



Full wwPDB EM Validation Report ⓘ

Feb 1, 2023 – 10:38 pm GMT

PDB ID : 7R44
EMDB ID : EMD-14266
Title : Bovine complex I in the presence of IM1761092, active class iv (Composite map)
Authors : Bridges, H.R.; Blaza, J.N.; Yin, Z.; Chung, I.; Hirst, J.
Deposited on : 2022-02-08
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
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 : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.1

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 2.40 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	100%
2	B	216	72% 28%
3	C	266	78% 22%
4	D	463	92% 7%
5	E	249	86% 14%
6	F	464	93% 7%
7	G	727	95% 5%
8	H	318	100%
9	I	212	83% 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	J	175	5% 99%
11	K	98	100%
12	L	606	98%
13	M	459	100%
14	N	347	100%
15	O	343	93% 7%
16	P	380	7% 90% 10%
17	Q	175	71% 29%
18	R	124	77% 23%
19	S	99	5% 83% 17%
20	T	156	25% 49% 51%
20	U	156	55% 45%
21	V	116	97%
22	W	128	5% 89% 11%
23	X	172	5% 99%
24	Y	141	32% 99%
25	Z	144	9% 97%
26	a	70	100%
27	b	84	13% 99%
28	c	76	7% 63% 37%
29	d	120	5% 93% 7%
30	e	106	14% 90% 10%
31	f	57	14% 91% 9%
32	g	154	5% 63% 36%
33	h	189	73% 27%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	i	127	<p>9% 79% 20%</p>
35	j	108	<p>5% 62% 38%</p>
36	k	98	<p>7% 82% 18%</p>
37	l	186	<p>5% 83% 17%</p>
38	m	129	<p>7% 88% 12%</p>
39	n	179	<p>5% 96%</p>
40	o	137	<p>8% 88% 12%</p>
41	p	176	<p>5% 97%</p>
42	q	145	<p>8% 99%</p>
43	r	113	<p>5% 81% 17%</p>
44	s	109	<p>39% 61%</p>

2 Entry composition i

There are 60 unique types of molecules in this entry. The entry contains 68213 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	115	921	622	133	159	7	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	155	1241	792	224	211	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	430	3459	2209	596	629	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	213	1655	1057	277	311	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	431	3319	2091	593	615	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	688	5279	3307	920	1013	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	318	2509	1681	385	420	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	174	1337	902	189	234	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	595	4692	3119	723	807	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	341	2747	1777	486	479	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	125	1016	641	181	191	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	95	730	448	137	142	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	82	663	416	124	121	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	76	612	393	90	124	5	0	0
20	U	86	693	447	102	139	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	112	911	589	154	165	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	114	971	622	180	165	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	140	1146	737	200	200	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	651	425	109	115	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	48	405	268	69	68	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	112	934	613	157	161	3	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	95	799	506	150	137	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	52	451	296	79	75	1	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	98	824	529	137	154	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	102	876	575	151	149	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	67	580	381	95	103	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	80	647	424	109	112	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	155	1304	844	213	239	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	113	954	613	167	174		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	172	1492	955	273	257	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	120	1035	645	199	183	8	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	170	1435	900	265	262	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	144	1201	773	215	209	4	0	0

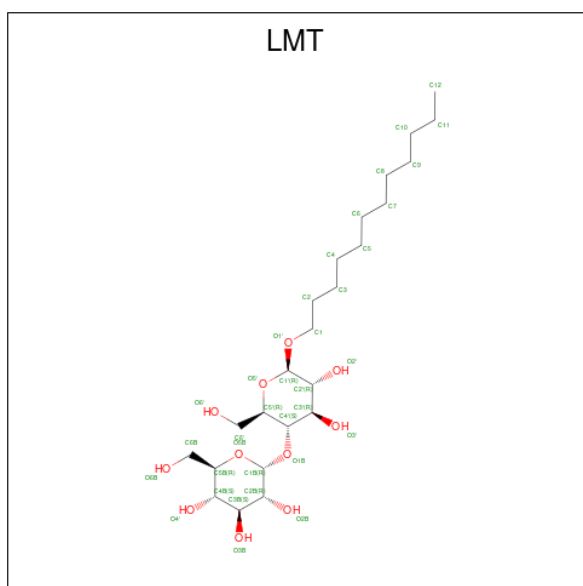
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	r	94	767	485	143	136	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	42	353	219	64	69	1	0	0

- Molecule 45 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



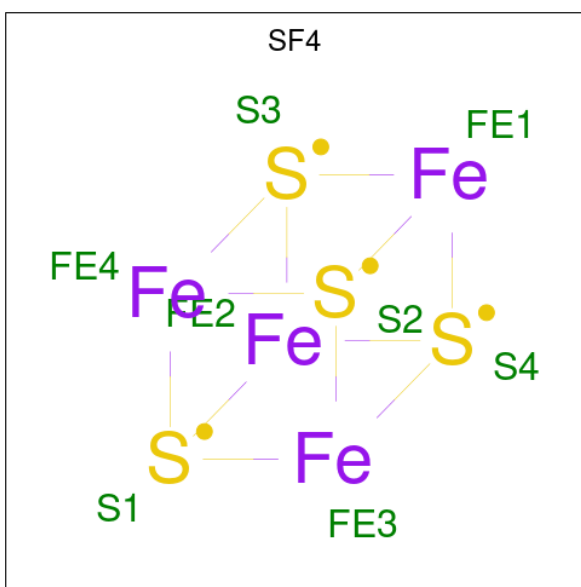
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
45	A	1	35	24	11	0
45	A	1	35	24	11	0
45	L	1	35	24	11	0
45	M	1	35	24	11	0
45	M	1	35	24	11	0
45	Y	1	35	24	11	0
45	Z	1	35	24	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
45	e	1	35	24	11	0
45	h	1	35	24	11	0
45	k	1	35	24	11	0
45	l	1	35	24	11	0

- Molecule 46 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



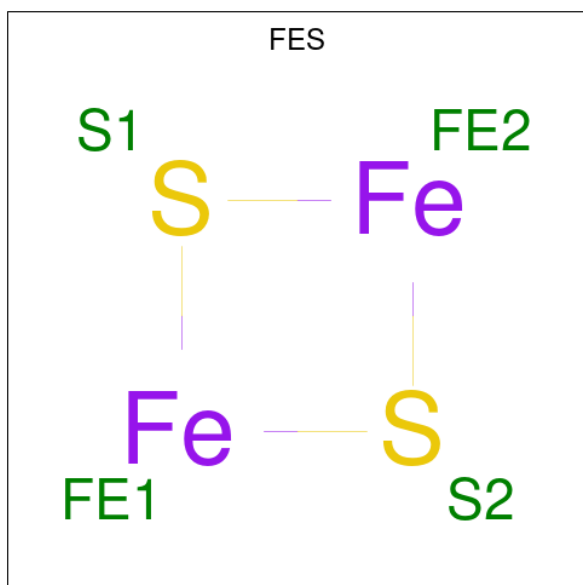
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
46	B	1	8	4	4	0
46	F	1	8	4	4	0
46	G	1	8	4	4	0
46	G	1	8	4	4	0
46	I	1	8	4	4	0
46	I	1	8	4	4	0

- Molecule 47 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: C₄₄H₈₈NO₈P).



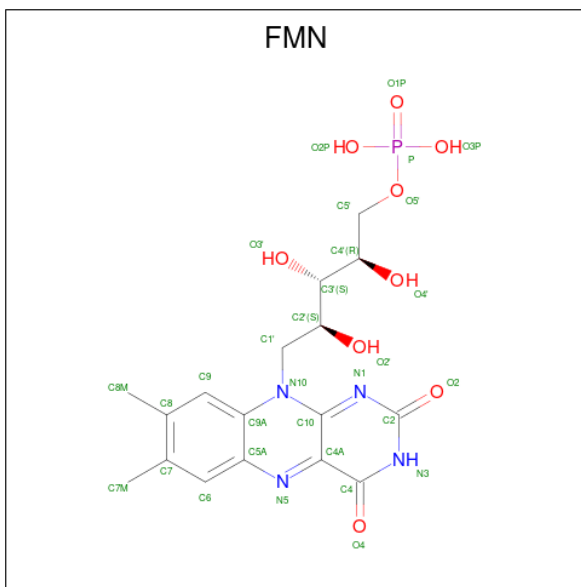
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
47	B	1	42	32	1	8	1	0
47	B	1	35	25	1	8	1	0
47	M	1	49	39	1	8	1	0
47	P	1	21	11	1	8	1	0

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



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

- Molecule 49 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).

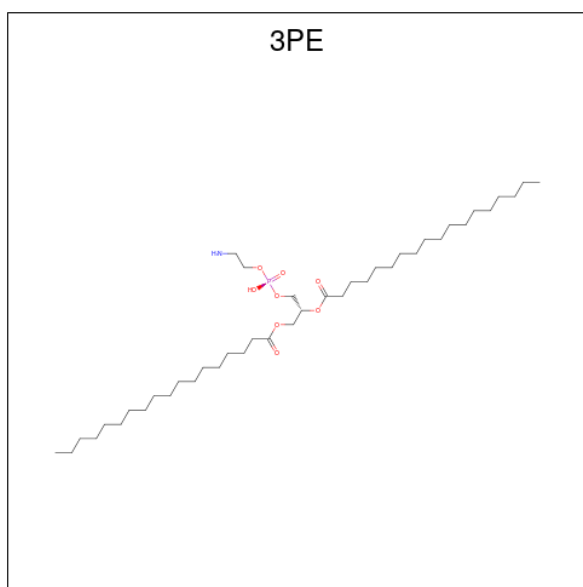


Mol	Chain	Residues	Atoms					AltConf
49	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 50 is POTASSIUM ION (three-letter code: K) (formula: K).

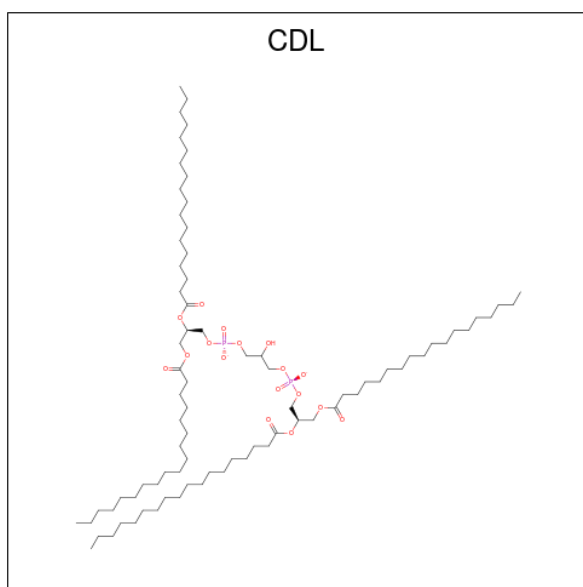
Mol	Chain	Residues	Atoms		AltConf
50	G	1	Total	K	0
			1	1	

- Molecule 51 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: C₄₁H₈₂NO₈P).



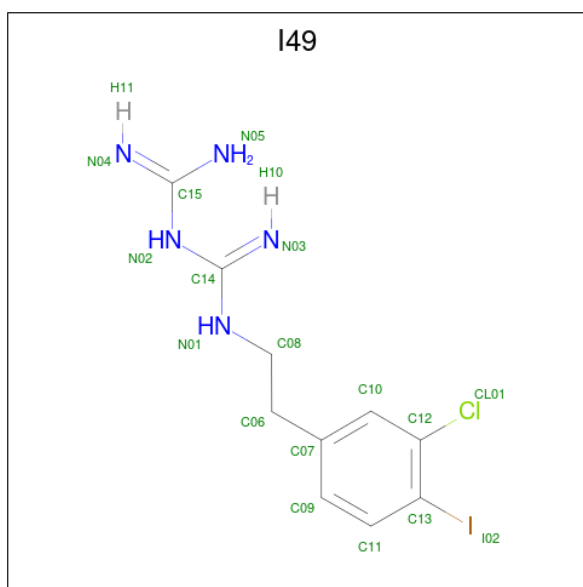
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
51	H	1	44	34	1	8	1	0
51	H	1	34	24	1	8	1	0
51	I	1	51	41	1	8	1	0
51	L	1	49	39	1	8	1	0
51	L	1	45	35	1	8	1	0
51	M	1	46	36	1	8	1	0
51	M	1	51	41	1	8	1	0
51	N	1	51	41	1	8	1	0
51	N	1	41	31	1	8	1	0
51	X	1	45	35	1	8	1	0
51	Y	1	35	25	1	8	1	0
51	d	1	51	41	1	8	1	0

- Molecule 52 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



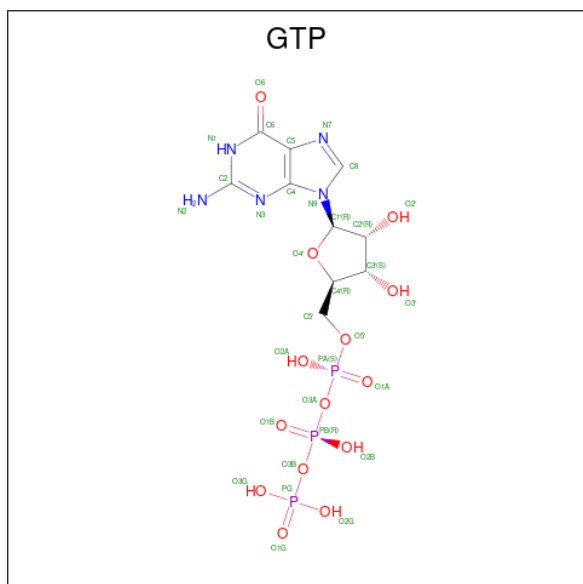
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
52	J	1	62	43	17	2	0
52	K	1	71	52	17	2	0
52	L	1	69	50	17	2	0
52	a	1	76	57	17	2	0
52	h	1	67	48	17	2	0

- Molecule 53 is 1-carbamimidoyl-3-[2-(3-chloranyl-4-iodanyl-phenyl)ethyl]guanidine (three-letter code: I49) (formula: $C_{10}H_{13}ClIN_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Cl	I	N	
53	N	1	17	10	1	1	5	0

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

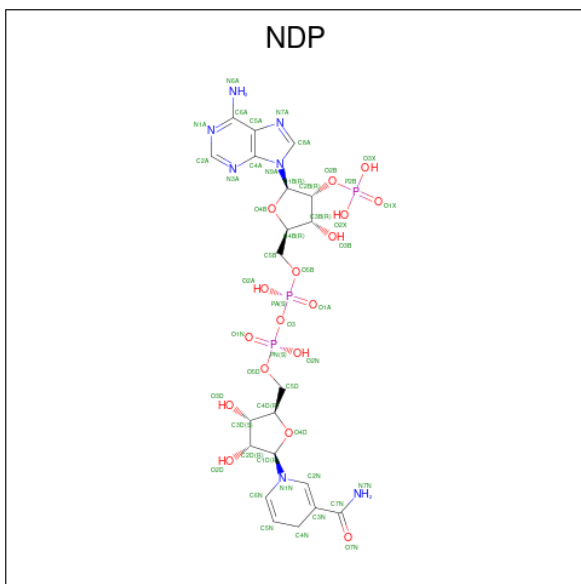


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
54	O	1	32	10	5	14	3	0

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

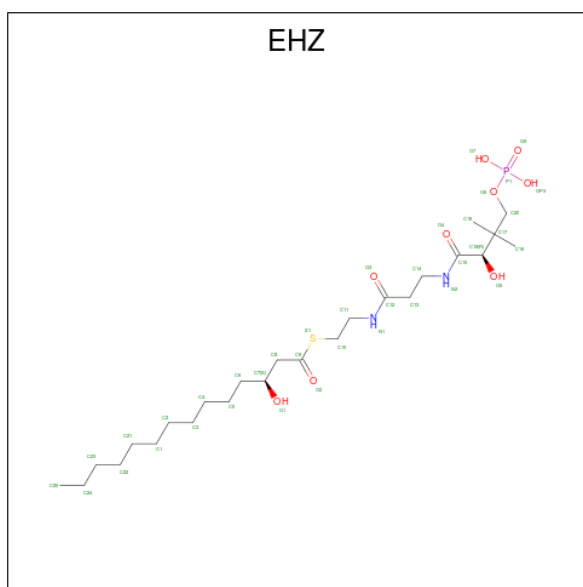


Mol	Chain	Residues	Atoms				AltConf	
56	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

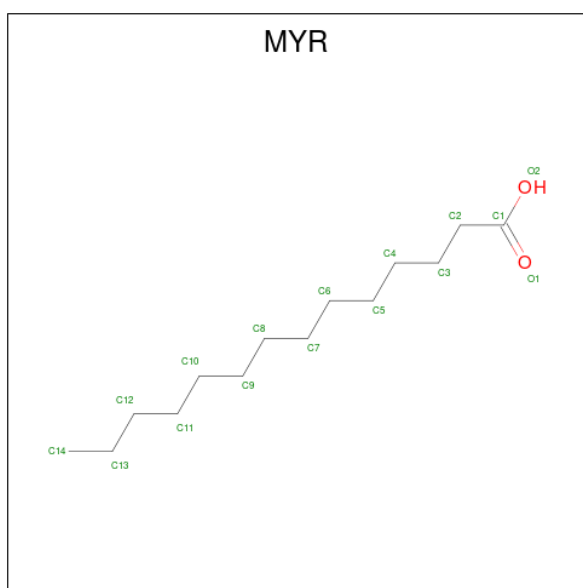
Mol	Chain	Residues	Atoms		AltConf
57	R	1	Total	Zn	0
			1	1	

- Molecule 58 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonoxy-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
			Total	C	O	
59	o	1	7	6	1	0

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	AltConf
60	A	16	Total O 16 16	0
60	B	48	Total O 48 48	0
60	C	61	Total O 61 61	0
60	D	123	Total O 123 123	0
60	E	7	Total O 7 7	0
60	F	36	Total O 36 36	0
60	G	132	Total O 132 132	0
60	H	42	Total O 42 42	0
60	I	76	Total O 76 76	0
60	J	10	Total O 10 10	0
60	K	11	Total O 11 11	0
60	L	23	Total O 23 23	0
60	M	28	Total O 28 28	0
60	N	30	Total O 30 30	0
60	O	10	Total O 10 10	0
60	P	35	Total O 35 35	0
60	Q	45	Total O 45 45	0
60	R	20	Total O 20 20	0
60	S	1	Total O 1 1	0
60	V	10	Total O 10 10	0
60	W	3	Total O 3 3	0
60	X	14	Total O 14 14	0

Continued on next page...

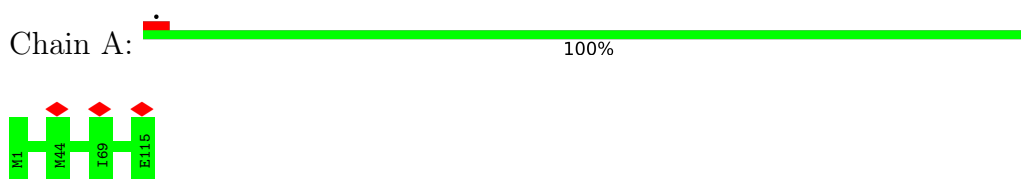
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
60	Y	1	Total 1	O 1	0
60	Z	13	Total 13	O 13	0
60	a	6	Total 6	O 6	0
60	d	8	Total 8	O 8	0
60	e	10	Total 10	O 10	0
60	f	1	Total 1	O 1	0
60	g	2	Total 2	O 2	0
60	h	8	Total 8	O 8	0
60	i	1	Total 1	O 1	0
60	j	1	Total 1	O 1	0
60	k	2	Total 2	O 2	0
60	l	7	Total 7	O 7	0
60	m	4	Total 4	O 4	0
60	n	10	Total 10	O 10	0
60	o	1	Total 1	O 1	0
60	p	10	Total 10	O 10	0
60	q	22	Total 22	O 22	0
60	r	15	Total 15	O 15	0
60	s	2	Total 2	O 2	0

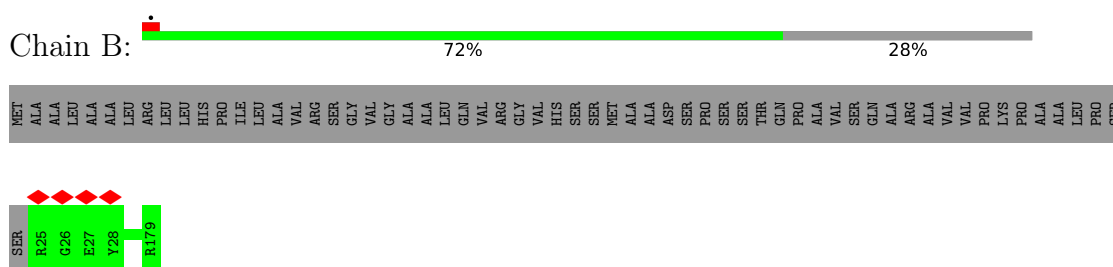
3 Residue-property plots [i](#)

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.

