201	PC1	C2A-C2B-C2C-C2D
45	L	701	PC1	C37-C38-C39-C3A
54	r	202	CDL	CB4-CB3-OB5-PB2
46	Y	203	3PE	C3D-C3E-C3F-C3G
54	i	201	CDL	C52-C53-C54-C55
54	M	606	CDL	C11-C12-C13-C14
50	F	502	FMN	O3'-C3'-C4'-O4'
57	P	501	FVH	O1-C1-C2-C3
46	Y	208	3PE	C2E-C2F-C2G-C2H
46	K	101	3PE	C38-C39-C3A-C3B
46	Y	203	3PE	C37-C38-C39-C3A
54	d	204	CDL	C31-C32-C33-C34
46	b	104	3PE	C2F-C2G-C2H-C2I
46	Y	201	3PE	O13-C11-C12-N
46	f	101	3PE	O13-C11-C12-N
46	q	202	3PE	C3E-C3F-C3G-C3H

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Mol	Chain	Res	Type	Atoms
54	M	606	CDL	C62-C63-C64-C65
46	J	202	3PE	C2D-C2E-C2F-C2G
46	Y	203	3PE	C23-C24-C25-C26
46	K	101	3PE	C33-C34-C35-C36
46	f	102	3PE	C34-C35-C36-C37
46	J	202	3PE	O32-C31-C32-C33
54	r	202	CDL	C51-C52-C53-C54
46	m	202	3PE	C34-C35-C36-C37
54	d	204	CDL	C73-C74-C75-C76
46	Y	205	3PE	C31-C32-C33-C34
46	Z	203	3PE	C2A-C2B-C2C-C2D
46	b	104	3PE	C24-C25-C26-C27
54	M	606	CDL	C35-C36-C37-C38
45	A	201	PC1	C1-C2-C3-O31
46	A	202	3PE	C22-C23-C24-C25
46	q	202	3PE	C2C-C2D-C2E-C2F
58	U	101	EHZ	O3-C12-C13-C14
58	T	101	EHZ	C19-C17-C20-O6
58	U	101	EHZ	C19-C17-C20-O6
48	J	203	PLC	C3B-C4B-C5B-C6B
46	m	202	3PE	C35-C36-C37-C38
46	b	102	3PE	C21-C22-C23-C24
48	J	203	PLC	C5B-C6B-C7B-C8B
46	Y	204	3PE	C1-C2-O21-C21
46	Y	204	3PE	C3-C2-O21-C21
46	d	201	3PE	C3-C2-O21-C21
48	Y	207	PLC	C3-C2-O2-C'
48	Z	201	PLC	C1-C2-O2-C'
45	A	204	PC1	C11-C12-N-C14
45	H	402	PC1	C11-C12-N-C15
45	d	202	PC1	C11-C12-N-C13
45	d	202	PC1	C11-C12-N-C14
46	Y	203	3PE	C3C-C3D-C3E-C3F
54	d	204	CDL	C52-C51-CB5-OB6
46	Y	208	3PE	C36-C37-C38-C39
45	B	203	PC1	C38-C39-C3A-C3B
46	r	201	3PE	C32-C33-C34-C35
46	m	201	3PE	C2B-C2C-C2D-C2E
46	K	101	3PE	O11-C1-C2-O21
48	b	103	PLC	O3P-C1-C2-O2
45	M	604	PC1	O11-C1-C2-C3
46	r	201	3PE	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
48	h	201	PLC	O3P-C1-C2-C3
46	K	101	3PE	C21-C22-C23-C24
54	M	605	CDL	C63-C64-C65-C66
45	L	701	PC1	C36-C37-C38-C39
46	N	401	3PE	O22-C21-O21-C2
46	H	401	3PE	O21-C2-C3-O31
54	i	201	CDL	CA5-C11-C12-C13
48	Y	207	PLC	C6'-C7'-C8'-C9'
54	N	403	CDL	C17-C18-C19-C20
45	I	204	PC1	C34-C35-C36-C37
46	N	402	3PE	O21-C21-C22-C23
45	L	701	PC1	C28-C29-C2A-C2B
54	M	605	CDL	C64-C65-C66-C67
48	Z	201	PLC	C2-C1-O3P-P
46	Z	203	3PE	C2E-C2F-C2G-C2H
46	d	201	3PE	C23-C24-C25-C26
48	Z	201	PLC	C2B-C1B-CB-O3
45	M	604	PC1	C1-C2-C3-O31
45	g	201	PC1	C32-C33-C34-C35
46	Y	202	3PE	C22-C23-C24-C25
46	Y	203	3PE	C3F-C3G-C3H-C3I
46	Y	205	3PE	C2C-C2D-C2E-C2F
54	M	605	CDL	C58-C59-C60-C61
46	Y	205	3PE	C2B-C2C-C2D-C2E
46	A	203	3PE	C35-C36-C37-C38
46	Y	205	3PE	C39-C3A-C3B-C3C
46	b	102	3PE	C37-C38-C39-C3A
46	A	203	3PE	C31-C32-C33-C34
48	L	703	PLC	CB-C1B-C2B-C3B
52	L	702	CHD	C22-C23-C24-O26
46	Y	206	3PE	C37-C38-C39-C3A
46	A	202	3PE	C27-C28-C29-C2A
46	m	202	3PE	O13-C11-C12-N
46	q	202	3PE	C2A-C2B-C2C-C2D
45	q	201	PC1	O21-C21-C22-C23
52	L	702	CHD	C22-C23-C24-O25
46	Z	203	3PE	C36-C37-C38-C39
54	i	201	CDL	OB6-CB4-CB6-OB8
54	r	202	CDL	CA4-CA6-OA8-CA7
46	Z	203	3PE	C32-C33-C34-C35
54	r	202	CDL	C73-C74-C75-C76
46	A	202	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
46	N	401	3PE	C11-O13-P-O11
45	A	204	PC1	C11-C12-N-C13
45	A	201	PC1	O21-C21-C22-C23
45	A	201	PC1	C33-C34-C35-C36
46	Y	204	3PE	C2D-C2E-C2F-C2G
46	d	201	3PE	C2A-C2B-C2C-C2D
46	Y	205	3PE	O31-C31-C32-C33
54	M	606	CDL	C12-C11-CA5-OA6
46	d	201	3PE	C1-C2-O21-C21
48	Z	201	PLC	C3-C2-O2-C'
54	X	201	CDL	CA3-CA4-OA6-CA5
54	X	201	CDL	CA6-CA4-OA6-CA5
46	f	101	3PE	C32-C33-C34-C35
54	X	201	CDL	C63-C64-C65-C66
54	N	403	CDL	C24-C25-C26-C27
46	A	203	3PE	O31-C31-C32-C33
45	H	403	PC1	C3F-C3G-C3H-C3I
45	g	201	PC1	C2E-C2F-C2G-C2H
54	M	605	CDL	C36-C37-C38-C39
45	B	203	PC1	C1-C2-C3-O31
45	A	204	PC1	C3A-C3B-C3C-C3D
48	h	201	PLC	C2'-C3'-C4'-C5'
45	B	203	PC1	C35-C36-C37-C38
45	A	204	PC1	O11-C1-C2-O21
46	L	704	3PE	O11-C1-C2-O21
46	L	705	3PE	O11-C1-C2-O21
48	Y	207	PLC	O2-C'-C1'-C2'
54	i	201	CDL	C12-C11-CA5-OA6
46	Z	202	3PE	C24-C25-C26-C27
46	b	104	3PE	C2E-C2F-C2G-C2H
54	X	201	CDL	C62-C63-C64-C65
54	i	201	CDL	C15-C16-C17-C18
46	A	202	3PE	O31-C31-C32-C33
54	X	201	CDL	C52-C51-CB5-OB6
45	L	701	PC1	C22-C23-C24-C25
46	N	401	3PE	C2E-C2F-C2G-C2H
46	A	202	3PE	O21-C21-C22-C23
46	f	102	3PE	O31-C31-C32-C33
54	r	202	CDL	C18-C19-C20-C21
45	L	701	PC1	C3A-C3B-C3C-C3D
46	f	102	3PE	C23-C24-C25-C26
46	Y	201	3PE	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
45	h	202	PC1	C22-C23-C24-C25
46	L	705	3PE	O21-C2-C3-O31
54	r	202	CDL	OB6-CB4-CB6-OB8
45	H	403	PC1	C35-C36-C37-C38
46	m	201	3PE	C33-C34-C35-C36
46	Y	201	3PE	O31-C31-C32-C33
46	b	102	3PE	O31-C31-C32-C33
45	h	202	PC1	C24-C25-C26-C27
46	H	401	3PE	C38-C39-C3A-C3B
46	b	101	3PE	C26-C27-C28-C29
57	P	501	FVH	C9-O9-P2-O6
58	U	101	EHZ	N1-C12-C13-C14
54	r	202	CDL	C17-C18-C19-C20
46	N	401	3PE	C22-C21-O21-C2
46	L	705	3PE	O21-C21-C22-C23
46	f	101	3PE	O31-C31-C32-C33
46	q	202	3PE	O31-C31-C32-C33
54	M	605	CDL	C32-C33-C34-C35
54	X	201	CDL	C73-C74-C75-C76
48	Y	207	PLC	C2B-C3B-C4B-C5B
54	i	201	CDL	C31-C32-C33-C34
57	P	501	FVH	O10-C10-C9-O9
46	Z	203	3PE	O31-C31-C32-C33
55	O	401	DGT	PA-O3A-PB-O2B
46	A	202	3PE	C3F-C3G-C3H-C3I
48	Y	207	PLC	C1B-C2B-C3B-C4B
48	Z	201	PLC	C1B-CB-O3-C3
45	d	202	PC1	C31-C32-C33-C34
54	X	201	CDL	C75-C76-C77-C78
45	A	201	PC1	O22-C21-C22-C23
46	f	102	3PE	O11-C1-C2-O21
46	L	704	3PE	C32-C33-C34-C35
46	b	101	3PE	C3A-C3B-C3C-C3D
54	M	606	CDL	C12-C13-C14-C15
46	A	202	3PE	O22-C21-C22-C23
48	Z	201	PLC	OB-CB-O3-C3
46	A	203	3PE	O32-C31-C32-C33
54	i	201	CDL	C12-C11-CA5-OA7
46	M	602	3PE	C22-C23-C24-C25
54	X	201	CDL	C74-C75-C76-C77
45	I	204	PC1	C1-C2-C3-O31
46	N	401	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
46	f	102	3PE	C1-C2-C3-O31
46	N	401	3PE	C2F-C2G-C2H-C2I
46	b	102	3PE	O32-C31-C32-C33
48	Y	207	PLC	O'-C'-C1'-C2'
45	g	201	PC1	C2-C1-O11-P
54	X	201	CDL	C1-CB2-OB2-PB2
46	A	202	3PE	O32-C31-C32-C33
46	Y	201	3PE	O32-C31-C32-C33
46	f	102	3PE	O32-C31-C32-C33
54	N	403	CDL	C13-C14-C15-C16
45	A	201	PC1	C11-C12-N-C14
45	A	204	PC1	C11-O13-P-O14
45	H	403	PC1	C11-O13-P-O14
45	I	203	PC1	C11-O13-P-O12
45	I	203	PC1	C11-C12-N-C14
45	I	204	PC1	C11-O13-P-O14
45	g	201	PC1	C11-O13-P-O14
46	M	602	3PE	C1-O11-P-O14
46	Y	204	3PE	C1-O11-P-O14
46	Y	206	3PE	C1-O11-P-O14
46	f	102	3PE	C11-O13-P-O12
48	O	403	PLC	C1-O3P-P-O1P
48	Y	207	PLC	C4-O4P-P-O1P
48	d	203	PLC	C1-O3P-P-O1P
54	M	605	CDL	CB3-OB5-PB2-OB3
54	d	204	CDL	CB2-OB2-PB2-OB3
54	i	201	CDL	CA3-OA5-PA1-OA3
46	L	705	3PE	O22-C21-C22-C23
46	Y	201	3PE	O22-C21-C22-C23
54	X	201	CDL	C52-C51-CB5-OB7
54	X	201	CDL	C72-C71-CB7-OB8
46	L	704	3PE	O11-C1-C2-C3
48	L	703	PLC	O3P-C1-C2-C3
48	b	103	PLC	O3P-C1-C2-C3
46	m	201	3PE	C32-C33-C34-C35
45	I	203	PC1	C28-C29-C2A-C2B
46	Z	202	3PE	O13-C11-C12-N
46	m	201	3PE	O13-C11-C12-N
46	b	101	3PE	C2B-C2C-C2D-C2E
54	X	201	CDL	C61-C62-C63-C64
46	Y	203	3PE	O31-C31-C32-C33
46	b	102	3PE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
45	H	402	PC1	O22-C21-C22-C23
46	Y	205	3PE	O32-C31-C32-C33
45	M	604	PC1	C12-C11-O13-P
45	h	202	PC1	C12-C11-O13-P
46	K	101	3PE	C12-C11-O13-P
46	Y	201	3PE	C12-C11-O13-P
46	Y	202	3PE	C12-C11-O13-P
46	Y	206	3PE	C12-C11-O13-P
46	Y	206	3PE	C1-C2-O21-C21
46	Y	206	3PE	C3-C2-O21-C21
46	Z	203	3PE	C12-C11-O13-P
46	f	101	3PE	O32-C31-C32-C33
46	q	202	3PE	O32-C31-C32-C33
48	L	703	PLC	C2B-C3B-C4B-C5B
46	Y	204	3PE	O21-C21-C22-C23
45	d	202	PC1	C3A-C3B-C3C-C3D
54	M	606	CDL	C39-C40-C41-C42
46	L	704	3PE	C37-C38-C39-C3A
46	f	102	3PE	C2B-C2C-C2D-C2E
46	b	101	3PE	O22-C21-C22-C23
45	A	201	PC1	C11-C12-N-C13
45	I	203	PC1	C11-C12-N-C13
46	L	704	3PE	O31-C31-C32-C33
46	L	704	3PE	O21-C21-C22-C23
46	M	602	3PE	O21-C21-C22-C23
46	r	201	3PE	O21-C21-C22-C23
48	L	703	PLC	O2-C'-C1'-C2'
54	M	605	CDL	C32-C31-CA7-OA8
46	b	101	3PE	C33-C34-C35-C36
46	J	201	3PE	O21-C21-C22-C23
46	N	401	3PE	O31-C31-C32-C33
46	Y	208	3PE	O31-C31-C32-C33
48	J	203	PLC	O2-C'-C1'-C2'
46	Z	203	3PE	O32-C31-C32-C33
46	Y	208	3PE	C3E-C3F-C3G-C3H
46	L	704	3PE	C34-C35-C36-C37
48	h	201	PLC	C4'-C5'-C6'-C7'
50	F	502	FMN	N10-C1'-C2'-O2'
46	d	201	3PE	O21-C21-C22-C23
46	f	102	3PE	O21-C21-C22-C23
46	Y	202	3PE	C35-C36-C37-C38
46	r	201	3PE	O22-C21-C22-C23

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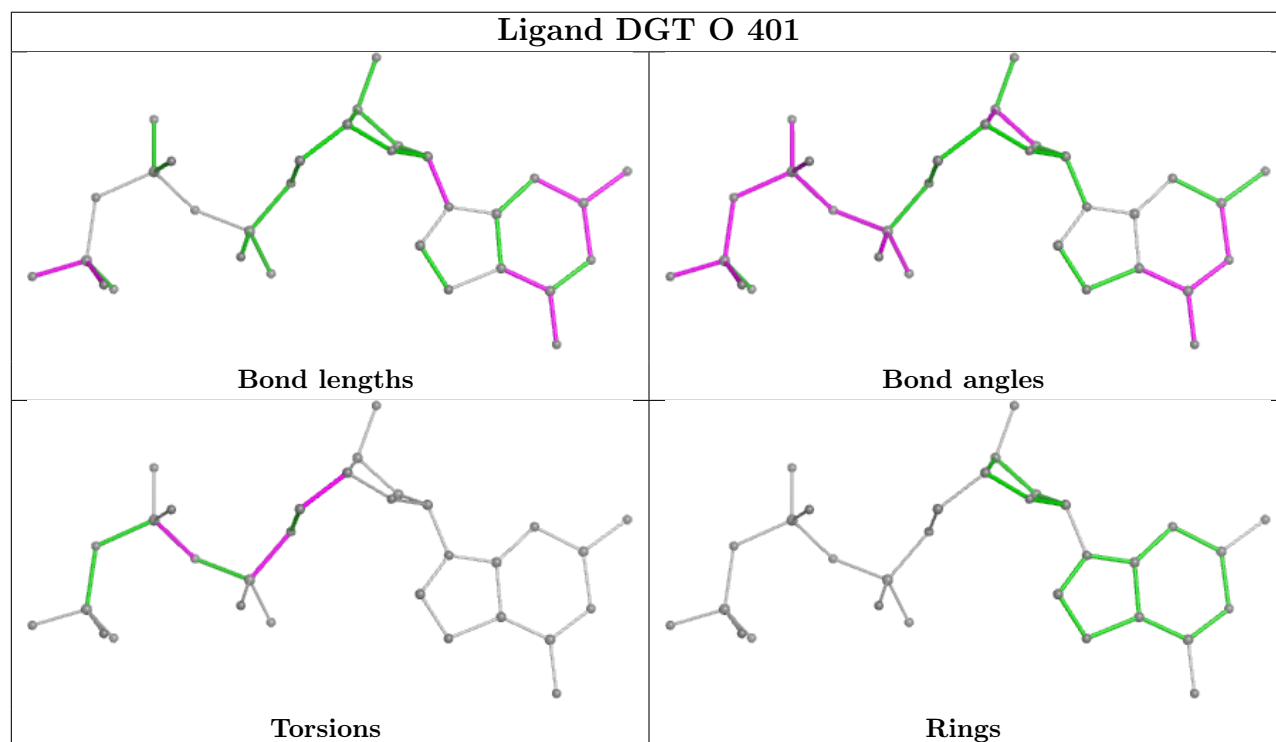
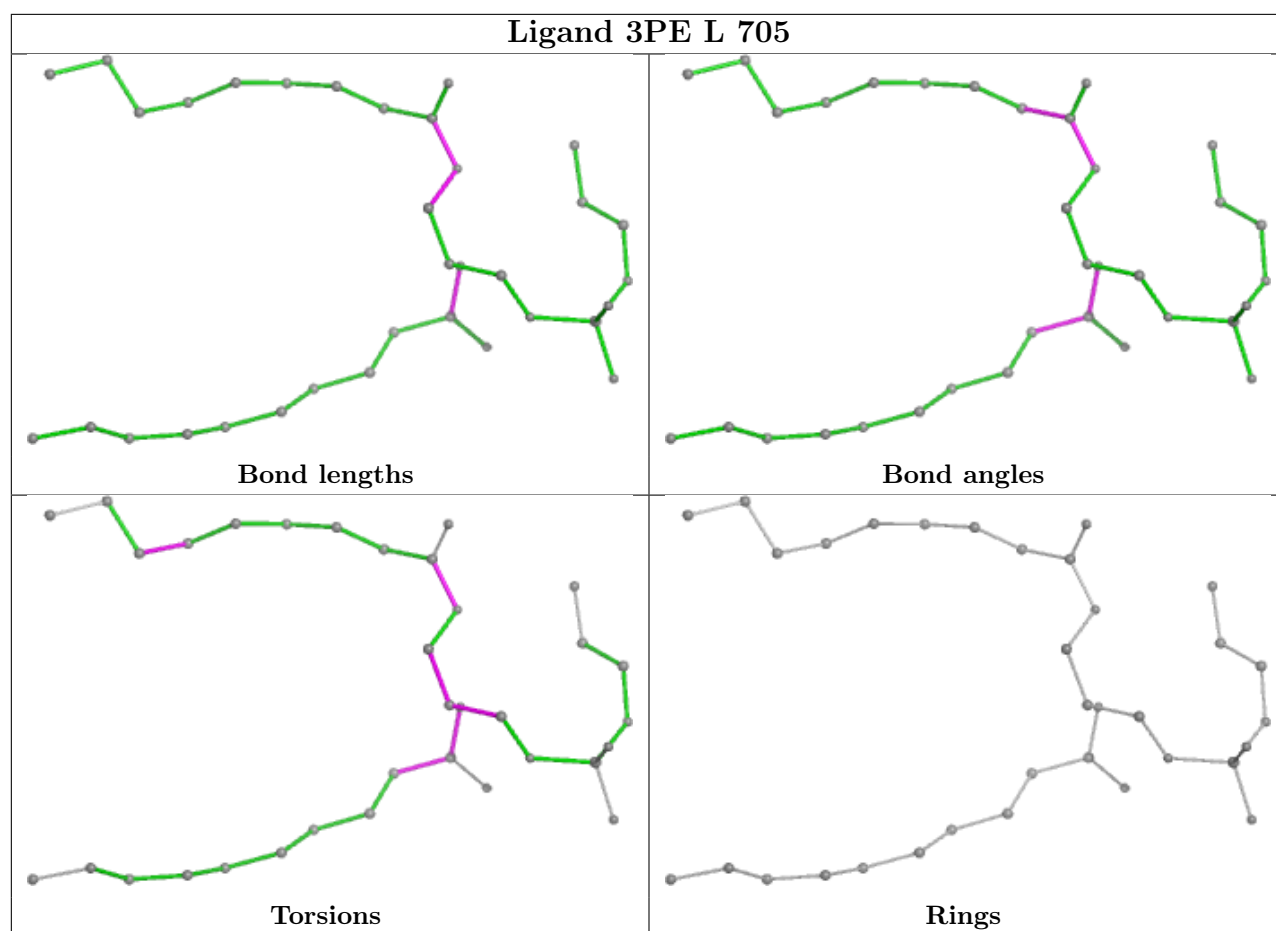
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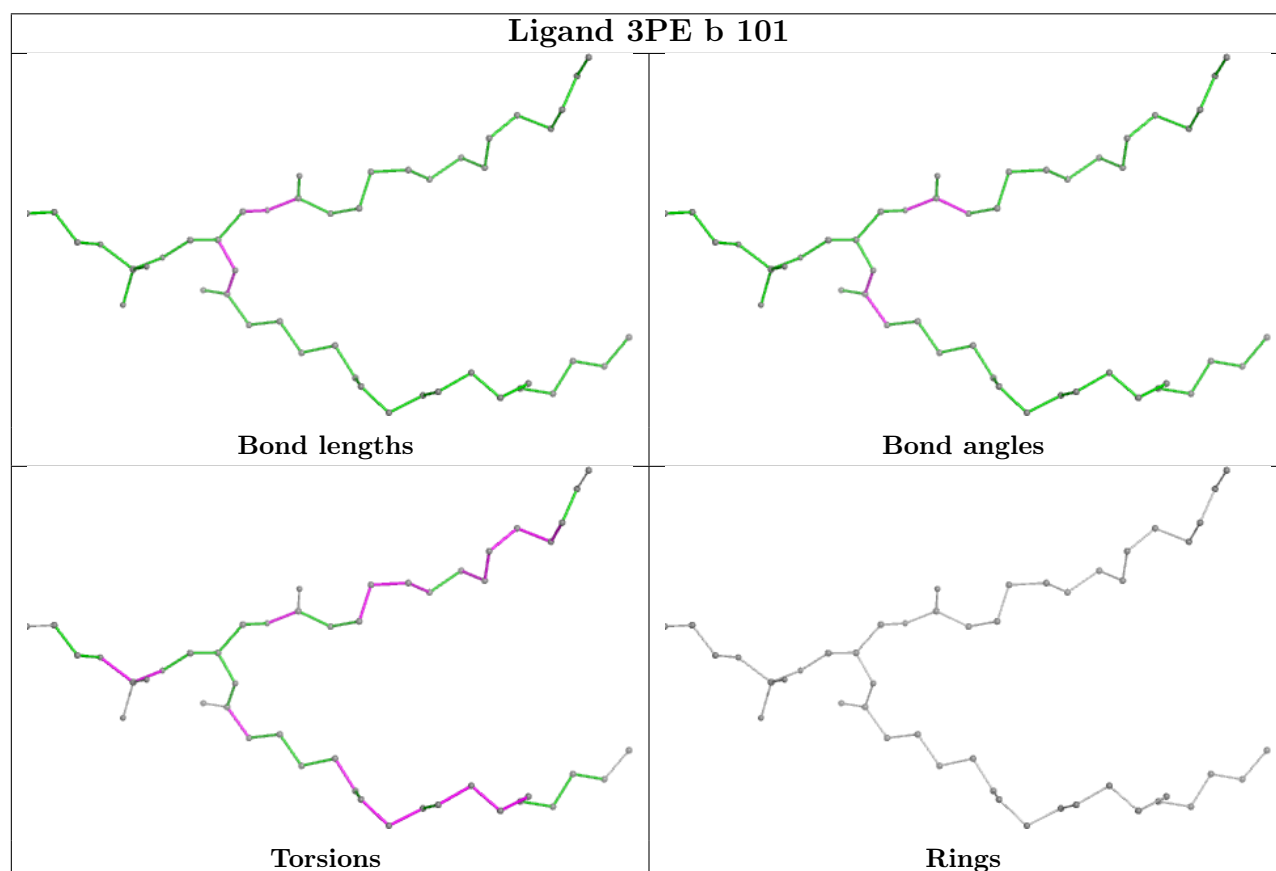
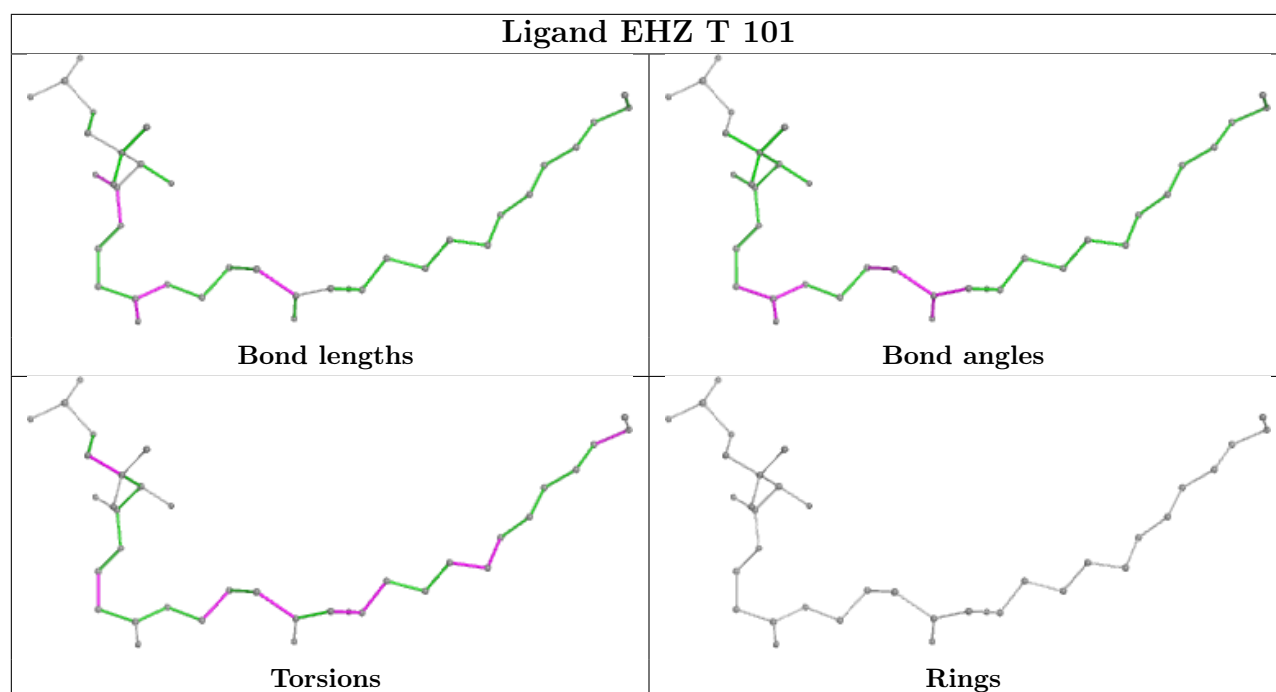
Mol	Chain	Res	Type	Atoms
48	J	203	PLC	O'-C'-C1'-C2'
45	I	204	PC1	C37-C38-C39-C3A
46	Y	208	3PE	C3F-C3G-C3H-C3I
54	d	204	CDL	C72-C71-CB7-OB8
48	L	703	PLC	O'-C'-C1'-C2'
46	m	201	3PE	C28-C29-C2A-C2B
46	r	201	3PE	O31-C31-C32-C33
54	M	606	CDL	C72-C71-CB7-OB8
46	L	704	3PE	O22-C21-C22-C23
54	X	201	CDL	C72-C71-CB7-OB9
58	U	101	EHZ	C21-C1-C2-C3
46	A	202	3PE	C3D-C3E-C3F-C3G
46	J	201	3PE	O22-C21-C22-C23
46	L	704	3PE	O32-C31-C32-C33

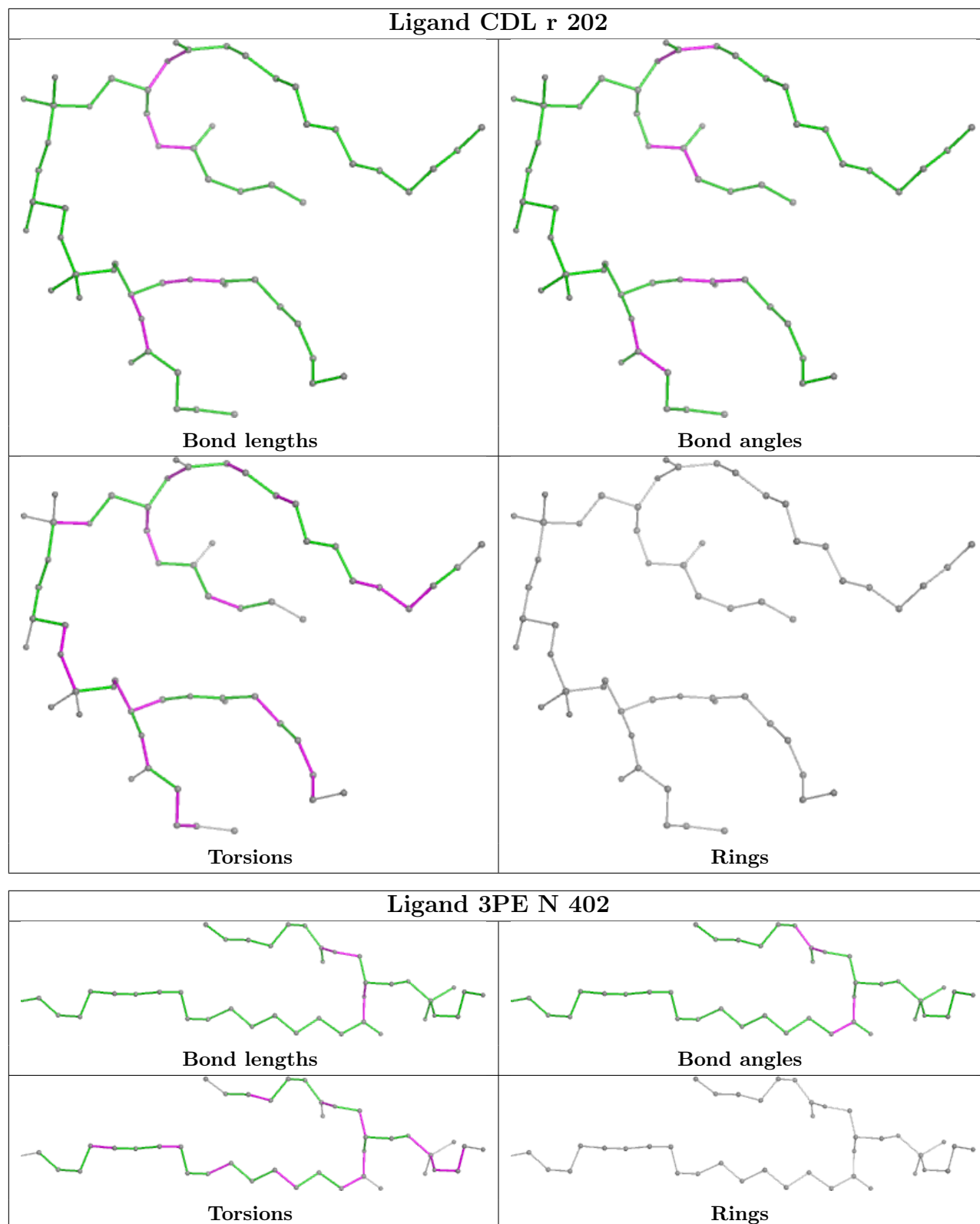
There are no ring outliers.