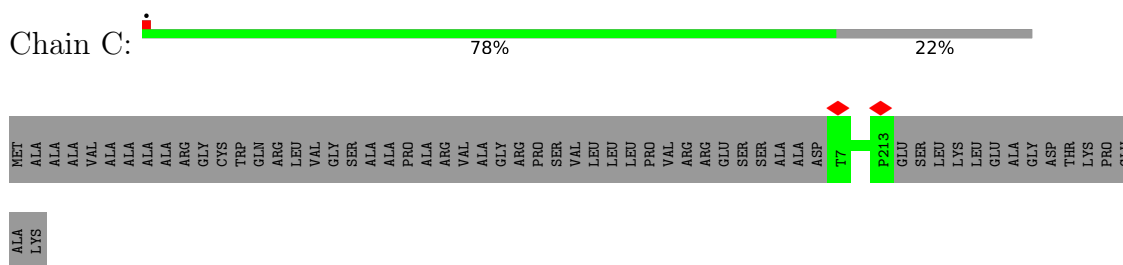
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



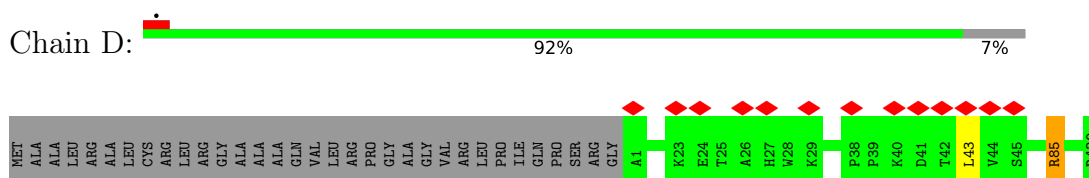
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



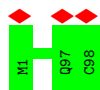
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



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

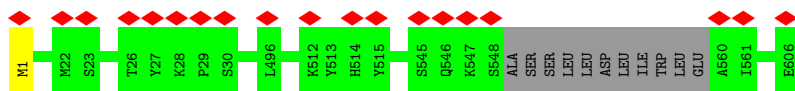


- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L: 98%



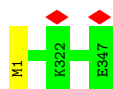
- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M: 100%



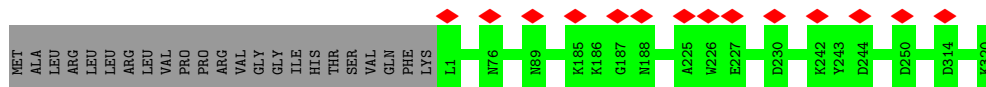
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N: 100%



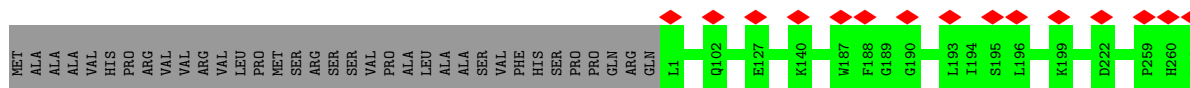
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O: 93%



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

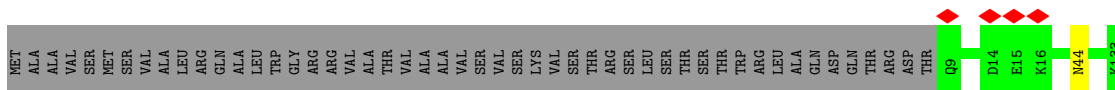
Chain P: 7%



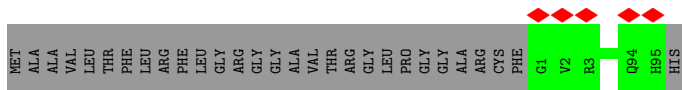
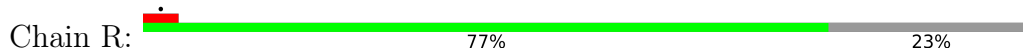
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q: 71%

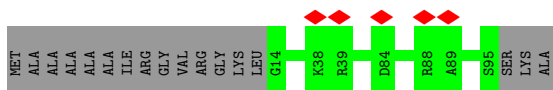
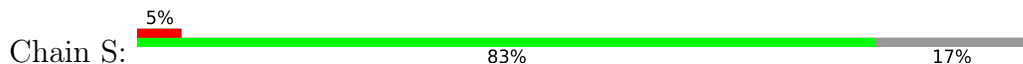




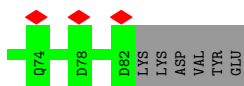
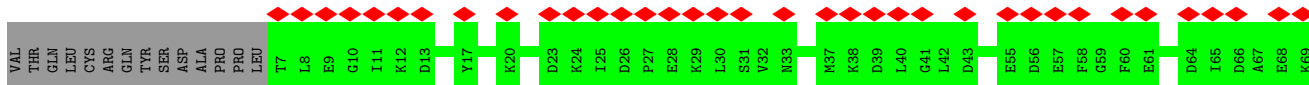
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



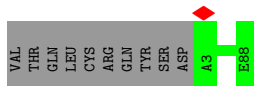
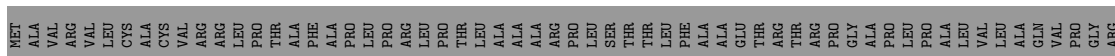
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



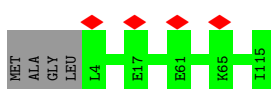
• Molecule 20: Acyl carrier protein, mitochondrial



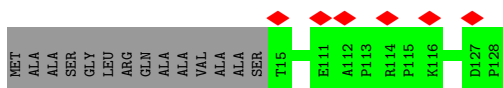
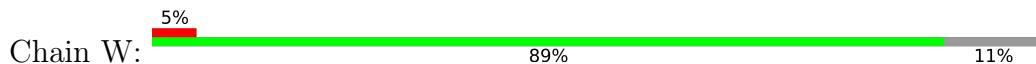
• Molecule 20: Acyl carrier protein, mitochondrial



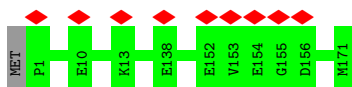
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



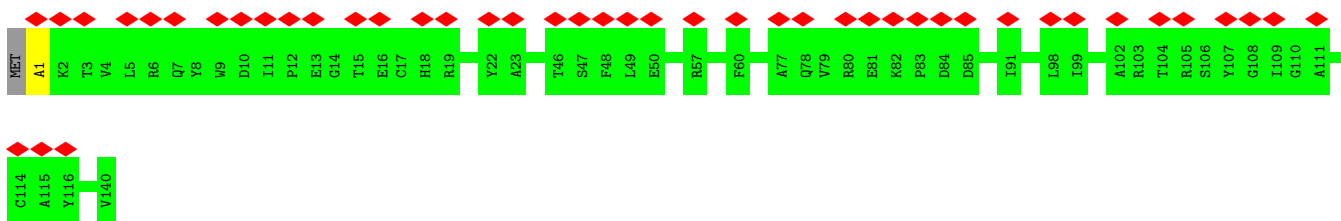
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



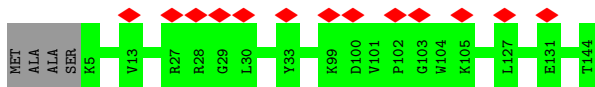
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



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



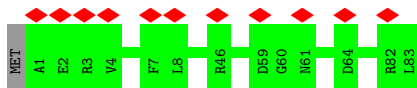
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



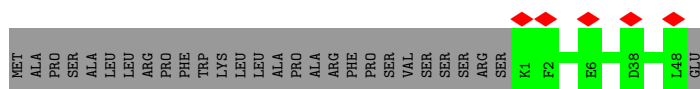
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



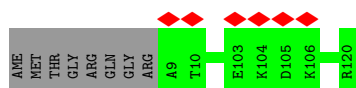
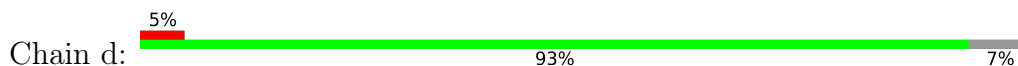
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



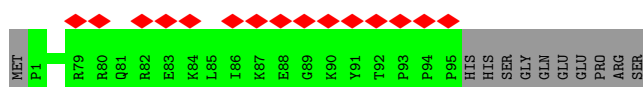
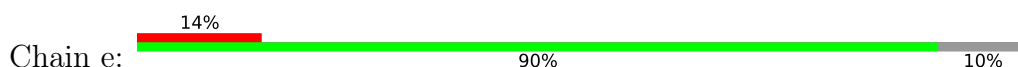
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



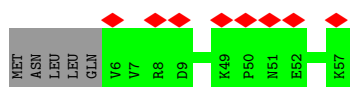
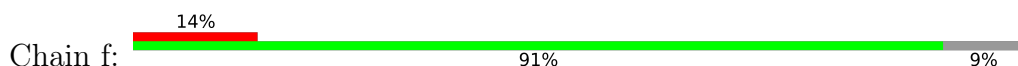
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



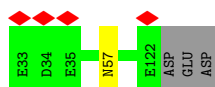
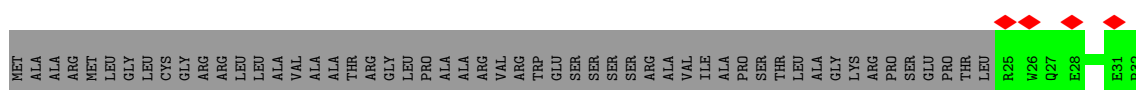
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



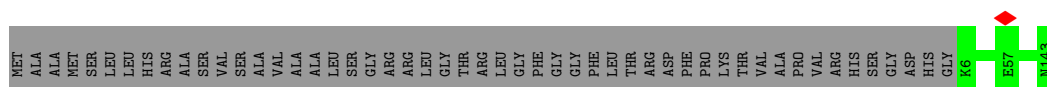
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



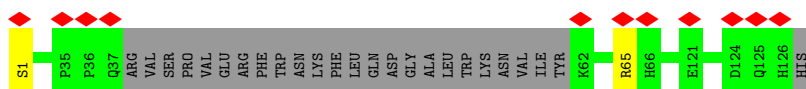
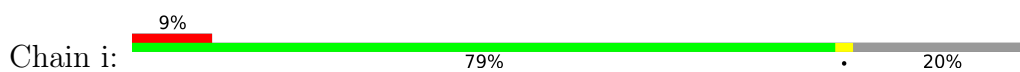
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



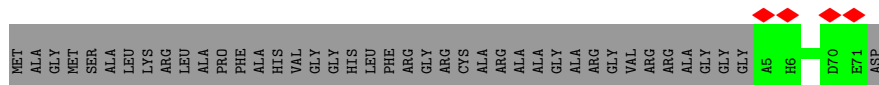
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



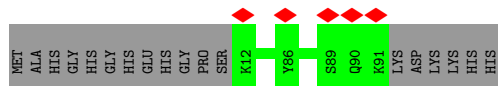
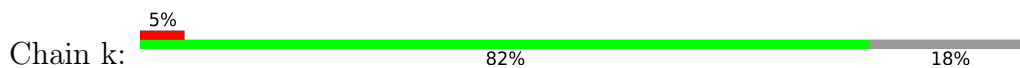
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



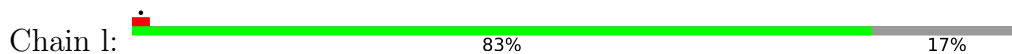
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



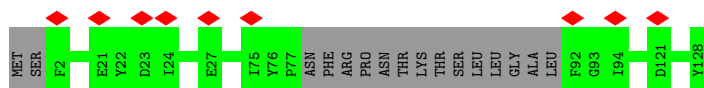
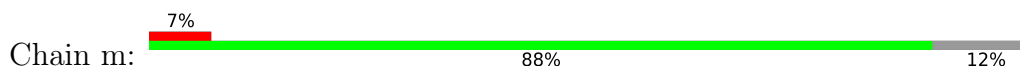
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



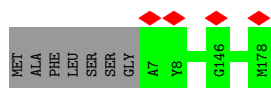
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



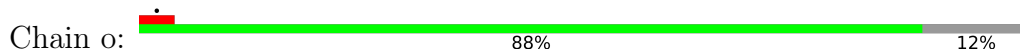
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

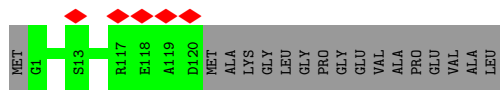


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

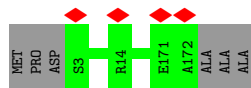


- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

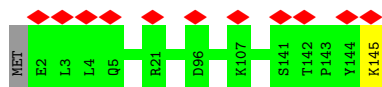




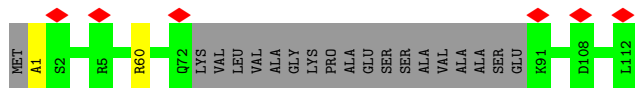
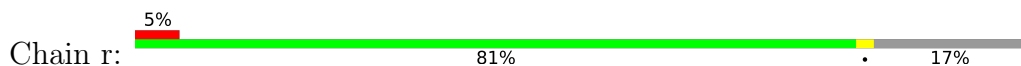
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



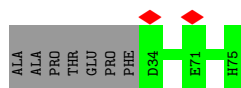
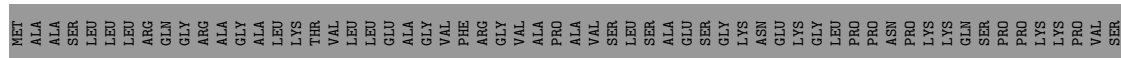
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- 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, Not provided	
Number of particles used	31957	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	30.444	Depositor
Minimum map value	-11.792	Depositor
Average map value	0.008	Depositor
Map value standard deviation	1.039	Depositor
Recommended contour level	6.0	Depositor
Map size (\AA)	482.46, 482.46, 482.46	wwPDB
Map dimensions	660, 660, 660	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.731, 0.731, 0.731	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, SF4, K, AYA, FMN, 3PE, I49, 2MR, GTP, NDP, PC1, FME, SAC, ZN, LMT, MYR, FES, MG, EHZ

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	0.30	0/936	0.42	0/1281
2	B	0.41	0/1272	0.49	0/1720
3	C	0.35	0/1772	0.45	0/2413
4	D	0.34	0/3537	0.46	0/4794
5	E	0.34	0/1695	0.44	0/2307
6	F	0.32	0/3393	0.46	0/4584
7	G	0.32	0/5367	0.46	0/7274
8	H	0.33	0/2571	0.43	0/3513
9	I	0.37	0/1445	0.48	0/1956
10	J	0.34	0/1362	0.42	0/1848
11	K	0.30	0/745	0.47	0/1008
12	L	0.33	0/4805	0.43	0/6536
13	M	0.32	0/3738	0.42	0/5097
14	N	0.31	0/2792	0.44	0/3800
15	O	0.34	0/2651	0.42	0/3587
16	P	0.31	0/2824	0.45	0/3831
17	Q	0.32	0/1039	0.46	0/1404
18	R	0.35	0/742	0.46	0/999
19	S	0.29	0/674	0.45	0/908
20	T	0.30	0/621	0.42	0/837
20	U	0.38	0/705	0.40	0/952
21	V	0.30	0/931	0.39	0/1261
22	W	0.31	0/995	0.42	0/1337
23	X	0.32	0/1439	0.41	0/1942
24	Y	0.27	0/1042	0.42	0/1414
25	Z	0.32	0/1175	0.42	0/1584
26	a	0.33	0/584	0.41	0/786
27	b	0.31	0/672	0.40	0/923
28	c	0.31	0/418	0.38	0/567
29	d	0.36	0/964	0.39	0/1305
30	e	0.31	0/818	0.43	0/1093

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.32	0/464	0.38	0/626
32	g	0.35	0/850	0.39	0/1154
33	h	0.34	0/1188	0.41	0/1607
34	i	0.36	0/896	0.43	0/1218
35	j	0.37	0/607	0.38	0/833
36	k	0.35	0/666	0.42	0/898
37	l	0.38	0/1358	0.41	0/1858
38	m	0.36	0/978	0.40	0/1321
39	n	0.37	0/1545	0.39	0/2092
40	o	0.38	0/1060	0.39	0/1420
41	p	0.35	0/1468	0.40	0/1979
42	q	0.33	0/1242	0.43	0/1688
43	r	0.33	0/780	0.44	0/1056
44	s	0.30	0/363	0.45	0/491
All	All	0.33	0/67189	0.43	0/91102

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	85	2MR	Mainchain

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	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
2	B	153/216 (71%)	147 (96%)	6 (4%)	0	100	100
3	C	205/266 (77%)	199 (97%)	6 (3%)	0	100	100
4	D	427/463 (92%)	411 (96%)	15 (4%)	1 (0%)	47	62
5	E	211/249 (85%)	205 (97%)	6 (3%)	0	100	100
6	F	429/464 (92%)	420 (98%)	9 (2%)	0	100	100
7	G	686/727 (94%)	668 (97%)	18 (3%)	0	100	100
8	H	316/318 (99%)	304 (96%)	12 (4%)	0	100	100
9	I	174/212 (82%)	169 (97%)	5 (3%)	0	100	100
10	J	172/175 (98%)	162 (94%)	10 (6%)	0	100	100
11	K	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
12	L	591/606 (98%)	568 (96%)	23 (4%)	0	100	100
13	M	457/459 (100%)	453 (99%)	4 (1%)	0	100	100
14	N	345/347 (99%)	340 (99%)	5 (1%)	0	100	100
15	O	318/343 (93%)	313 (98%)	5 (2%)	0	100	100
16	P	339/380 (89%)	335 (99%)	4 (1%)	0	100	100
17	Q	123/175 (70%)	121 (98%)	2 (2%)	0	100	100
18	R	93/124 (75%)	89 (96%)	4 (4%)	0	100	100
19	S	80/99 (81%)	77 (96%)	3 (4%)	0	100	100
20	T	74/156 (47%)	73 (99%)	1 (1%)	0	100	100
20	U	84/156 (54%)	84 (100%)	0	0	100	100
21	V	110/116 (95%)	109 (99%)	1 (1%)	0	100	100
22	W	112/128 (88%)	110 (98%)	2 (2%)	0	100	100
23	X	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
24	Y	138/141 (98%)	135 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Z	138/144 (96%)	134 (97%)	4 (3%)	0	100	100
26	a	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
27	b	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
28	c	46/76 (60%)	45 (98%)	1 (2%)	0	100	100
29	d	110/120 (92%)	109 (99%)	1 (1%)	0	100	100
30	e	93/106 (88%)	91 (98%)	2 (2%)	0	100	100
31	f	50/57 (88%)	50 (100%)	0	0	100	100
32	g	96/154 (62%)	91 (95%)	5 (5%)	0	100	100
33	h	136/189 (72%)	135 (99%)	1 (1%)	0	100	100
34	i	98/127 (77%)	94 (96%)	4 (4%)	0	100	100
35	j	65/108 (60%)	64 (98%)	1 (2%)	0	100	100
36	k	78/98 (80%)	76 (97%)	2 (3%)	0	100	100
37	l	153/186 (82%)	148 (97%)	5 (3%)	0	100	100
38	m	109/129 (84%)	105 (96%)	4 (4%)	0	100	100
39	n	170/179 (95%)	168 (99%)	2 (1%)	0	100	100
40	o	118/137 (86%)	113 (96%)	5 (4%)	0	100	100
41	p	168/176 (96%)	167 (99%)	1 (1%)	0	100	100
42	q	142/145 (98%)	141 (99%)	1 (1%)	0	100	100
43	r	90/113 (80%)	86 (96%)	4 (4%)	0	100	100
44	s	40/109 (37%)	39 (98%)	1 (2%)	0	100	100
All	All	8064/9212 (88%)	7860 (98%)	203 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	43	LEU

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	100/100 (100%)	100 (100%)	0	100	100
2	B	131/175 (75%)	131 (100%)	0	100	100
3	C	188/228 (82%)	188 (100%)	0	100	100
4	D	370/392 (94%)	370 (100%)	0	100	100
5	E	183/205 (89%)	183 (100%)	0	100	100
6	F	345/368 (94%)	345 (100%)	0	100	100
7	G	578/608 (95%)	578 (100%)	0	100	100
8	H	274/274 (100%)	274 (100%)	0	100	100
9	I	151/175 (86%)	151 (100%)	0	100	100
10	J	140/141 (99%)	140 (100%)	0	100	100
11	K	85/85 (100%)	85 (100%)	0	100	100
12	L	518/533 (97%)	518 (100%)	0	100	100
13	M	412/412 (100%)	412 (100%)	0	100	100
14	N	315/315 (100%)	315 (100%)	0	100	100
15	O	283/303 (93%)	283 (100%)	0	100	100
16	P	295/327 (90%)	295 (100%)	0	100	100
17	Q	112/153 (73%)	111 (99%)	1 (1%)	78	90
18	R	78/97 (80%)	78 (100%)	0	100	100
19	S	73/82 (89%)	73 (100%)	0	100	100
20	T	70/135 (52%)	70 (100%)	0	100	100
20	U	79/135 (58%)	79 (100%)	0	100	100
21	V	100/102 (98%)	100 (100%)	0	100	100
22	W	107/114 (94%)	107 (100%)	0	100	100
23	X	154/155 (99%)	154 (100%)	0	100	100
24	Y	101/102 (99%)	101 (100%)	0	100	100
25	Z	119/121 (98%)	119 (100%)	0	100	100
26	a	59/59 (100%)	59 (100%)	0	100	100
27	b	71/72 (99%)	71 (100%)	0	100	100
28	c	44/68 (65%)	44 (100%)	0	100	100
29	d	100/105 (95%)	100 (100%)	0	100	100
30	e	86/96 (90%)	86 (100%)	0	100	100
31	f	49/54 (91%)	49 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	g	89/131 (68%)	88 (99%)	1 (1%)	73	87
33	h	121/158 (77%)	121 (100%)	0	100	100
34	i	97/120 (81%)	96 (99%)	1 (1%)	76	88
35	j	61/84 (73%)	61 (100%)	0	100	100
36	k	62/76 (82%)	62 (100%)	0	100	100
37	l	139/159 (87%)	139 (100%)	0	100	100
38	m	101/115 (88%)	101 (100%)	0	100	100
39	n	156/161 (97%)	156 (100%)	0	100	100
40	o	109/120 (91%)	109 (100%)	0	100	100
41	p	154/157 (98%)	154 (100%)	0	100	100
42	q	130/131 (99%)	129 (99%)	1 (1%)	81	91
43	r	84/97 (87%)	83 (99%)	1 (1%)	71	85
44	s	41/92 (45%)	41 (100%)	0	100	100
All	All	7114/7892 (90%)	7109 (100%)	5 (0%)	93	98