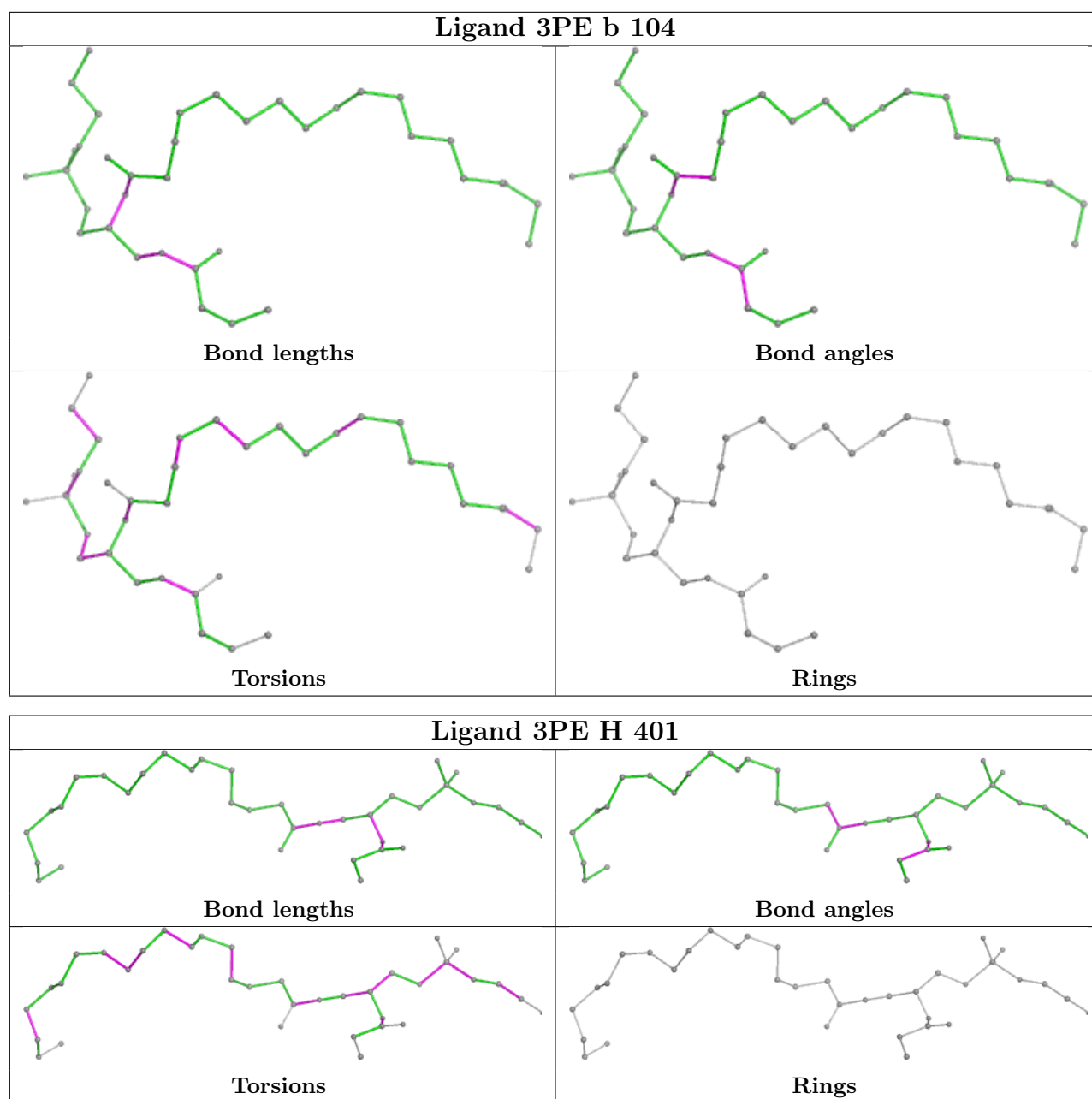
No monomer is involved in short contacts.

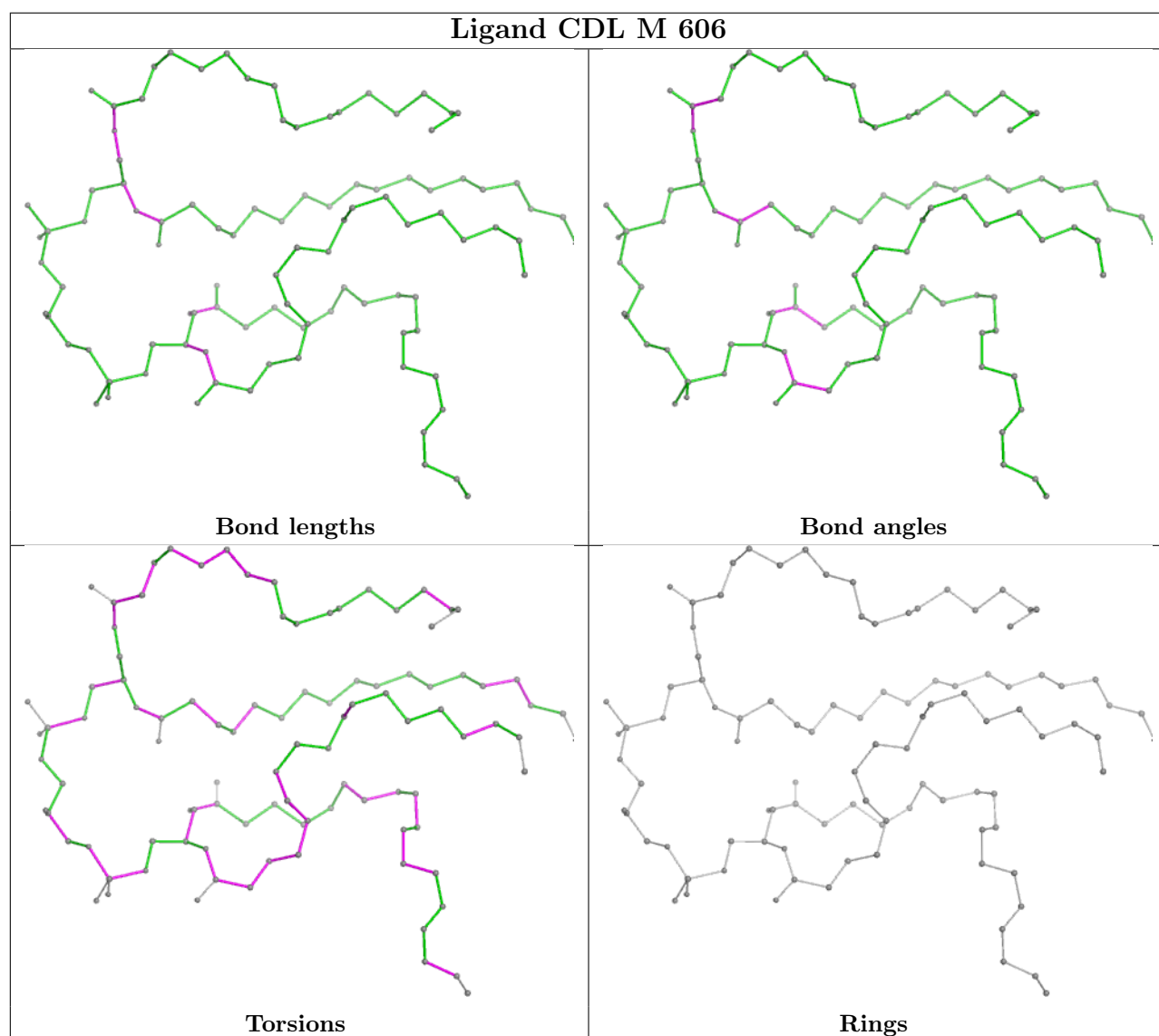
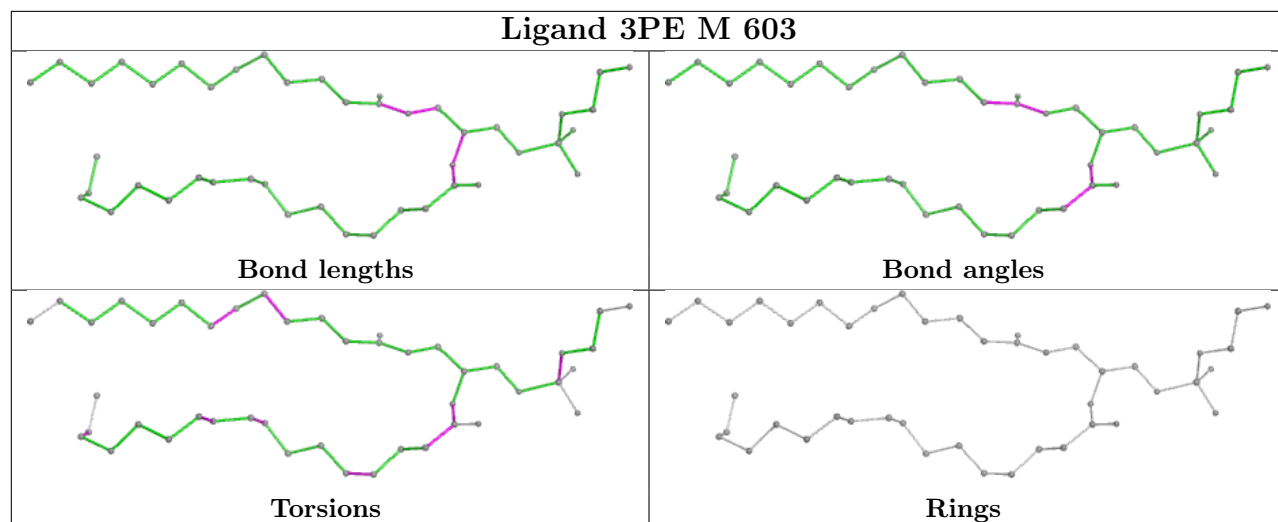
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

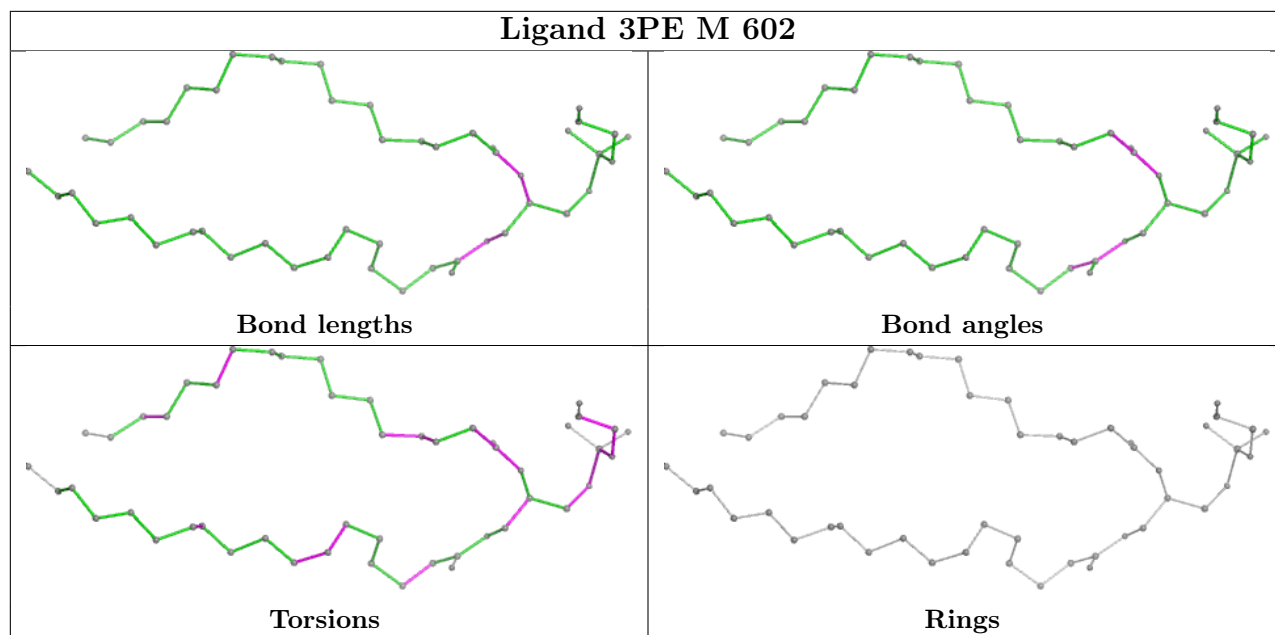


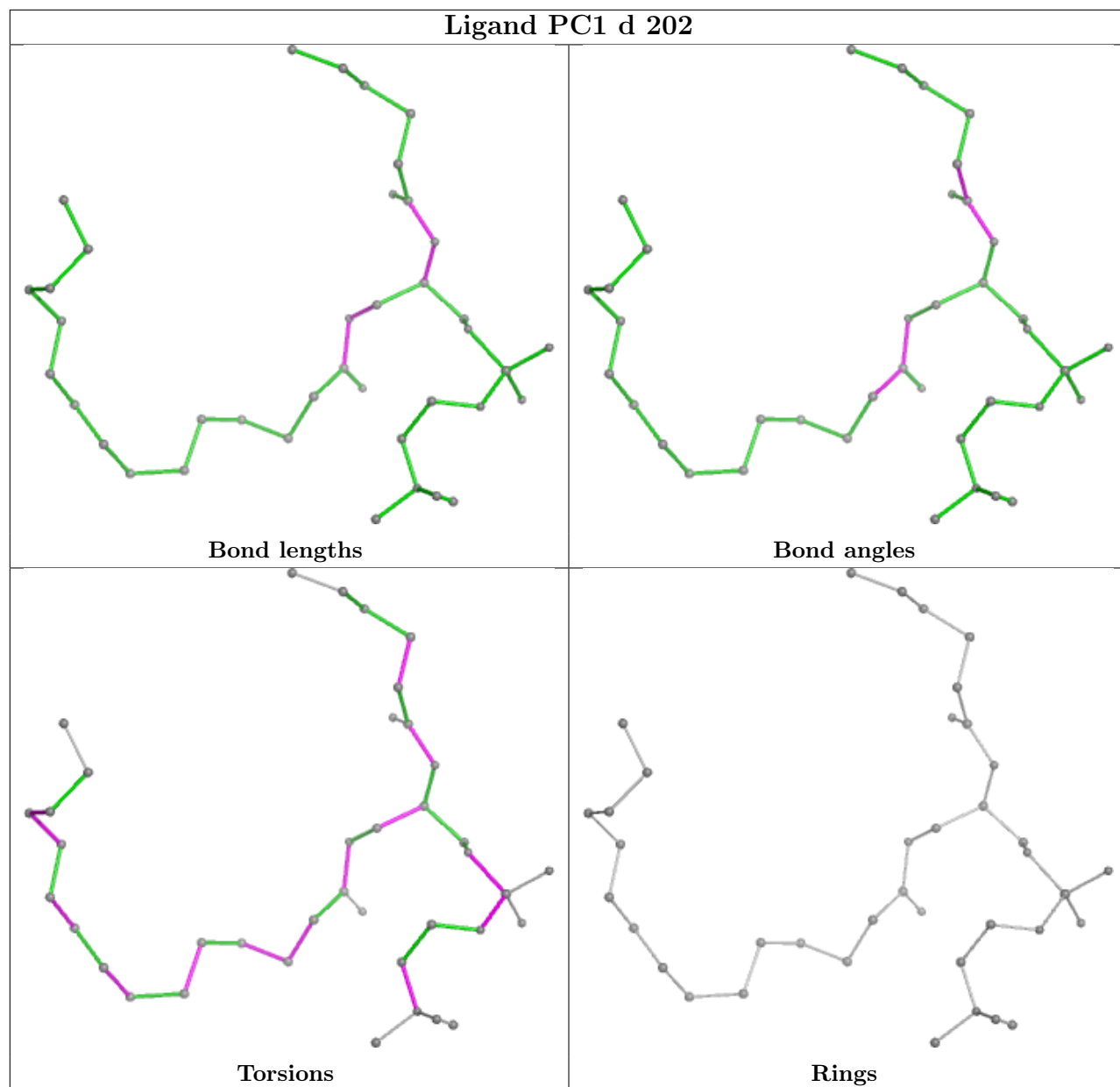


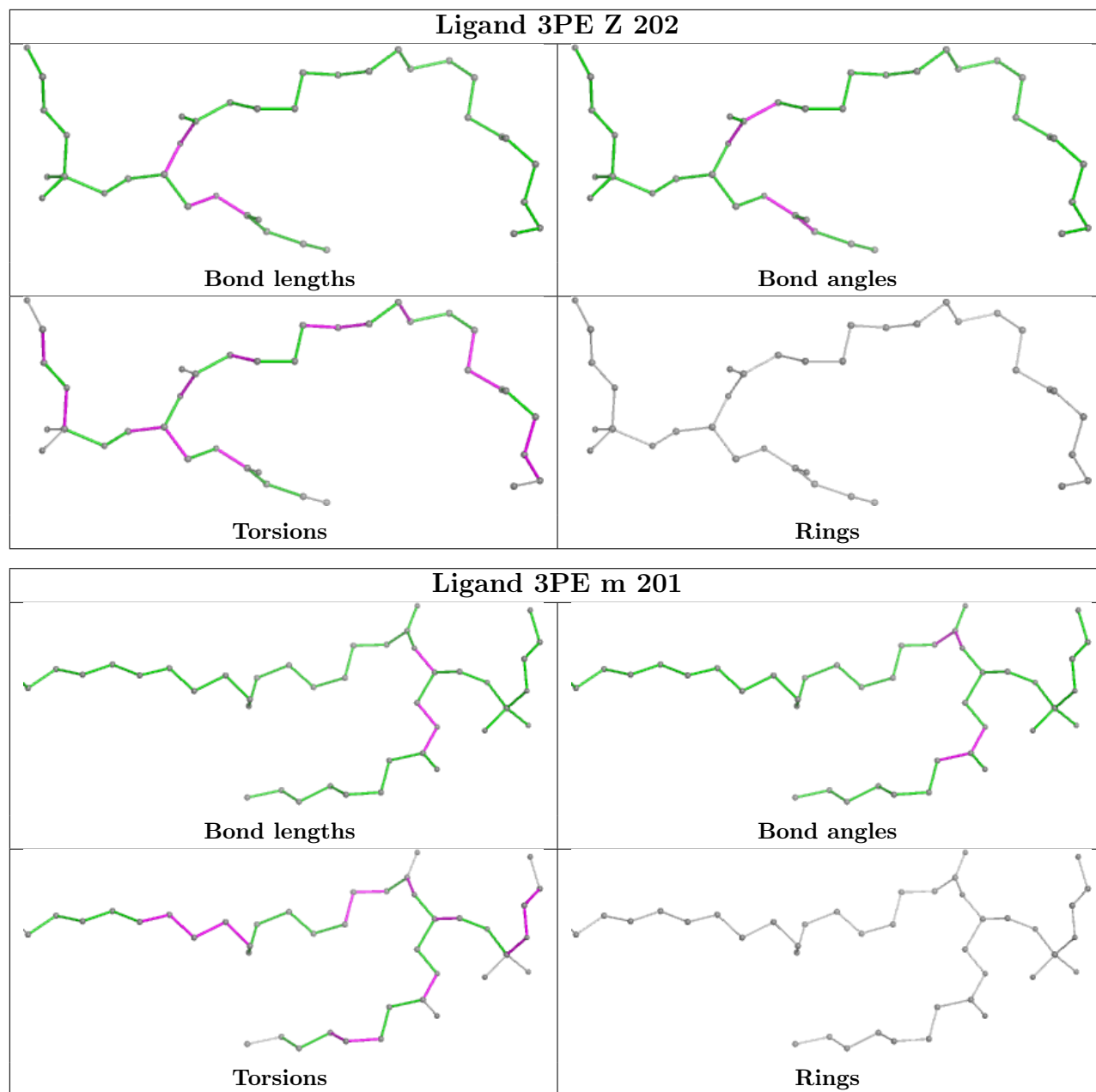


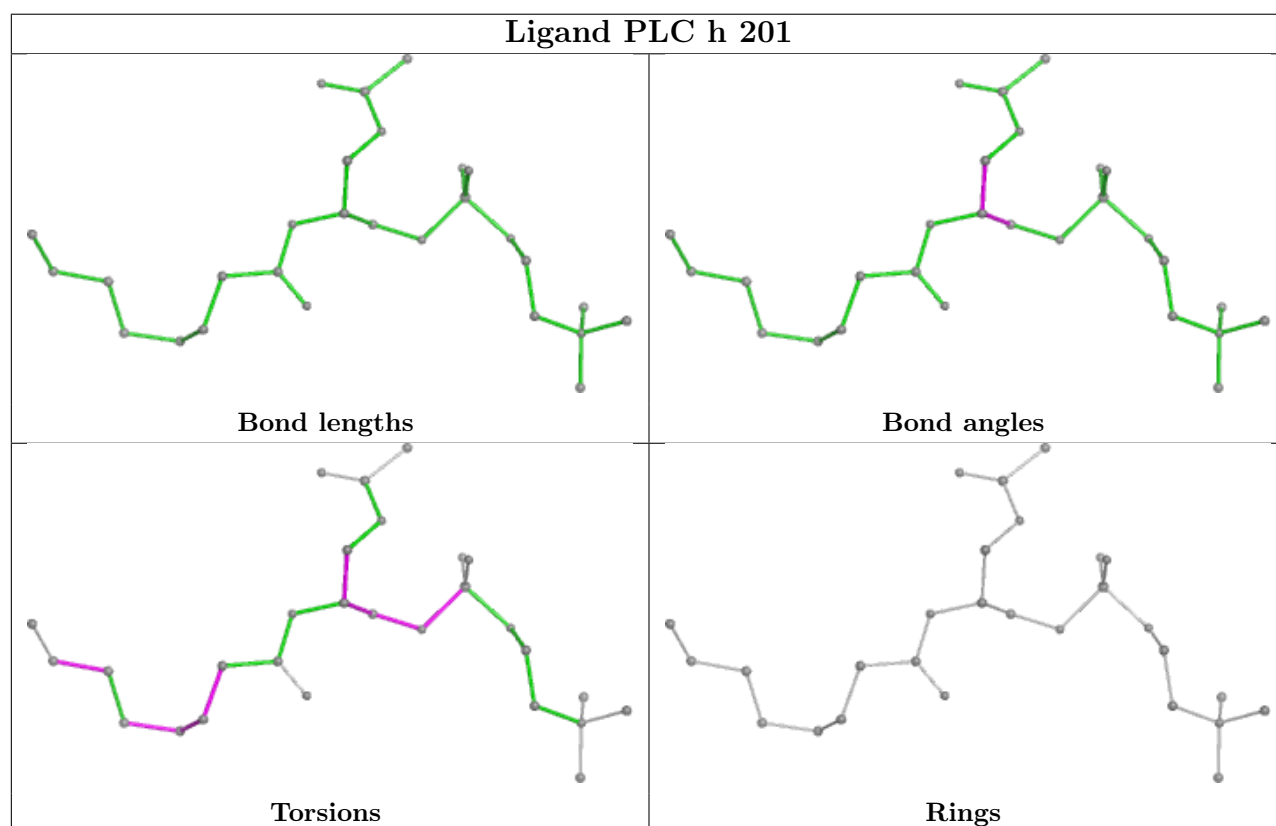
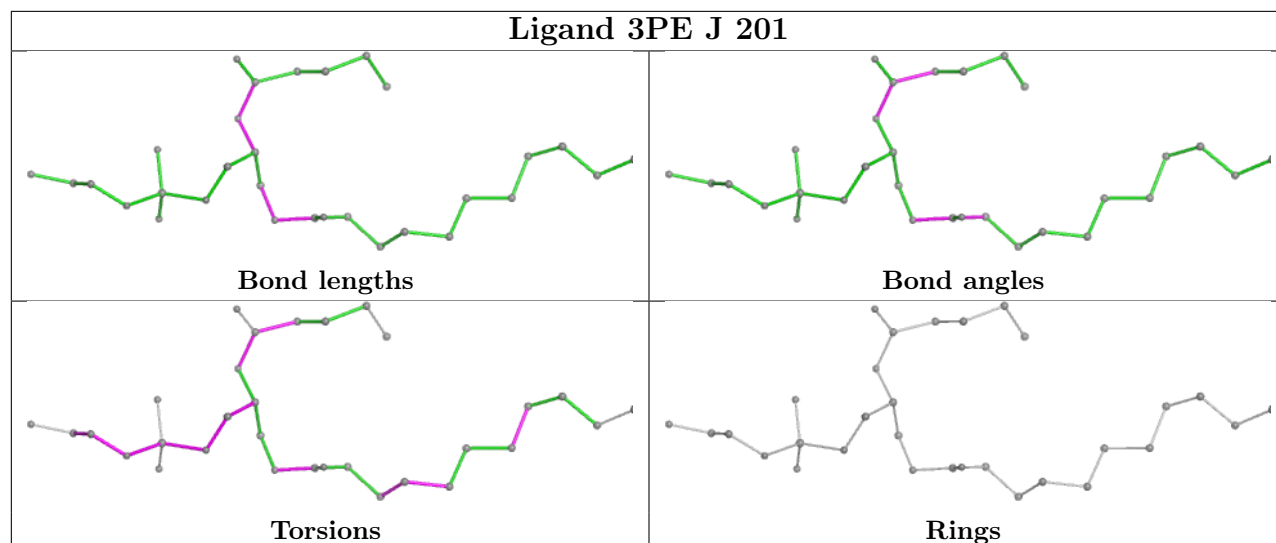