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	Q	44	ASN
32	g	57	ASN
34	i	65	ARG
42	q	145	LYS
43	r	60	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	200	ASN
4	D	150	HIS
6	F	438	GLN
12	L	570	GLN
15	O	180	GLN
17	Q	44	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

11 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
4	2MR	D	85	4	10,12,13	2.66	3 (30%)	5,13,15	1.13	1 (20%)
8	FME	H	1	8	8,9,10	0.96	0	7,9,11	0.91	0
12	FME	L	1	12	8,9,10	1.02	1 (12%)	7,9,11	0.74	0
14	FME	N	1	14	8,9,10	0.88	0	7,9,11	1.05	1 (14%)
24	AYA	Y	1	24	6,7,8	1.77	1 (16%)	5,8,10	1.40	1 (20%)
1	FME	A	1	1	8,9,10	0.95	0	7,9,11	0.82	0
34	SAC	i	1	34	7,8,9	0.94	0	8,9,11	1.33	2 (25%)
13	FME	M	1	13	8,9,10	1.01	1 (12%)	7,9,11	0.92	0
11	FME	K	1	11	8,9,10	0.93	0	7,9,11	0.73	0
43	AYA	r	1	43	6,7,8	1.81	2 (33%)	5,8,10	1.20	1 (20%)
10	FME	J	1	10	8,9,10	0.94	0	7,9,11	1.21	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	2MR	D	85	4	-	0/10/13/15	-
8	FME	H	1	8	-	3/7/9/11	-
12	FME	L	1	12	-	4/7/9/11	-
14	FME	N	1	14	-	3/7/9/11	-
24	AYA	Y	1	24	-	0/4/6/8	-
1	FME	A	1	1	-	2/7/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	SAC	i	1	34	-	2/7/8/10	-
13	FME	M	1	13	-	0/7/9/11	-
11	FME	K	1	11	-	1/7/9/11	-
43	AYA	r	1	43	-	0/4/6/8	-
10	FME	J	1	10	-	3/7/9/11	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	4.97	1.44	1.33
4	D	85	2MR	CZ-NE	4.75	1.44	1.34
4	D	85	2MR	O-C	3.93	1.35	1.19
24	Y	1	AYA	CT-N	3.26	1.45	1.34
43	r	1	AYA	CT-N	3.20	1.45	1.34
12	L	1	FME	CA-N	-2.13	1.43	1.46
43	r	1	AYA	OT-CT	-2.11	1.18	1.23
13	M	1	FME	CA-N	-2.09	1.43	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	i	1	SAC	C-CA-N	2.83	114.85	109.73
10	J	1	FME	C-CA-N	2.50	114.25	109.73
24	Y	1	AYA	CM-CT-N	2.41	120.18	116.10
34	i	1	SAC	OG-CB-CA	-2.33	105.02	110.97
43	r	1	AYA	CM-CT-N	2.17	119.78	116.10
4	D	85	2MR	NE-CZ-NH2	-2.17	117.49	119.48
14	N	1	FME	C-CA-N	2.11	113.54	109.73

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	C-CA-CB-CG
8	H	1	FME	C-CA-CB-CG
10	J	1	FME	O1-CN-N-CA
10	J	1	FME	N-CA-CB-CG
12	L	1	FME	O1-CN-N-CA
14	N	1	FME	O1-CN-N-CA
14	N	1	FME	CB-CA-N-CN
8	H	1	FME	CA-CB-CG-SD

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	L	1	FME	N-CA-CB-CG
14	N	1	FME	N-CA-CB-CG
10	J	1	FME	CB-CG-SD-CE
12	L	1	FME	CA-CB-CG-SD
1	A	1	FME	N-CA-CB-CG
34	i	1	SAC	CB-CA-N-C1A
11	K	1	FME	CB-CG-SD-CE
12	L	1	FME	CB-CG-SD-CE
34	i	1	SAC	C-CA-N-C1A
8	H	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 50 ligands modelled in this entry, 3 are monoatomic - leaving 47 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	$\# Z > 2$
51	3PE	L	704	-	44,44,50	0.91	4 (9%)	47,49,55	1.15	2 (4%)
51	3PE	H	401	-	43,43,50	0.92	3 (6%)	46,48,55	1.13	2 (4%)
46	SF4	I	203	9	0,12,12	-	-	-		
45	LMT	M	602	-	36,36,36	1.21	3 (8%)	47,47,47	0.93	0
45	LMT	A	301	-	36,36,36	1.15	2 (5%)	47,47,47	0.97	1 (2%)
45	LMT	e	501	-	36,36,36	1.21	3 (8%)	47,47,47	1.04	3 (6%)
47	PC1	B	203	-	34,34,53	1.16	4 (11%)	40,42,61	1.10	2 (5%)
51	3PE	d	301	-	50,50,50	0.84	4 (8%)	53,55,55	1.16	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	CDL	J	701	-	61,61,99	1.08	6 (9%)	67,73,111	1.24	4 (5%)
52	CDL	a	101	-	75,75,99	0.99	6 (8%)	81,87,111	1.12	5 (6%)
51	3PE	Y	802	-	34,34,50	1.03	4 (11%)	37,39,55	1.21	2 (5%)
52	CDL	L	703	-	68,68,99	1.03	5 (7%)	74,80,111	1.12	4 (5%)
56	NDP	P	501	-	45,52,52	2.15	4 (8%)	53,80,80	1.70	11 (20%)
52	CDL	h	1001	-	66,66,99	1.05	7 (10%)	72,78,111	1.20	4 (5%)
52	CDL	K	401	-	70,70,99	1.02	7 (10%)	76,82,111	1.09	4 (5%)
51	3PE	X	401	-	44,44,50	0.91	4 (9%)	47,49,55	1.15	2 (4%)
45	LMT	h	1002	-	36,36,36	1.12	2 (5%)	47,47,47	1.22	4 (8%)
48	FES	G	803	7	0,4,4	-	-	-	-	-
45	LMT	Y	801	-	36,36,36	1.20	4 (11%)	47,47,47	1.19	4 (8%)
45	LMT	L	702	-	36,36,36	1.16	3 (8%)	47,47,47	0.82	0
51	3PE	N	1301	-	50,50,50	0.87	4 (8%)	53,55,55	1.10	2 (3%)
46	SF4	I	202	9	0,12,12	-	-	-	-	-
45	LMT	k	101	-	36,36,36	1.18	3 (8%)	47,47,47	1.00	1 (2%)
54	GTP	O	401	55	26,34,34	2.90	10 (38%)	32,54,54	1.73	11 (34%)
48	FES	E	301	5	0,4,4	-	-	-	-	-
49	FMN	F	501	-	33,33,33	1.08	1 (3%)	48,50,50	1.26	6 (12%)
46	SF4	B	201	2	0,12,12	-	-	-	-	-
58	EHZ	T	101	20	29,36,37	1.67	6 (20%)	35,44,47	1.68	6 (17%)
47	PC1	M	605	-	48,48,53	0.98	4 (8%)	54,56,61	1.07	2 (3%)
47	PC1	B	202	-	41,41,53	1.04	3 (7%)	47,49,61	1.04	2 (4%)
45	LMT	l	201	-	36,36,36	1.21	3 (8%)	47,47,47	1.09	4 (8%)
46	SF4	G	801	7	0,12,12	-	-	-	-	-
51	3PE	M	604	-	50,50,50	0.85	3 (6%)	53,55,55	1.08	2 (3%)
46	SF4	G	802	7	0,12,12	-	-	-	-	-
51	3PE	H	402	-	33,33,50	1.37	4 (12%)	34,37,55	1.22	2 (5%)
51	3PE	M	601	-	45,45,50	0.91	3 (6%)	48,50,55	1.03	2 (4%)
47	PC1	P	502	-	20,20,53	1.86	3 (15%)	24,27,61	1.15	1 (4%)
59	MYR	o	201	40	6,6,15	0.93	0	5,5,15	0.96	0
45	LMT	Z	301	-	36,36,36	1.27	3 (8%)	47,47,47	1.33	5 (10%)
51	3PE	I	201	-	50,50,50	0.87	4 (8%)	53,55,55	0.98	2 (3%)
58	EHZ	U	101	20	29,36,37	1.65	6 (20%)	35,44,47	1.60	3 (8%)
45	LMT	M	603	-	36,36,36	1.22	4 (11%)	47,47,47	1.22	4 (8%)
51	3PE	L	701	-	48,48,50	0.89	3 (6%)	51,53,55	1.10	2 (3%)
51	3PE	N	1302	-	40,40,50	0.97	4 (10%)	43,45,55	1.00	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	SF4	F	502	6	0,12,12	-	-	-	-	-
45	LMT	A	302	-	36,36,36	1.18	3 (8%)	47,47,47	1.40	3 (6%)
53	I49	N	1303	-	15,17,17	1.51	2 (13%)	21,22,22	1.69	3 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	3PE	L	704	-	-	20/48/48/54	-
51	3PE	H	401	-	-	16/47/47/54	-
46	SF4	I	203	9	-	-	0/6/5/5
45	LMT	M	602	-	-	9/21/61/61	0/2/2/2
45	LMT	A	301	-	-	7/21/61/61	0/2/2/2
45	LMT	e	501	-	-	11/21/61/61	0/2/2/2
47	PC1	B	203	-	-	19/38/38/57	-
51	3PE	d	301	-	-	18/54/54/54	-
52	CDL	J	701	-	-	28/71/71/110	-
52	CDL	a	101	-	-	34/86/86/110	-
51	3PE	Y	802	-	-	16/38/38/54	-
52	CDL	L	703	-	-	35/79/79/110	-
56	NDP	P	501	-	-	7/30/77/77	0/5/5/5
52	CDL	h	1001	-	-	34/77/77/110	-
52	CDL	K	401	-	-	40/81/81/110	-
51	3PE	X	401	-	-	22/48/48/54	-
45	LMT	h	1002	-	-	8/21/61/61	0/2/2/2
51	3PE	N	1301	-	-	21/54/54/54	-
45	LMT	Y	801	-	-	10/21/61/61	0/2/2/2
45	LMT	L	702	-	-	9/21/61/61	0/2/2/2
48	FES	G	803	7	-	-	0/1/1/1
54	GTP	O	401	55	-	6/18/38/38	0/3/3/3
45	LMT	k	101	-	-	4/21/61/61	0/2/2/2
46	SF4	I	202	9	-	-	0/6/5/5
48	FES	E	301	5	-	-	0/1/1/1
49	FMN	F	501	-	-	1/18/18/18	0/3/3/3
46	SF4	B	201	2	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	EHZ	T	101	20	-	14/42/44/45	-
47	PC1	M	605	-	-	23/52/52/57	-
47	PC1	B	202	-	-	14/45/45/57	-
45	LMT	l	201	-	-	4/21/61/61	0/2/2/2
46	SF4	G	801	7	-	-	0/6/5/5
51	3PE	M	604	-	-	29/54/54/54	-
46	SF4	G	802	7	-	-	0/6/5/5
51	3PE	H	402	-	-	20/36/36/54	-
51	3PE	M	601	-	-	21/49/49/54	-
47	PC1	P	502	-	-	8/22/22/57	-
59	MYR	o	201	40	-	3/3/4/13	-
45	LMT	Z	301	-	-	7/21/61/61	0/2/2/2
51	3PE	I	201	-	-	25/54/54/54	-
58	EHZ	U	101	20	-	7/42/44/45	-
45	LMT	M	603	-	-	8/21/61/61	0/2/2/2
51	3PE	L	701	-	-	26/52/52/54	-
51	3PE	N	1302	-	-	21/44/44/54	-
46	SF4	F	502	6	-	-	0/6/5/5
45	LMT	A	302	-	-	13/21/61/61	0/2/2/2
53	I49	N	1303	-	-	3/10/10/10	0/1/1/1

All (151) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	501	NDP	P2B-O2B	11.96	1.81	1.59
54	O	401	GTP	O6-C6	8.06	1.39	1.23
47	P	502	PC1	O21-C2	-5.77	1.40	1.46
54	O	401	GTP	O4'-C1'	5.45	1.48	1.41
58	T	101	EHZ	C15-N2	5.25	1.45	1.33
58	U	101	EHZ	C15-N2	5.22	1.45	1.33
51	H	402	3PE	O21-C2	-5.20	1.40	1.46
58	T	101	EHZ	C12-N1	5.12	1.45	1.33
58	U	101	EHZ	C12-N1	4.91	1.44	1.33
54	O	401	GTP	C2-N1	4.74	1.49	1.37
54	O	401	GTP	C2-N3	4.63	1.44	1.33
53	N	1303	I49	C15-N02	-4.59	1.31	1.37
54	O	401	GTP	C2-N2	4.44	1.44	1.34
45	Z	301	LMT	O5B-C1B	3.60	1.51	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	M	602	LMT	O5B-C1B	3.52	1.50	1.41
45	e	501	LMT	O5B-C1B	3.51	1.50	1.41
45	Z	301	LMT	O5'-C1'	3.45	1.50	1.41
49	F	501	FMN	C4A-N5	3.44	1.37	1.30
45	M	603	LMT	O5B-C1B	3.42	1.50	1.41
45	k	101	LMT	O5B-C1B	3.40	1.50	1.41
45	A	302	LMT	O5B-C1B	3.38	1.50	1.41
56	P	501	NDP	PN-O5D	3.38	1.73	1.59
45	l	201	LMT	O5B-C1B	3.34	1.50	1.41
54	O	401	GTP	C2'-C1'	-3.33	1.48	1.53
45	L	702	LMT	O5B-C1B	3.32	1.50	1.41
45	A	301	LMT	O5B-C1B	3.32	1.50	1.41
45	l	201	LMT	O5'-C1'	3.31	1.50	1.41
45	e	501	LMT	O5'-C1'	3.25	1.50	1.41
45	h	1002	LMT	O5B-C1B	3.24	1.50	1.41
45	Y	801	LMT	O5B-C1B	3.21	1.50	1.41
56	P	501	NDP	O2B-C2B	-3.17	1.32	1.44
45	A	302	LMT	O5'-C1'	3.14	1.49	1.41
45	M	602	LMT	O5'-C1'	3.09	1.49	1.41
45	M	603	LMT	O5'-C1'	3.08	1.49	1.41
51	H	402	3PE	O21-C21	3.08	1.40	1.33
54	O	401	GTP	C5-C6	-3.06	1.41	1.47
45	Y	801	LMT	O5'-C1'	3.05	1.49	1.41
45	A	301	LMT	O5'-C1'	3.03	1.49	1.41
53	N	1303	I49	C14-N03	3.03	1.38	1.29
45	k	101	LMT	O5'-C1'	3.03	1.49	1.41
47	P	502	PC1	O21-C21	2.99	1.40	1.33
45	L	702	LMT	O5'-C1'	2.93	1.49	1.41
45	h	1002	LMT	O5'-C1'	2.89	1.49	1.41
51	L	701	3PE	O21-C2	-2.84	1.39	1.46
51	M	601	3PE	O21-C2	-2.78	1.39	1.46
51	N	1301	3PE	O21-C2	-2.77	1.39	1.46
52	K	401	CDL	OA6-CA4	-2.74	1.39	1.46
51	H	401	3PE	O21-C2	-2.72	1.39	1.46
52	a	101	CDL	OB6-CB4	-2.68	1.39	1.46
52	h	1001	CDL	OA6-CA4	-2.67	1.39	1.46
51	N	1302	3PE	O21-C2	-2.65	1.40	1.46
52	L	703	CDL	OB6-CB4	-2.64	1.40	1.46
52	J	701	CDL	OB6-CB4	-2.63	1.40	1.46
52	a	101	CDL	OA8-CA6	-2.62	1.39	1.45
51	H	402	3PE	O31-C31	2.60	1.40	1.33
52	L	703	CDL	OA6-CA4	-2.60	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	a	101	CDL	OA6-CA4	-2.58	1.40	1.46
47	B	202	PC1	O21-C2	-2.58	1.40	1.46
51	X	401	3PE	O21-C2	-2.56	1.40	1.46
52	K	401	CDL	OB6-CB4	-2.54	1.40	1.46
51	Y	802	3PE	O21-C2	-2.54	1.40	1.46
52	J	701	CDL	OA6-CA5	2.53	1.40	1.35
51	M	604	3PE	O31-C31	2.53	1.40	1.33
52	K	401	CDL	OA8-CA6	-2.52	1.39	1.45
58	U	101	EHZ	O4-C15	-2.51	1.18	1.23
52	J	701	CDL	OA8-CA7	2.50	1.40	1.33
51	L	701	3PE	O31-C3	-2.50	1.39	1.45
47	B	203	PC1	O21-C2	-2.49	1.40	1.46
52	h	1001	CDL	OB6-CB4	-2.47	1.40	1.46
51	I	201	3PE	O31-C3	-2.47	1.39	1.45
51	L	704	3PE	O21-C2	-2.47	1.40	1.46
51	H	401	3PE	O31-C3	-2.45	1.39	1.45
52	L	703	CDL	OB8-CB7	2.45	1.40	1.33
51	M	601	3PE	O31-C3	-2.45	1.39	1.45
51	I	201	3PE	O21-C2	-2.42	1.40	1.46
58	T	101	EHZ	O4-C15	-2.42	1.18	1.23
51	L	704	3PE	O31-C3	-2.41	1.39	1.45
51	N	1301	3PE	O31-C3	-2.41	1.39	1.45
51	N	1302	3PE	O31-C31	2.40	1.40	1.33
47	M	605	PC1	O21-C2	-2.35	1.40	1.46
51	Y	802	3PE	O31-C31	2.35	1.40	1.33
52	a	101	CDL	OB8-CB7	2.34	1.40	1.33
54	O	401	GTP	PG-O3G	-2.32	1.45	1.54
47	B	203	PC1	O31-C31	2.32	1.40	1.33
52	L	703	CDL	OA8-CA7	2.32	1.40	1.33
51	d	301	3PE	O31-C3	-2.32	1.39	1.45
54	O	401	GTP	PG-O2G	-2.30	1.46	1.54
54	O	401	GTP	C2'-C3'	-2.30	1.47	1.53
45	Z	301	LMT	O5'-C5'	2.30	1.49	1.44
52	h	1001	CDL	OA8-CA7	2.28	1.40	1.33
51	Y	802	3PE	O31-C3	-2.28	1.40	1.45
58	T	101	EHZ	O3-C12	-2.28	1.18	1.23
52	L	703	CDL	OA8-CA6	-2.28	1.40	1.45
58	U	101	EHZ	O3-C12	-2.27	1.18	1.23
47	M	605	PC1	O31-C3	-2.27	1.40	1.45
51	X	401	3PE	O31-C3	-2.26	1.40	1.45
52	J	701	CDL	OB8-CB6	-2.25	1.40	1.45
52	h	1001	CDL	OB8-CB7	2.25	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	K	401	CDL	OB8-CB7	2.25	1.39	1.33
52	h	1001	CDL	OA8-CA6	-2.24	1.40	1.45
51	I	201	3PE	O21-C21	2.22	1.40	1.34
51	H	401	3PE	O31-C31	2.22	1.39	1.33
47	M	605	PC1	O31-C31	2.21	1.39	1.33
51	M	604	3PE	O21-C21	2.21	1.40	1.34
47	B	202	PC1	O31-C3	-2.21	1.40	1.45
47	B	202	PC1	O31-C31	2.21	1.39	1.33
51	L	704	3PE	O31-C31	2.20	1.39	1.33
52	a	101	CDL	OB8-CB6	-2.20	1.40	1.45
52	h	1001	CDL	OB8-CB6	-2.20	1.40	1.45
52	K	401	CDL	OB8-CB6	-2.20	1.40	1.45
51	X	401	3PE	O31-C31	2.18	1.39	1.33
52	K	401	CDL	OB6-CB5	2.17	1.40	1.34
52	h	1001	CDL	OB6-CB5	2.17	1.40	1.34
45	M	603	LMT	O5B-C5B	2.16	1.49	1.44
45	M	603	LMT	O5'-C5'	2.16	1.49	1.44
45	e	501	LMT	O5B-C5B	2.16	1.49	1.44
45	A	302	LMT	O1B-C4'	2.16	1.49	1.43
47	B	203	PC1	O21-C21	2.15	1.40	1.34
51	d	301	3PE	O21-C21	2.14	1.40	1.34
52	J	701	CDL	OB8-CB7	2.14	1.39	1.33
47	M	605	PC1	O21-C21	2.14	1.40	1.34
58	T	101	EHZ	O6-C20	-2.13	1.39	1.44
51	M	604	3PE	O21-C2	-2.13	1.41	1.46
51	X	401	3PE	O21-C21	2.13	1.40	1.34
51	M	601	3PE	O31-C31	2.12	1.39	1.33
52	a	101	CDL	OA6-CA5	2.12	1.40	1.34
51	d	301	3PE	O31-C31	2.12	1.39	1.33
45	l	201	LMT	O5B-C5B	2.12	1.49	1.44
51	I	201	3PE	O31-C31	2.11	1.39	1.33
52	J	701	CDL	OA6-CA4	-2.11	1.41	1.46
56	P	501	NDP	O3D-C3D	-2.11	1.38	1.43
51	d	301	3PE	O21-C2	-2.11	1.41	1.46
45	L	702	LMT	O5B-C5B	2.10	1.49	1.44
51	N	1302	3PE	O21-C21	2.10	1.40	1.34
45	k	101	LMT	O5B-C5B	2.10	1.49	1.44
51	N	1301	3PE	O31-C31	2.09	1.39	1.33
51	L	701	3PE	O31-C31	2.09	1.39	1.33
51	Y	802	3PE	O21-C21	2.09	1.40	1.34
47	P	502	PC1	O31-C3	-2.06	1.40	1.45
58	U	101	EHZ	O6-C20	-2.06	1.39	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	B	203	PC1	O31-C3	-2.05	1.40	1.45
51	H	402	3PE	O31-C3	-2.05	1.40	1.45
51	L	704	3PE	O21-C21	2.05	1.40	1.34
45	M	602	LMT	O5B-C5B	2.04	1.49	1.44
51	N	1302	3PE	O31-C3	-2.04	1.40	1.45
52	K	401	CDL	OA8-CA7	2.04	1.39	1.33
58	T	101	EHZ	C9-S1	2.04	1.81	1.76
51	N	1301	3PE	O21-C21	2.03	1.40	1.34
45	Y	801	LMT	O5'-C5'	2.03	1.49	1.44
45	Y	801	LMT	O5B-C5B	2.02	1.49	1.44
58	U	101	EHZ	C9-S1	2.00	1.81	1.76