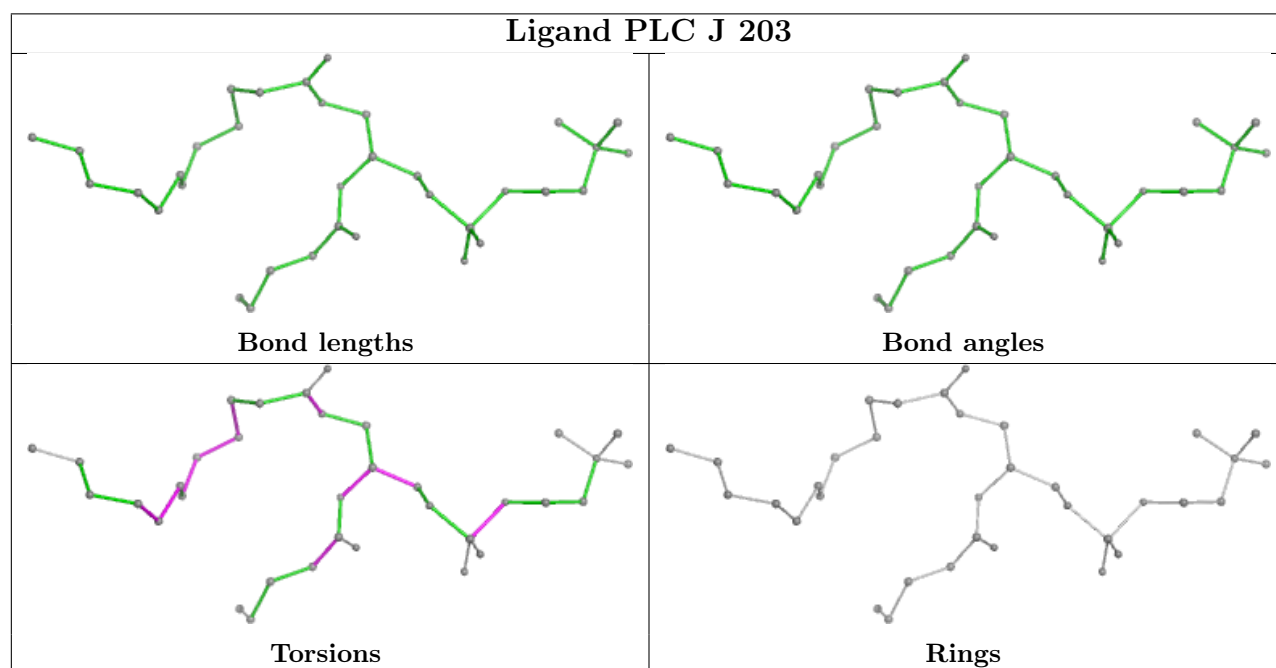
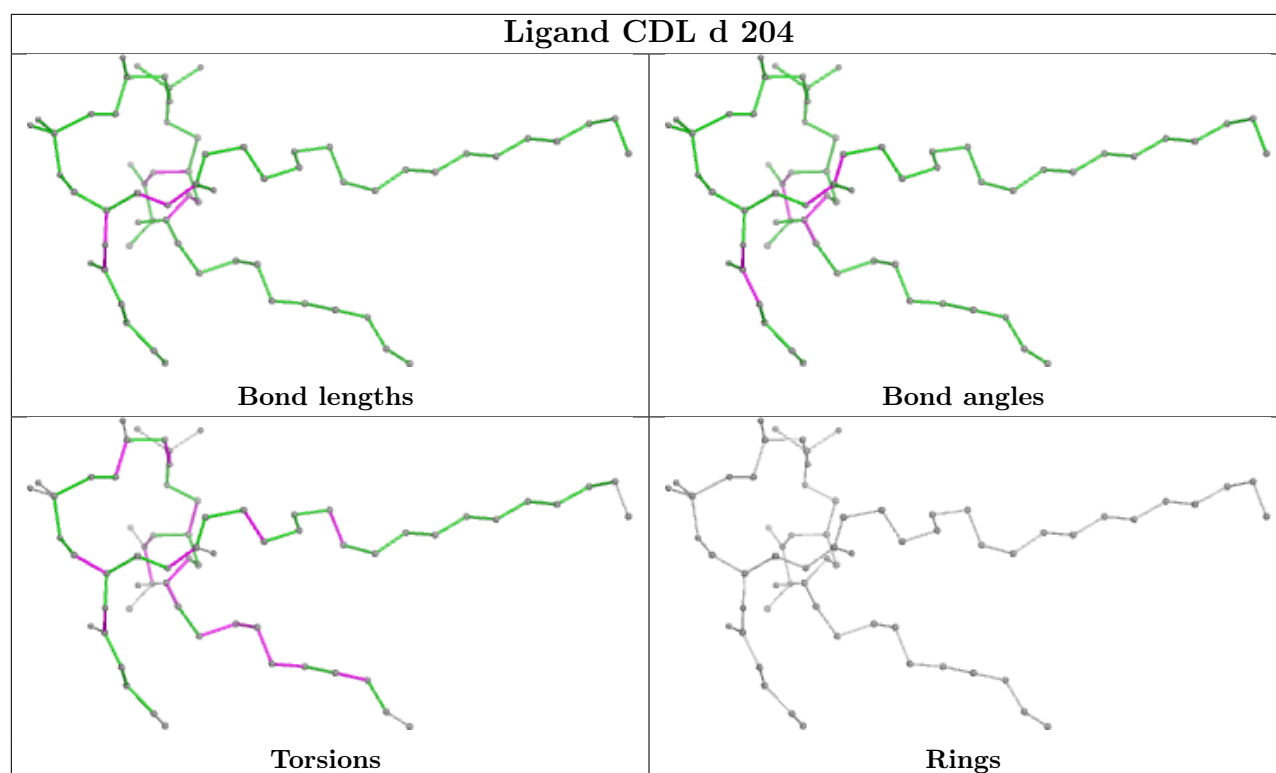


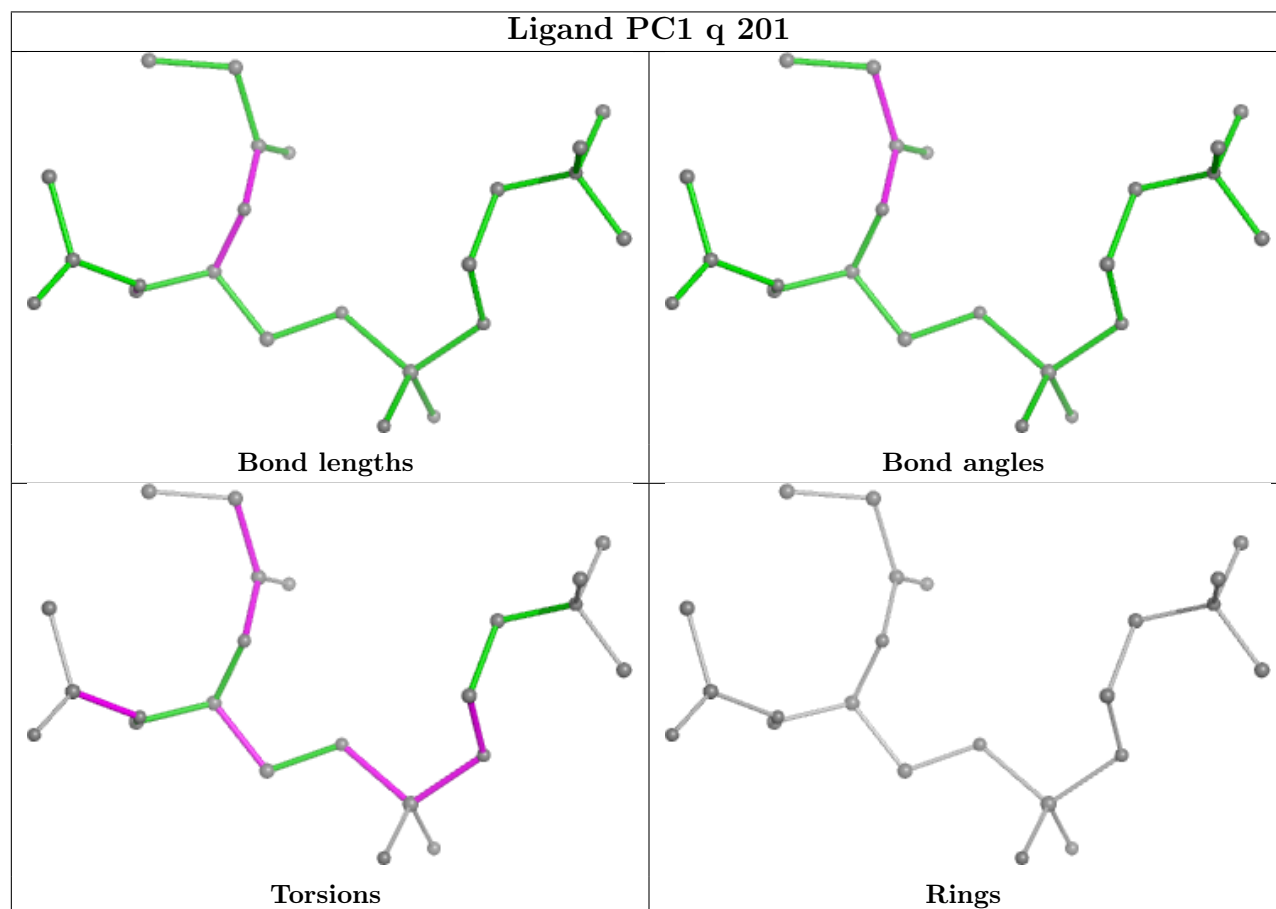
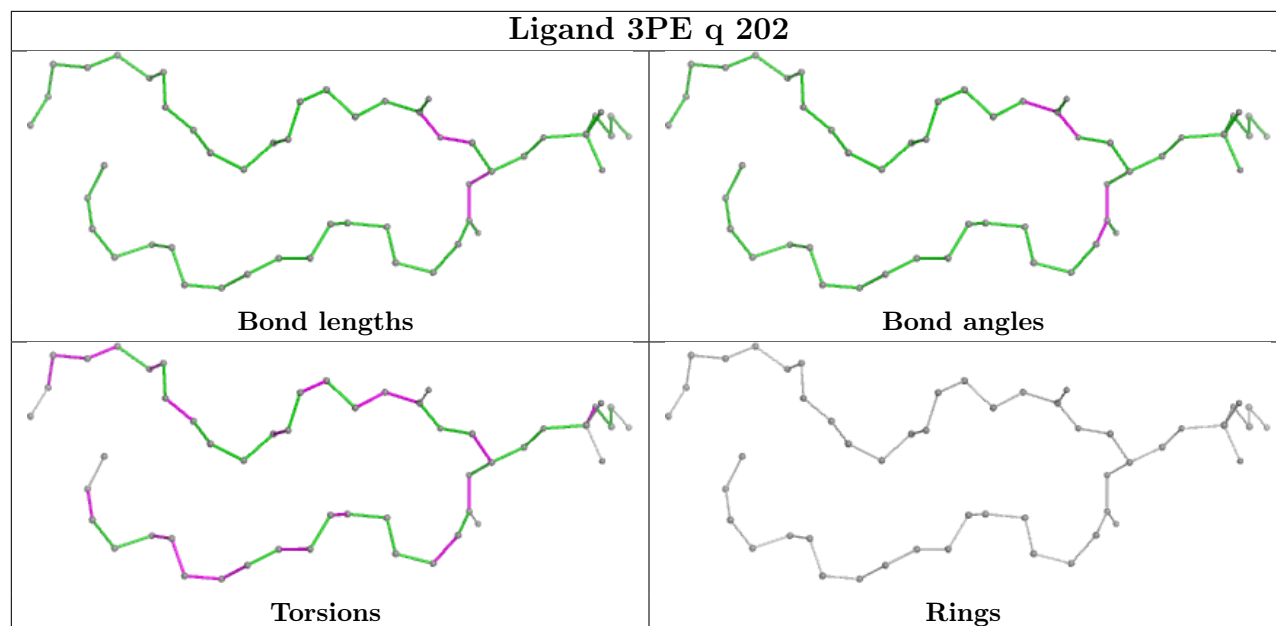


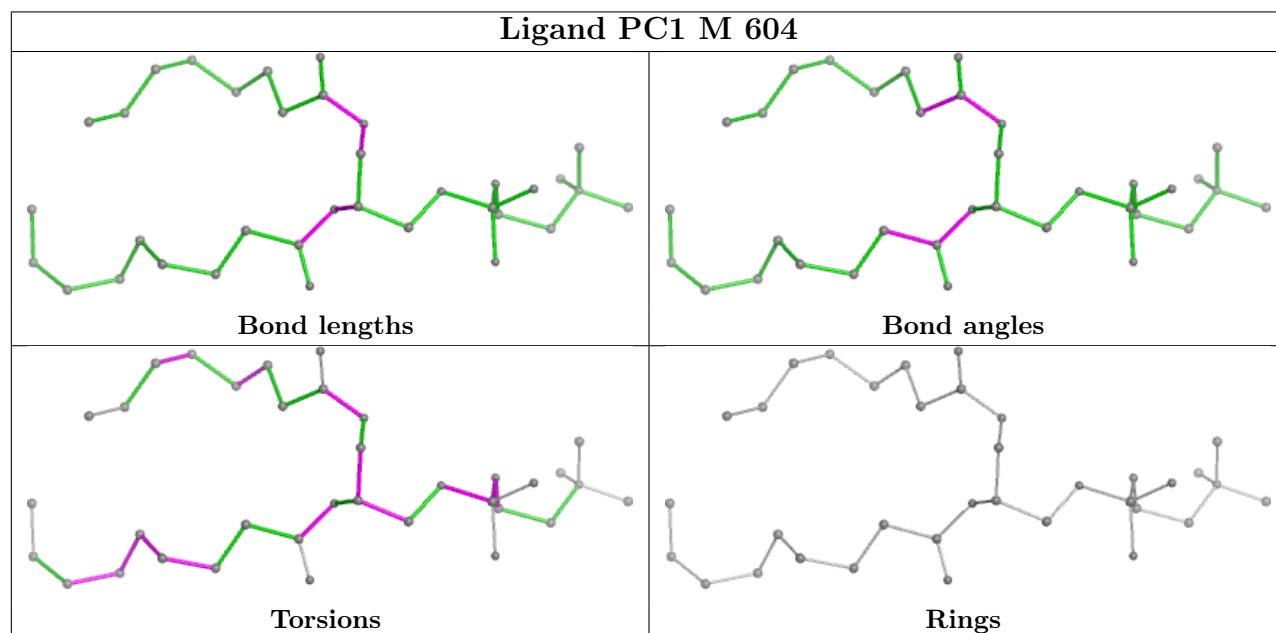
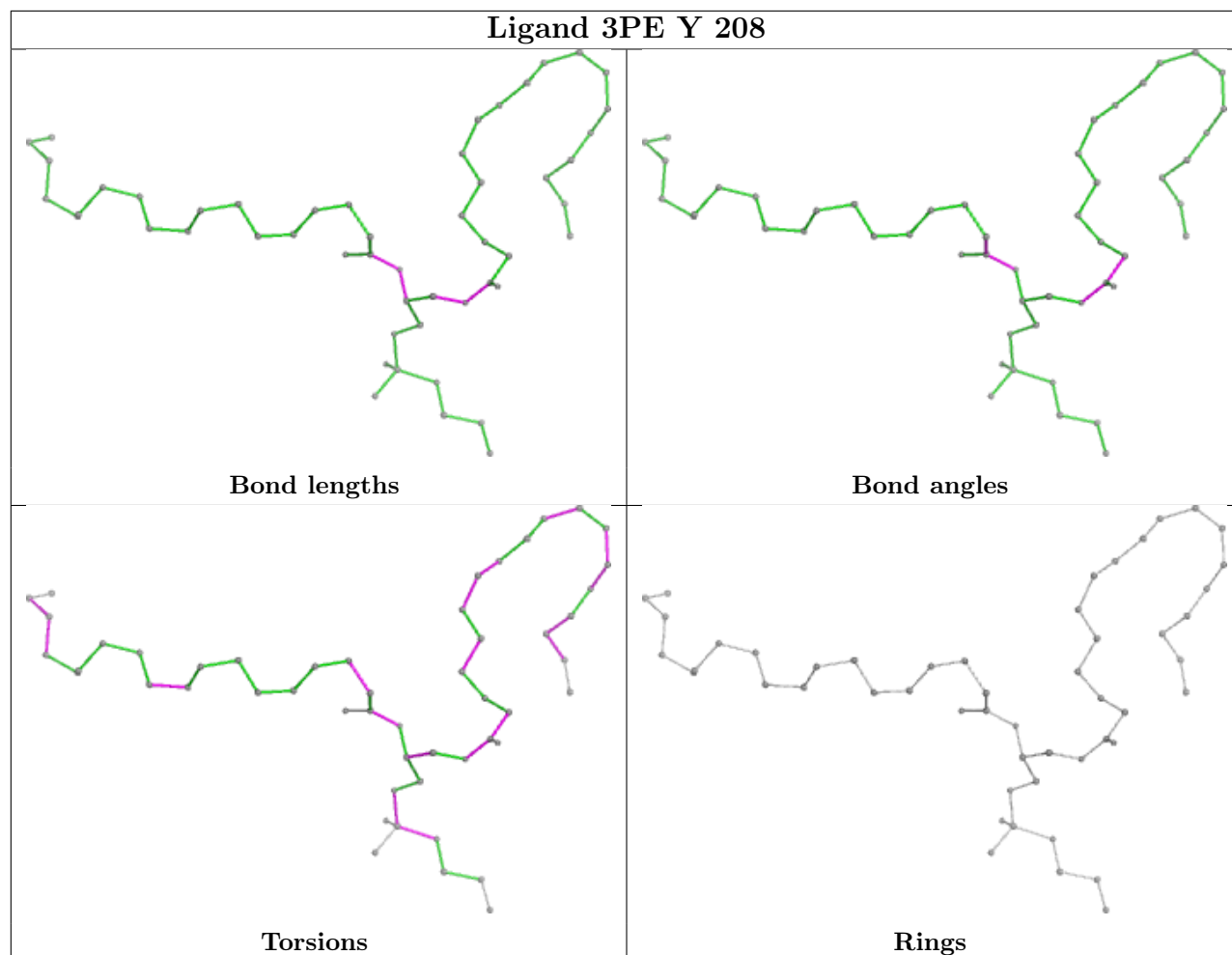


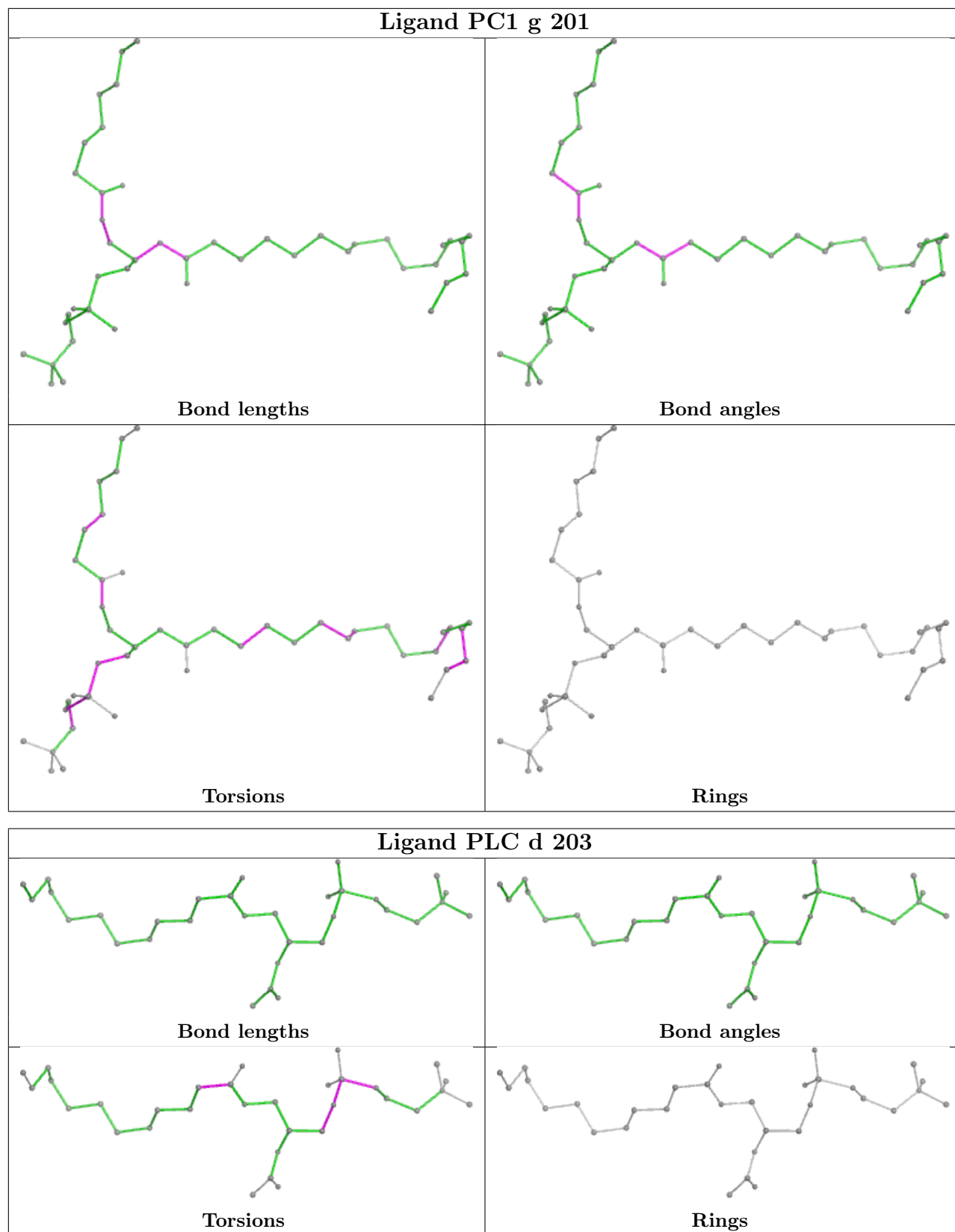


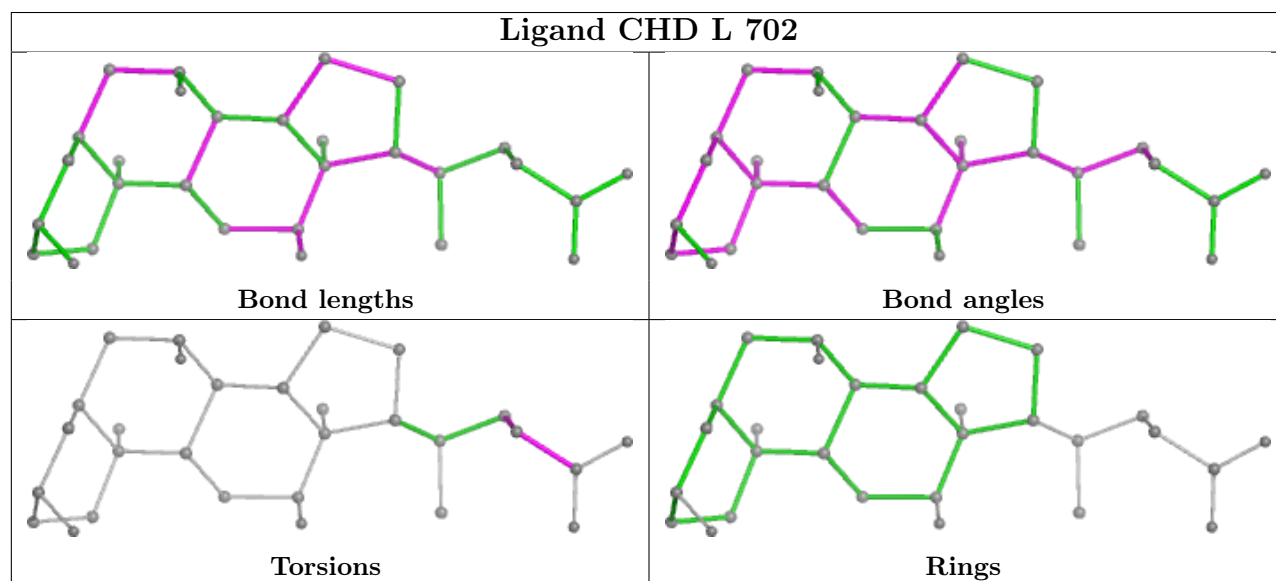
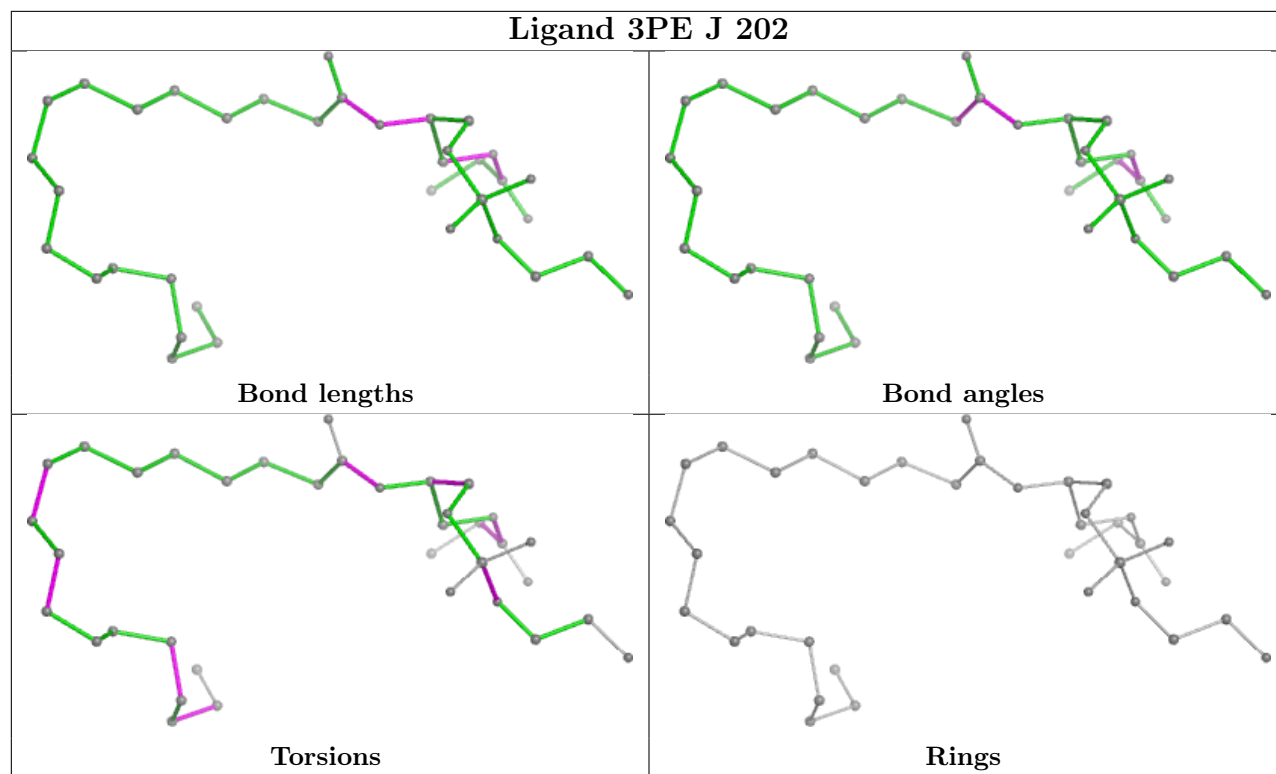