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	P	501	NDP	PN-O3-PA	-6.86	109.27	132.83
58	U	101	EHZ	C8-C9-S1	6.70	121.92	113.63
58	T	101	EHZ	C8-C9-S1	6.44	121.59	113.63
45	A	302	LMT	C1-O1'-C1'	5.14	122.36	113.84
51	d	301	3PE	O21-C21-C22	4.64	121.50	111.50
52	J	701	CDL	OA6-CA5-C11	4.61	119.57	111.09
47	P	502	PC1	O21-C21-O22	-4.55	119.78	125.57
52	J	701	CDL	OB6-CB5-C51	4.51	121.22	111.50
51	L	704	3PE	O21-C21-C22	4.38	120.93	111.50
51	H	402	3PE	O21-C21-O22	-4.35	120.04	125.57
52	h	1001	CDL	OB6-CB5-C51	4.32	120.82	111.50
51	X	401	3PE	O21-C21-C22	4.27	120.71	111.50
47	M	605	PC1	O21-C21-C22	4.26	120.69	111.50
51	M	604	3PE	O21-C21-C22	4.24	120.65	111.50
47	B	203	PC1	O21-C21-C22	4.24	120.63	111.50
51	Y	802	3PE	O21-C21-C22	4.18	120.51	111.50
47	B	202	PC1	O21-C21-C22	4.14	120.43	111.50
52	a	101	CDL	OA6-CA5-C11	4.09	120.31	111.50
45	A	302	LMT	O1'-C1'-C2'	4.05	114.63	108.30
52	h	1001	CDL	OA6-CA5-C11	4.01	120.15	111.50
51	L	701	3PE	O21-C21-C22	4.01	120.15	111.50
53	N	1303	I49	C14-N02-C15	-4.00	118.54	125.21
52	L	703	CDL	OA6-CA5-C11	3.91	119.93	111.50
52	a	101	CDL	OB6-CB5-C51	3.84	119.78	111.50
52	K	401	CDL	OA6-CA5-C11	3.82	119.74	111.50
51	N	1301	3PE	O21-C21-C22	3.81	119.71	111.50
51	I	201	3PE	O21-C21-C22	3.66	119.39	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	K	401	CDL	OB6-CB5-C51	3.65	119.36	111.50
51	N	1302	3PE	O21-C21-C22	3.64	119.35	111.50
45	M	603	LMT	O5'-C5'-C4'	3.61	117.36	109.75
56	P	501	NDP	O2B-P2B-O1X	-3.60	95.51	109.39
51	H	401	3PE	O21-C21-C22	3.56	119.17	111.50
45	Z	301	LMT	C1B-C2B-C3B	3.50	117.28	110.00
52	L	703	CDL	OB6-CB5-C51	3.49	119.03	111.50
54	O	401	GTP	C3'-C2'-C1'	3.45	106.18	100.98
45	Z	301	LMT	O5B-C1B-C2B	3.44	117.64	110.35
51	M	601	3PE	O21-C21-C22	3.42	118.88	111.50
51	H	402	3PE	O31-C31-C32	3.37	122.47	111.91
53	N	1303	I49	N01-C14-N03	3.35	126.53	120.26
49	F	501	FMN	C4-N3-C2	-3.32	119.51	125.64
54	O	401	GTP	C2-N1-C6	-3.26	119.09	125.10
54	O	401	GTP	C5-C6-N1	3.17	119.56	113.95
51	H	401	3PE	O31-C31-C32	3.07	121.55	111.91
51	M	604	3PE	O31-C31-C32	3.07	121.54	111.91
45	Z	301	LMT	O5'-C5'-C4'	3.04	116.16	109.75
49	F	501	FMN	C4A-C10-N10	2.95	120.80	116.48
51	Y	802	3PE	O31-C31-C32	2.93	121.09	111.91
54	O	401	GTP	O2G-PG-O3B	2.90	114.36	104.64
51	N	1301	3PE	O31-C31-C32	2.89	120.97	111.91
45	Y	801	LMT	O5'-C5'-C4'	2.88	115.82	109.75
52	J	701	CDL	OA8-CA7-C31	2.88	120.94	111.91
45	h	1002	LMT	C1B-C2B-C3B	2.87	115.98	110.00
56	P	501	NDP	PA-O5B-C5B	-2.85	104.96	121.68
45	Y	801	LMT	C3B-C4B-C5B	2.85	115.32	110.24
47	B	203	PC1	O31-C31-C32	2.84	120.81	111.91
45	h	1002	LMT	C4B-C3B-C2B	2.83	115.77	110.82
52	h	1001	CDL	OB8-CB7-C71	2.80	120.71	111.91
58	T	101	EHZ	O2-C9-S1	-2.80	118.97	122.61
54	O	401	GTP	PB-O3B-PG	-2.80	123.22	132.83
58	U	101	EHZ	C10-S1-C9	2.78	110.53	101.87
58	T	101	EHZ	C10-S1-C9	2.78	110.52	101.87
58	T	101	EHZ	C13-C12-N1	2.76	121.07	116.42
51	X	401	3PE	O31-C31-C32	2.75	120.55	111.91
52	h	1001	CDL	OA8-CA7-C31	2.75	120.54	111.91
58	T	101	EHZ	C13-C14-N2	-2.74	106.37	111.90
52	K	401	CDL	OB8-CB7-C71	2.73	120.47	111.91
45	Z	301	LMT	C1'-O5'-C5'	2.72	119.03	113.69
47	B	202	PC1	O31-C31-C32	2.71	120.42	111.91
45	A	302	LMT	C1B-C2B-C3B	2.70	115.62	110.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	P	501	NDP	O4B-C4B-C3B	2.70	110.45	105.11
49	F	501	FMN	C4A-C4-N3	2.68	119.99	113.19
45	l	201	LMT	O5B-C5B-C4B	2.66	114.52	109.69
56	P	501	NDP	PN-O5D-C5D	-2.65	106.13	121.68
45	M	603	LMT	C3'-C4'-C5'	2.65	116.99	110.93
52	L	703	CDL	OB8-CB7-C71	2.64	120.20	111.91
53	N	1303	I49	N05-C15-N04	-2.63	112.15	120.26
47	M	605	PC1	O31-C31-C32	2.62	120.12	111.91
52	J	701	CDL	OB8-CB7-C71	2.60	120.06	111.91
51	L	704	3PE	O31-C31-C32	2.59	120.04	111.91
52	a	101	CDL	OB8-CB7-C71	2.56	119.95	111.91
56	P	501	NDP	O3X-P2B-O2X	2.55	117.40	107.64
51	L	701	3PE	O31-C31-C32	2.55	119.90	111.91
51	d	301	3PE	O31-C31-C32	2.54	119.89	111.91
54	O	401	GTP	PA-O3A-PB	-2.54	124.11	132.83
51	M	601	3PE	O31-C31-C32	2.54	119.87	111.91
49	F	501	FMN	O4-C4-C4A	-2.53	119.89	126.60
52	L	703	CDL	OA8-CA7-C31	2.53	119.85	111.91
58	U	101	EHZ	O2-C9-S1	-2.50	119.36	122.61
54	O	401	GTP	O3G-PG-O3B	2.49	113.00	104.64
56	P	501	NDP	O5D-PN-O1N	-2.48	99.39	109.07
51	N	1302	3PE	O31-C31-C32	2.47	119.67	111.91
54	O	401	GTP	C2'-C3'-C4'	2.44	107.39	102.64
51	I	201	3PE	O31-C31-C32	2.43	119.53	111.91
45	k	101	LMT	O5B-C5B-C4B	2.41	114.08	109.69
54	O	401	GTP	O2A-PA-O1A	-2.39	100.43	112.24
52	a	101	CDL	OA8-CA7-C31	2.35	119.29	111.91
45	l	201	LMT	C3B-C4B-C5B	2.33	114.39	110.24
56	P	501	NDP	O2N-PN-O1N	2.32	123.72	112.24
45	M	603	LMT	C6'-C5'-C4'	-2.29	106.67	113.33
52	K	401	CDL	OA8-CA7-C31	2.27	119.03	111.91
49	F	501	FMN	C4A-C10-N1	-2.26	119.48	124.73
56	P	501	NDP	C2A-N1A-C6A	-2.24	114.92	118.75
56	P	501	NDP	C5B-C4B-C3B	-2.22	106.86	115.18
49	F	501	FMN	C10-C4A-N5	-2.22	120.15	124.86
45	l	201	LMT	O5'-C1'-C2'	2.21	115.02	110.35
45	e	501	LMT	O5B-C5B-C4B	2.16	113.62	109.69
45	M	603	LMT	C1-O1'-C1'	2.15	117.41	113.84
45	Z	301	LMT	C1B-O1B-C4'	-2.12	112.72	117.96
45	l	201	LMT	C4B-C3B-C2B	2.11	114.50	110.82
45	Y	801	LMT	C1'-O5'-C5'	2.10	117.81	113.69
45	h	1002	LMT	C3B-C4B-C5B	2.10	113.98	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	d	301	3PE	O21-C21-O22	-2.10	118.64	123.70
45	Y	801	LMT	O5B-C5B-C4B	2.09	113.50	109.69
54	O	401	GTP	O2B-PB-O1B	-2.09	101.90	112.24
45	h	1002	LMT	C1B-O5B-C5B	-2.08	109.61	113.69
52	a	101	CDL	CA6-CA4-CA3	-2.07	106.88	111.79
45	A	301	LMT	C1B-O1B-C4'	-2.07	112.84	117.96
56	P	501	NDP	O7N-C7N-C3N	2.04	124.74	120.90
45	e	501	LMT	O5'-C5'-C4'	2.03	114.04	109.75
58	T	101	EHZ	C19-C17-C16	2.01	112.31	108.82
45	e	501	LMT	C1B-C2B-C3B	2.01	114.18	110.00
54	O	401	GTP	O6-C6-C5	-2.00	120.46	124.37

There are no chirality outliers.

All (621) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	302	LMT	C2'-C1'-O1'-C1
45	L	702	LMT	C2'-C1'-O1'-C1
45	L	702	LMT	C2-C1-O1'-C1'
45	M	603	LMT	O5'-C1'-O1'-C1
45	Z	301	LMT	O5'-C1'-O1'-C1
45	Z	301	LMT	C2-C1-O1'-C1'
45	e	501	LMT	C2'-C1'-O1'-C1
45	e	501	LMT	O5'-C1'-O1'-C1
45	l	201	LMT	C2'-C1'-O1'-C1
45	l	201	LMT	O5'-C1'-O1'-C1
47	B	203	PC1	C11-O13-P-O14
47	M	605	PC1	C11-O13-P-O12
47	M	605	PC1	C11-O13-P-O14
47	M	605	PC1	C22-C21-O21-C2
47	P	502	PC1	C11-O13-P-O12
47	P	502	PC1	C11-O13-P-O14
47	P	502	PC1	C11-O13-P-O11
47	P	502	PC1	C1-O11-P-O13
51	H	401	3PE	O13-C11-C12-N
51	H	402	3PE	O13-C11-C12-N
51	H	402	3PE	C1-C2-O21-C21
51	H	402	3PE	O22-C21-O21-C2
51	I	201	3PE	O11-C1-C2-O21
51	L	701	3PE	C1-O11-P-O14
51	L	701	3PE	C11-O13-P-O14
51	L	701	3PE	O13-C11-C12-N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
51	L	701	3PE	C22-C21-O21-C2
51	L	704	3PE	C1-O11-P-O12
51	L	704	3PE	C11-O13-P-O14
51	M	601	3PE	O13-C11-C12-N
51	M	604	3PE	O13-C11-C12-N
51	M	604	3PE	O32-C31-O31-C3
51	M	604	3PE	C32-C31-O31-C3
51	N	1301	3PE	C1-O11-P-O14
51	N	1301	3PE	O13-C11-C12-N
51	N	1301	3PE	O21-C2-C3-O31
51	N	1302	3PE	O13-C11-C12-N
51	X	401	3PE	C1-O11-P-O12
51	X	401	3PE	C1-O11-P-O14
51	X	401	3PE	C12-C11-O13-P
51	X	401	3PE	C22-C21-O21-C2
51	Y	802	3PE	C1-O11-P-O12
51	Y	802	3PE	C1-O11-P-O14
51	Y	802	3PE	C11-O13-P-O14
51	Y	802	3PE	C22-C21-O21-C2
51	d	301	3PE	O22-C21-O21-C2
52	J	701	CDL	CA2-OA2-PA1-OA3
52	J	701	CDL	OB7-CB5-OB6-CB4
52	J	701	CDL	C51-CB5-OB6-CB4
52	K	401	CDL	CA2-C1-CB2-OB2
52	K	401	CDL	CA3-OA5-PA1-OA3
52	K	401	CDL	CB2-OB2-PB2-OB3
52	K	401	CDL	CB2-OB2-PB2-OB4
52	L	703	CDL	CA2-OA2-PA1-OA3
52	a	101	CDL	CA2-OA2-PA1-OA3
52	a	101	CDL	CA3-OA5-PA1-OA4
52	a	101	CDL	CB2-OB2-PB2-OB3
52	a	101	CDL	CB2-OB2-PB2-OB4
52	a	101	CDL	CB2-OB2-PB2-OB5
52	h	1001	CDL	CA2-OA2-PA1-OA5
52	h	1001	CDL	CB3-OB5-PB2-OB3
52	h	1001	CDL	C51-CB5-OB6-CB4
53	N	1303	I49	N01-C14-N02-C15
53	N	1303	I49	N03-C14-N02-C15
54	O	401	GTP	PB-O3B-PG-O2G
54	O	401	GTP	C5'-O5'-PA-O3A
54	O	401	GTP	C5'-O5'-PA-O1A
54	O	401	GTP	C5'-O5'-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
56	P	501	NDP	C2B-O2B-P2B-O3X
58	T	101	EHZ	C11-C10-S1-C9
58	T	101	EHZ	N2-C15-C16-O5
58	T	101	EHZ	C16-C17-C20-O6
58	T	101	EHZ	O2-C9-S1-C10
58	T	101	EHZ	C8-C9-S1-C10
58	U	101	EHZ	C5-C6-C7-O1
58	U	101	EHZ	C5-C6-C7-C8
58	U	101	EHZ	O2-C9-S1-C10
58	U	101	EHZ	C8-C9-S1-C10
52	J	701	CDL	C11-CA5-OA6-CA4
51	H	402	3PE	O32-C31-O31-C3
51	H	402	3PE	C32-C31-O31-C3
51	H	401	3PE	O32-C31-O31-C3
45	k	101	LMT	O5B-C1B-O1B-C4'
45	A	302	LMT	C5'-C4'-O1B-C1B
45	e	501	LMT	O5B-C1B-O1B-C4'
47	M	605	PC1	O22-C21-O21-C2
51	X	401	3PE	O22-C21-O21-C2
51	Y	802	3PE	O22-C21-O21-C2
52	h	1001	CDL	OB7-CB5-OB6-CB4
51	H	401	3PE	C32-C31-O31-C3
51	N	1301	3PE	C32-C31-O31-C3
45	M	602	LMT	O5'-C5'-C6'-O6'
51	d	301	3PE	C22-C21-O21-C2
52	L	703	CDL	OA9-CA7-OA8-CA6
47	P	502	PC1	C32-C31-O31-C3
52	K	401	CDL	C71-CB7-OB8-CB6
52	a	101	CDL	C31-CA7-OA8-CA6
45	A	301	LMT	O5'-C5'-C6'-O6'
45	h	1002	LMT	O5'-C5'-C6'-O6'
45	k	101	LMT	C2B-C1B-O1B-C4'
52	J	701	CDL	OA7-CA5-OA6-CA4
51	L	701	3PE	O22-C21-O21-C2
51	N	1301	3PE	O32-C31-O31-C3
51	Y	802	3PE	O32-C31-O31-C3
52	J	701	CDL	CA4-CA6-OA8-CA7
45	M	602	LMT	O5B-C5B-C6B-O6B
45	Y	801	LMT	O5B-C5B-C6B-O6B
45	e	501	LMT	O5B-C5B-C6B-O6B
52	K	401	CDL	O1-C1-CB2-OB2
51	Y	802	3PE	C32-C31-O31-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	J	701	CDL	C31-CA7-OA8-CA6
52	L	703	CDL	C31-CA7-OA8-CA6
52	a	101	CDL	OA9-CA7-OA8-CA6
45	e	501	LMT	C3'-C4'-O1B-C1B
45	e	501	LMT	O5'-C5'-C6'-O6'
45	h	1002	LMT	C4'-C5'-C6'-O6'
52	J	701	CDL	OA9-CA7-OA8-CA6
45	A	301	LMT	C4'-C5'-C6'-O6'
45	M	602	LMT	C4'-C5'-C6'-O6'
45	Y	801	LMT	C4'-C5'-C6'-O6'
45	A	302	LMT	C4'-C5'-C6'-O6'
45	A	302	LMT	O5'-C5'-C6'-O6'
52	K	401	CDL	OB9-CB7-OB8-CB6
45	L	702	LMT	O5'-C1'-O1'-C1
45	Y	801	LMT	O5'-C5'-C6'-O6'
52	a	101	CDL	C11-CA5-OA6-CA4
45	M	603	LMT	C4B-C5B-C6B-O6B
47	B	203	PC1	C32-C31-O31-C3
47	M	605	PC1	C32-C31-O31-C3
51	L	701	3PE	C32-C31-O31-C3
52	L	703	CDL	CB4-CB6-OB8-CB7
51	N	1301	3PE	C31-C32-C33-C34
45	M	602	LMT	C4B-C5B-C6B-O6B
45	A	301	LMT	O5B-C5B-C6B-O6B
52	J	701	CDL	O1-C1-CA2-OA2
52	h	1001	CDL	O1-C1-CB2-OB2
45	M	603	LMT	C2'-C1'-O1'-C1
51	M	604	3PE	C22-C21-O21-C2
47	M	605	PC1	O32-C31-O31-C3
51	L	701	3PE	O32-C31-O31-C3
52	K	401	CDL	CA5-C11-C12-C13
47	B	202	PC1	C31-C32-C33-C34
51	L	704	3PE	C21-C22-C23-C24
51	d	301	3PE	C31-C32-C33-C34
52	L	703	CDL	CA5-C11-C12-C13
47	P	502	PC1	O32-C31-O31-C3
51	M	604	3PE	O22-C21-O21-C2
47	B	203	PC1	C21-C22-C23-C24
52	L	703	CDL	CB5-C51-C52-C53
53	N	1303	I49	C07-C06-C08-N01
47	B	203	PC1	O32-C31-O31-C3
45	A	301	LMT	O5'-C1'-O1'-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	L	702	LMT	O5B-C5B-C6B-O6B
52	a	101	CDL	OA7-CA5-OA6-CA4
45	e	501	LMT	C4B-C5B-C6B-O6B
45	Y	801	LMT	C4B-C5B-C6B-O6B
47	M	605	PC1	C11-O13-P-O11
51	H	402	3PE	C11-O13-P-O11
51	I	201	3PE	C1-O11-P-O13
51	L	704	3PE	C1-O11-P-O13
51	M	601	3PE	C11-O13-P-O11
51	M	604	3PE	C1-O11-P-O13
51	X	401	3PE	C1-O11-P-O13
51	Y	802	3PE	C1-O11-P-O13
52	K	401	CDL	CB2-OB2-PB2-OB5
52	L	703	CDL	CB3-OB5-PB2-OB2
52	a	101	CDL	CA2-OA2-PA1-OA5
52	a	101	CDL	CA3-OA5-PA1-OA2
52	h	1001	CDL	CA3-OA5-PA1-OA2
52	h	1001	CDL	CB2-OB2-PB2-OB5
52	h	1001	CDL	CB3-OB5-PB2-OB2
52	h	1001	CDL	C31-CA7-OA8-CA6
52	K	401	CDL	C51-CB5-OB6-CB4
45	M	603	LMT	O5B-C5B-C6B-O6B
45	L	702	LMT	C5-C6-C7-C8
45	e	501	LMT	C5'-C4'-O1B-C1B
47	M	605	PC1	C2D-C2E-C2F-C2G
58	T	101	EHZ	C18-C17-C20-O6
47	M	605	PC1	C24-C25-C26-C27
51	L	704	3PE	C34-C35-C36-C37
51	M	604	3PE	C29-C2A-C2B-C2C
51	X	401	3PE	C36-C37-C38-C39
52	h	1001	CDL	C22-C23-C24-C25
52	K	401	CDL	OB7-CB5-OB6-CB4
51	I	201	3PE	C2B-C2C-C2D-C2E
51	I	201	3PE	C33-C34-C35-C36
51	M	604	3PE	C3E-C3F-C3G-C3H
51	N	1301	3PE	C2D-C2E-C2F-C2G
52	L	703	CDL	C38-C39-C40-C41
52	h	1001	CDL	C72-C73-C74-C75
51	X	401	3PE	C23-C24-C25-C26
51	X	401	3PE	C28-C29-C2A-C2B
52	K	401	CDL	CB7-C71-C72-C73
45	Y	801	LMT	C2'-C1'-O1'-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	J	701	CDL	C76-C77-C78-C79
51	M	601	3PE	C33-C34-C35-C36
51	X	401	3PE	C38-C39-C3A-C3B
47	B	203	PC1	C23-C24-C25-C26
51	L	704	3PE	C36-C37-C38-C39
52	h	1001	CDL	C14-C15-C16-C17
51	d	301	3PE	C27-C28-C29-C2A
52	L	703	CDL	OA7-CA5-OA6-CA4
52	L	703	CDL	C11-CA5-OA6-CA4
45	Z	301	LMT	C2-C3-C4-C5
51	L	701	3PE	C28-C29-C2A-C2B
51	L	701	3PE	C2D-C2E-C2F-C2G
52	J	701	CDL	C73-C74-C75-C76
52	a	101	CDL	C51-C52-C53-C54
45	A	302	LMT	C11-C10-C9-C8
47	B	203	PC1	C32-C33-C34-C35
47	M	605	PC1	C2B-C2C-C2D-C2E
51	L	704	3PE	C3C-C3D-C3E-C3F
51	M	601	3PE	C37-C38-C39-C3A
51	X	401	3PE	C32-C33-C34-C35
52	K	401	CDL	C11-C12-C13-C14
52	a	101	CDL	C58-C59-C60-C61
58	U	101	EHZ	C21-C1-C2-C3
59	o	201	MYR	C2-C3-C4-C5
45	A	302	LMT	O5B-C5B-C6B-O6B
45	Y	801	LMT	O5'-C1'-O1'-C1
45	A	302	LMT	C7-C8-C9-C10
51	N	1302	3PE	C32-C33-C34-C35
51	X	401	3PE	O13-C11-C12-N
51	L	701	3PE	C33-C34-C35-C36
52	a	101	CDL	C11-C12-C13-C14
51	M	601	3PE	C31-C32-C33-C34
51	M	604	3PE	C34-C35-C36-C37
51	X	401	3PE	C3C-C3D-C3E-C3F
45	h	1002	LMT	C2-C1-O1'-C1'
45	l	201	LMT	C2-C1-O1'-C1'
51	N	1301	3PE	C35-C36-C37-C38
51	d	301	3PE	C32-C33-C34-C35
51	d	301	3PE	C24-C25-C26-C27
45	A	302	LMT	C4B-C5B-C6B-O6B
52	h	1001	CDL	OA9-CA7-OA8-CA6
51	M	601	3PE	C38-C39-C3A-C3B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	L	703	CDL	CA3-CA4-CA6-OA8
45	M	603	LMT	O1'-C1-C2-C3
52	K	401	CDL	C40-C41-C42-C43
51	I	201	3PE	C3B-C3C-C3D-C3E
51	N	1301	3PE	C22-C21-O21-C2
51	M	604	3PE	C32-C33-C34-C35
51	M	604	3PE	C2B-C2C-C2D-C2E
52	J	701	CDL	C78-C79-C80-C81
45	M	603	LMT	C3'-C4'-O1B-C1B
45	Z	301	LMT	C1-C2-C3-C4
51	N	1302	3PE	C36-C37-C38-C39
47	B	203	PC1	C31-C32-C33-C34
45	M	603	LMT	C5'-C4'-O1B-C1B
51	d	301	3PE	C26-C27-C28-C29
52	J	701	CDL	C77-C78-C79-C80
51	M	601	3PE	C35-C36-C37-C38
52	h	1001	CDL	C13-C14-C15-C16
47	B	203	PC1	C22-C21-O21-C2
51	N	1302	3PE	C22-C21-O21-C2
51	d	301	3PE	C23-C24-C25-C26
52	K	401	CDL	C36-C37-C38-C39
47	M	605	PC1	C29-C2A-C2B-C2C
51	d	301	3PE	C3E-C3F-C3G-C3H
52	J	701	CDL	C72-C73-C74-C75
51	L	704	3PE	O22-C21-O21-C2
51	d	301	3PE	C35-C36-C37-C38
45	A	301	LMT	C4B-C5B-C6B-O6B
51	Y	802	3PE	C37-C38-C39-C3A
51	M	604	3PE	C2D-C2E-C2F-C2G
52	a	101	CDL	C39-C40-C41-C42
51	M	604	3PE	C21-C22-C23-C24
47	M	605	PC1	C26-C27-C28-C29
51	d	301	3PE	C39-C3A-C3B-C3C
58	U	101	EHZ	C2-C3-C4-C5
47	M	605	PC1	C27-C28-C29-C2A
51	L	701	3PE	C23-C24-C25-C26
45	M	603	LMT	C2-C3-C4-C5
51	L	704	3PE	C22-C21-O21-C2
52	K	401	CDL	C11-CA5-OA6-CA4
52	h	1001	CDL	C11-CA5-OA6-CA4
52	a	101	CDL	O1-C1-CB2-OB2
51	N	1301	3PE	O22-C21-O21-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	K	401	CDL	OA7-CA5-OA6-CA4
45	M	602	LMT	C2'-C1'-O1'-C1
52	L	703	CDL	OA6-CA4-CA6-OA8
51	L	704	3PE	C38-C39-C3A-C3B
58	U	101	EHZ	C21-C22-C23-C24
47	B	203	PC1	O22-C21-O21-C2
51	N	1302	3PE	O22-C21-O21-C2
52	h	1001	CDL	OA7-CA5-OA6-CA4
52	J	701	CDL	C74-C75-C76-C77
51	L	701	3PE	C1-O11-P-O13
51	L	701	3PE	C11-O13-P-O11
51	L	704	3PE	C11-O13-P-O11
51	N	1301	3PE	C1-O11-P-O13
51	Y	802	3PE	C11-O13-P-O11
52	J	701	CDL	CA2-OA2-PA1-OA5
52	K	401	CDL	CA3-OA5-PA1-OA2
51	N	1302	3PE	C23-C24-C25-C26
45	L	702	LMT	O5'-C5'-C6'-O6'
45	Z	301	LMT	O5'-C5'-C6'-O6'
52	L	703	CDL	C71-CB7-OB8-CB6
51	I	201	3PE	O11-C1-C2-C3
51	I	201	3PE	C21-C22-C23-C24
45	A	302	LMT	O1'-C1-C2-C3
52	K	401	CDL	C16-C17-C18-C19
52	L	703	CDL	C31-C32-C33-C34
45	Z	301	LMT	C5-C6-C7-C8
51	L	701	3PE	C3B-C3C-C3D-C3E
51	N	1302	3PE	C35-C36-C37-C38
51	L	704	3PE	C1-C2-C3-O31
51	N	1301	3PE	C36-C37-C38-C39
52	a	101	CDL	CA3-CA4-CA6-OA8
45	M	602	LMT	C9-C10-C11-C12
51	M	601	3PE	C22-C23-C24-C25
52	L	703	CDL	C13-C14-C15-C16
51	N	1301	3PE	C3D-C3E-C3F-C3G
58	T	101	EHZ	O4-C15-C16-O5
47	M	605	PC1	C39-C3A-C3B-C3C
51	L	701	3PE	C2F-C2G-C2H-C2I
58	T	101	EHZ	C21-C22-C23-C24
51	L	704	3PE	C33-C34-C35-C36
51	M	601	3PE	C26-C27-C28-C29
51	N	1301	3PE	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
51	Y	802	3PE	C3B-C3C-C3D-C3E
52	h	1001	CDL	C52-C53-C54-C55
58	T	101	EHZ	C2-C1-C21-C22
47	B	202	PC1	C35-C36-C37-C38
58	T	101	EHZ	C19-C17-C20-O6
51	H	401	3PE	C31-C32-C33-C34
51	N	1301	3PE	C26-C27-C28-C29
47	M	605	PC1	C1-C2-O21-C21
47	M	605	PC1	C37-C38-C39-C3A
47	M	605	PC1	C23-C24-C25-C26
51	I	201	3PE	C32-C31-O31-C3
51	X	401	3PE	C3F-C3G-C3H-C3I
52	a	101	CDL	OA6-CA4-CA6-OA8
52	a	101	CDL	C56-C57-C58-C59
45	L	702	LMT	C6-C7-C8-C9
52	L	703	CDL	C54-C55-C56-C57
56	P	501	NDP	PN-O3-PA-O1A
51	H	401	3PE	C23-C24-C25-C26
47	B	203	PC1	C36-C37-C38-C39
45	M	602	LMT	C6-C7-C8-C9
51	M	604	3PE	C2F-C2G-C2H-C2I
52	h	1001	CDL	C11-C12-C13-C14
52	a	101	CDL	CA2-C1-CB2-OB2
52	L	703	CDL	C51-CB5-OB6-CB4
45	h	1002	LMT	C4B-C5B-C6B-O6B
51	X	401	3PE	C3E-C3F-C3G-C3H
51	L	701	3PE	C29-C2A-C2B-C2C
52	L	703	CDL	C34-C35-C36-C37
52	K	401	CDL	OB5-CB3-CB4-CB6
51	I	201	3PE	O13-C11-C12-N
47	B	203	PC1	C24-C25-C26-C27
51	M	601	3PE	C34-C35-C36-C37
52	h	1001	CDL	CB7-C71-C72-C73
52	K	401	CDL	C31-CA7-OA8-CA6
52	a	101	CDL	C1-CB2-OB2-PB2
52	L	703	CDL	OB9-CB7-OB8-CB6
51	H	402	3PE	C33-C34-C35-C36
51	M	604	3PE	C23-C24-C25-C26
45	A	302	LMT	C2-C1-O1'-C1'
45	M	602	LMT	C2-C1-O1'-C1'
45	Y	801	LMT	C2-C1-O1'-C1'
45	k	101	LMT	C2-C1-O1'-C1'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
51	M	601	3PE	C32-C31-O31-C3
52	h	1001	CDL	C71-CB7-OB8-CB6
52	L	703	CDL	C71-C72-C73-C74
52	h	1001	CDL	C16-C17-C18-C19
47	B	202	PC1	C1-C2-C3-O31
47	M	605	PC1	C1-C2-C3-O31
47	P	502	PC1	C1-C2-C3-O31
51	H	401	3PE	C1-C2-C3-O31
51	H	402	3PE	C1-C2-C3-O31
51	M	604	3PE	C1-C2-C3-O31
52	J	701	CDL	CA3-CA4-CA6-OA8
52	J	701	CDL	CB3-CB4-CB6-OB8
52	L	703	CDL	CB3-CB4-CB6-OB8
51	X	401	3PE	C31-C32-C33-C34
51	I	201	3PE	O32-C31-O31-C3
51	L	701	3PE	C25-C26-C27-C28
47	B	202	PC1	C33-C34-C35-C36
51	X	401	3PE	C11-O13-P-O11
45	h	1002	LMT	C7-C8-C9-C10
51	N	1302	3PE	C21-C22-C23-C24
52	K	401	CDL	C41-C42-C43-C44
47	P	502	PC1	O21-C2-C3-O31
51	H	401	3PE	O21-C2-C3-O31
51	H	402	3PE	O21-C2-C3-O31
51	H	402	3PE	C3B-C3C-C3D-C3E
51	Y	802	3PE	C32-C33-C34-C35
52	L	703	CDL	OB7-CB5-OB6-CB4
51	Y	802	3PE	C34-C35-C36-C37
51	N	1301	3PE	C3B-C3C-C3D-C3E
52	K	401	CDL	C1-CB2-OB2-PB2
52	K	401	CDL	CB4-CB3-OB5-PB2
52	L	703	CDL	C58-C59-C60-C61
45	e	501	LMT	C4'-C5'-C6'-O6'
51	L	701	3PE	C21-C22-C23-C24
47	B	202	PC1	C23-C24-C25-C26
52	L	703	CDL	C35-C36-C37-C38
45	l	201	LMT	O1'-C1-C2-C3
51	I	201	3PE	C3C-C3D-C3E-C3F
51	M	601	3PE	O11-C1-C2-C3
52	h	1001	CDL	OB5-CB3-CB4-CB6
45	A	302	LMT	C3-C4-C5-C6
51	L	704	3PE	C3A-C3B-C3C-C3D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
51	H	402	3PE	C31-C32-C33-C34
51	M	604	3PE	O21-C21-C22-C23
51	d	301	3PE	C1-C2-O21-C21
51	N	1301	3PE	C3A-C3B-C3C-C3D
45	A	302	LMT	O5'-C1'-O1'-C1
47	B	203	PC1	C1-C2-C3-O31
51	H	402	3PE	C2-C1-O11-P
51	N	1301	3PE	C1-C2-C3-O31
51	Y	802	3PE	C1-C2-C3-O31
51	L	701	3PE	C34-C35-C36-C37
51	M	601	3PE	O11-C1-C2-O21
51	I	201	3PE	C38-C39-C3A-C3B
51	M	601	3PE	O32-C31-O31-C3
51	H	402	3PE	C3C-C3D-C3E-C3F
47	B	202	PC1	O21-C2-C3-O31
51	N	1302	3PE	O21-C2-C3-O31
51	Y	802	3PE	O21-C2-C3-O31
52	J	701	CDL	OA6-CA4-CA6-OA8
52	J	701	CDL	OB6-CB4-CB6-OB8
52	L	703	CDL	OB6-CB4-CB6-OB8
52	h	1001	CDL	OA6-CA4-CA6-OA8
52	h	1001	CDL	OB9-CB7-OB8-CB6
52	K	401	CDL	OA9-CA7-OA8-CA6
51	I	201	3PE	C2E-C2F-C2G-C2H
52	L	703	CDL	C11-C12-C13-C14
51	H	401	3PE	C3D-C3E-C3F-C3G
51	M	604	3PE	C38-C39-C3A-C3B
47	B	203	PC1	C11-O13-P-O11
51	M	601	3PE	C1-O11-P-O13
52	L	703	CDL	CA2-OA2-PA1-OA5
52	L	703	CDL	C52-C53-C54-C55
47	M	605	PC1	C2-C1-O11-P
51	M	604	3PE	C2-C1-O11-P
52	J	701	CDL	C71-C72-C73-C74
51	H	402	3PE	C11-O13-P-O12
51	I	201	3PE	C1-O11-P-O12
51	I	201	3PE	C1-O11-P-O14
51	I	201	3PE	C11-O13-P-O12
51	L	701	3PE	C1-O11-P-O12
51	L	704	3PE	C1-O11-P-O14
51	L	704	3PE	C11-O13-P-O12
51	M	601	3PE	C11-O13-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
51	M	604	3PE	C1-O11-P-O12
51	M	604	3PE	C1-O11-P-O14
51	M	604	3PE	C11-O13-P-O12
51	N	1301	3PE	C1-O11-P-O12
51	Y	802	3PE	C11-O13-P-O12
52	J	701	CDL	CA2-OA2-PA1-OA4
52	L	703	CDL	CB3-OB5-PB2-OB4
52	a	101	CDL	CA3-OA5-PA1-OA3
52	h	1001	CDL	CA3-OA5-PA1-OA3
52	h	1001	CDL	CB2-OB2-PB2-OB3
52	h	1001	CDL	CB2-OB2-PB2-OB4
52	h	1001	CDL	CB3-OB5-PB2-OB4
51	L	701	3PE	O11-C1-C2-C3
51	M	604	3PE	C28-C29-C2A-C2B
51	M	601	3PE	C12-C11-O13-P
51	N	1301	3PE	C12-C11-O13-P
51	N	1302	3PE	C12-C11-O13-P
51	N	1302	3PE	C33-C34-C35-C36
52	a	101	CDL	C57-C58-C59-C60
51	L	701	3PE	O11-C1-C2-O21
52	K	401	CDL	OB5-CB3-CB4-OB6
52	h	1001	CDL	OB5-CB3-CB4-OB6
45	M	602	LMT	O1'-C1-C2-C3
51	d	301	3PE	C25-C26-C27-C28
52	K	401	CDL	C15-C16-C17-C18
51	d	301	3PE	C1-C2-C3-O31
52	h	1001	CDL	CA3-CA4-CA6-OA8
59	o	201	MYR	C1-C2-C3-C4
47	B	203	PC1	O21-C2-C3-O31
51	M	604	3PE	O21-C2-C3-O31
51	d	301	3PE	O21-C2-C3-O31
52	a	101	CDL	OB6-CB4-CB6-OB8
47	M	605	PC1	C35-C36-C37-C38
51	d	301	3PE	C3B-C3C-C3D-C3E
52	a	101	CDL	C33-C34-C35-C36
52	K	401	CDL	C71-C72-C73-C74
52	K	401	CDL	CB5-C51-C52-C53
52	J	701	CDL	CA3-CA4-OA6-CA5
52	J	701	CDL	CB2-C1-CA2-OA2
52	h	1001	CDL	CA2-C1-CB2-OB2
51	I	201	3PE	C29-C2A-C2B-C2C
52	a	101	CDL	CA4-CA3-OA5-PA1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
52	L	703	CDL	C53-C54-C55-C56
51	L	704	3PE	O21-C2-C3-O31
51	I	201	3PE	C11-O13-P-O11
51	d	301	3PE	C1-O11-P-O13
51	d	301	3PE	C11-O13-P-O11
52	K	401	CDL	CB3-OB5-PB2-OB2
47	M	605	PC1	C34-C35-C36-C37
52	K	401	CDL	C31-C32-C33-C34
52	J	701	CDL	C72-C71-CB7-OB8
56	P	501	NDP	O4D-C1D-N1N-C6N
51	I	201	3PE	C39-C3A-C3B-C3C
56	P	501	NDP	PN-O3-PA-O2A
51	I	201	3PE	C3A-C3B-C3C-C3D
51	N	1302	3PE	C2-C1-O11-P
54	O	401	GTP	C4'-C5'-O5'-PA
51	N	1302	3PE	C31-C32-C33-C34
45	L	702	LMT	C4B-C5B-C6B-O6B
45	A	301	LMT	C4-C5-C6-C7
58	T	101	EHZ	C12-C13-C14-N2
52	a	101	CDL	C13-C14-C15-C16
51	H	401	3PE	C37-C38-C39-C3A
45	k	101	LMT	C4-C5-C6-C7
52	a	101	CDL	CB3-CB4-CB6-OB8
52	a	101	CDL	C32-C33-C34-C35
51	L	704	3PE	C27-C28-C29-C2A
51	M	604	3PE	C1-C2-O21-C21
51	L	701	3PE	C3A-C3B-C3C-C3D
45	e	501	LMT	C7-C8-C9-C10
52	a	101	CDL	C38-C39-C40-C41
51	M	604	3PE	C11-O13-P-O11
51	H	402	3PE	C32-C33-C34-C35
52	L	703	CDL	CA7-C31-C32-C33
51	H	401	3PE	O11-C1-C2-C3
52	J	701	CDL	CA7-C31-C32-C33
51	H	402	3PE	C3E-C3F-C3G-C3H
51	M	604	3PE	C2E-C2F-C2G-C2H
52	L	703	CDL	C55-C56-C57-C58
52	a	101	CDL	C35-C36-C37-C38
52	a	101	CDL	CA5-C11-C12-C13
45	e	501	LMT	C4-C5-C6-C7
52	J	701	CDL	C75-C76-C77-C78
45	Y	801	LMT	C5'-C4'-O1B-C1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
51	L	701	3PE	C2E-C2F-C2G-C2H
45	A	301	LMT	C2-C3-C4-C5
47	M	605	PC1	C2F-C2G-C2H-C2I
59	o	201	MYR	C3-C4-C5-C6
56	P	501	NDP	O4D-C4D-C5D-O5D
51	N	1301	3PE	C27-C28-C29-C2A
51	L	701	3PE	C36-C37-C38-C39
51	H	401	3PE	O11-C1-C2-O21
51	N	1302	3PE	C27-C28-C29-C2A
52	K	401	CDL	C14-C15-C16-C17
51	N	1302	3PE	O11-C1-C2-C3
45	Y	801	LMT	C4-C5-C6-C7
58	T	101	EHZ	C3-C4-C5-C6
51	I	201	3PE	C22-C23-C24-C25
52	K	401	CDL	CB2-C1-CA2-OA2
52	h	1001	CDL	C31-C32-C33-C34
51	N	1302	3PE	O31-C31-C32-C33
47	B	202	PC1	C32-C31-O31-C3
51	X	401	3PE	O21-C21-C22-C23
51	X	401	3PE	C21-C22-C23-C24
51	H	402	3PE	C35-C36-C37-C38
45	Z	301	LMT	C4B-C5B-C6B-O6B
47	B	202	PC1	O32-C31-O31-C3
51	I	201	3PE	C34-C35-C36-C37
52	K	401	CDL	C53-C54-C55-C56
45	h	1002	LMT	C4-C5-C6-C7
51	I	201	3PE	C2F-C2G-C2H-C2I
51	N	1302	3PE	C29-C2A-C2B-C2C
45	h	1002	LMT	C11-C10-C9-C8
52	a	101	CDL	C34-C35-C36-C37
51	N	1302	3PE	C1-C2-C3-O31
51	N	1302	3PE	O11-C1-C2-O21
51	H	401	3PE	O21-C21-C22-C23
47	B	202	PC1	C22-C23-C24-C25
51	L	701	3PE	C3C-C3D-C3E-C3F
52	J	701	CDL	C33-C34-C35-C36
52	L	703	CDL	C12-C11-CA5-OA6
45	L	702	LMT	C1-C2-C3-C4
45	Y	801	LMT	C3'-C4'-O1B-C1B
47	B	202	PC1	O31-C31-C32-C33
51	M	601	3PE	O21-C2-C3-O31
52	K	401	CDL	OB6-CB4-CB6-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
51	M	601	3PE	C21-C22-C23-C24
45	A	302	LMT	C3'-C4'-O1B-C1B
47	B	203	PC1	O21-C21-C22-C23
52	K	401	CDL	C33-C34-C35-C36
52	h	1001	CDL	C12-C13-C14-C15
45	h	1002	LMT	O5B-C5B-C6B-O6B
56	P	501	NDP	C2D-C1D-N1N-C6N
51	H	401	3PE	C32-C33-C34-C35
51	I	201	3PE	C26-C27-C28-C29
56	P	501	NDP	O4B-C4B-C5B-O5B
51	M	604	3PE	C31-C32-C33-C34
51	H	401	3PE	O22-C21-C22-C23
54	O	401	GTP	PG-O3B-PB-O2B
51	N	1302	3PE	C3A-C3B-C3C-C3D
51	M	604	3PE	C37-C38-C39-C3A
51	X	401	3PE	O22-C21-C22-C23
52	L	703	CDL	C12-C11-CA5-OA7
47	B	202	PC1	C34-C35-C36-C37
52	a	101	CDL	C52-C53-C54-C55
47	B	203	PC1	C2-C3-O31-C31
47	B	202	PC1	C11-O13-P-O14
51	M	601	3PE	C1-O11-P-O14
51	X	401	3PE	C11-O13-P-O12
52	K	401	CDL	CA2-OA2-PA1-OA3
52	K	401	CDL	CB3-OB5-PB2-OB3
52	L	703	CDL	CB3-OB5-PB2-OB3
58	T	101	EHZ	C6-C7-C8-C9
47	B	202	PC1	O32-C31-C32-C33
47	M	605	PC1	C33-C34-C35-C36
52	h	1001	CDL	C71-C72-C73-C74
47	B	202	PC1	C12-C11-O13-P
51	H	401	3PE	C12-C11-O13-P
51	H	402	3PE	C12-C11-O13-P
58	T	101	EHZ	O4-C15-C16-C17
47	B	203	PC1	O22-C21-C22-C23
51	H	401	3PE	C36-C37-C38-C39
51	I	201	3PE	C24-C25-C26-C27
51	L	704	3PE	C28-C29-C2A-C2B
47	B	203	PC1	O31-C31-C32-C33
51	H	402	3PE	O31-C31-C32-C33
51	X	401	3PE	O31-C31-C32-C33
47	B	203	PC1	C2-C1-O11-P