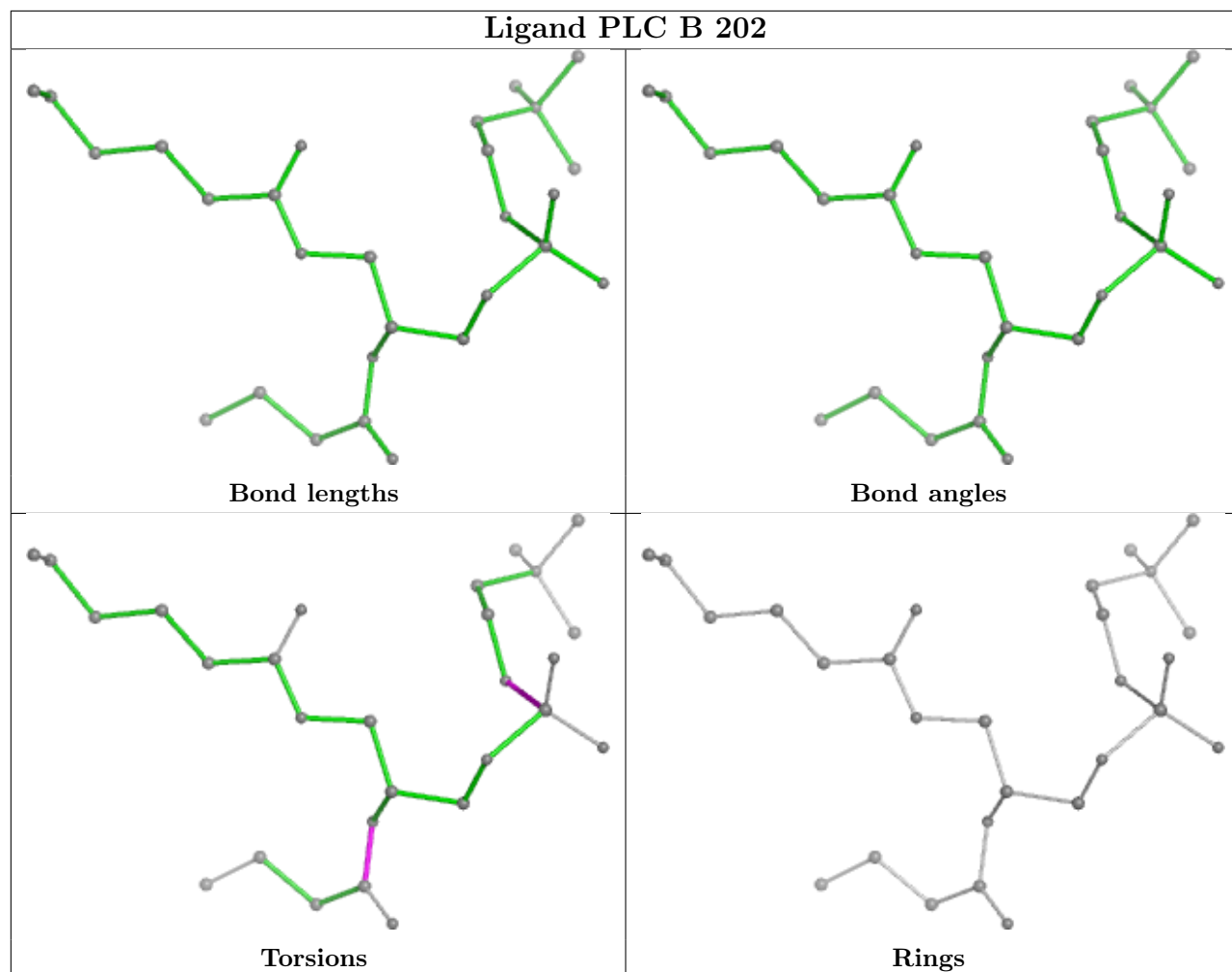


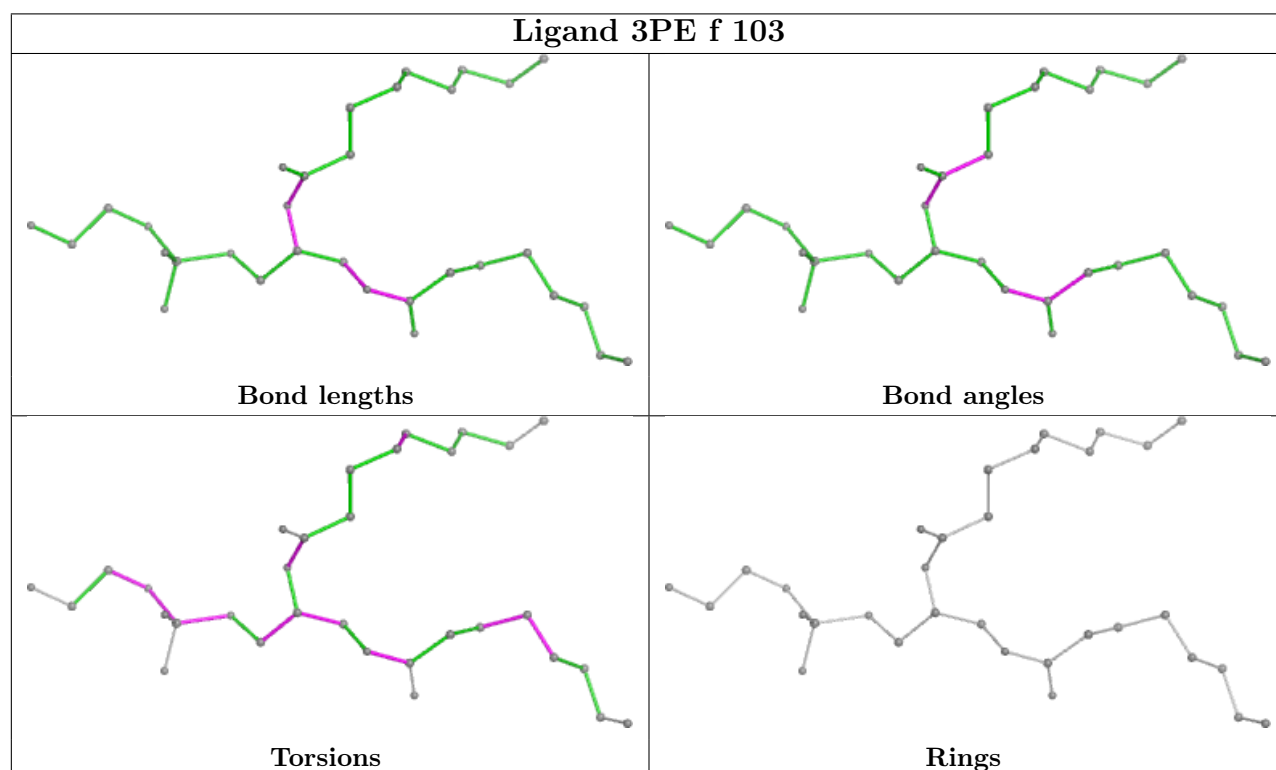
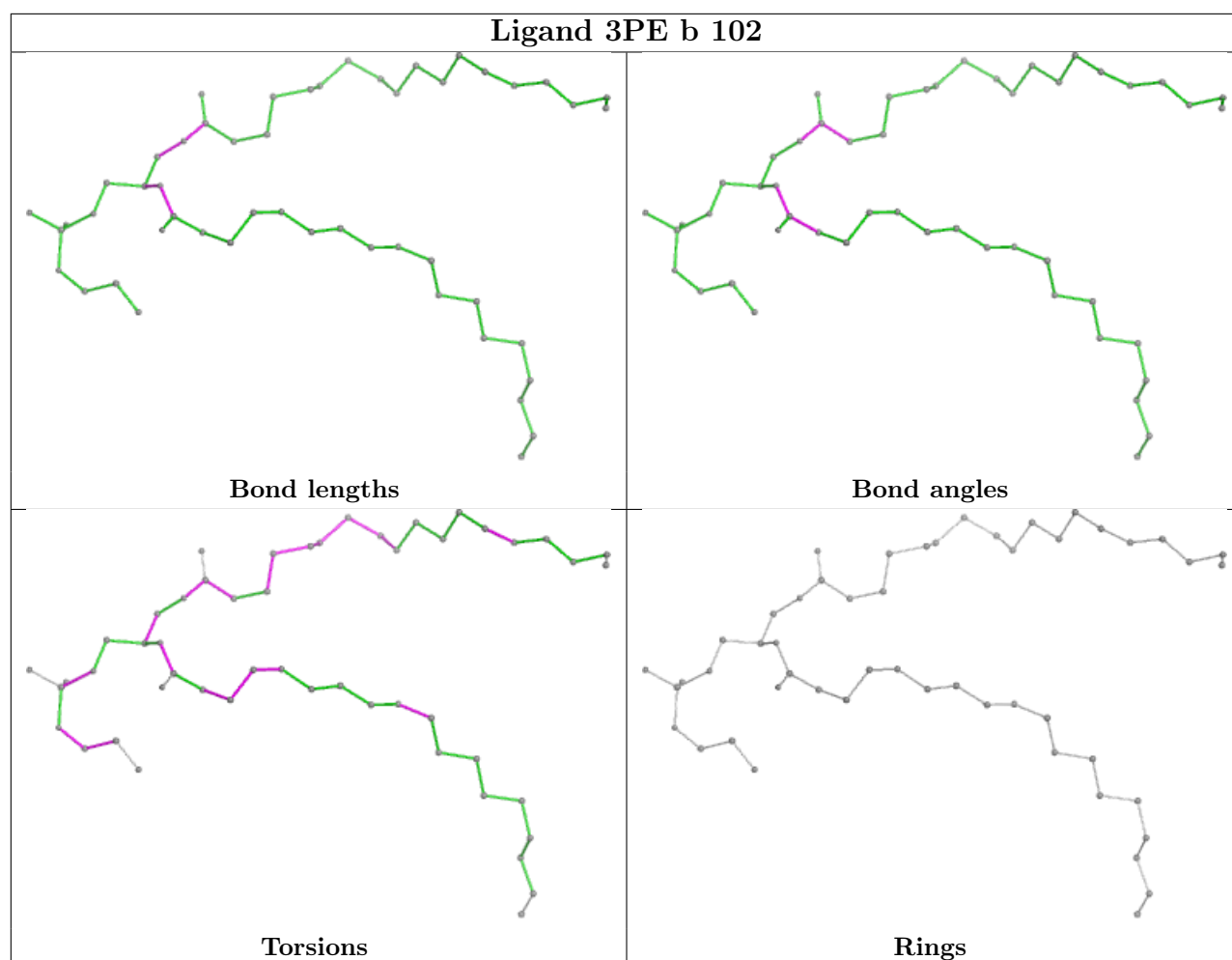


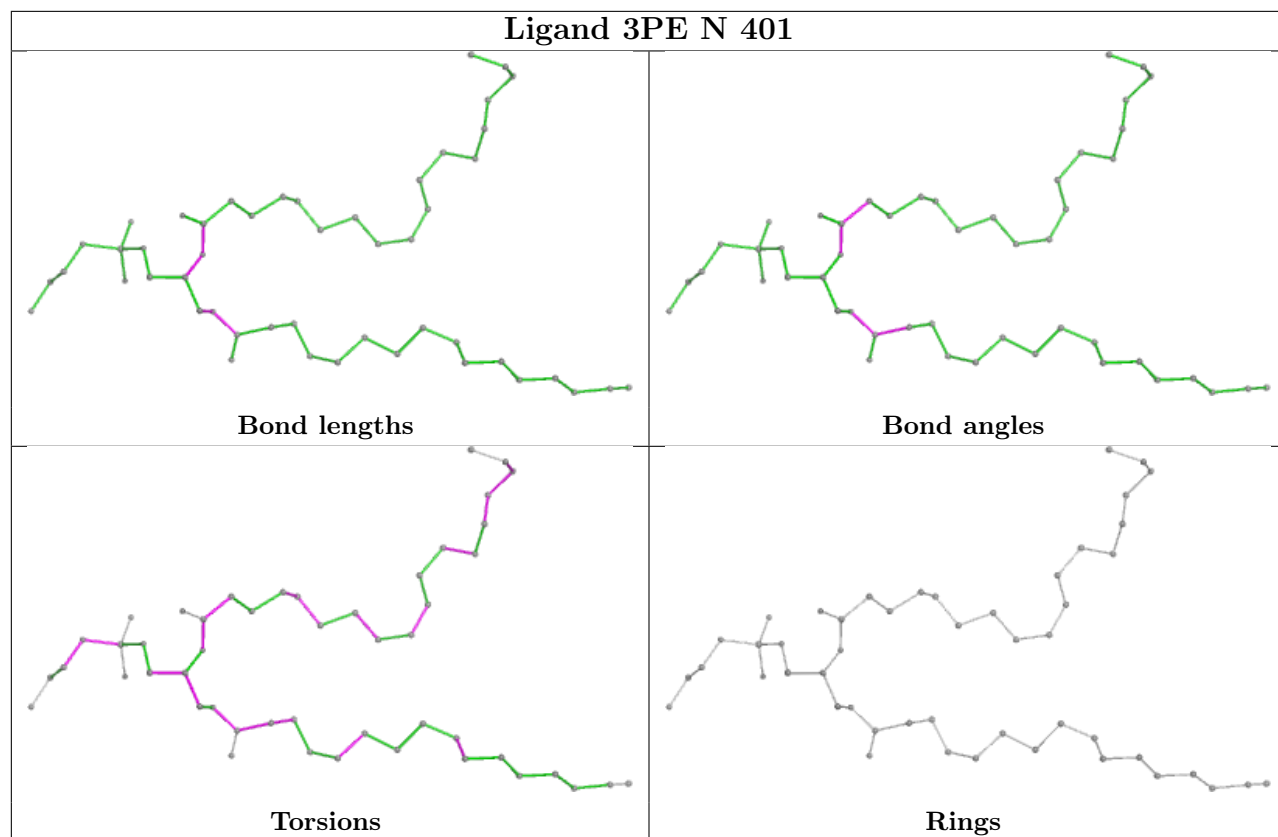


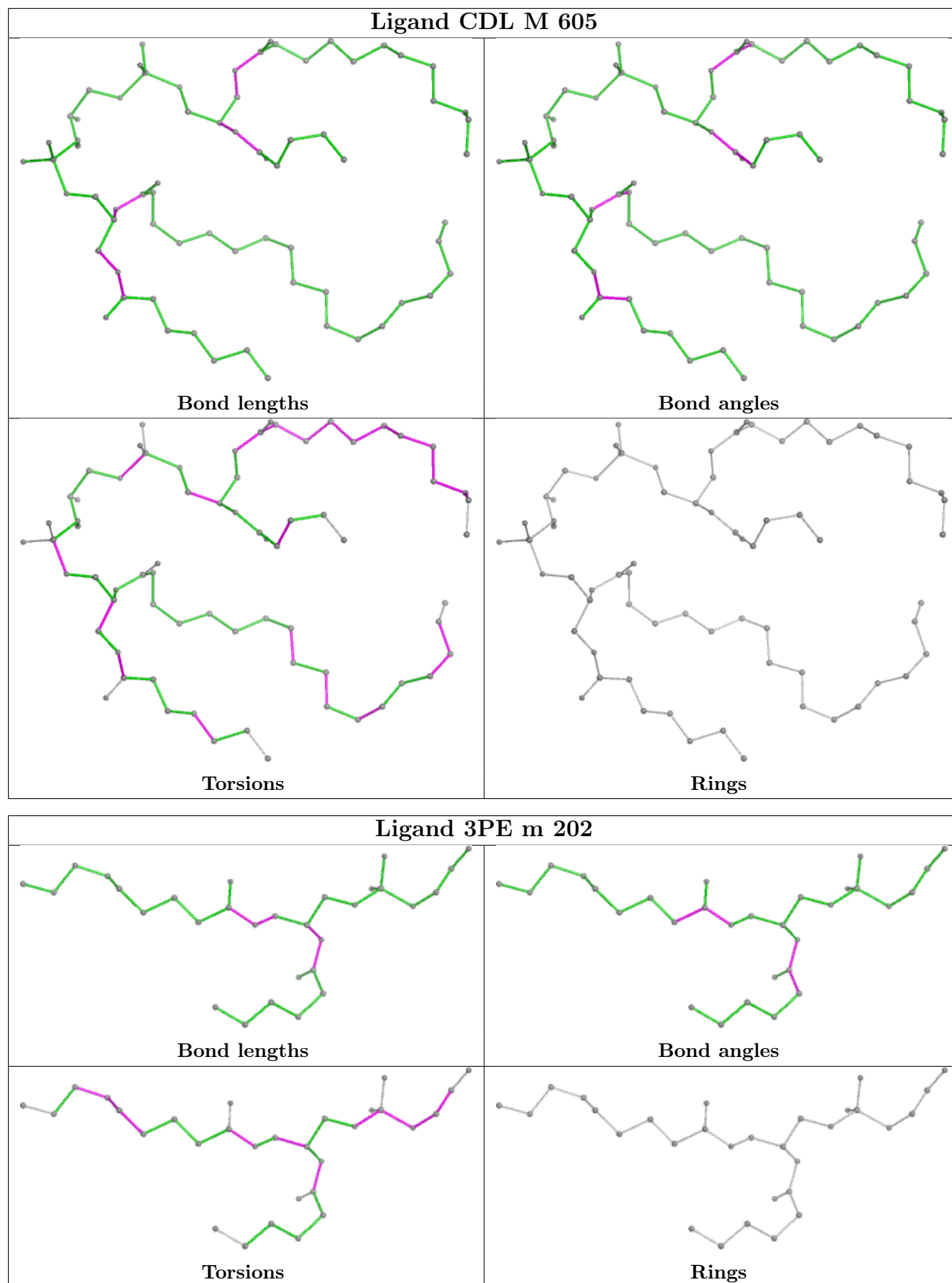


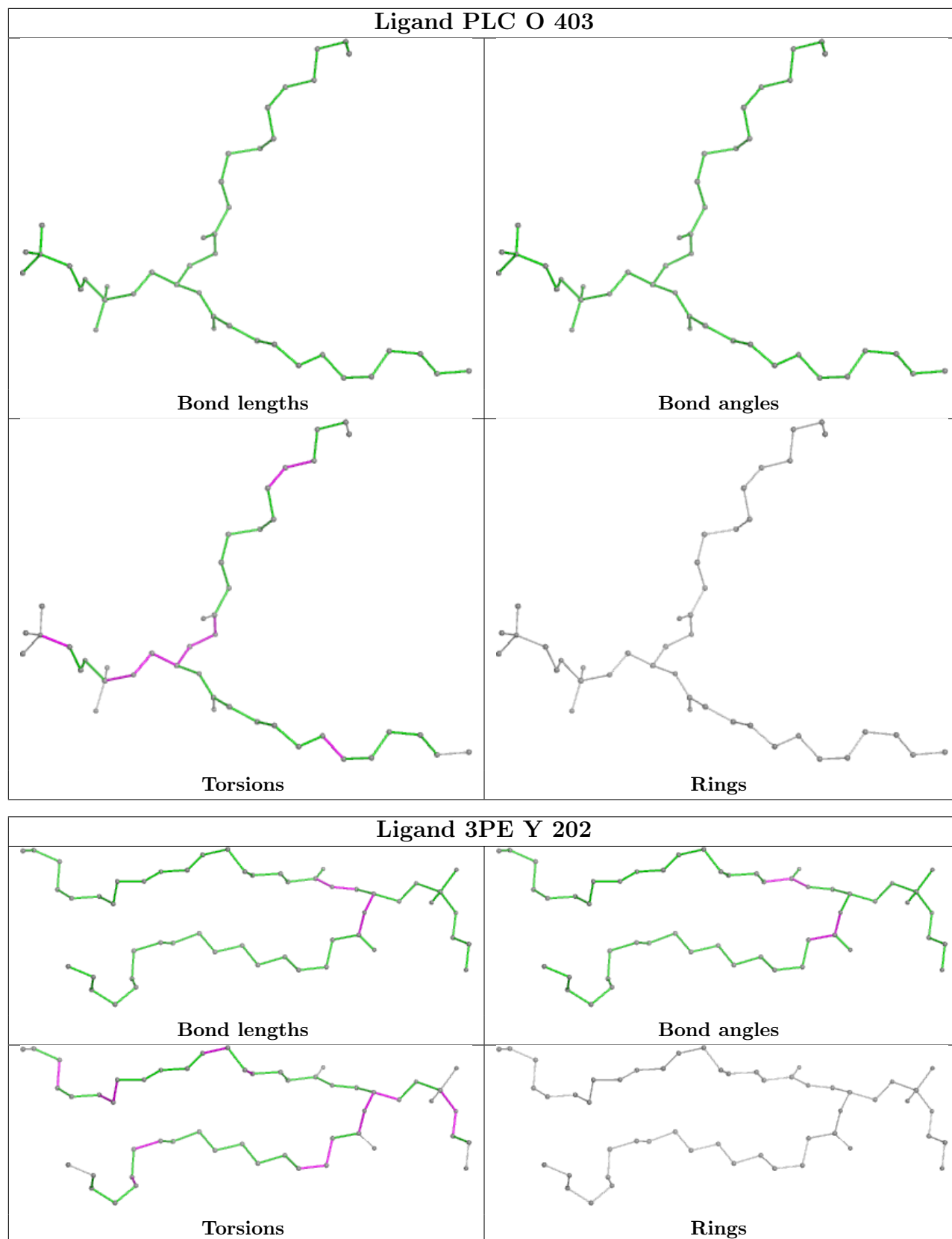


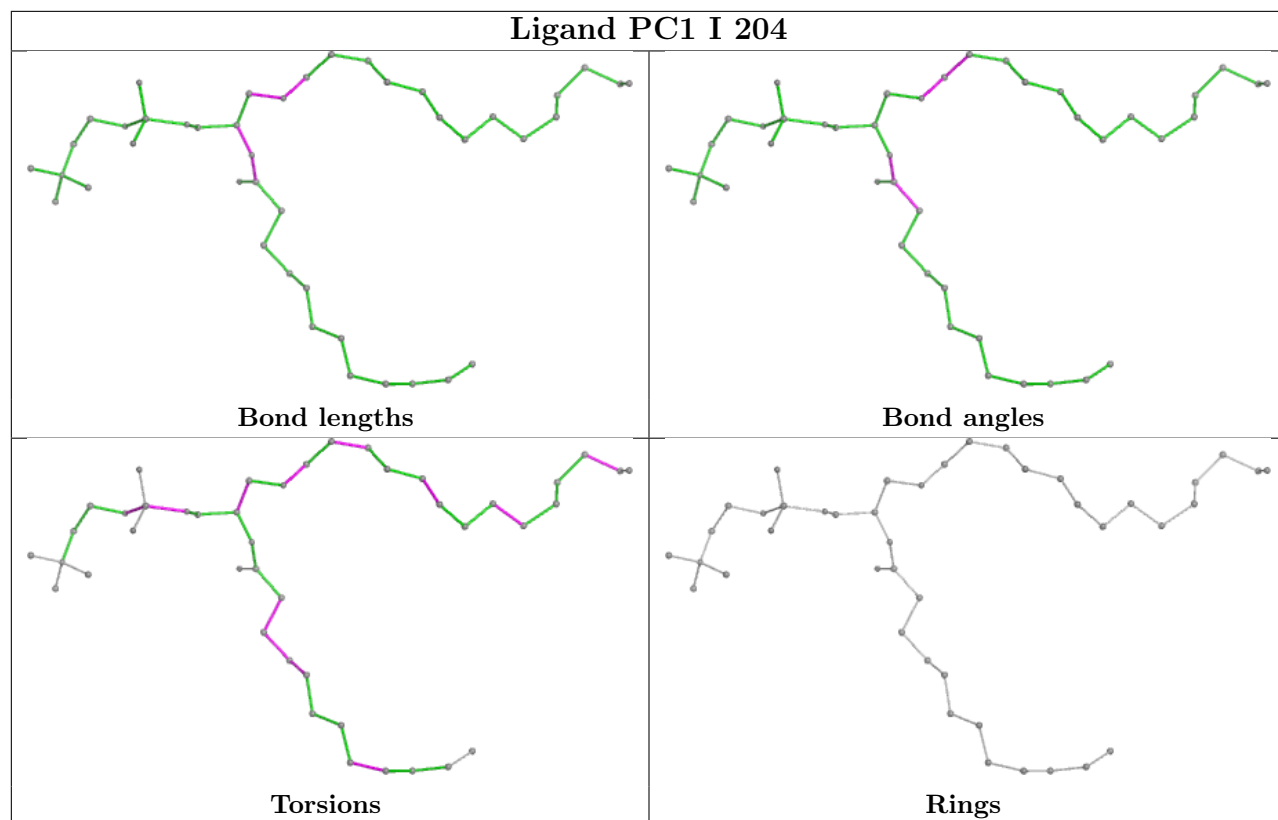


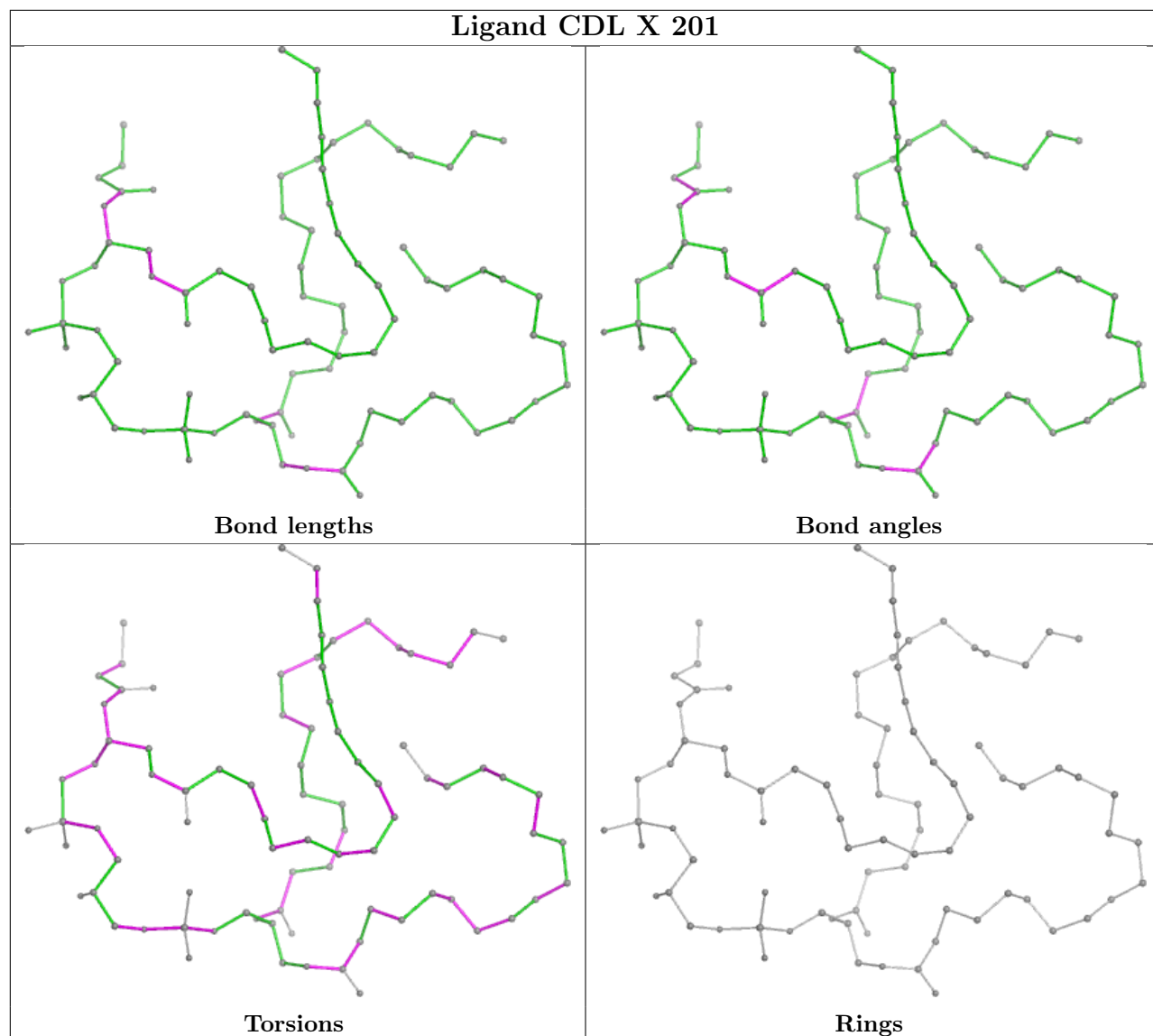


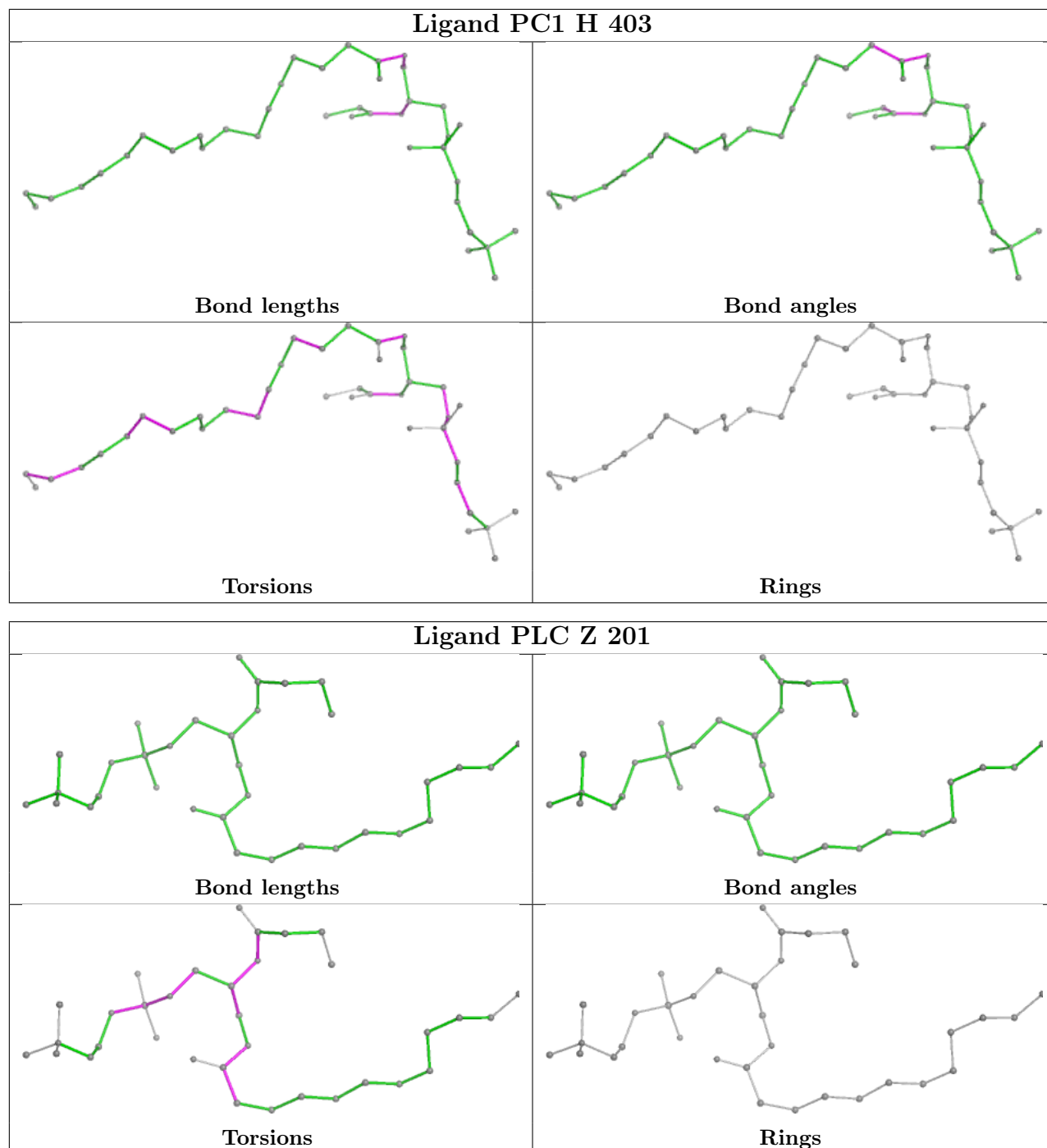


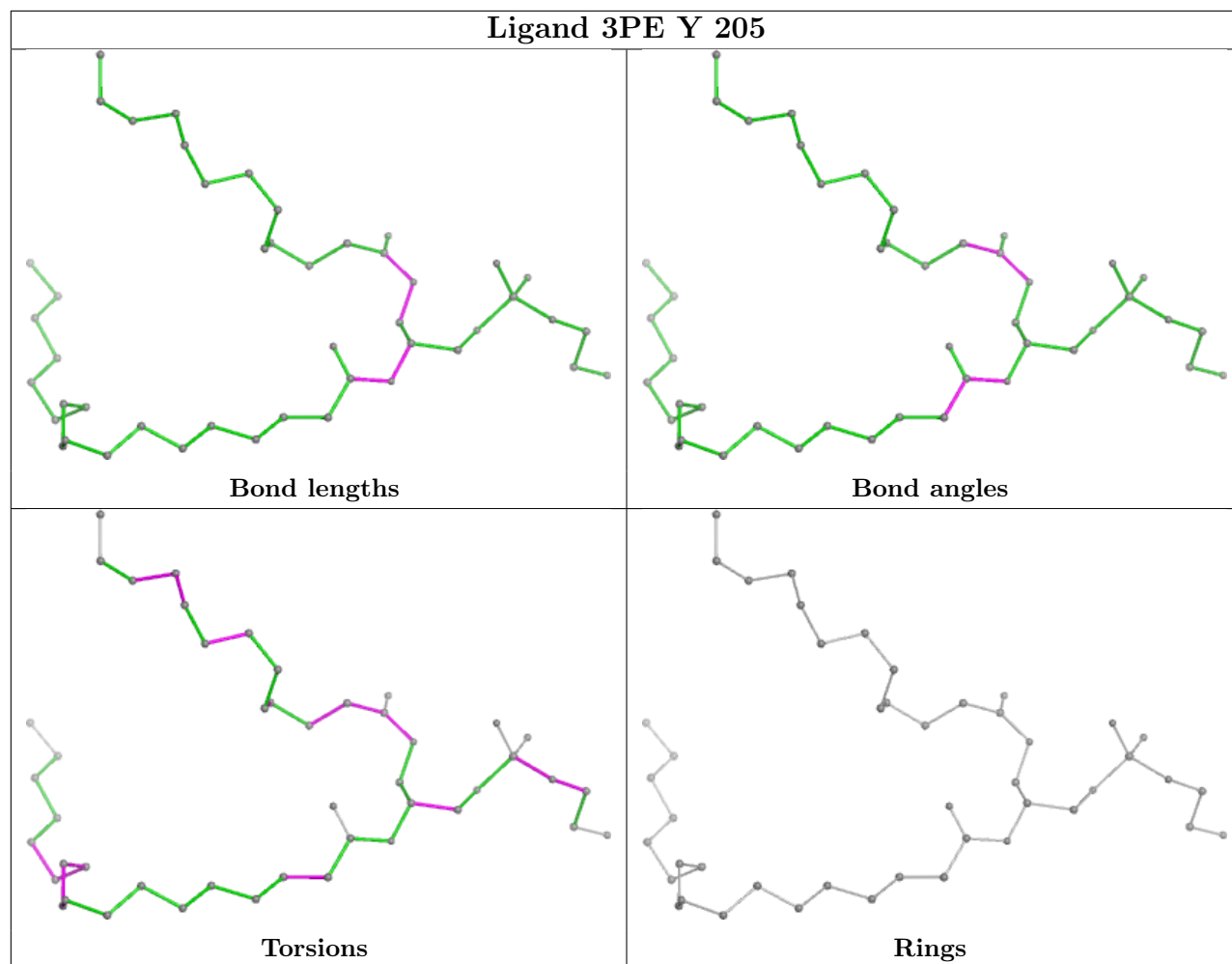


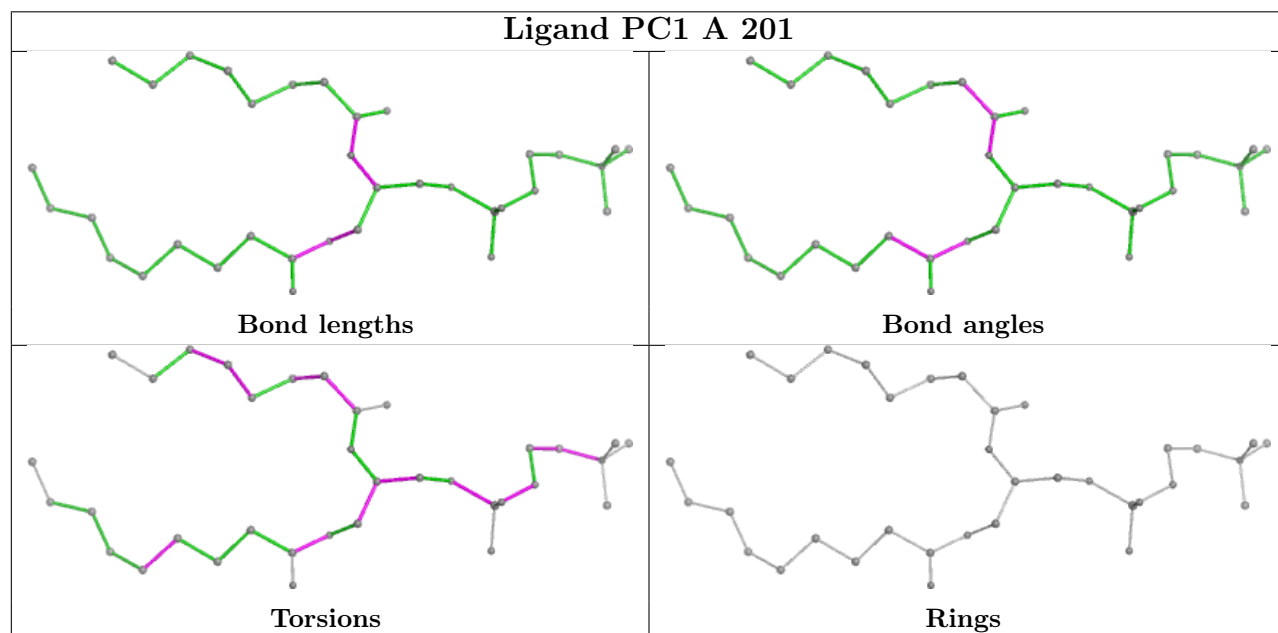
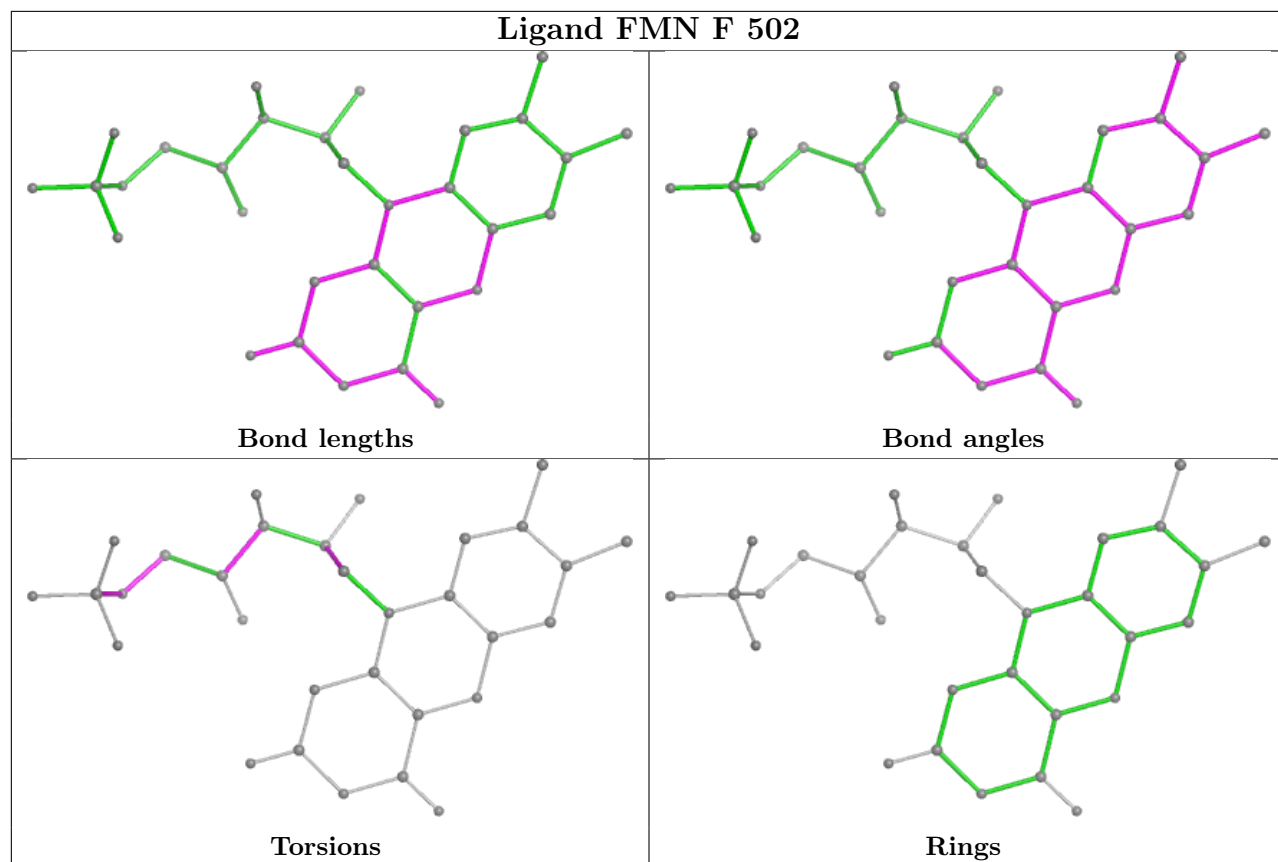


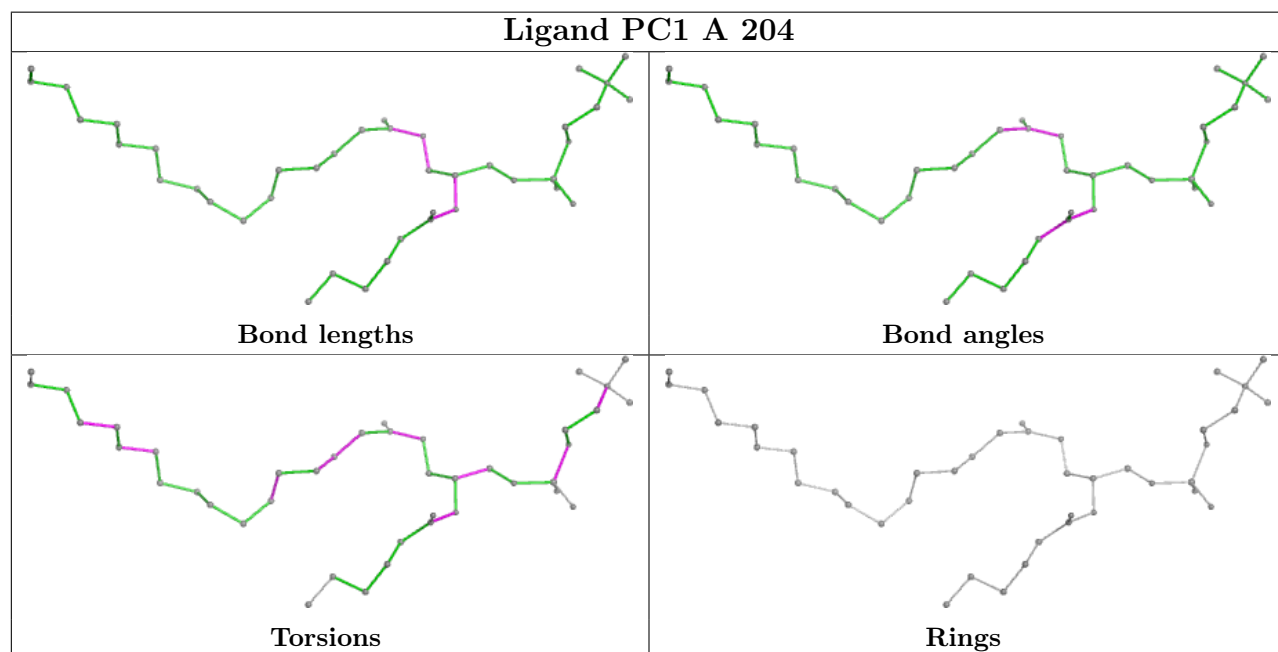
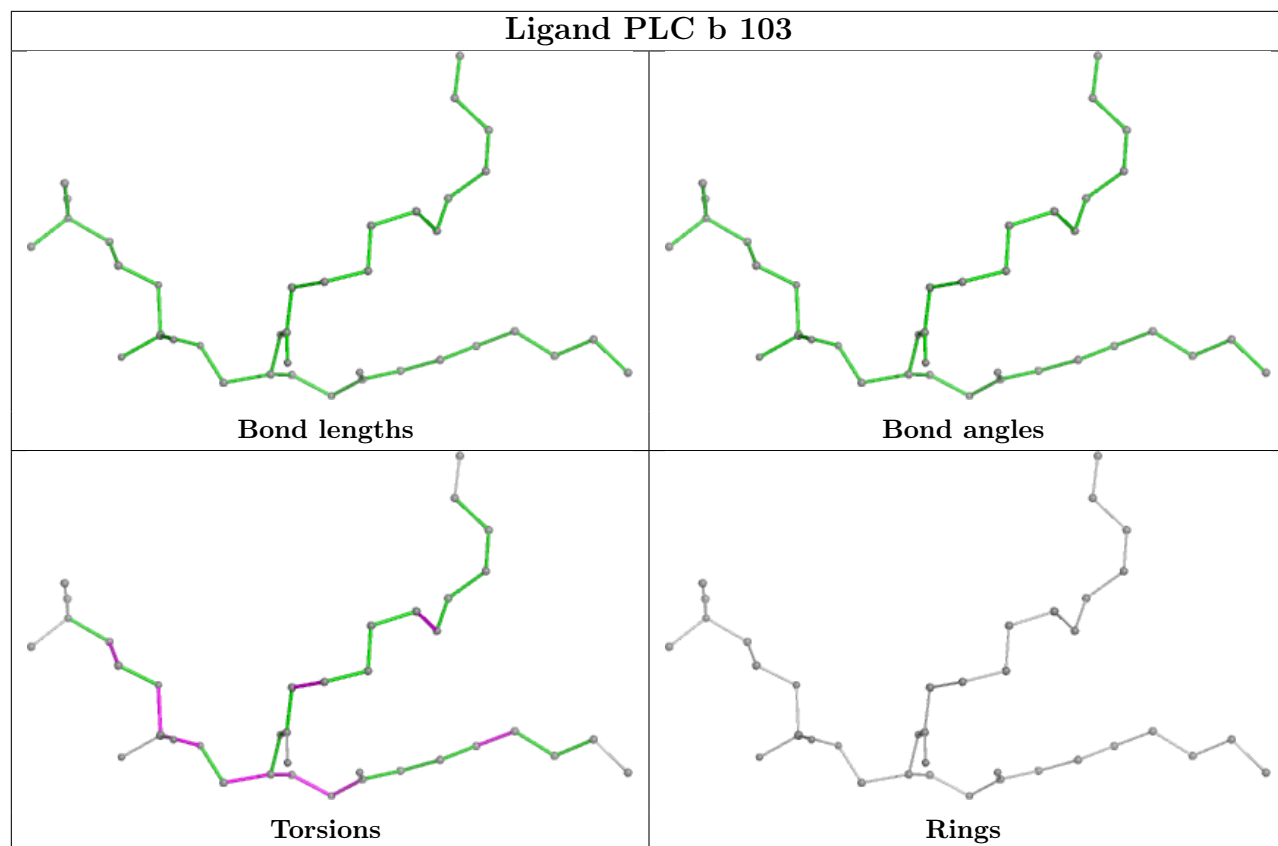


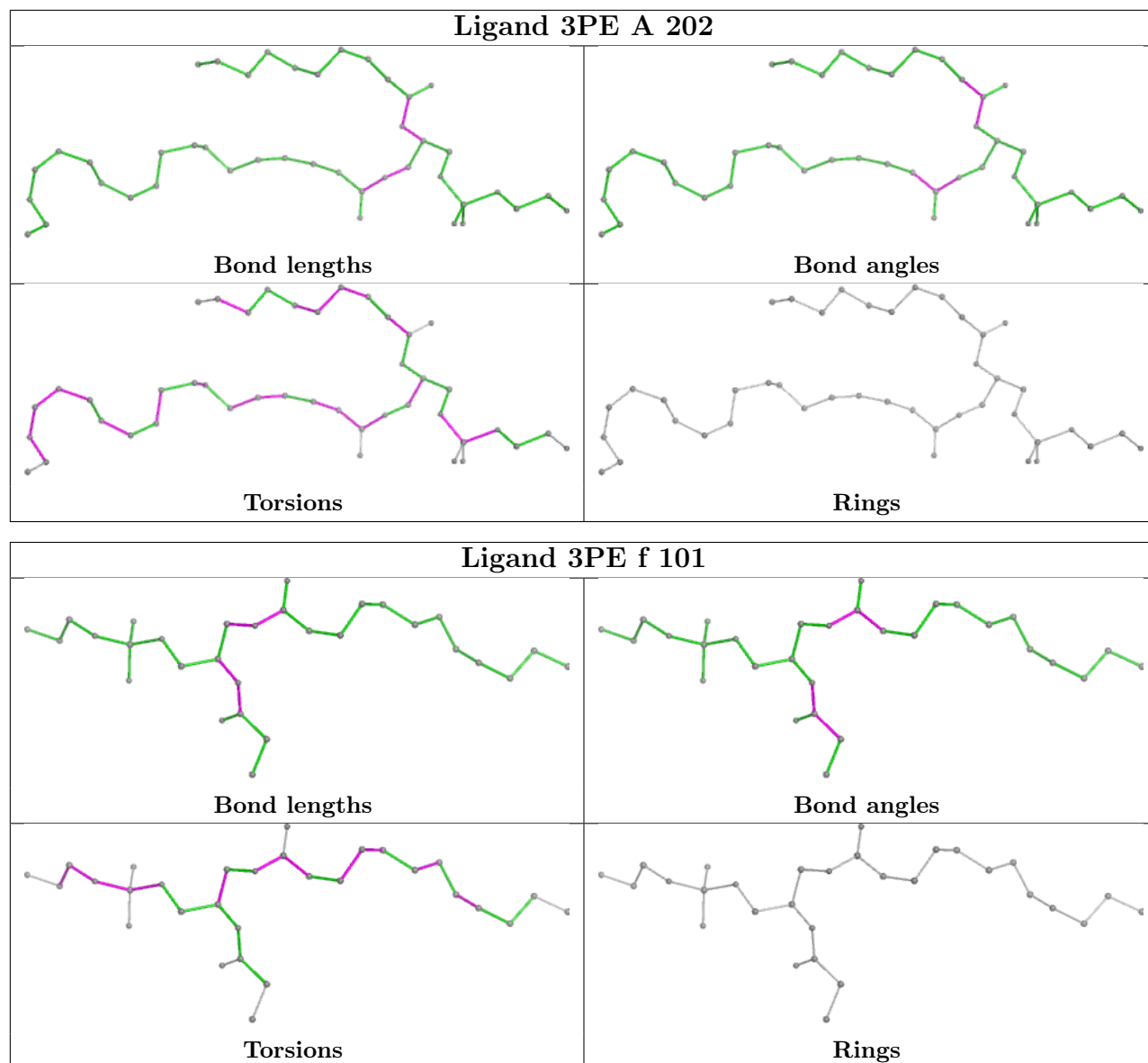


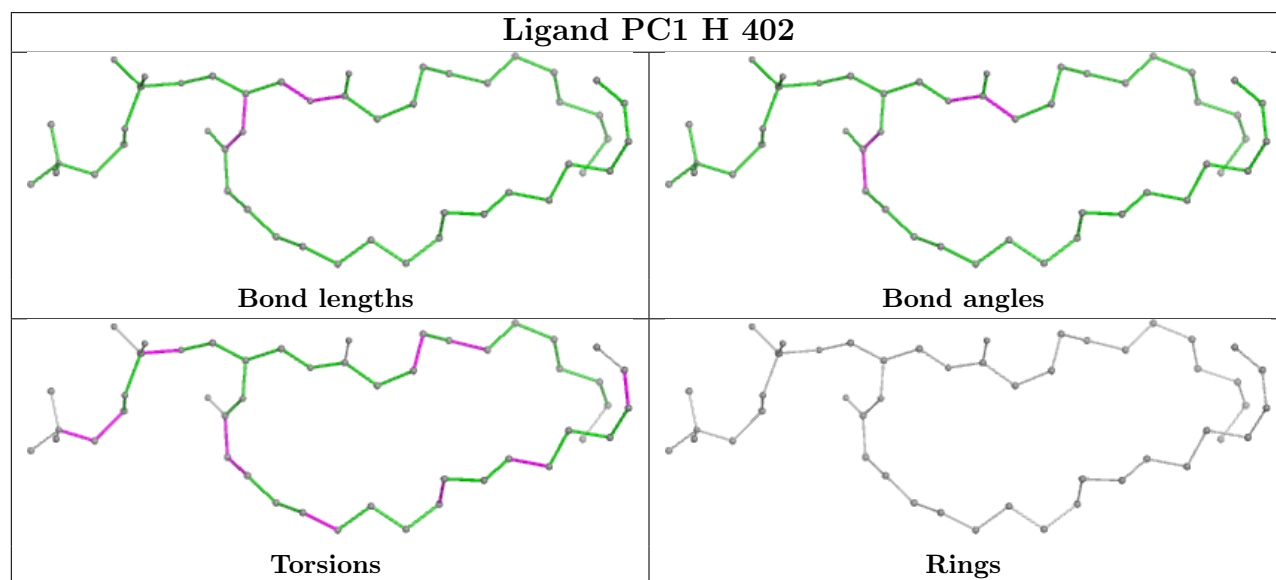
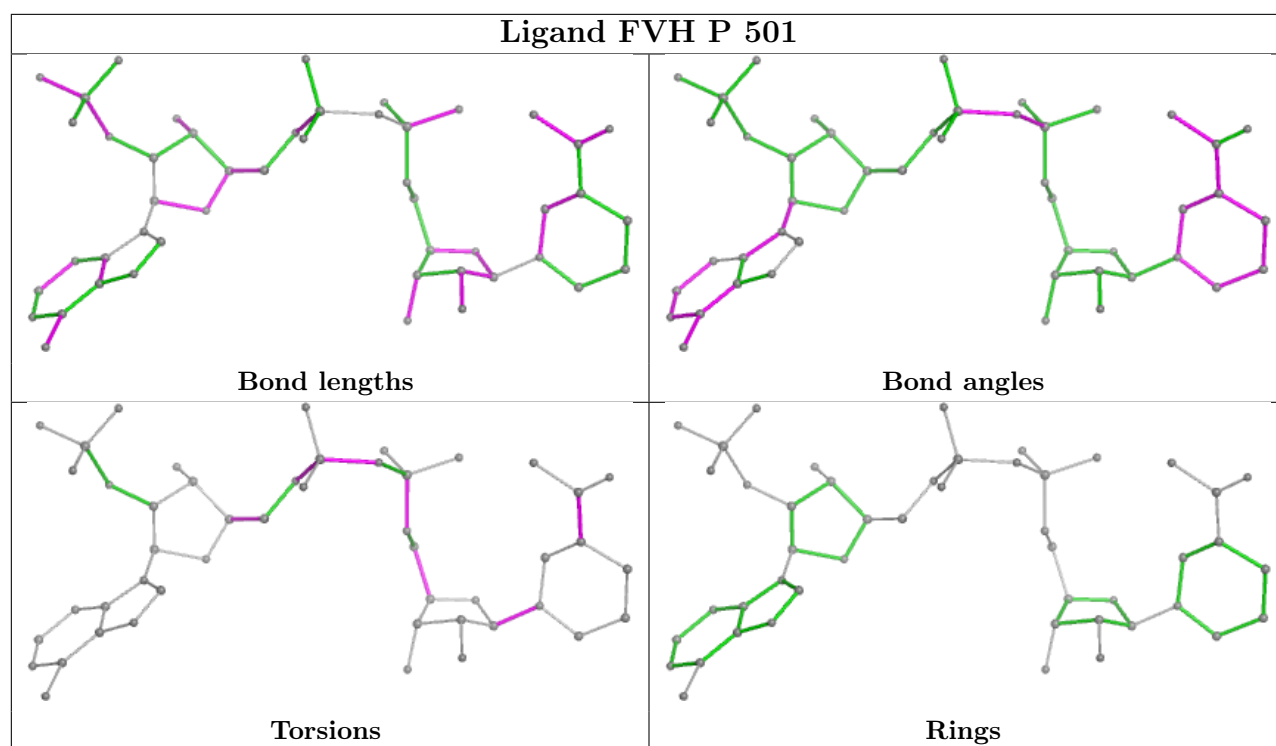


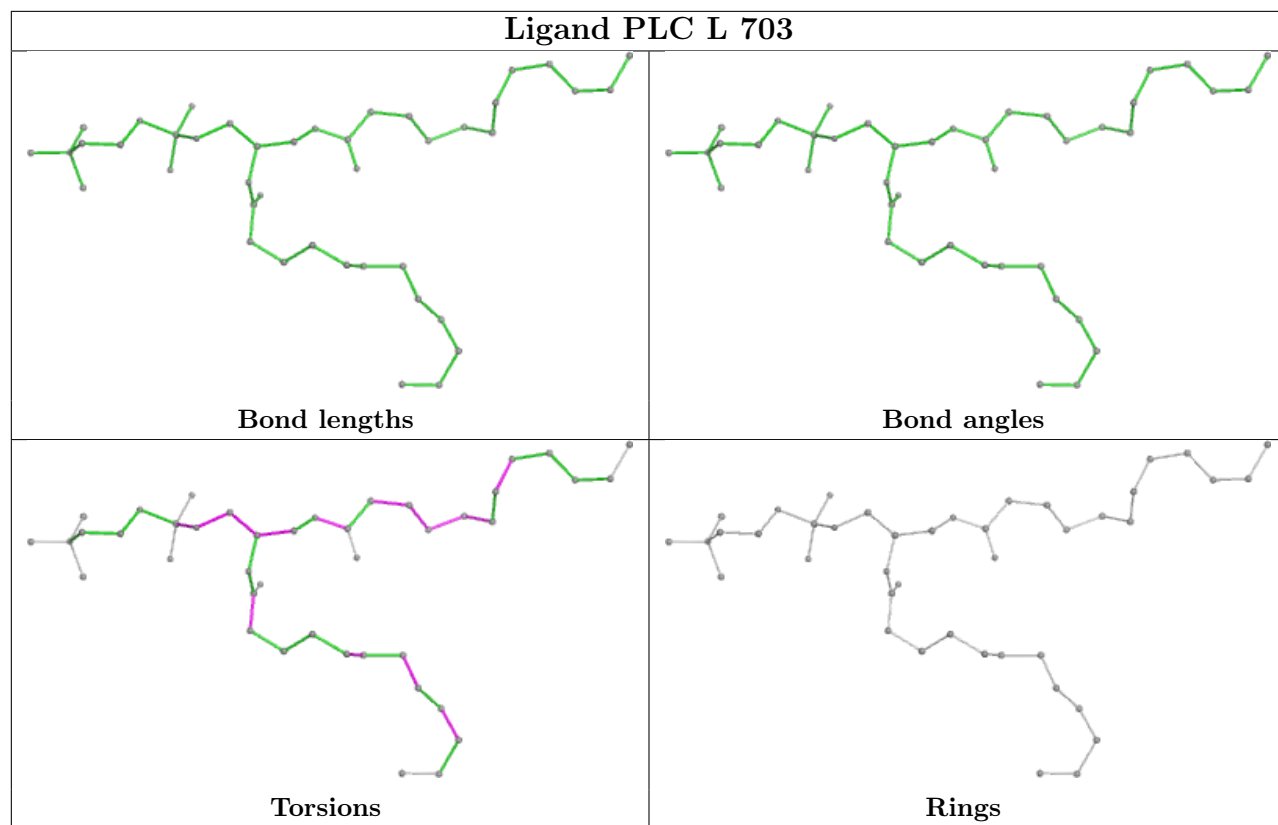


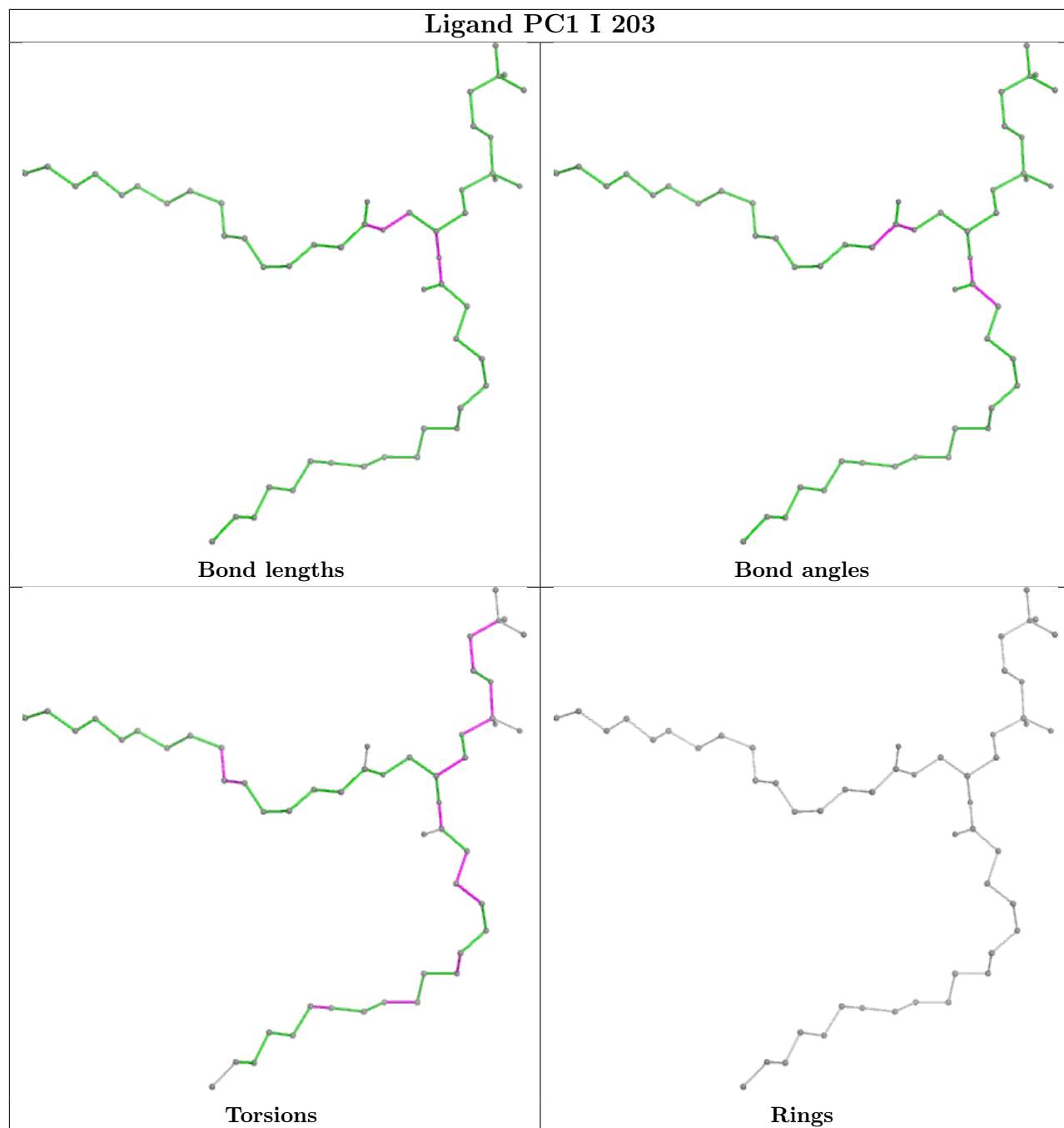


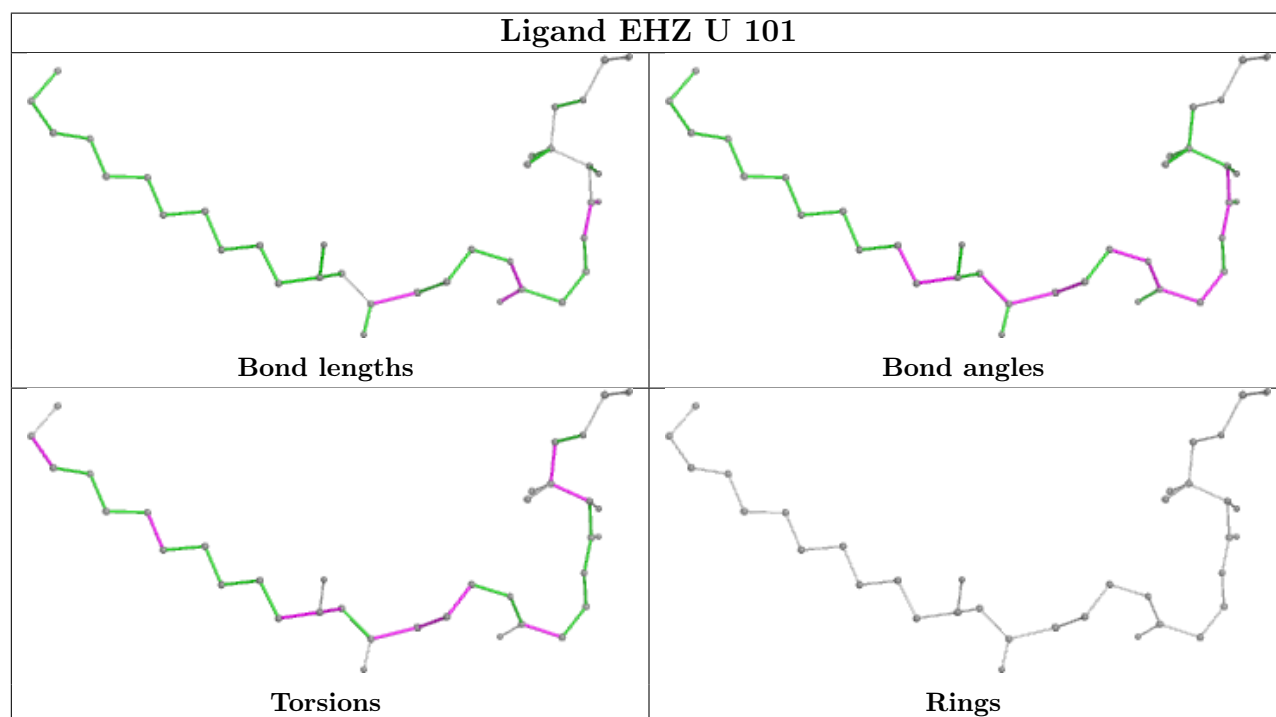
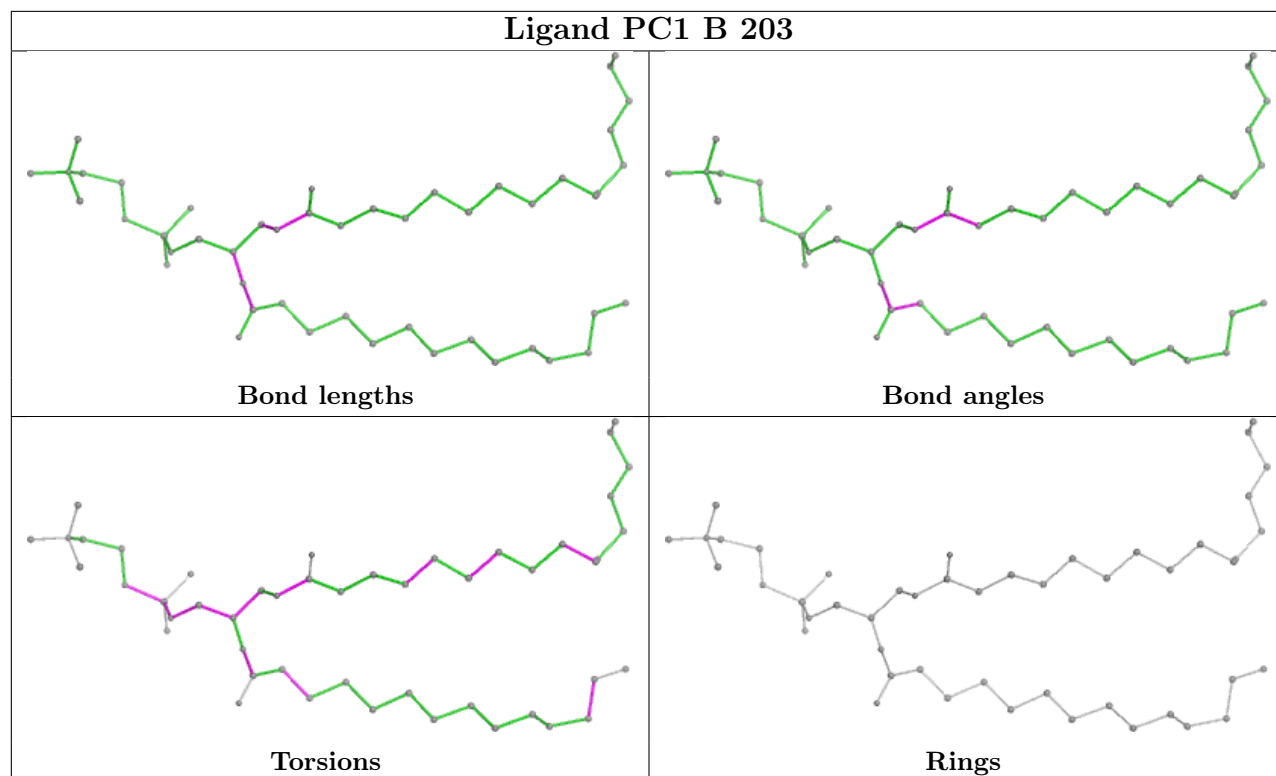