Continued on next page...

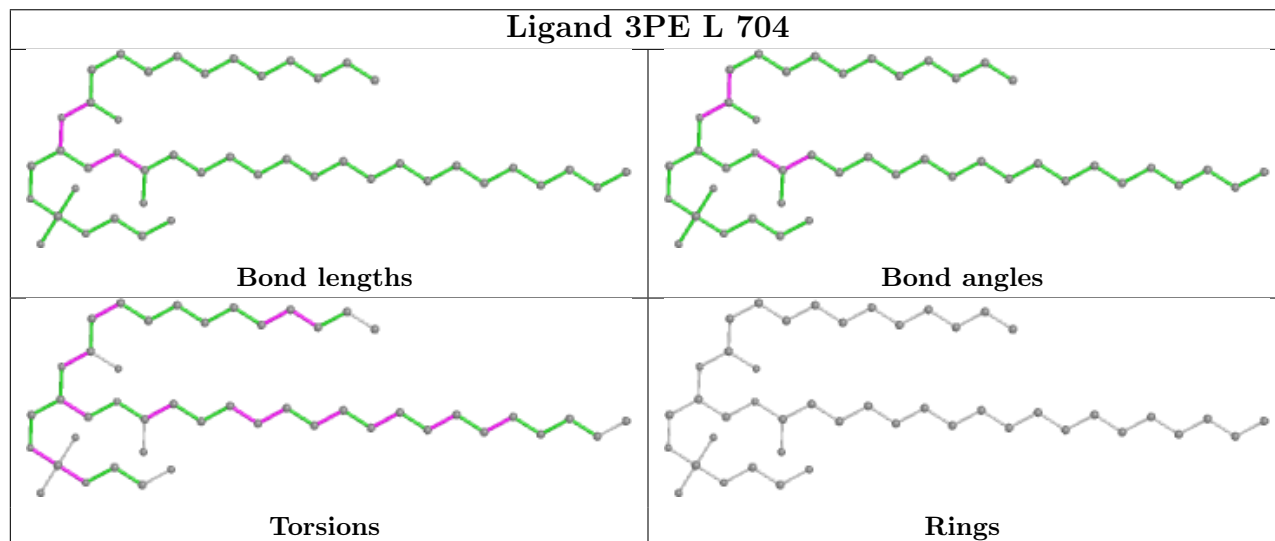
Continued from previous page...

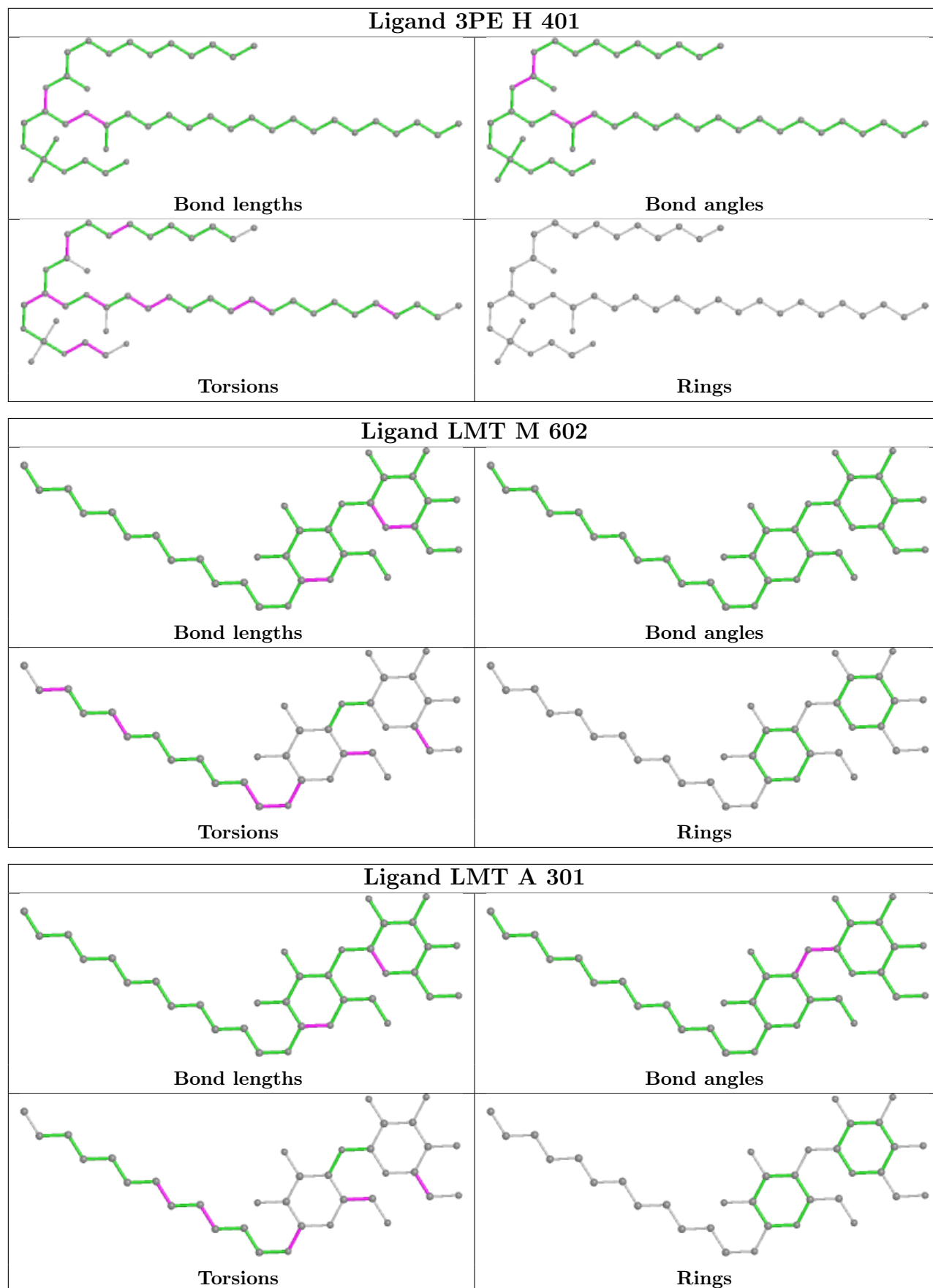
Mol	Chain	Res	Type	Atoms
49	F	501	FMN	N10-C1'-C2'-O2'
51	H	402	3PE	C3A-C3B-C3C-C3D
51	L	704	3PE	O31-C31-C32-C33
52	K	401	CDL	C72-C71-CB7-OB8
52	K	401	CDL	C35-C36-C37-C38
51	M	601	3PE	O21-C21-C22-C23
51	N	1302	3PE	O21-C21-C22-C23

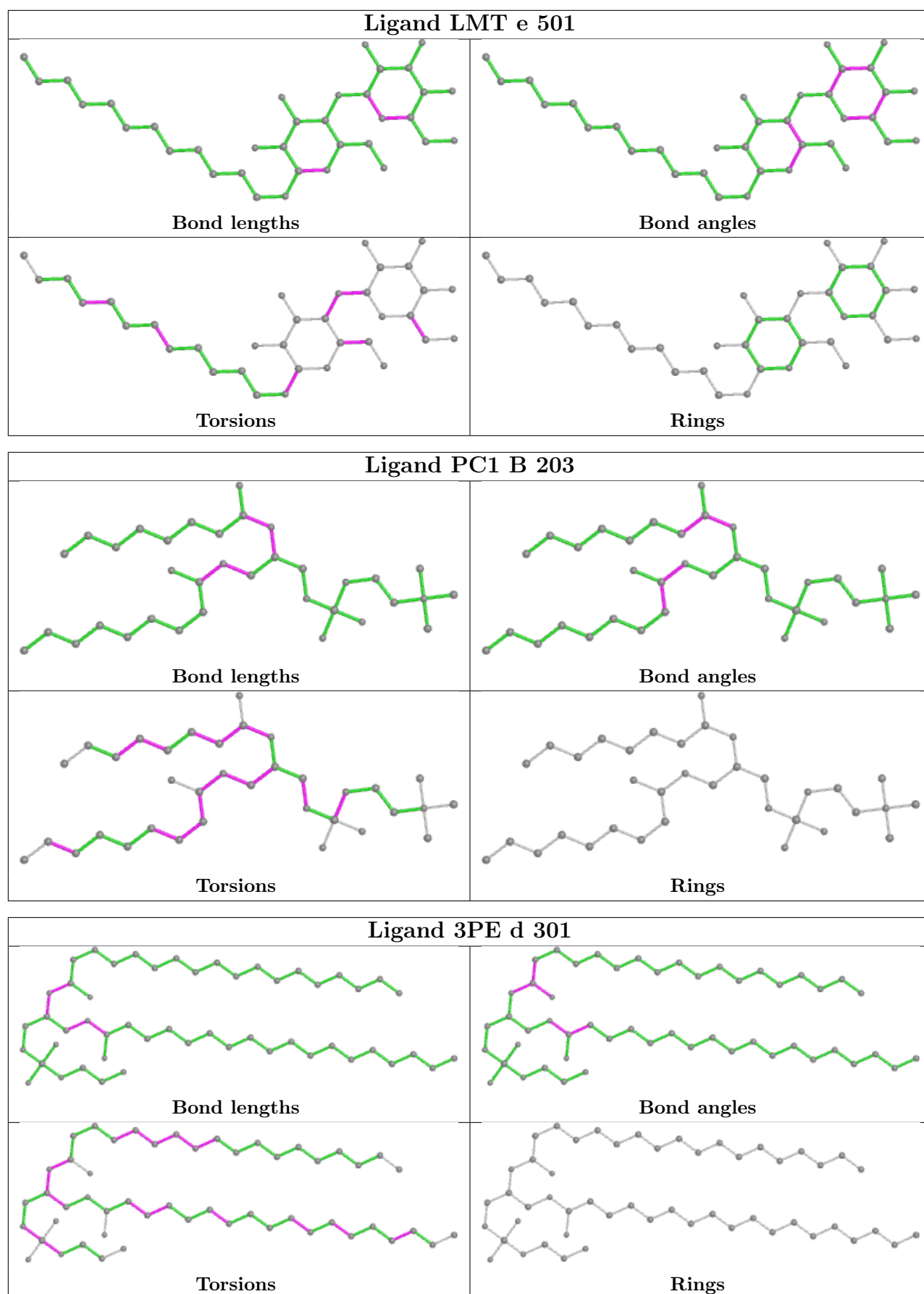
There are no ring outliers.

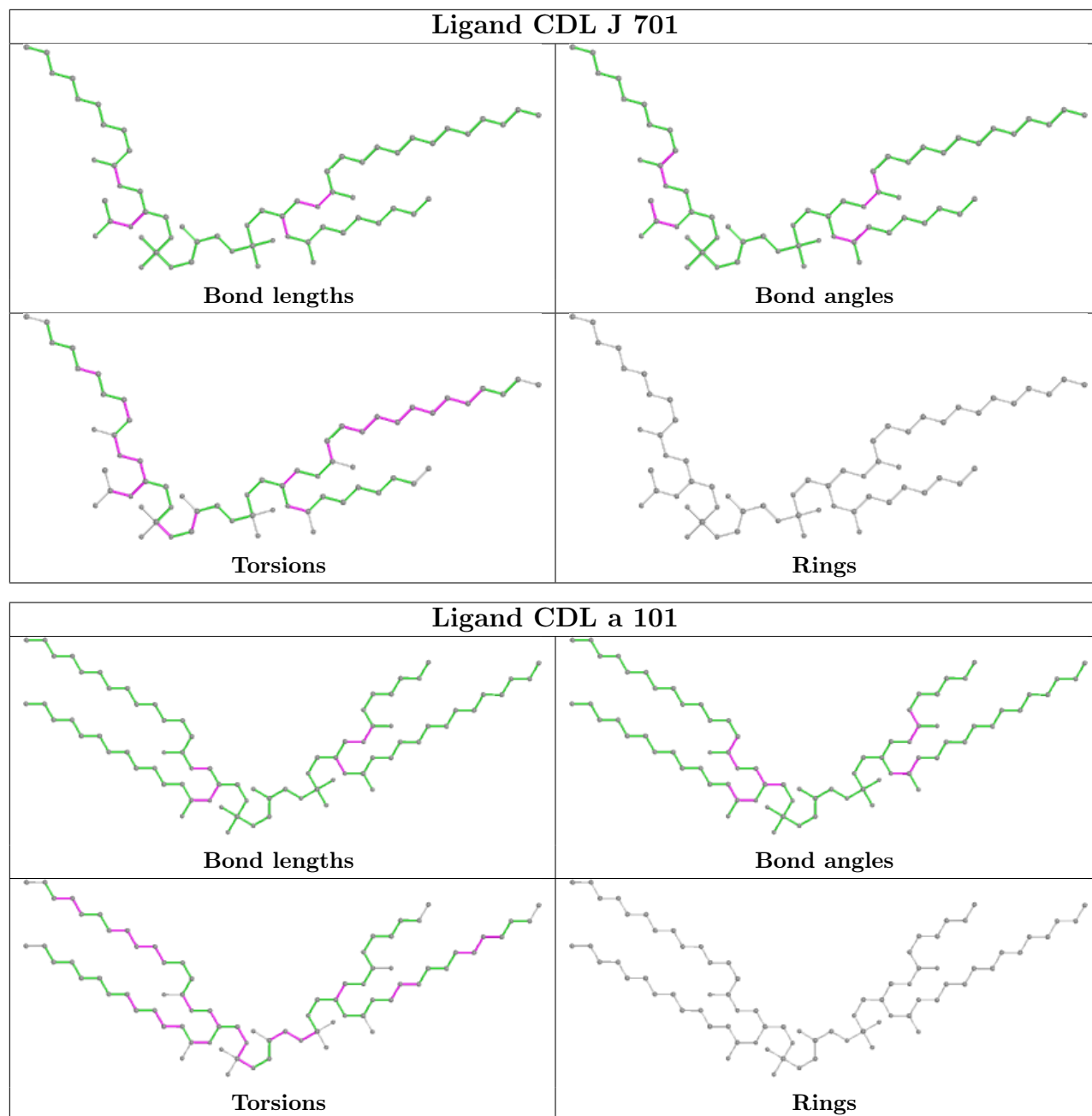
No monomer is involved in short contacts.