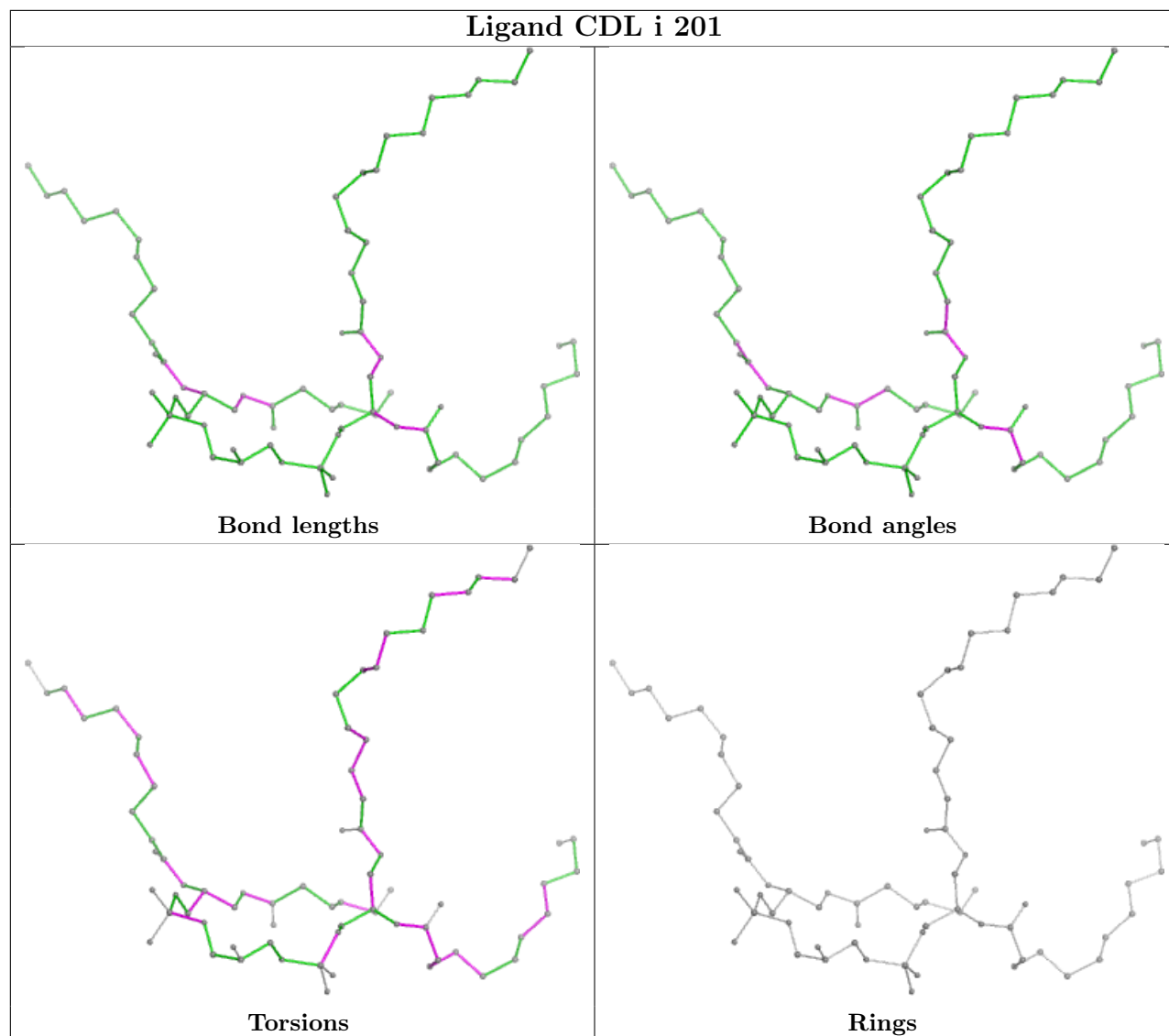


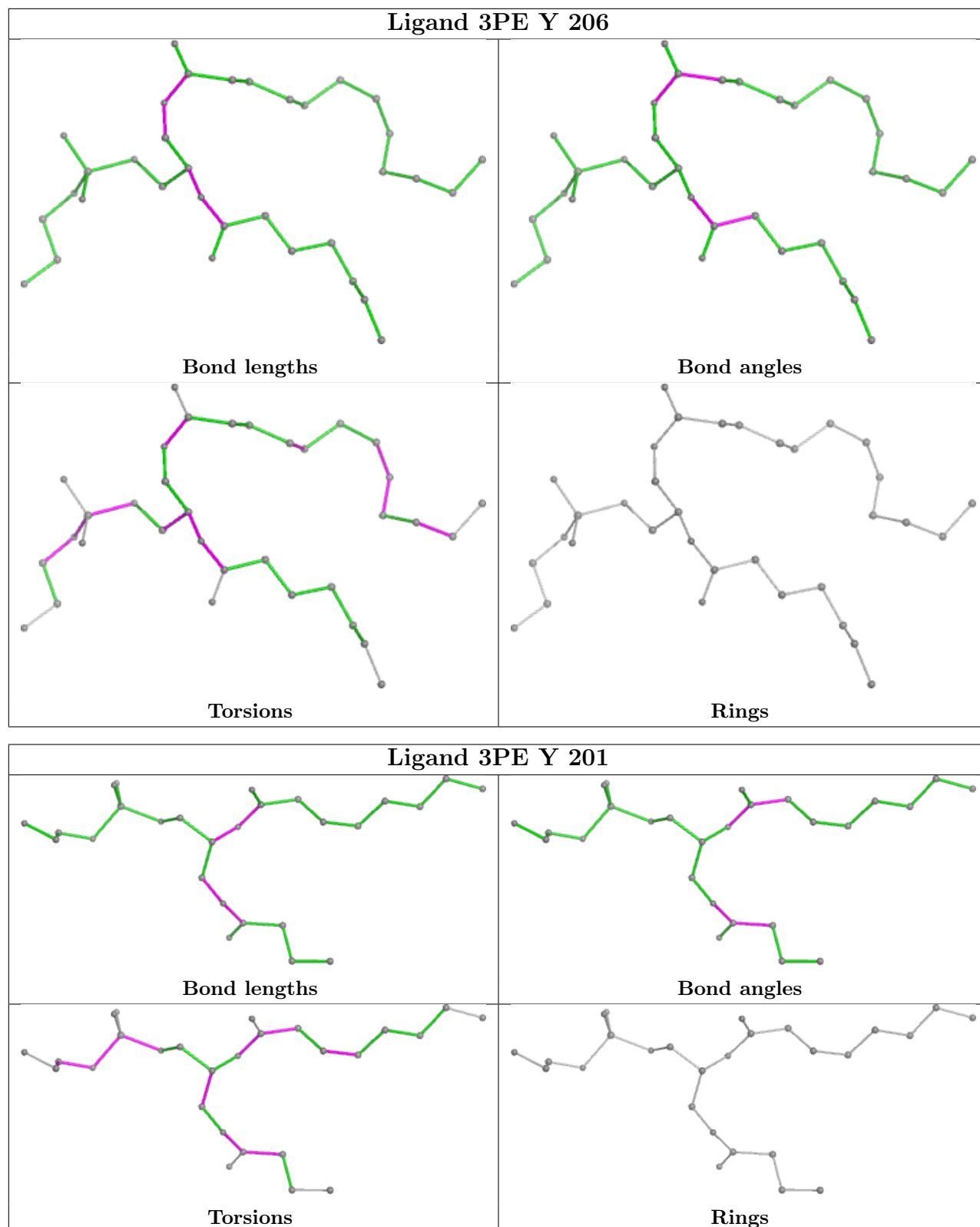


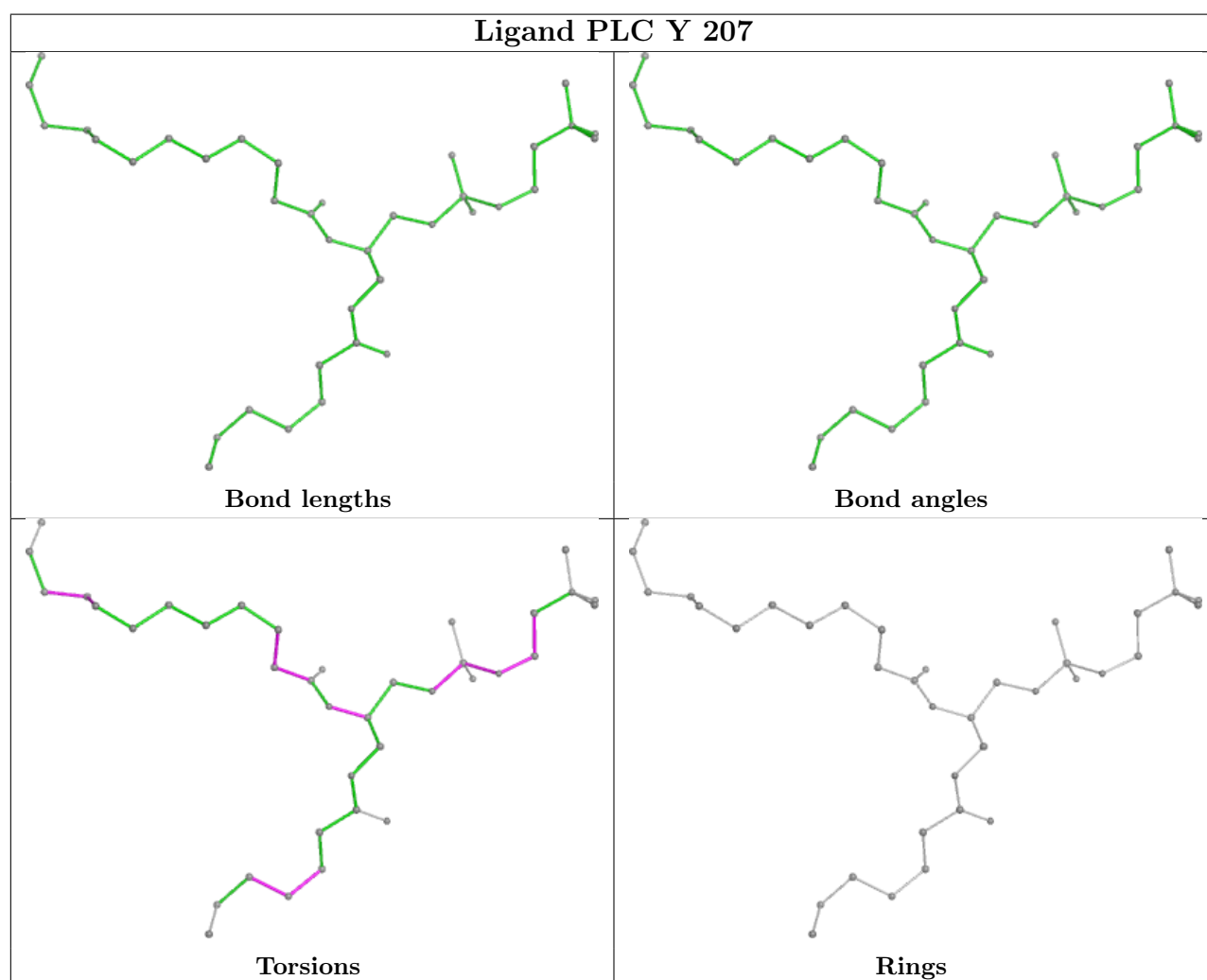
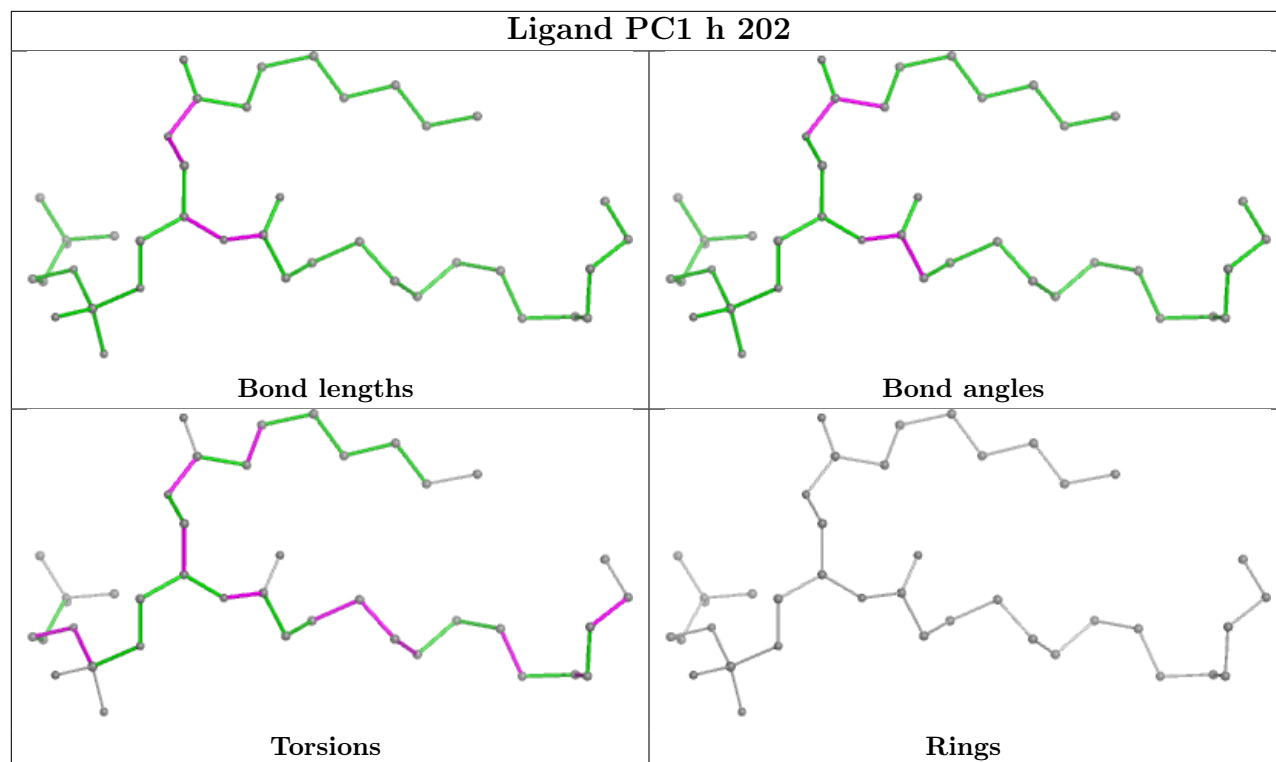


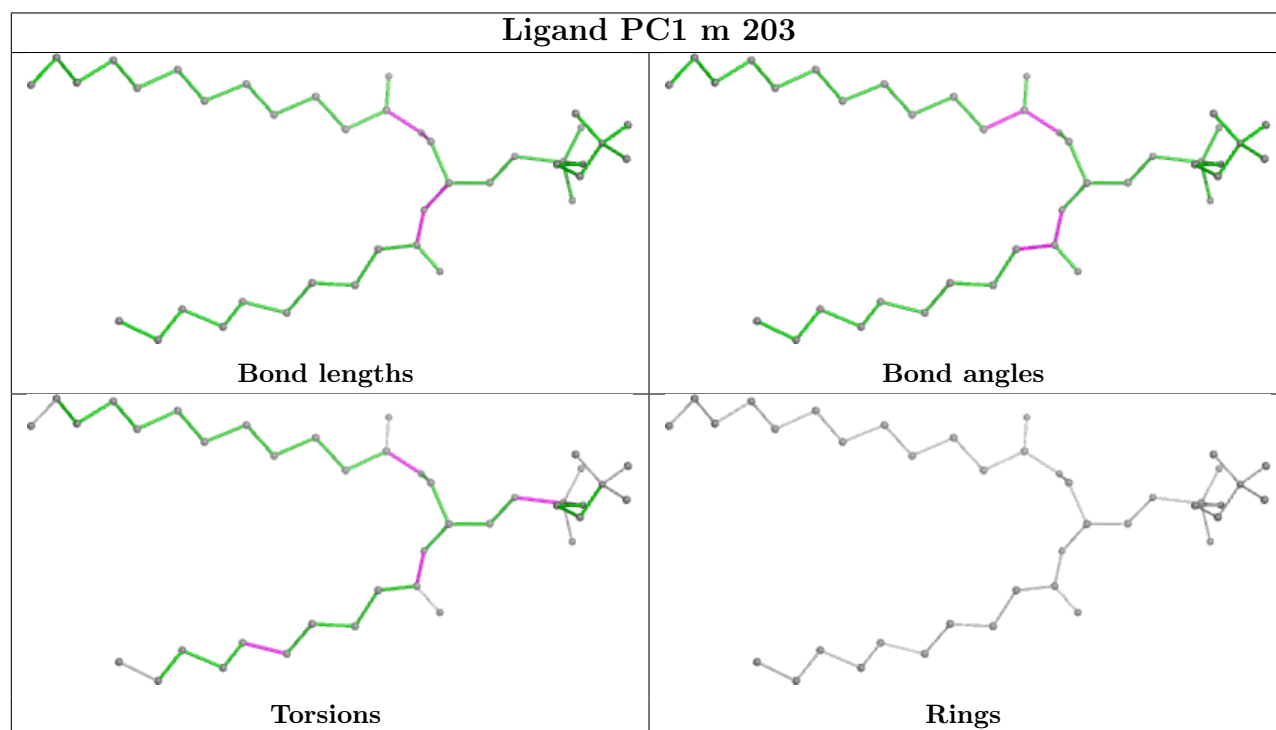
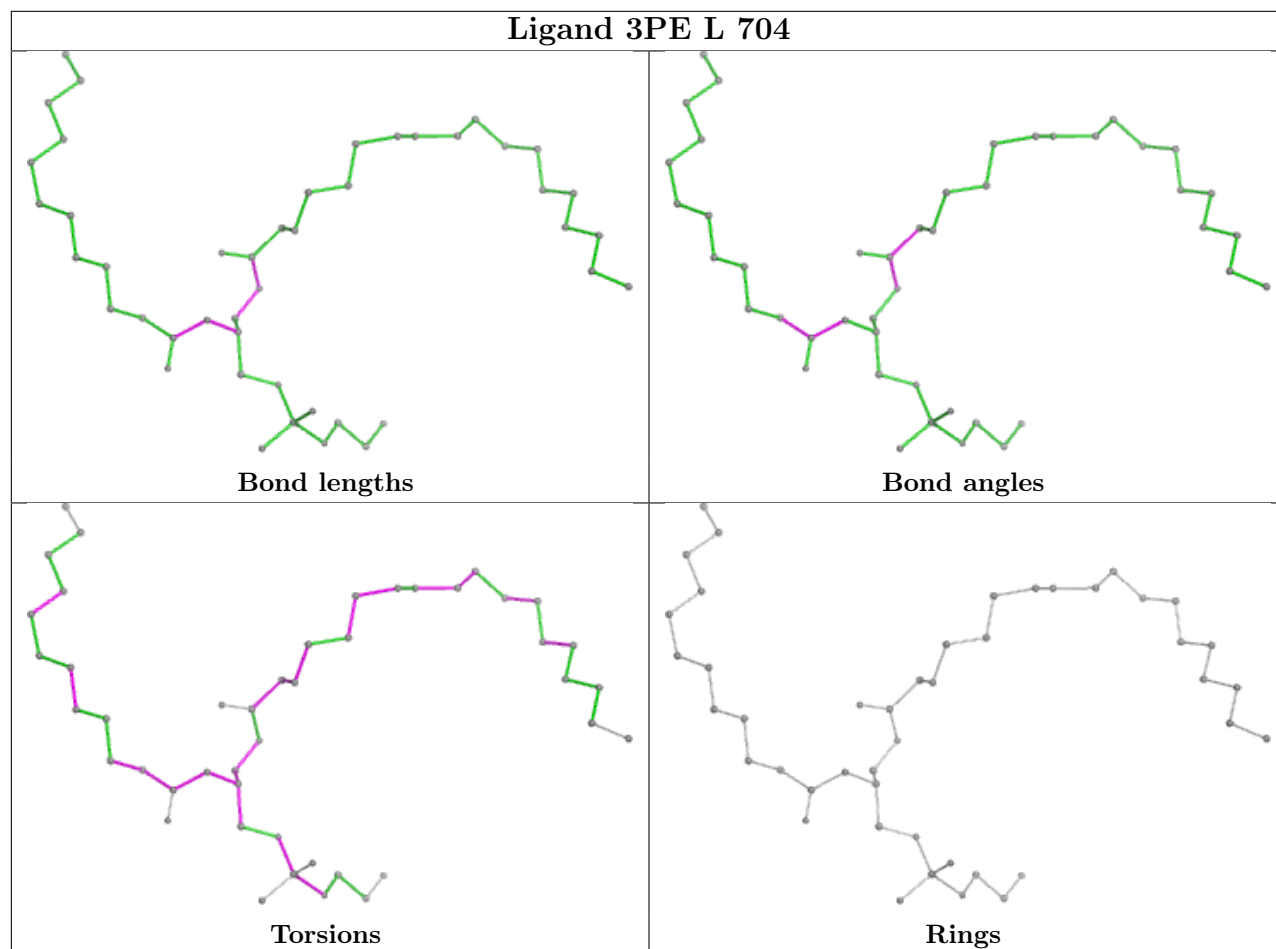


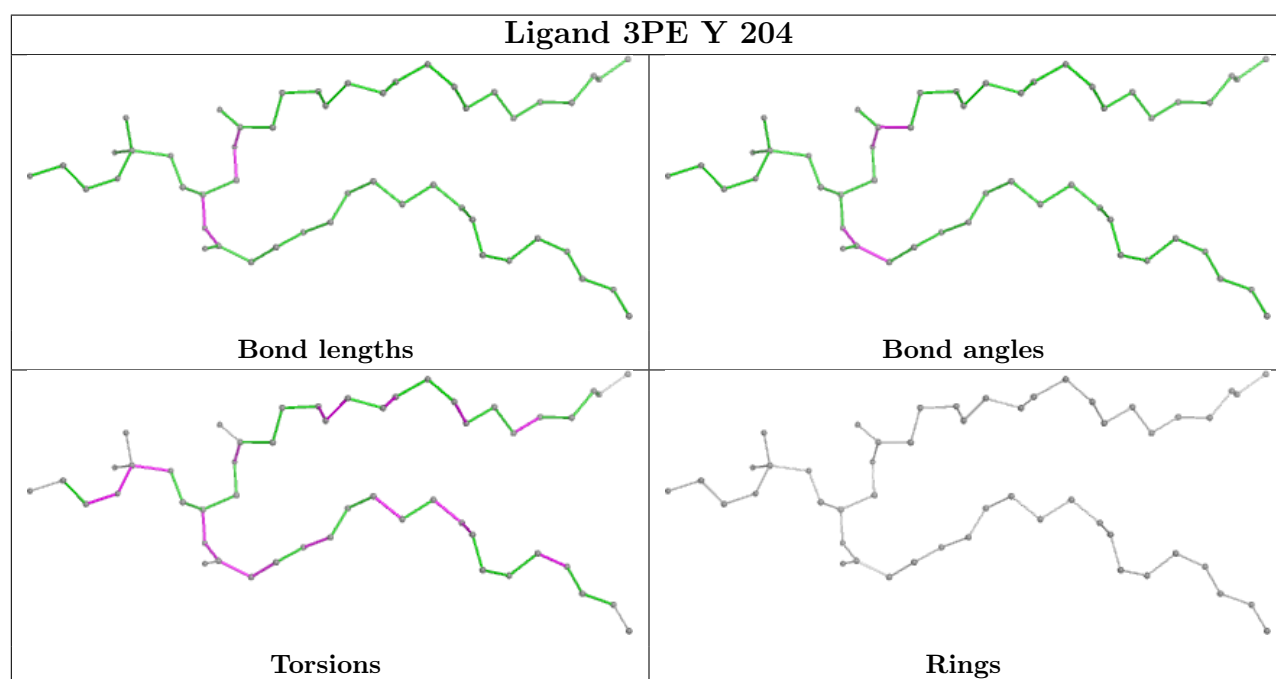
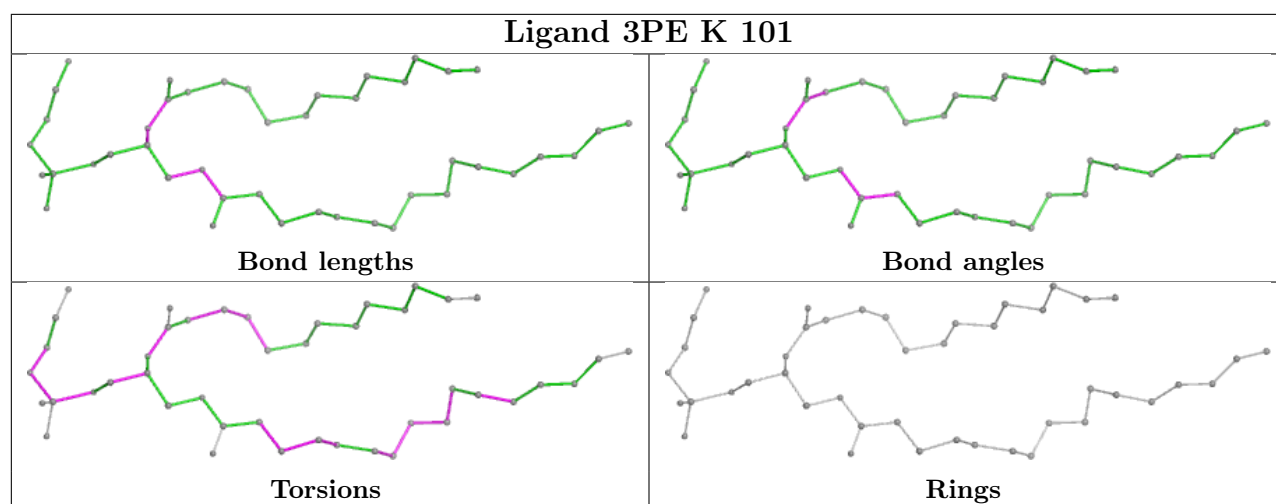


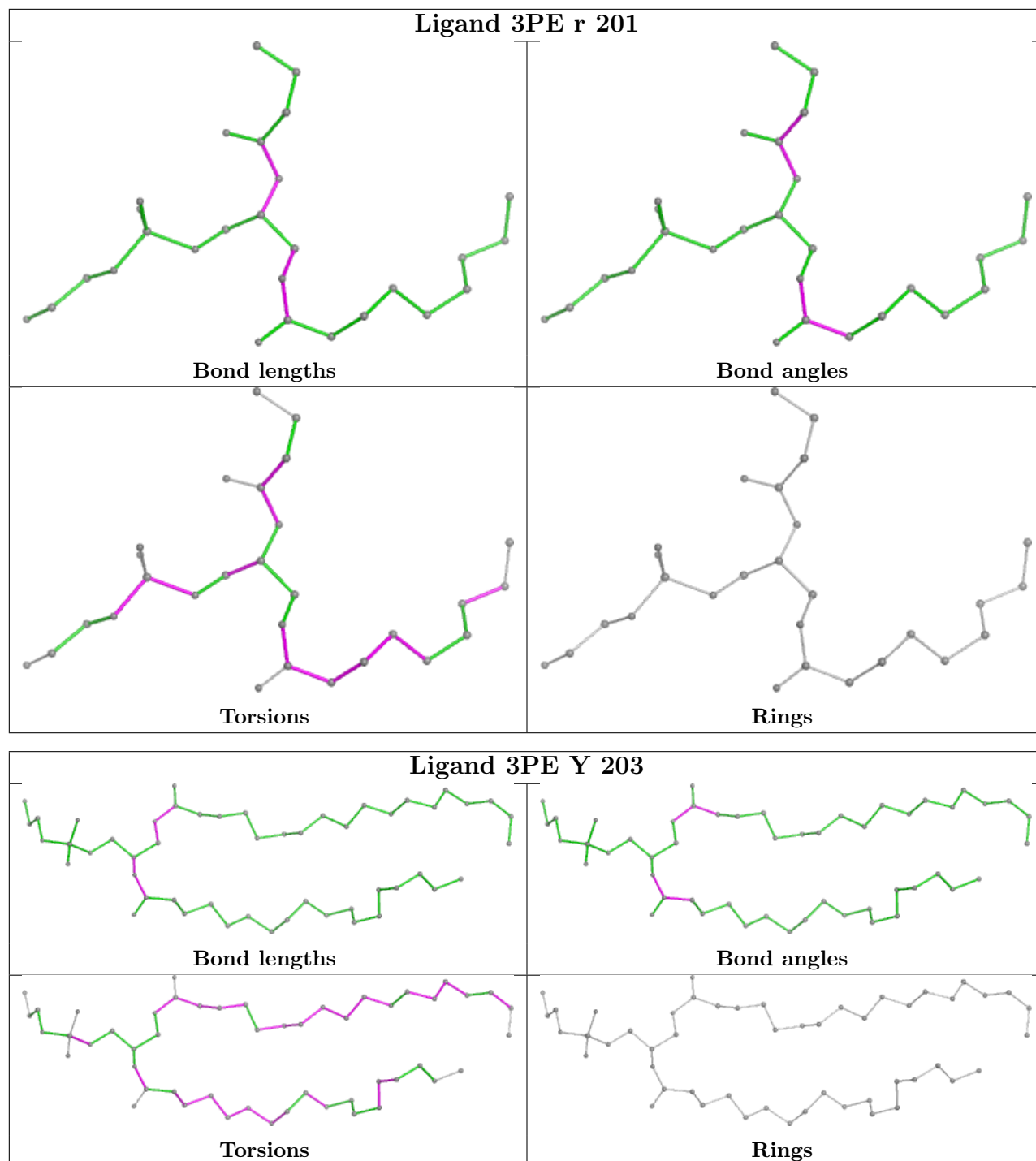


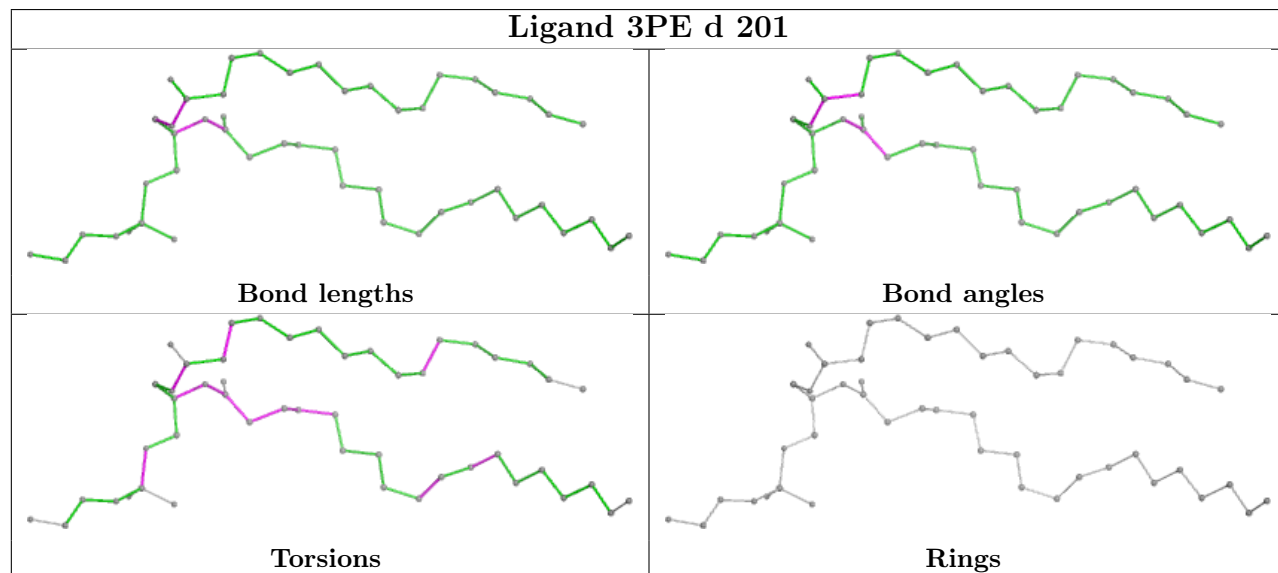
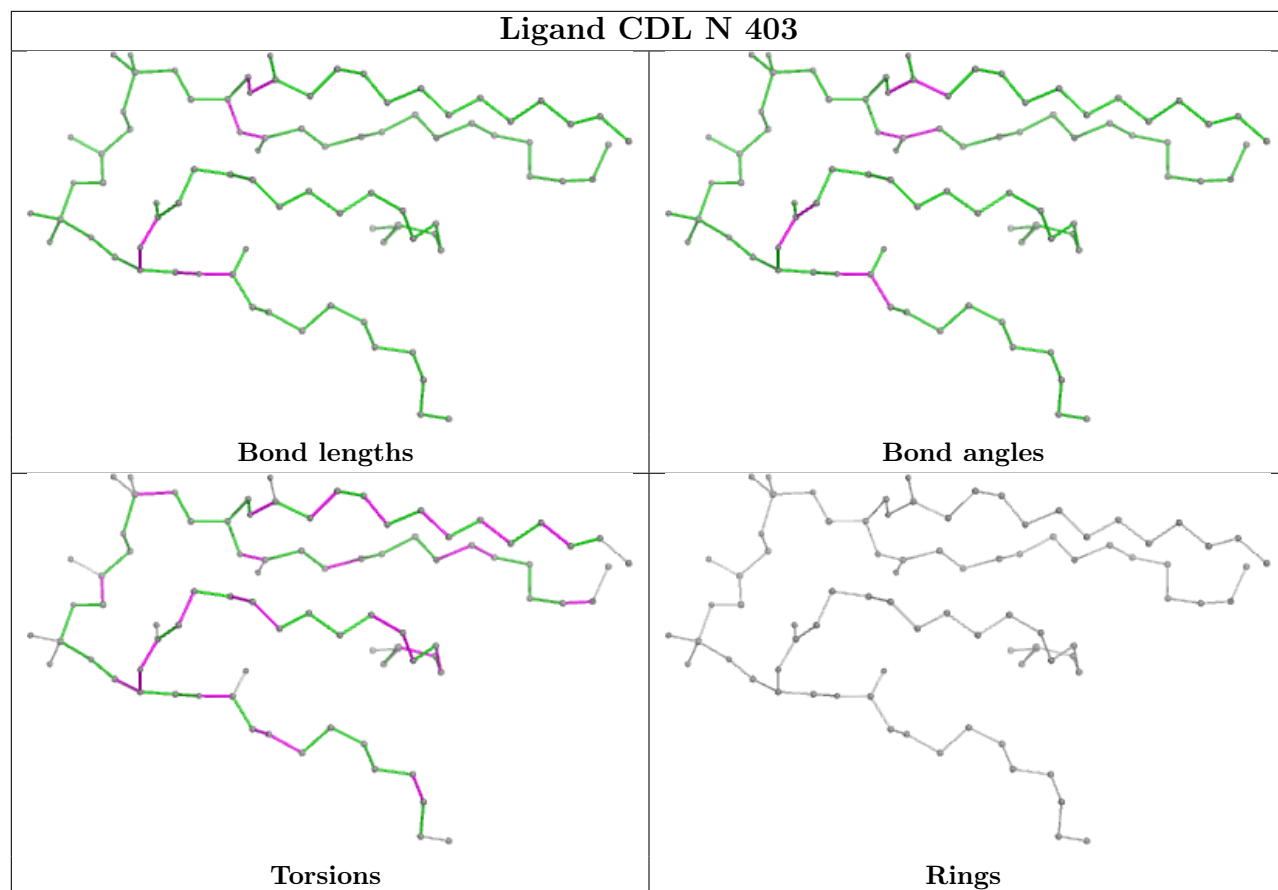


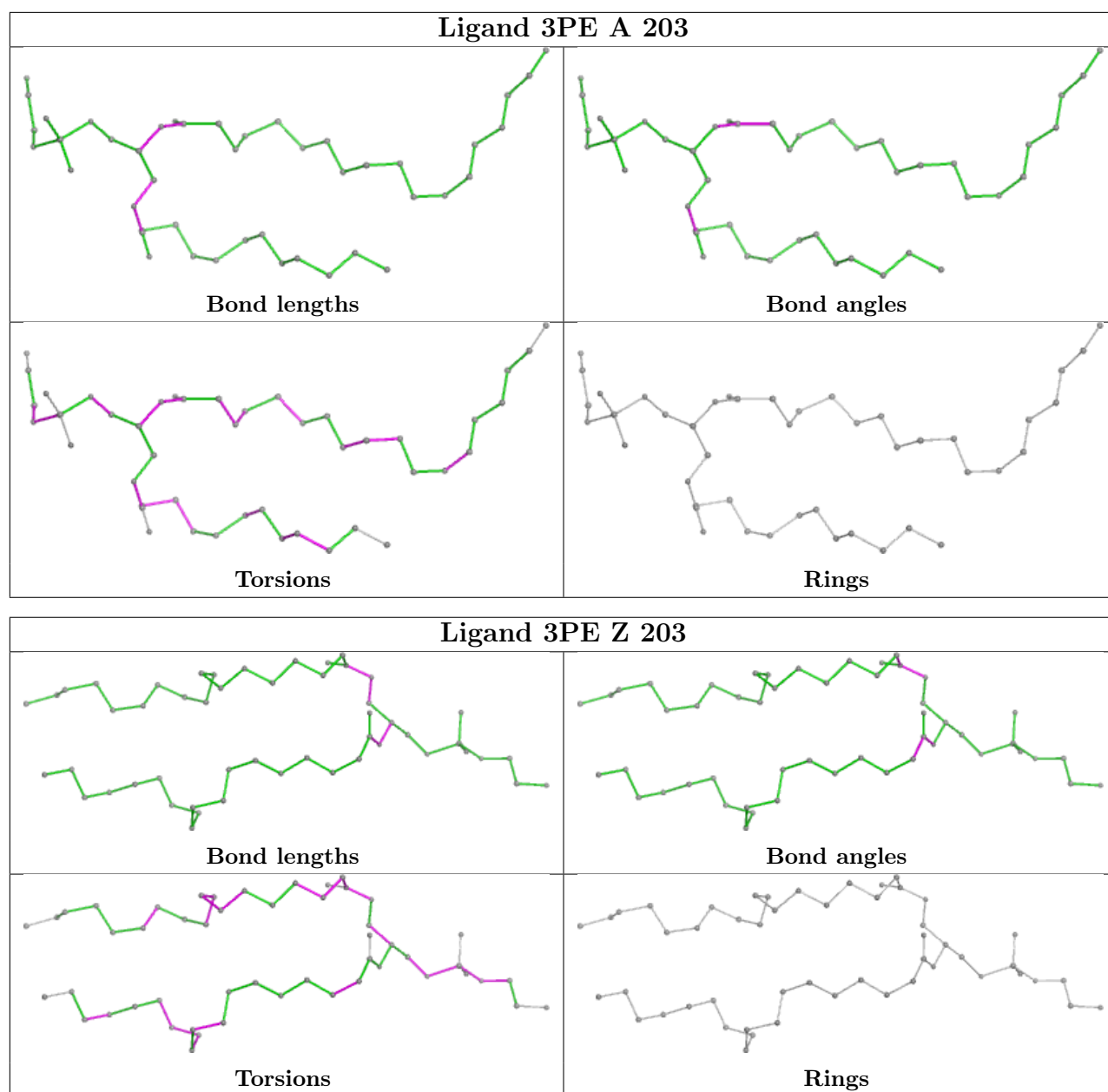


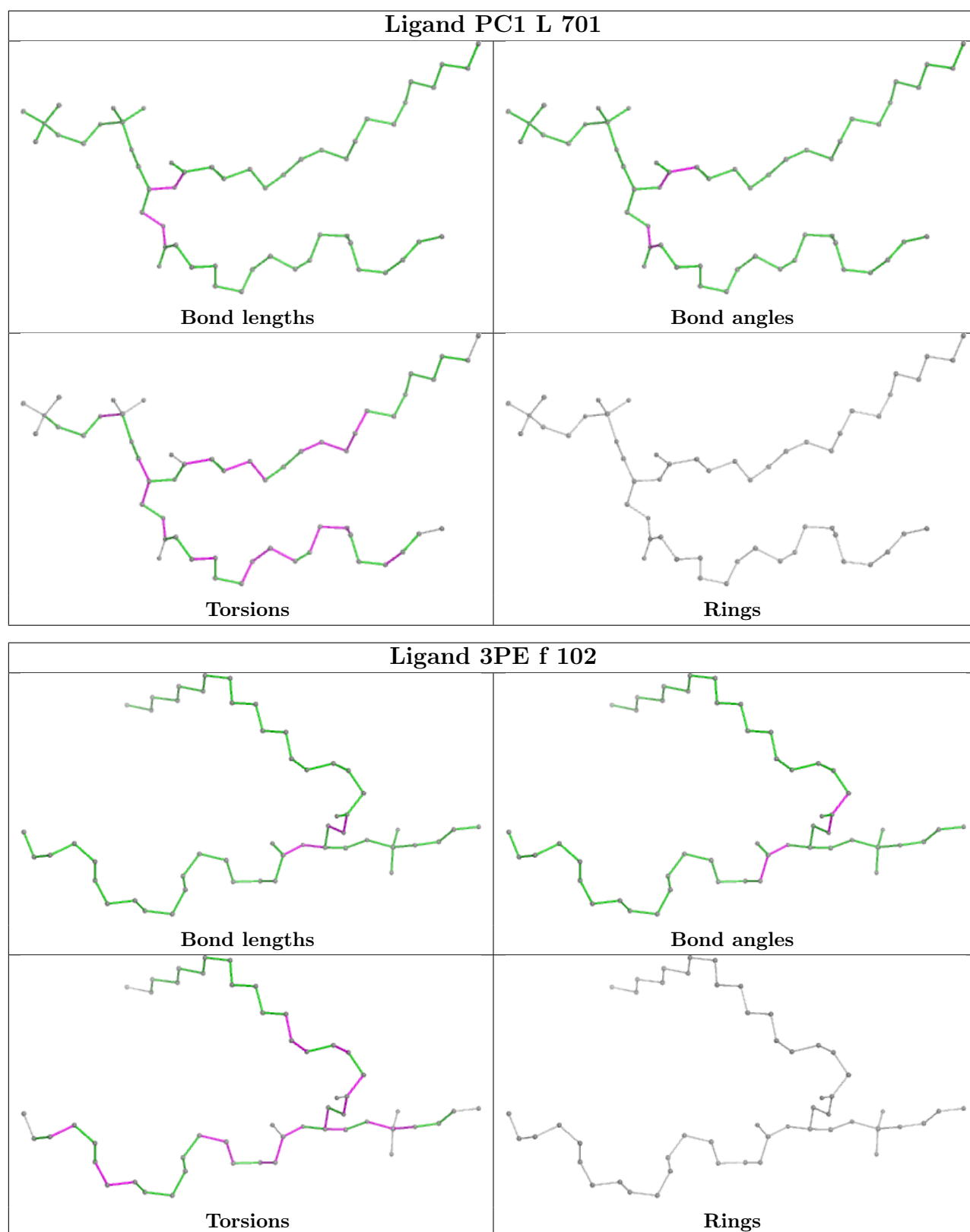












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

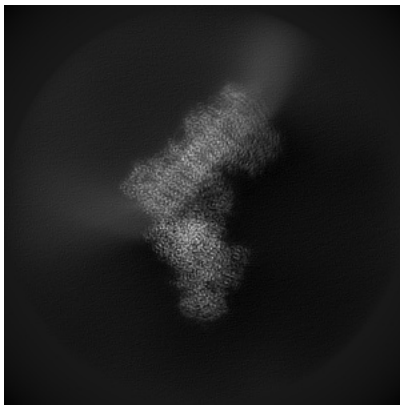
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18142. These allow visual inspection of the internal detail of the map and identification of artifacts.

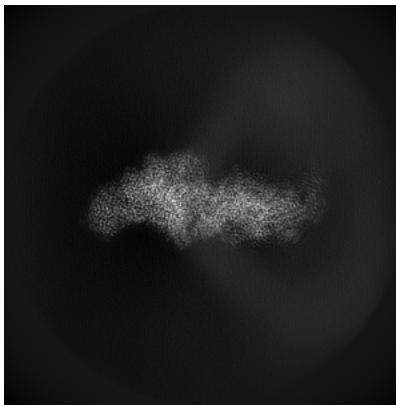
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

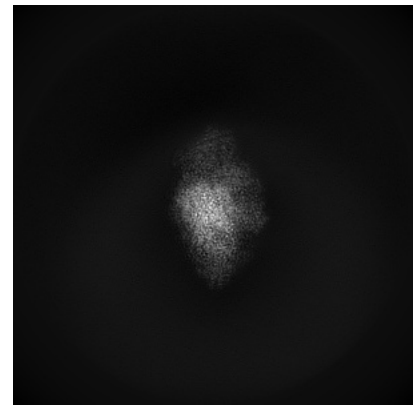
6.1.1 Primary map



X

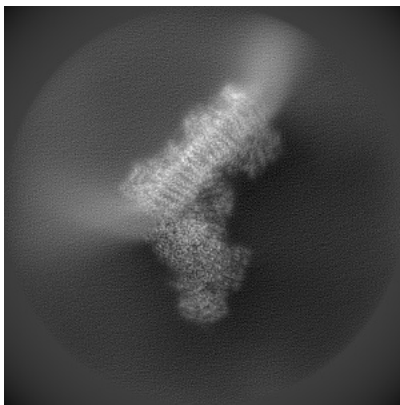


Y

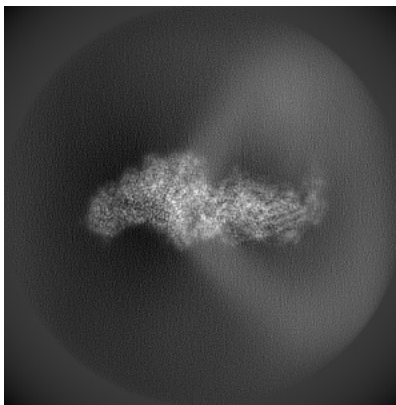


Z

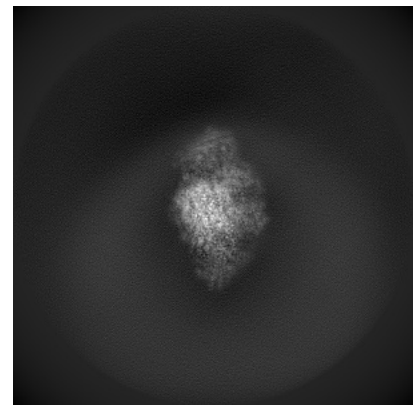
6.1.2 Raw map



X



Y

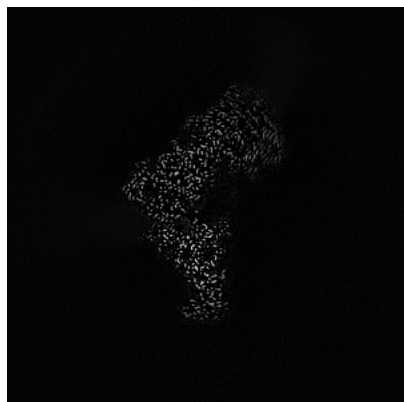


Z

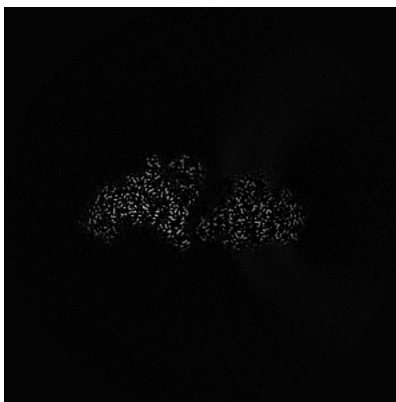
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

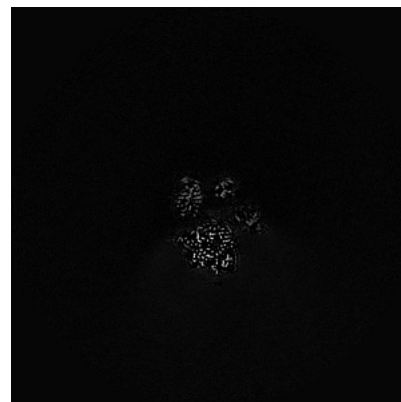
6.2.1 Primary map



X Index: 225

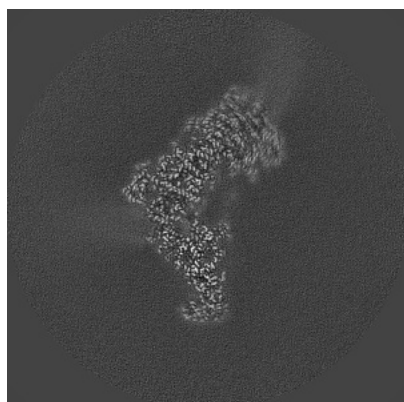


Y Index: 225

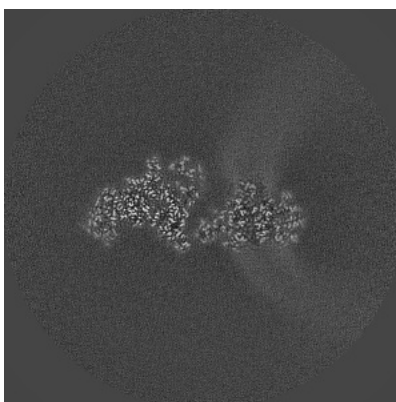


Z Index: 225

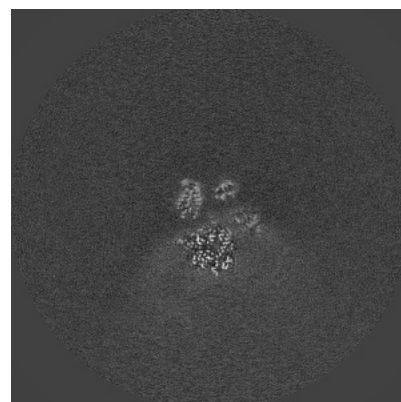
6.2.2 Raw map



X Index: 225



Y Index: 225

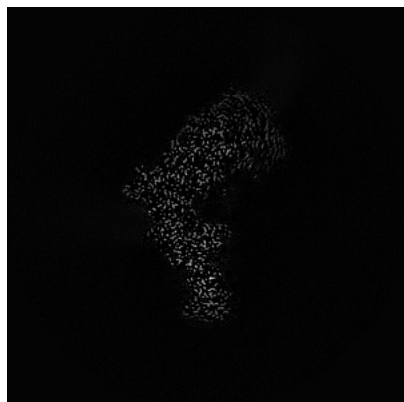


Z Index: 225

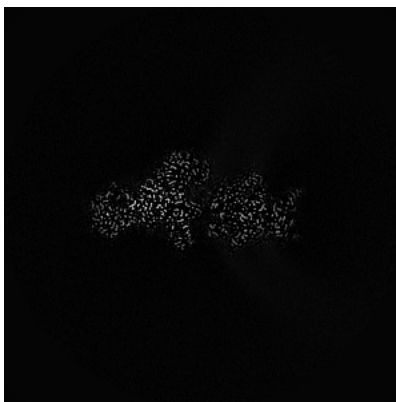
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 221

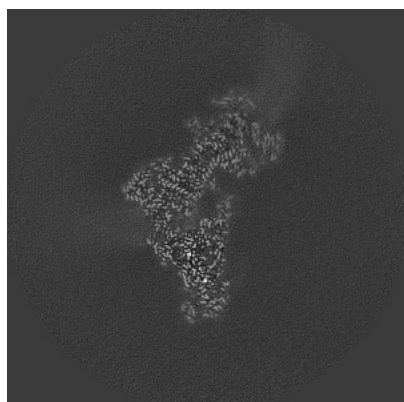


Y Index: 211

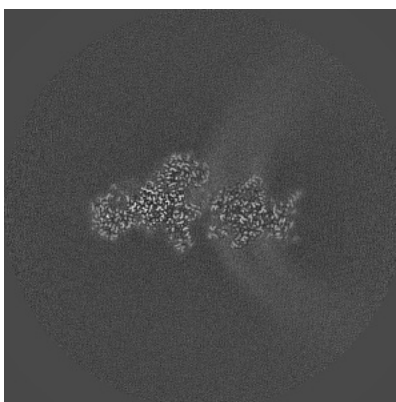


Z Index: 186

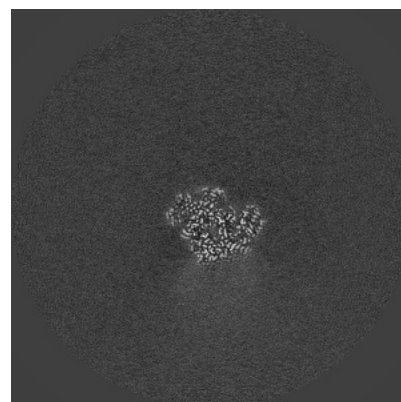
6.3.2 Raw map



X Index: 233



Y Index: 211

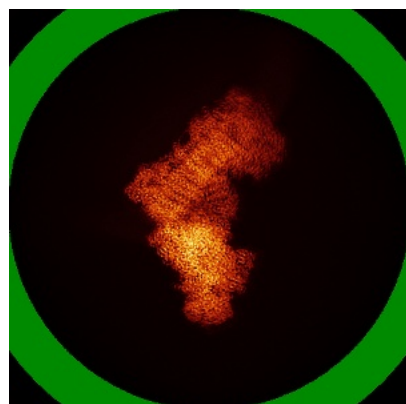


Z Index: 198

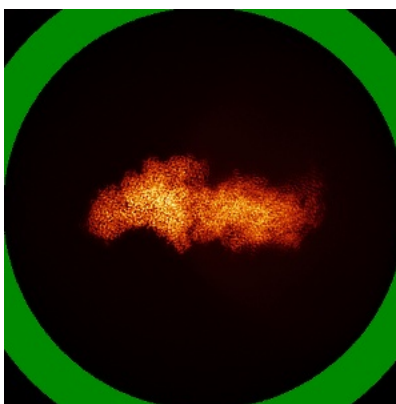
The images above show the largest variance slices of the map in three orthogonal directions.