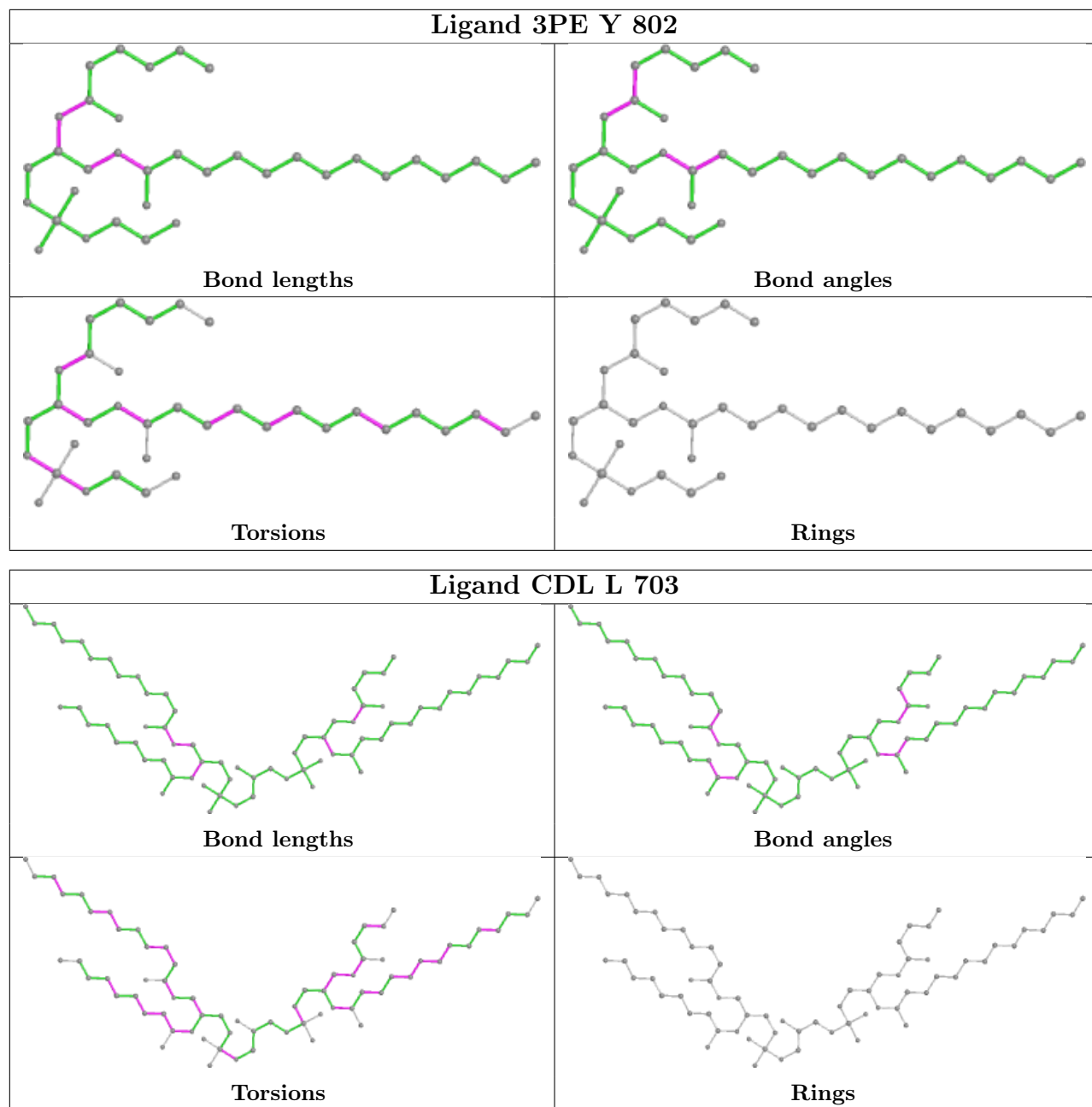
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

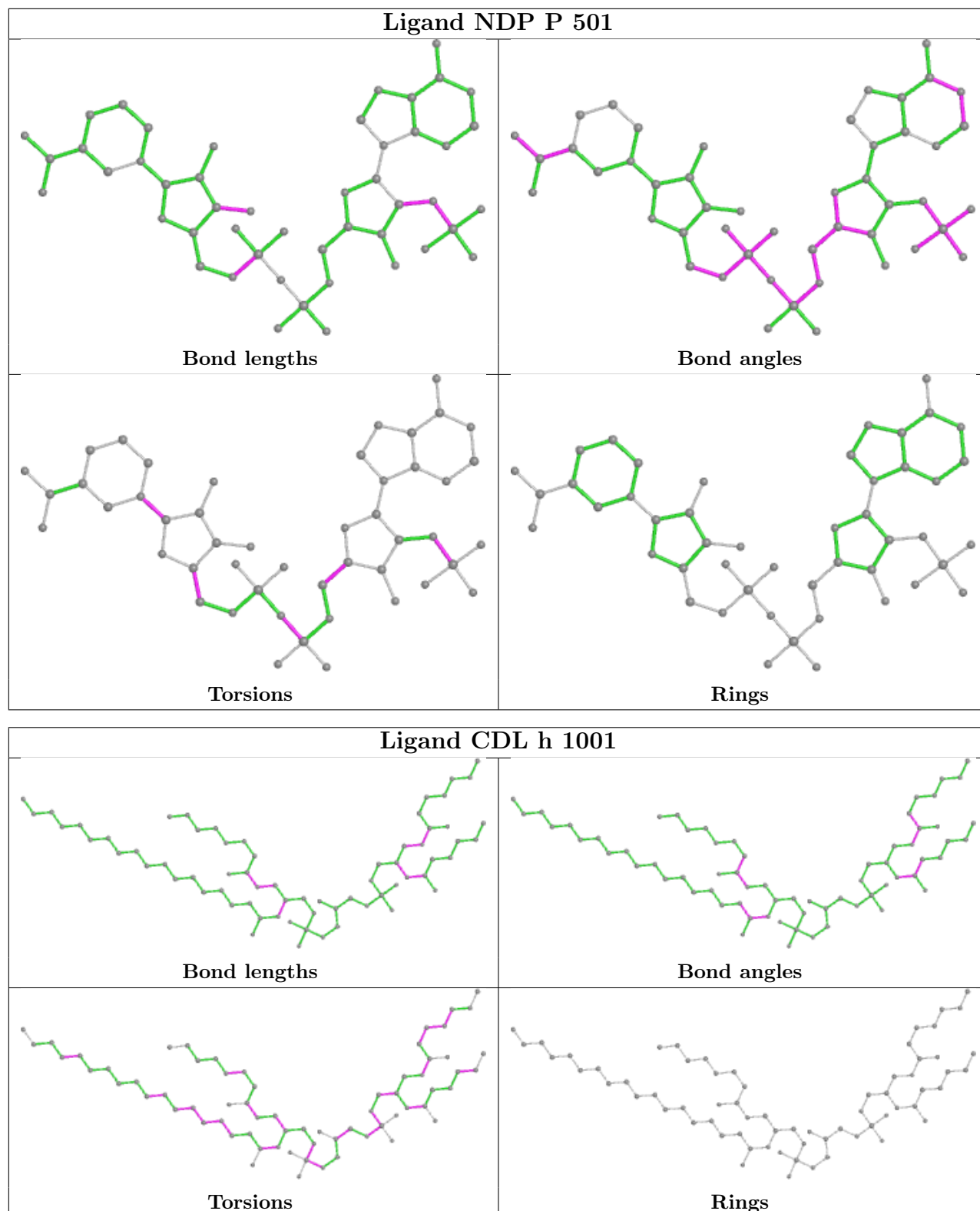


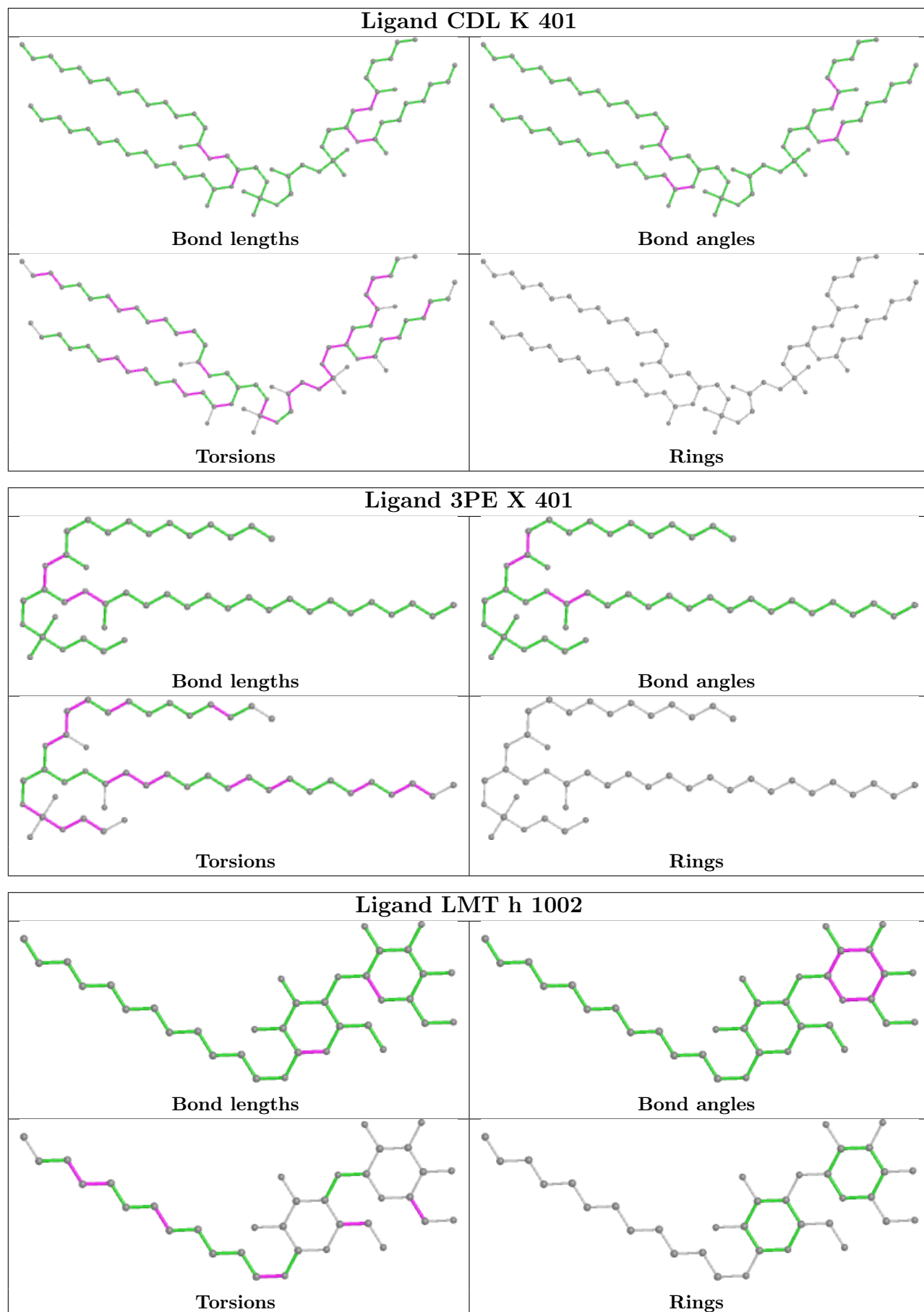


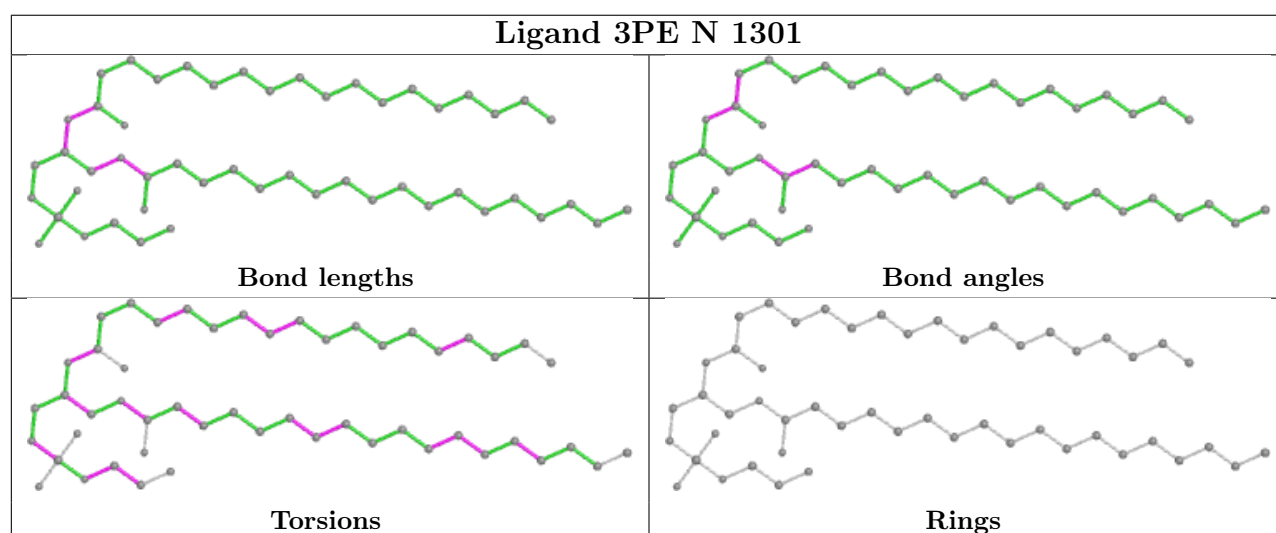
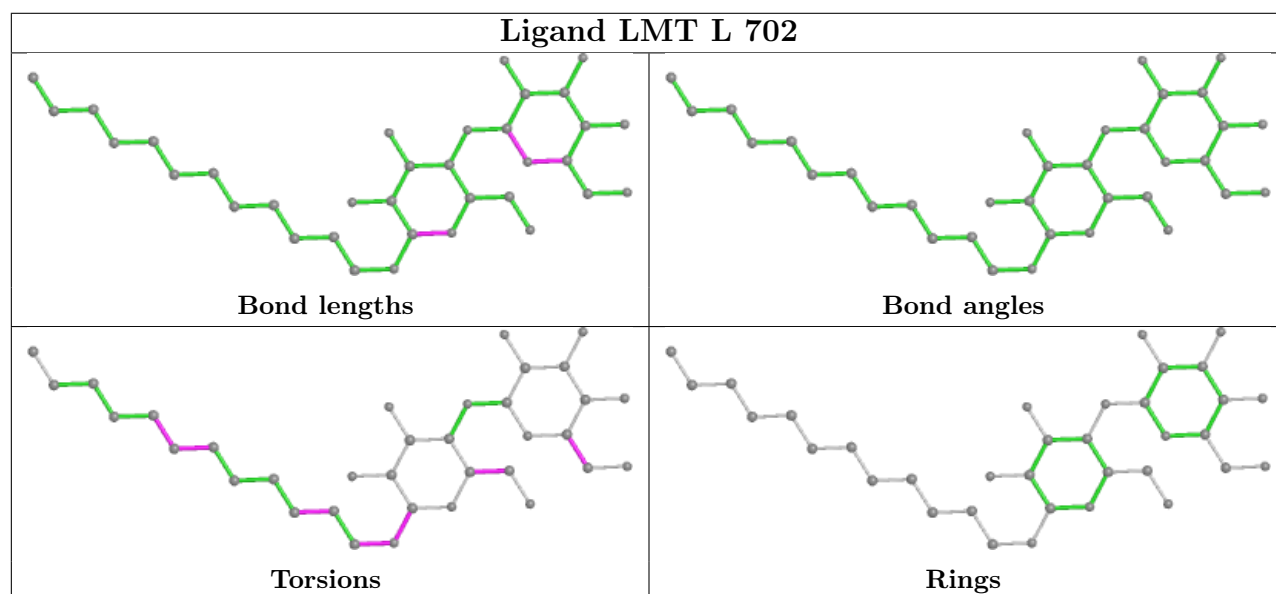
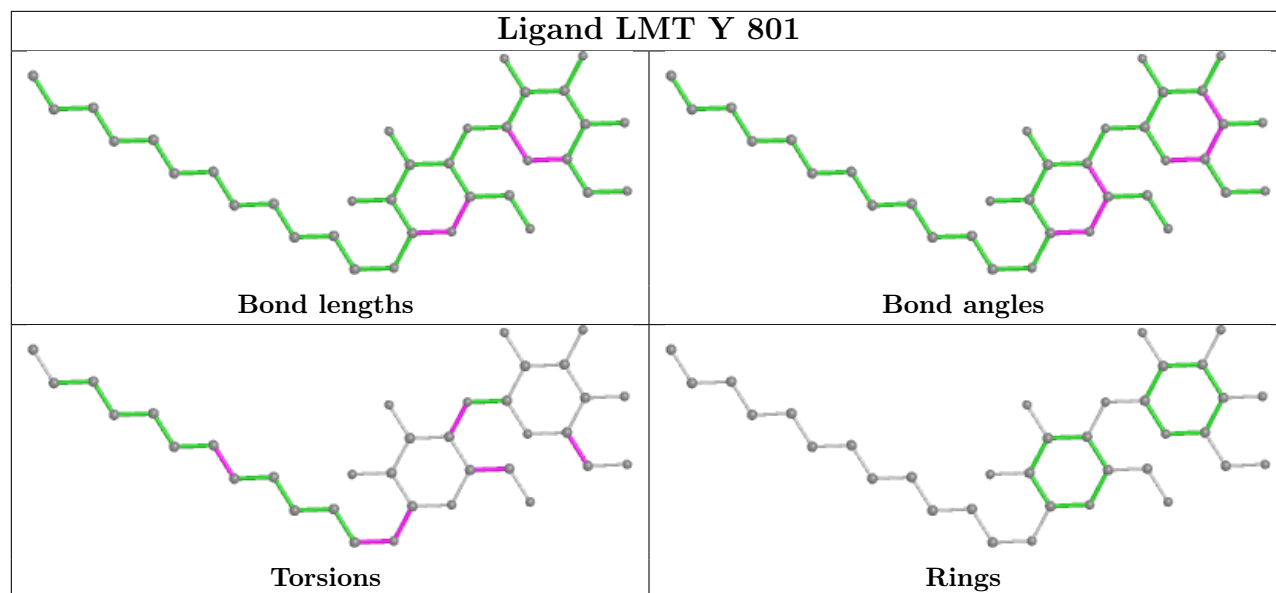


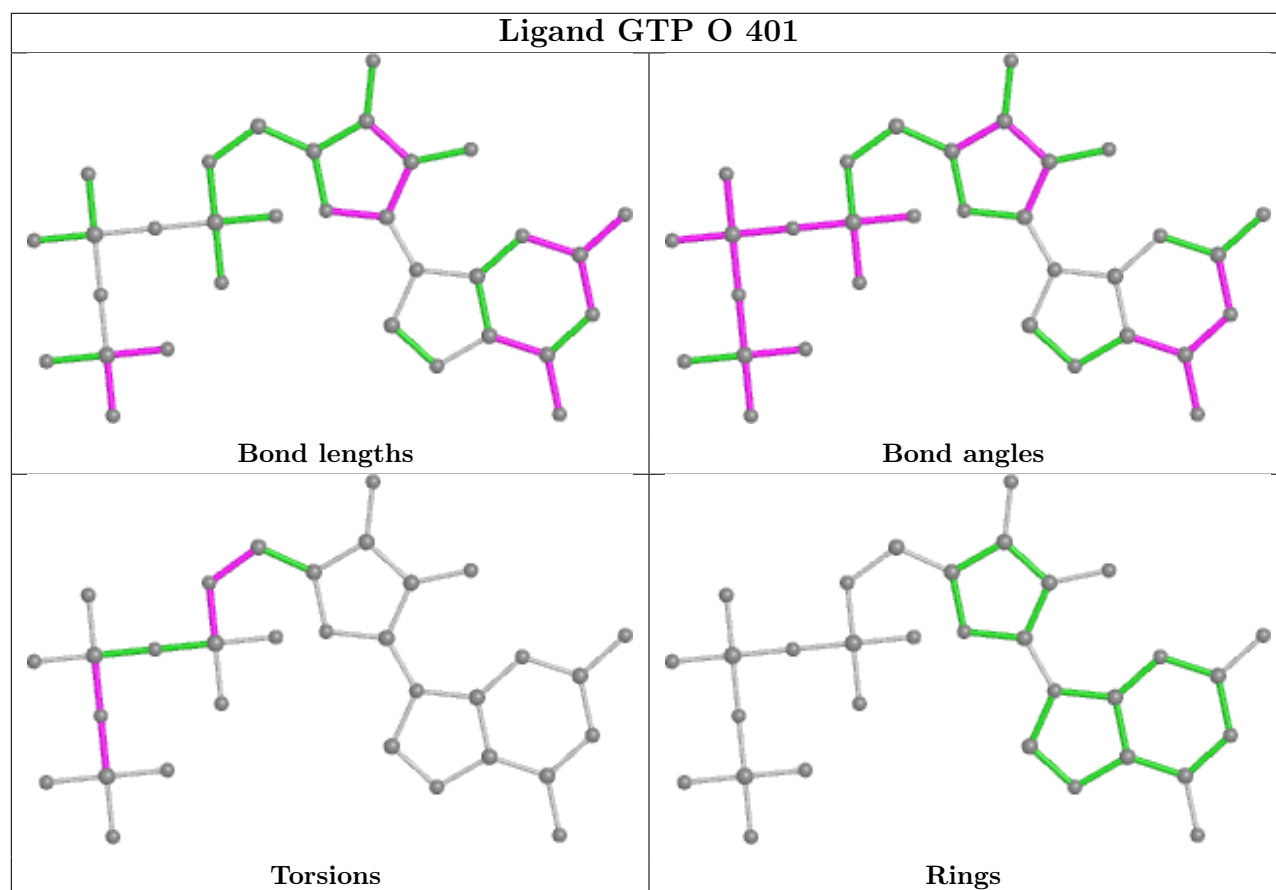
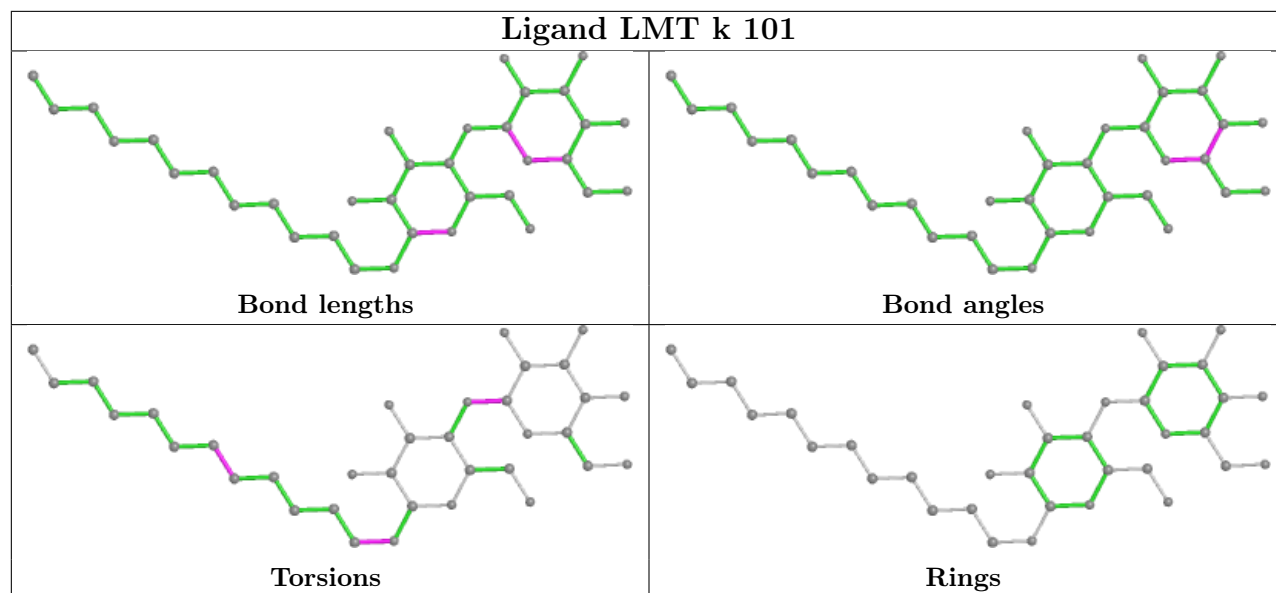