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

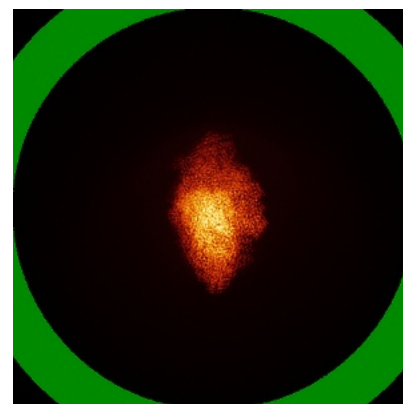
6.4.1 Primary map



X

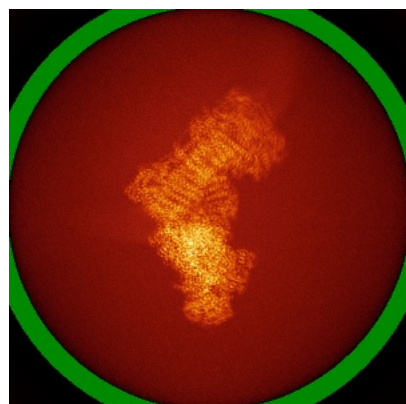


Y

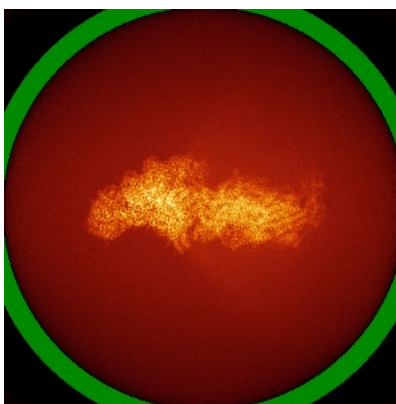


Z

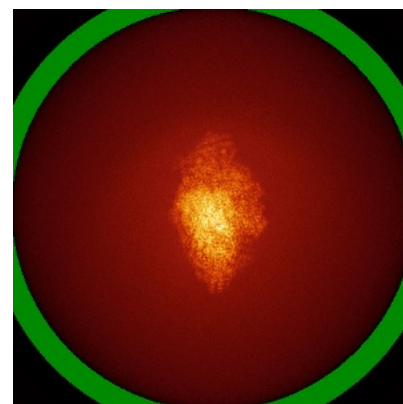
6.4.2 Raw map



X



Y

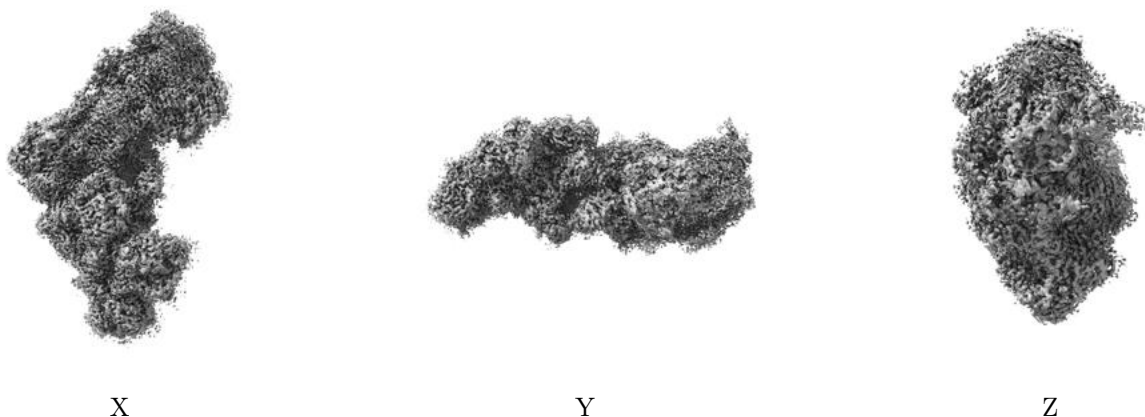


Z

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

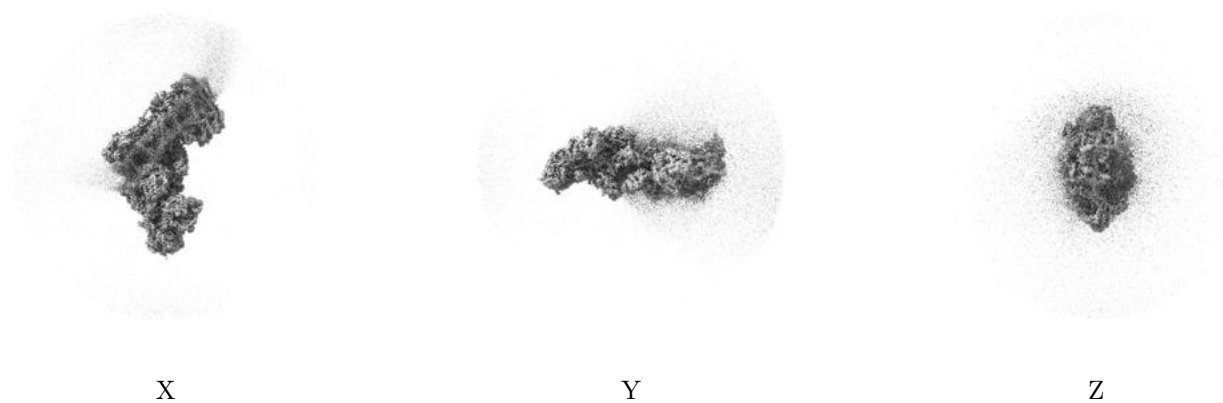
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

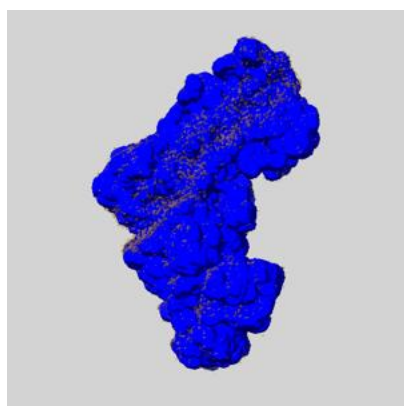
6.6 Mask visualisation [i](#)

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

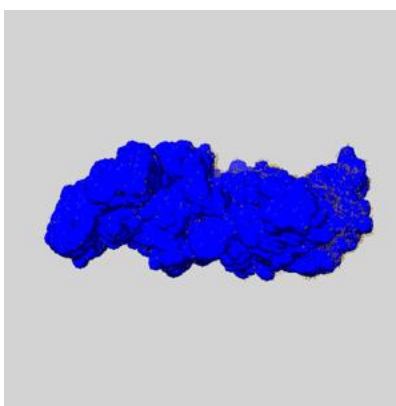
A mask typically either:

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

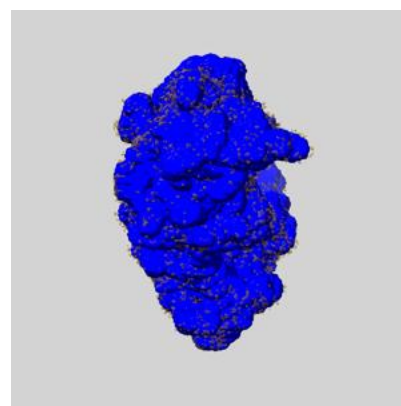
6.6.1 emd_18142_msk_1.map [i](#)



X



Y

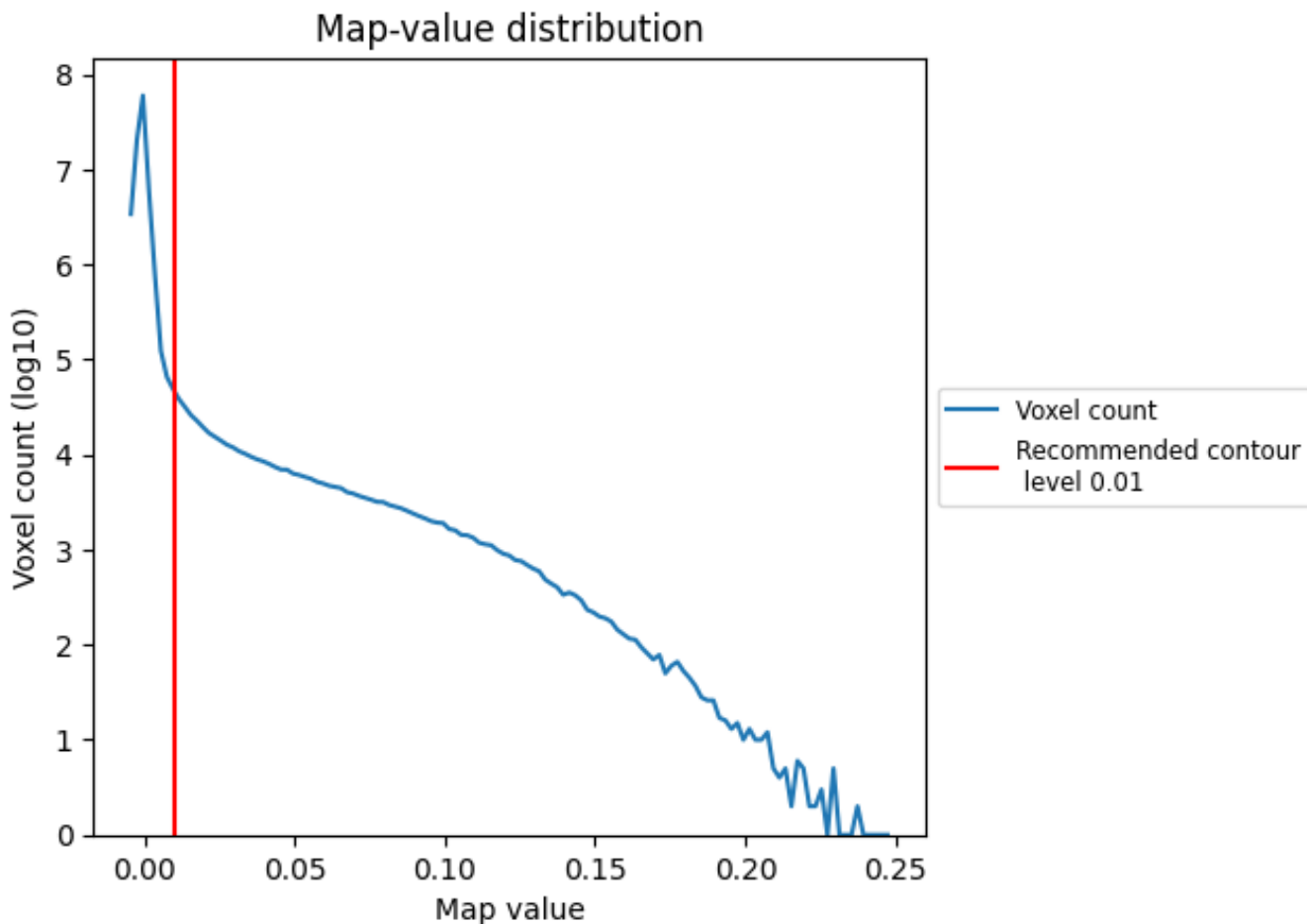


Z

7 Map analysis [i](#)

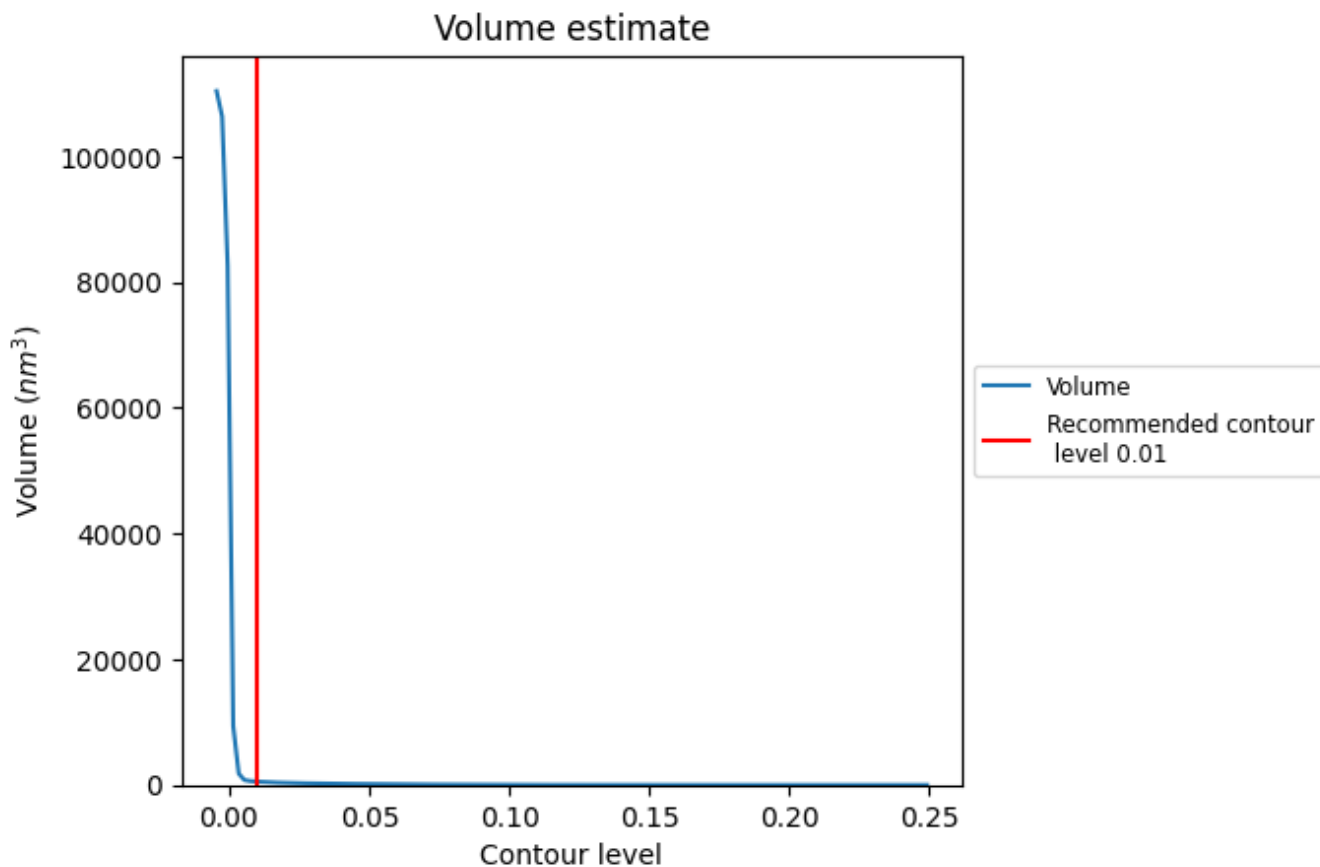
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

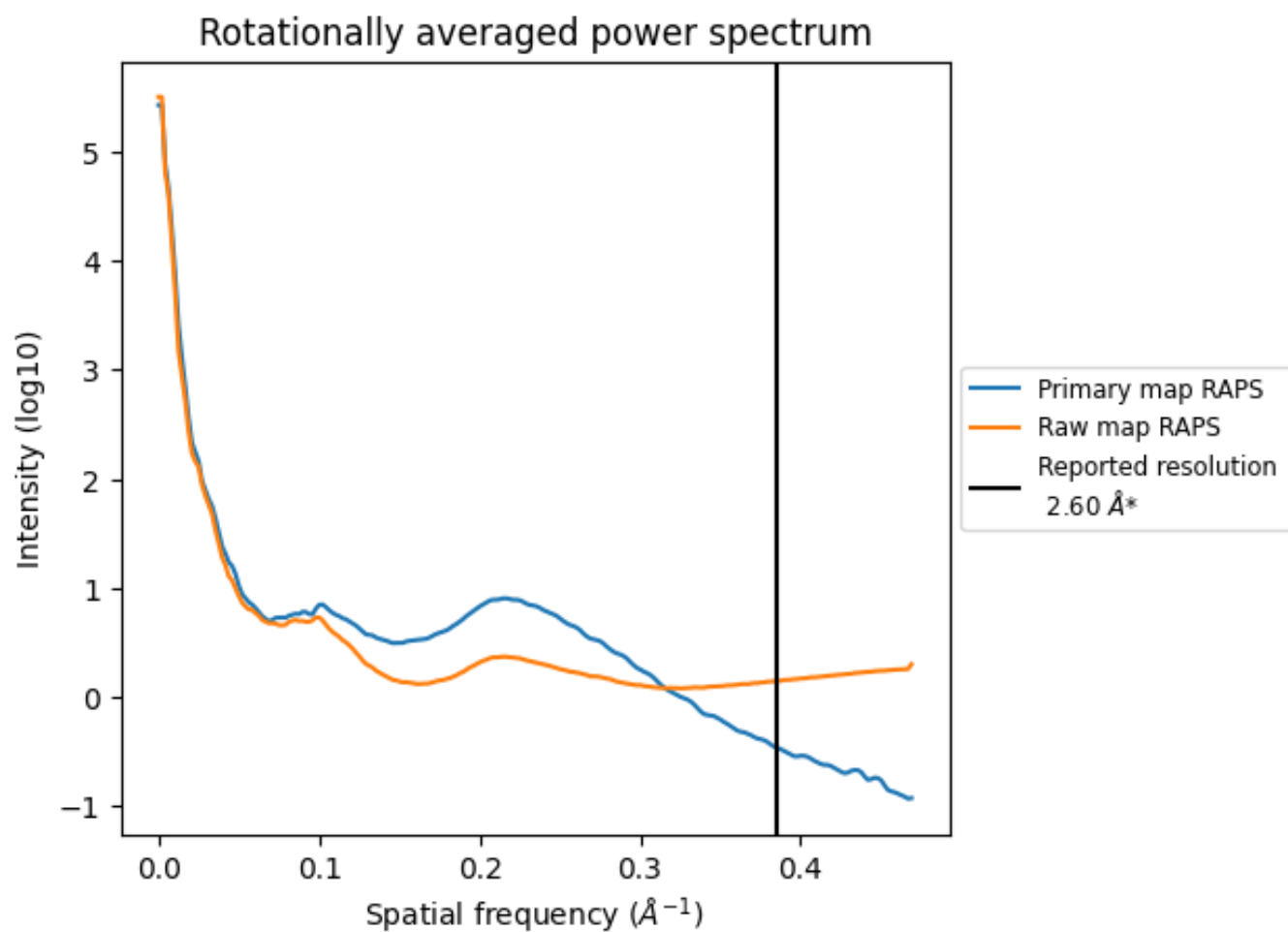
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 535 nm^3 ; this corresponds to an approximate mass of 483 kDa.

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

7.3 Rotationally averaged power spectrum i

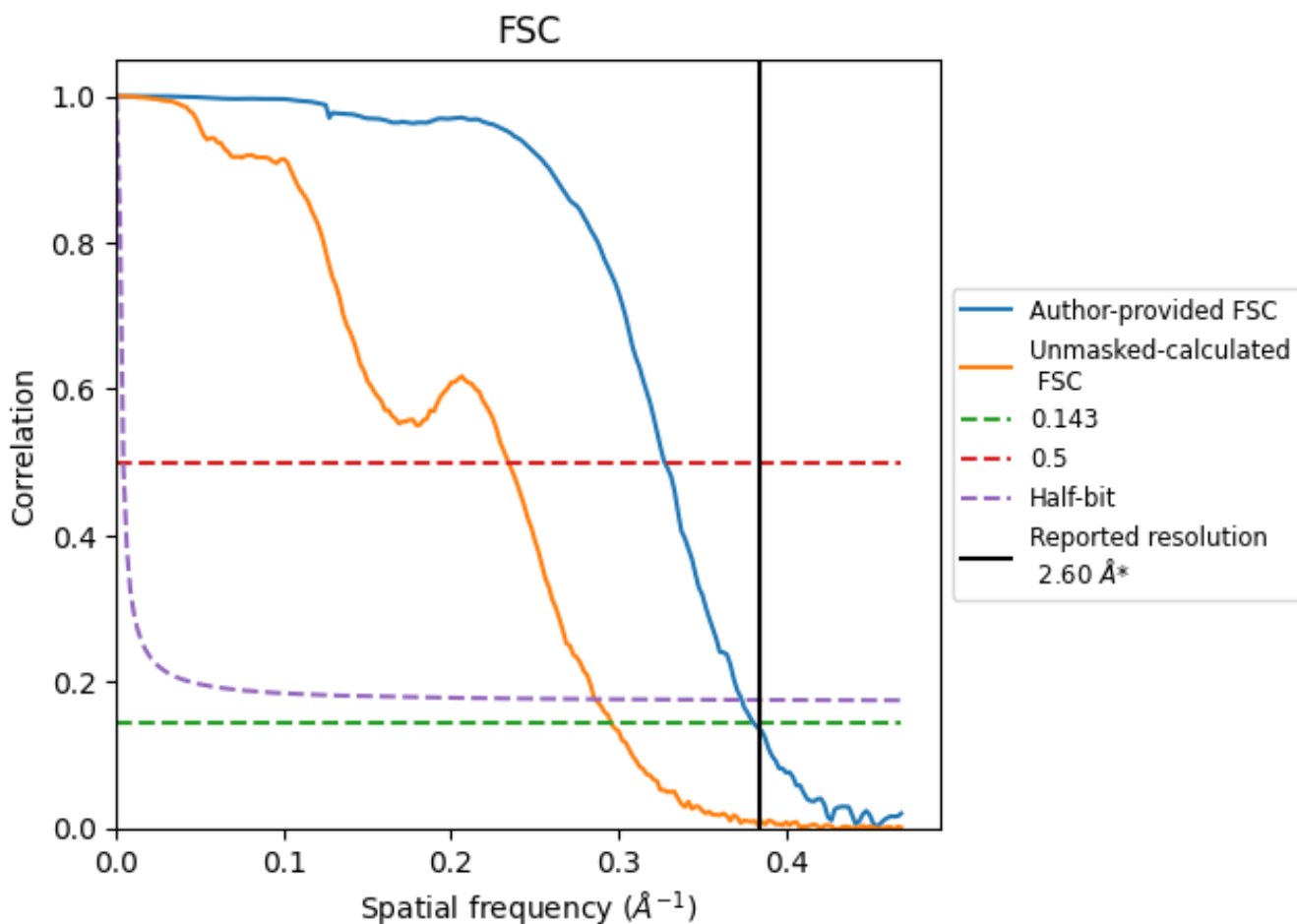


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

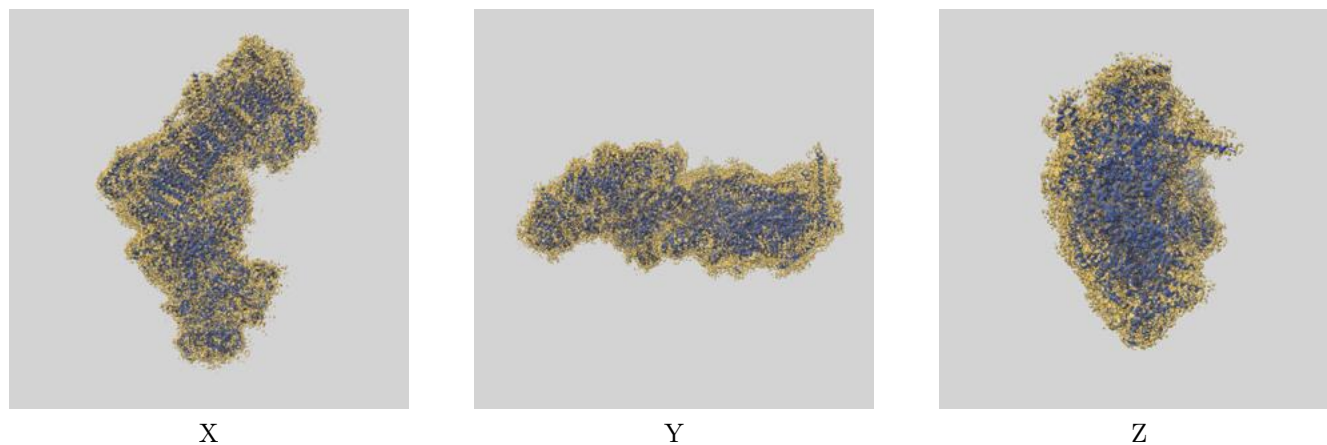
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.62	3.05	2.68
Unmasked-calculated*	3.38	4.27	3.50

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.38 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

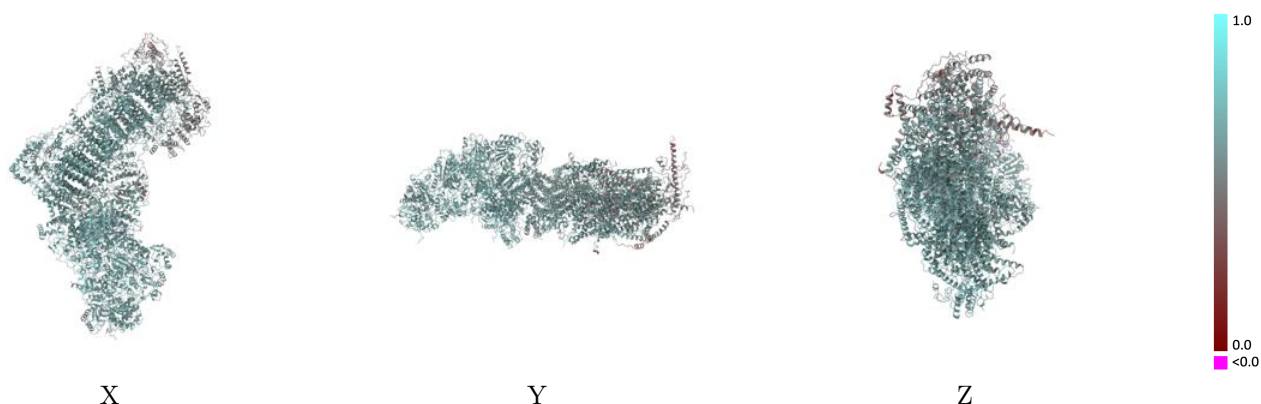
This section contains information regarding the fit between EMDB map EMD-18142 and PDB model 8Q49. Per-residue inclusion information can be found in section 3 on page 25.

9.1 Map-model overlay [i](#)



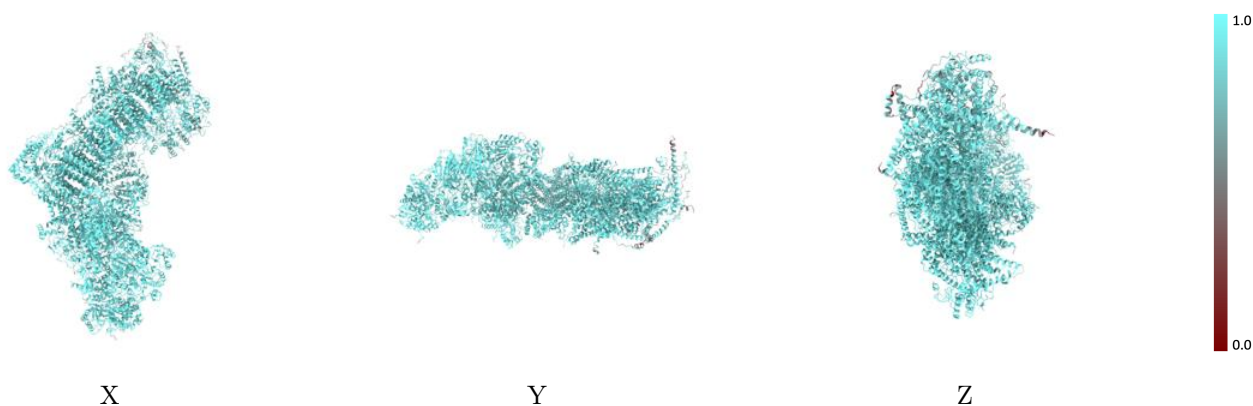
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



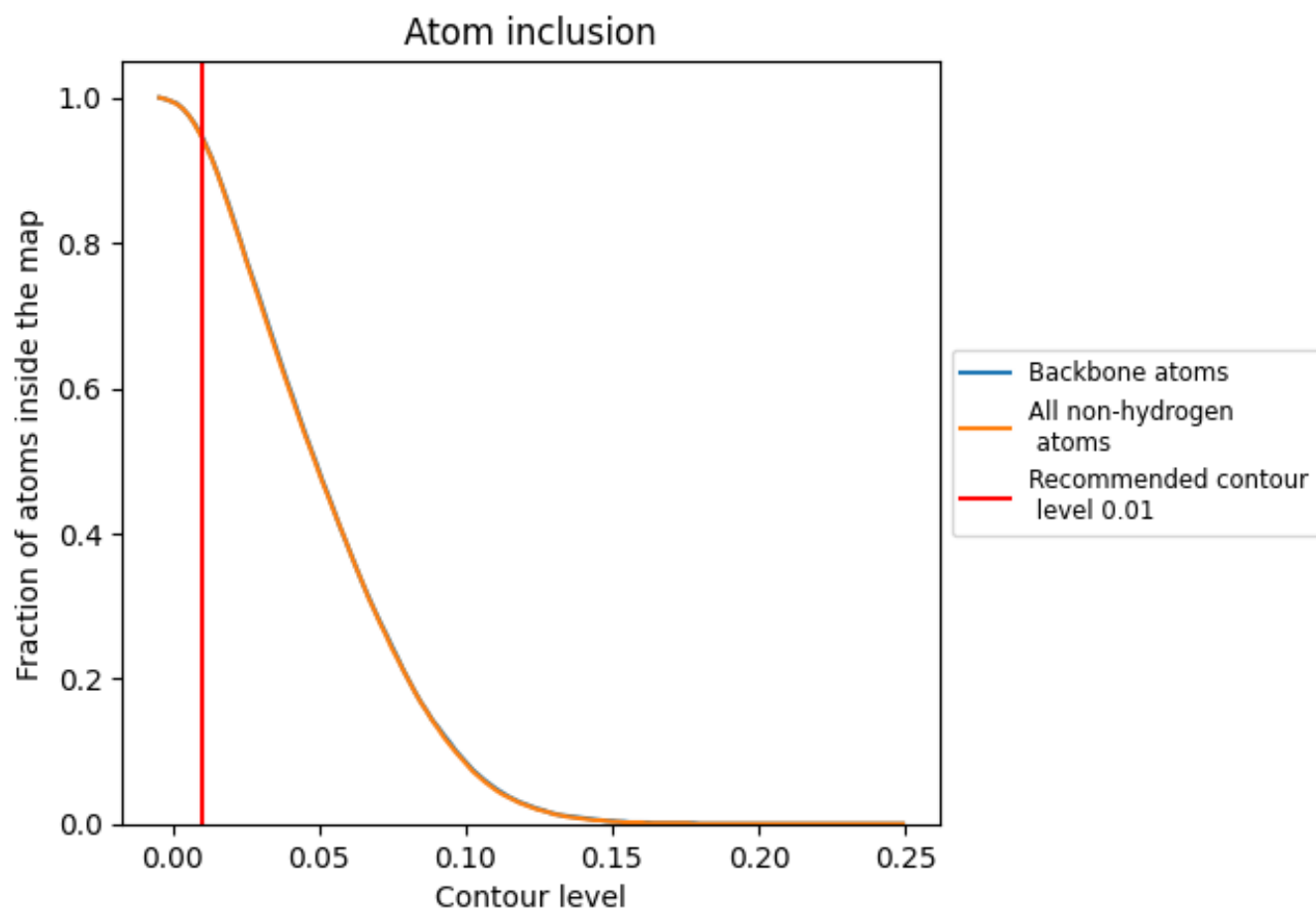
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary























The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9450	 0.6170
A	 0.9610	 0.6280
B	 0.9760	 0.6610
C	 0.9930	 0.6760
D	 0.9850	 0.6720
E	 0.9510	 0.6130
F	 0.9680	 0.6330
G	 0.9700	 0.6460
H	 0.9750	 0.6470
I	 0.9930	 0.6820
J	 0.9530	 0.6310
K	 0.9890	 0.6550
L	 0.9370	 0.5890
M	 0.9820	 0.6500
N	 0.9900	 0.6630
O	 0.9390	 0.6000
P	 0.9430	 0.6150
Q	 0.9600	 0.6550
R	 0.9570	 0.6490
S	 0.9260	 0.5980
T	 0.8860	 0.5470
U	 0.8180	 0.4640
V	 0.9670	 0.6420
W	 0.9610	 0.6460
X	 0.9600	 0.6300
Y	 0.9340	 0.6090
Z	 0.9560	 0.6290
a	 0.9800	 0.6530
b	 0.9600	 0.6320
c	 0.9360	 0.6180
d	 0.9520	 0.6320
e	 0.9480	 0.6210
f	 0.8680	 0.5640
g	 0.9270	 0.5900
h	 0.9670	 0.6280



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Chain	Atom inclusion	Q-score
i	 0.8120	 0.4920
j	 0.8160	 0.4670
k	 0.7570	 0.4500
l	 0.9020	 0.5570
m	 0.9100	 0.5770
n	 0.8860	 0.5150
o	 0.7500	 0.4390
p	 0.9060	 0.5690
q	 0.9680	 0.6510
r	 0.9760	 0.6530
s	 0.9030	 0.5800