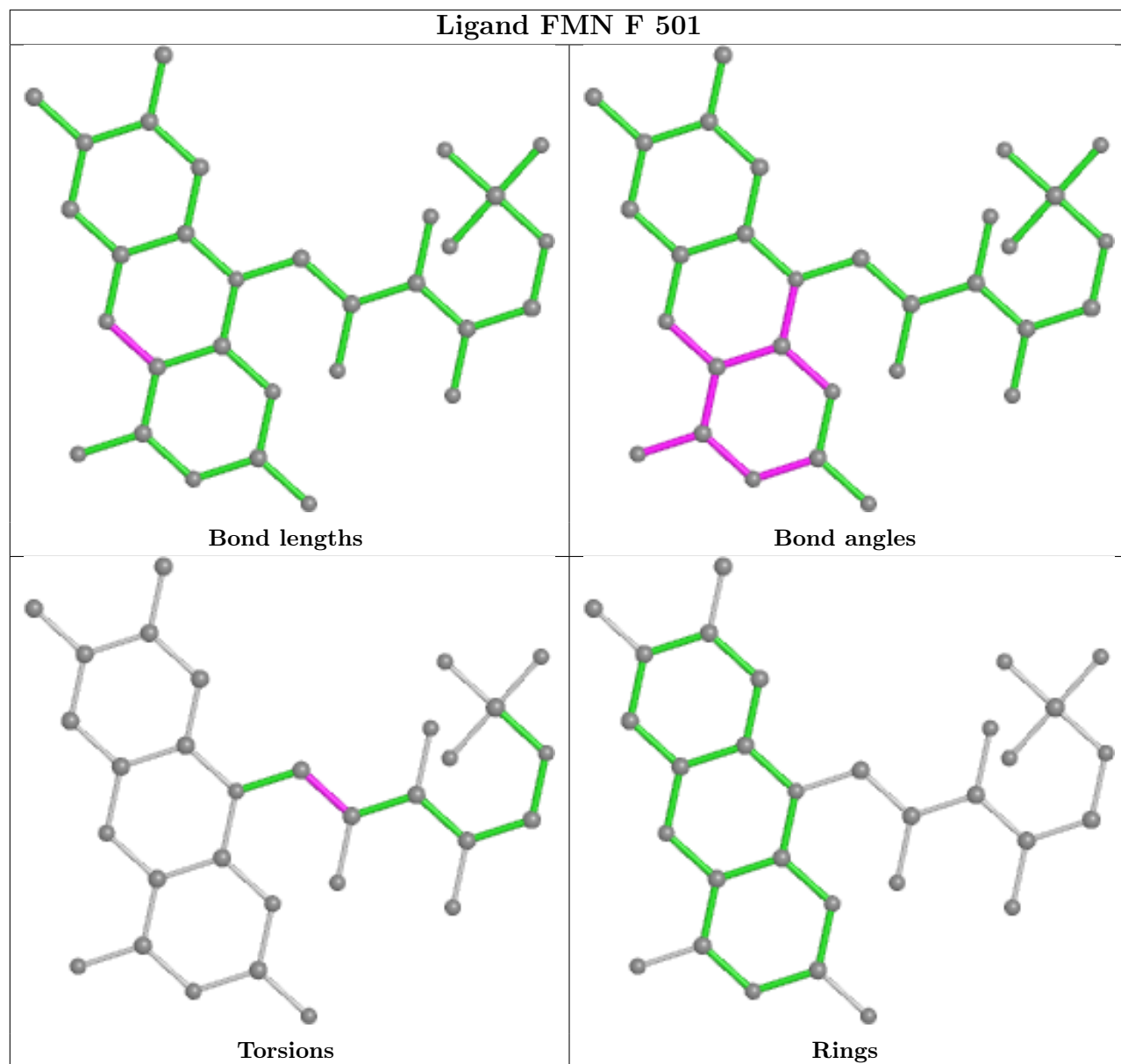


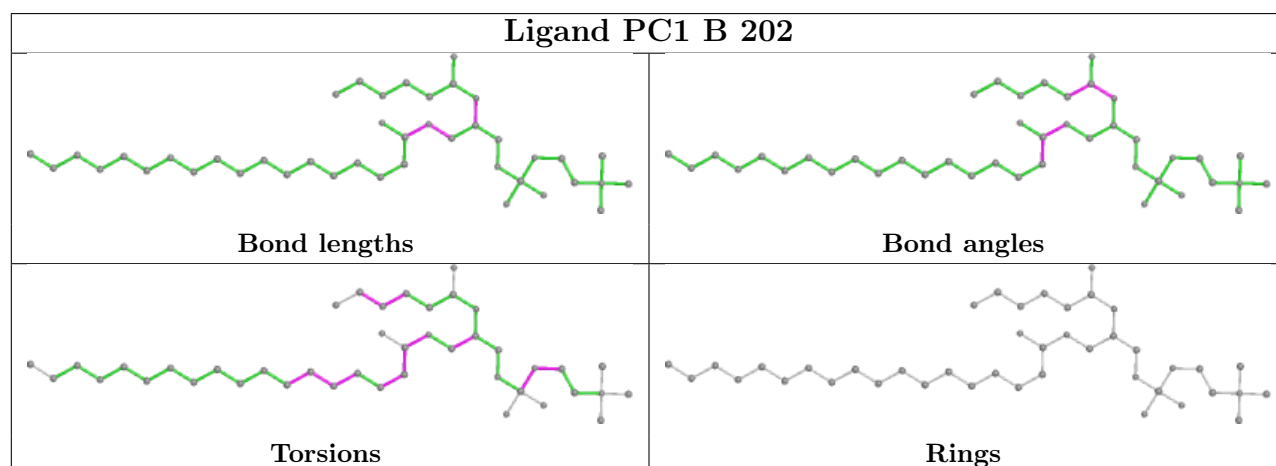
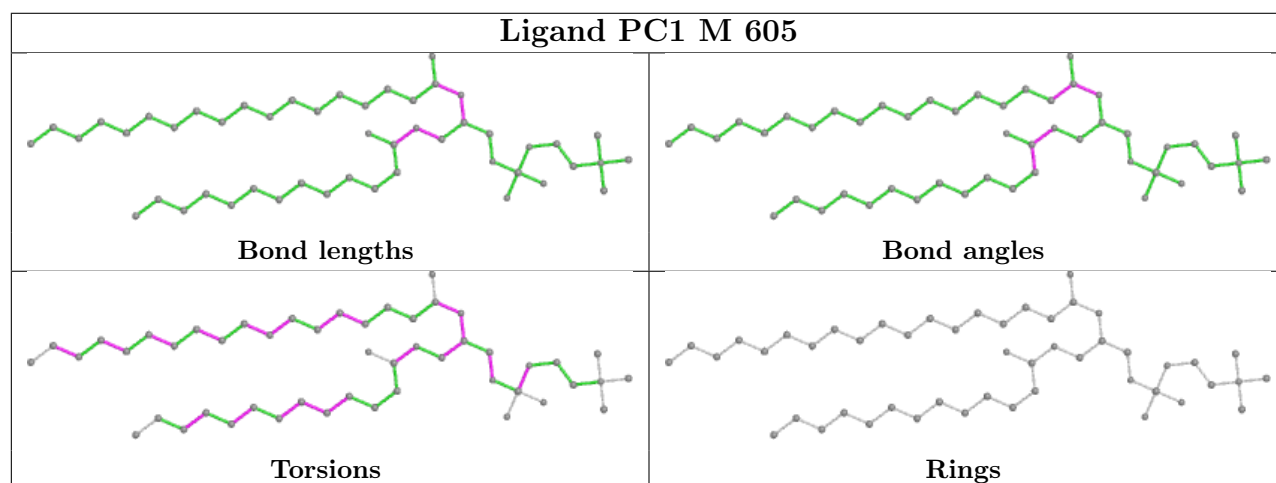
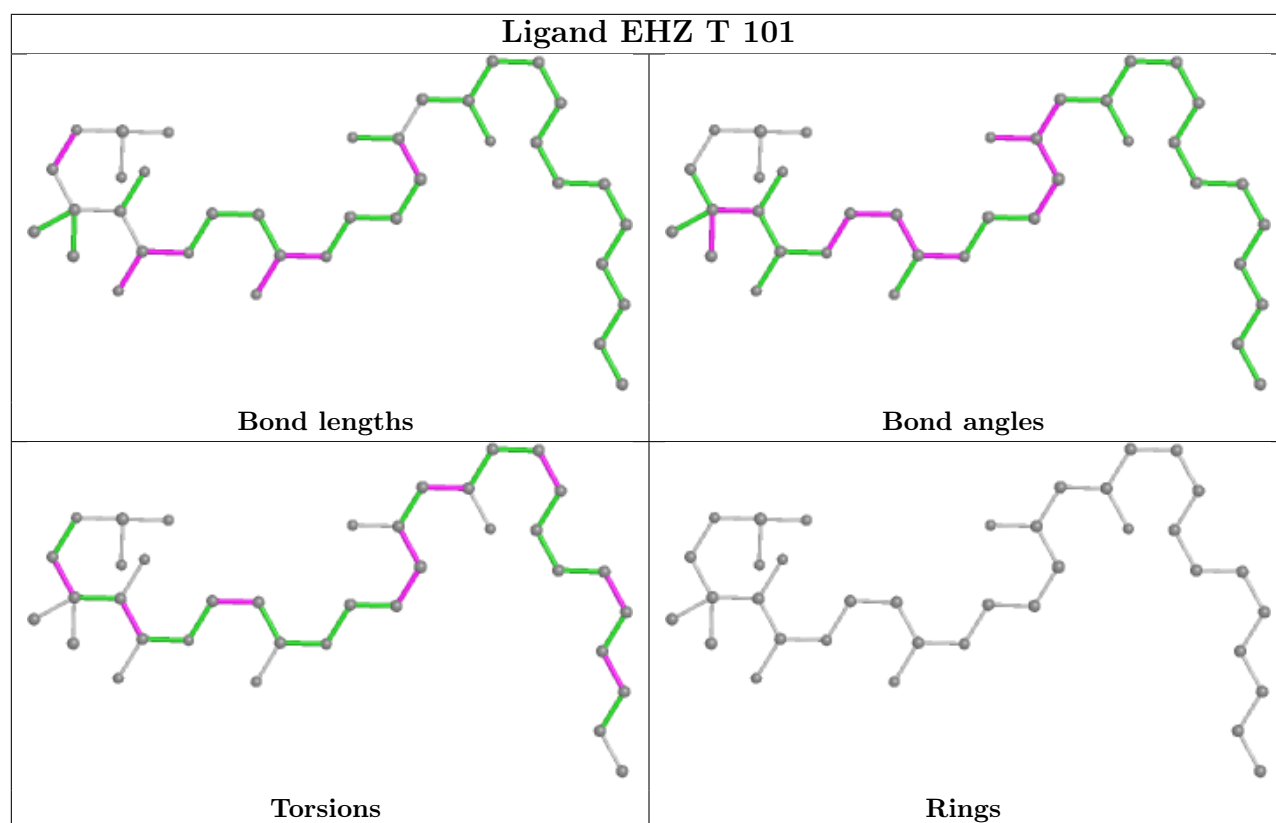


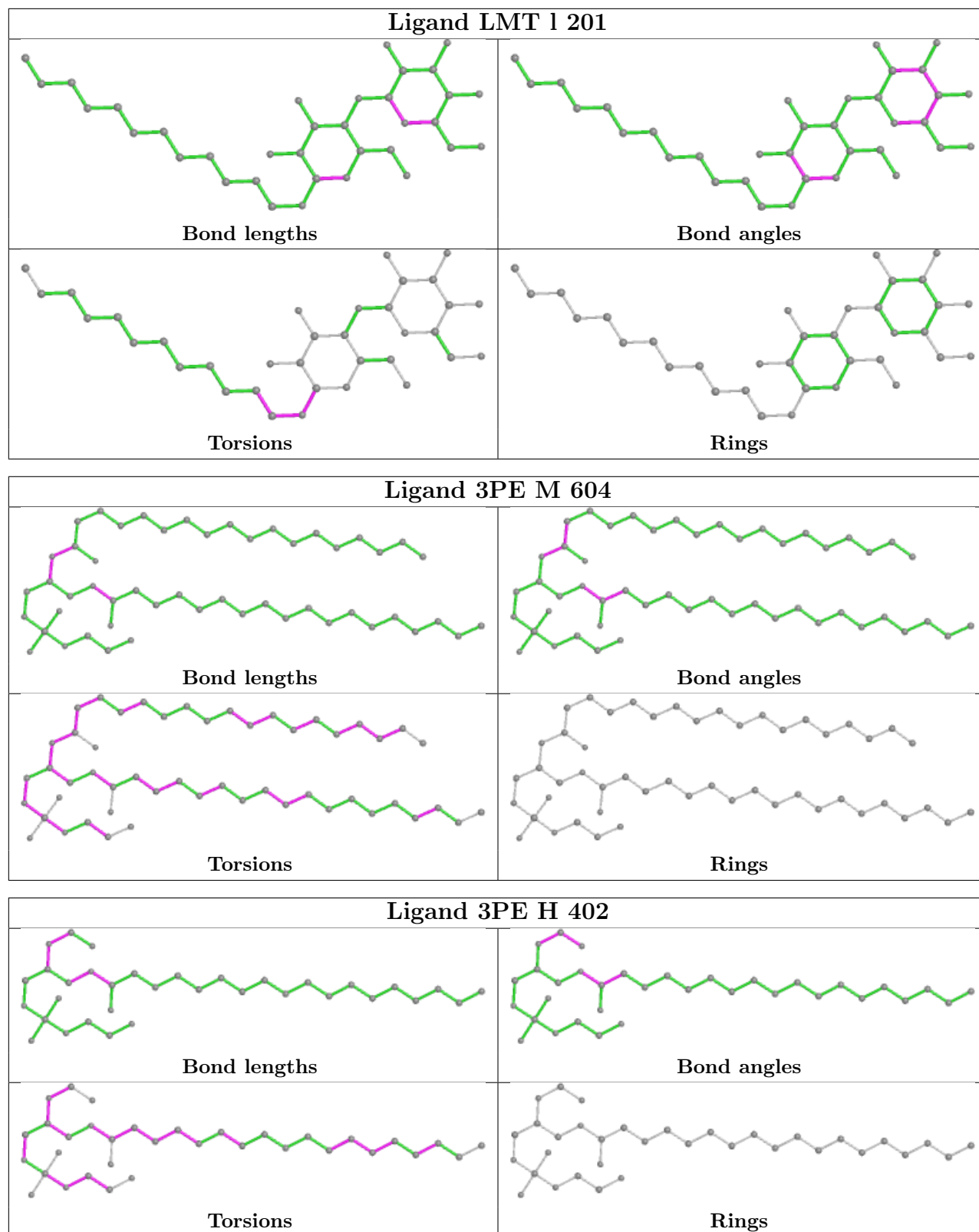


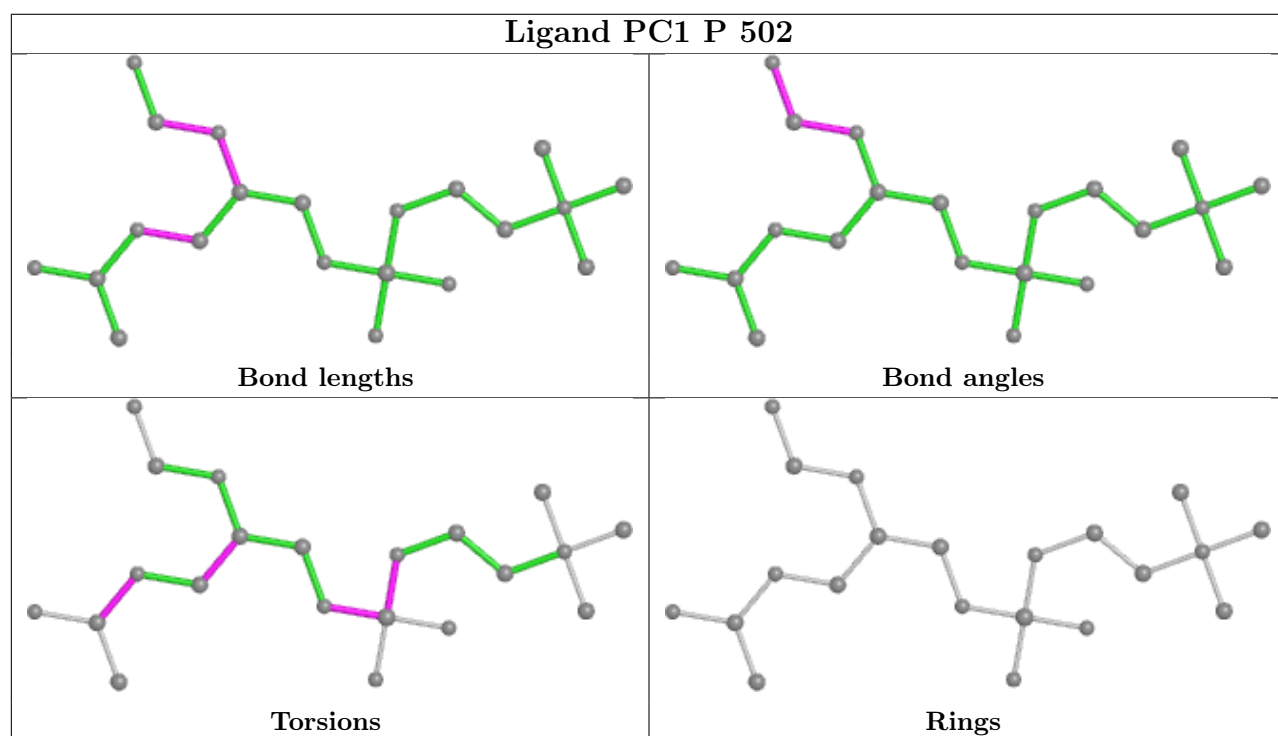
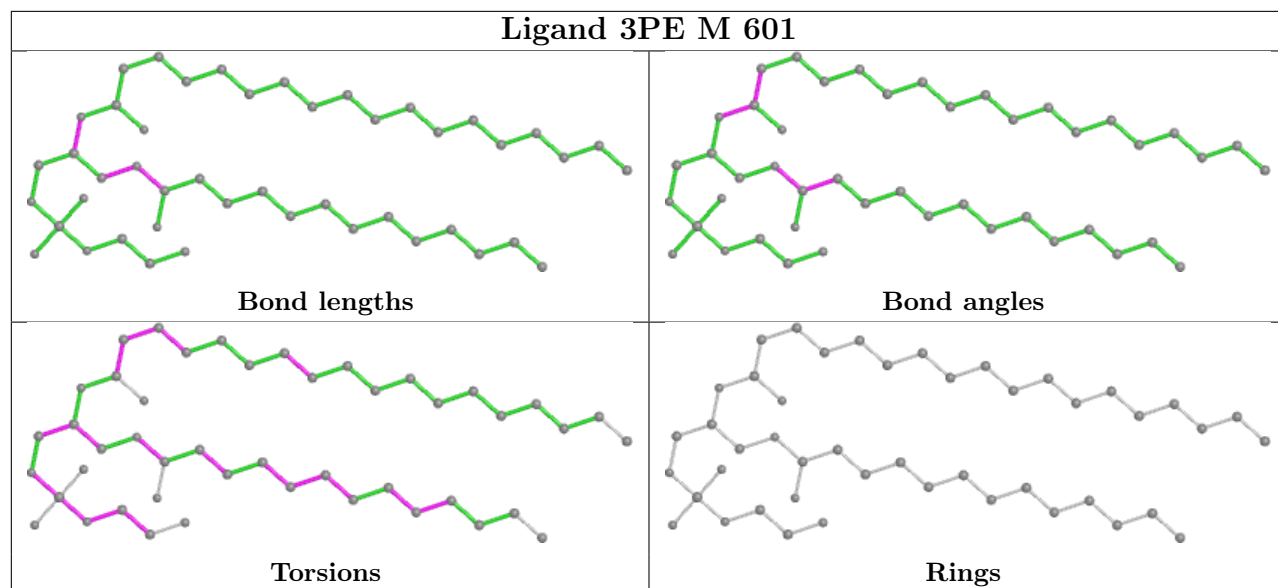


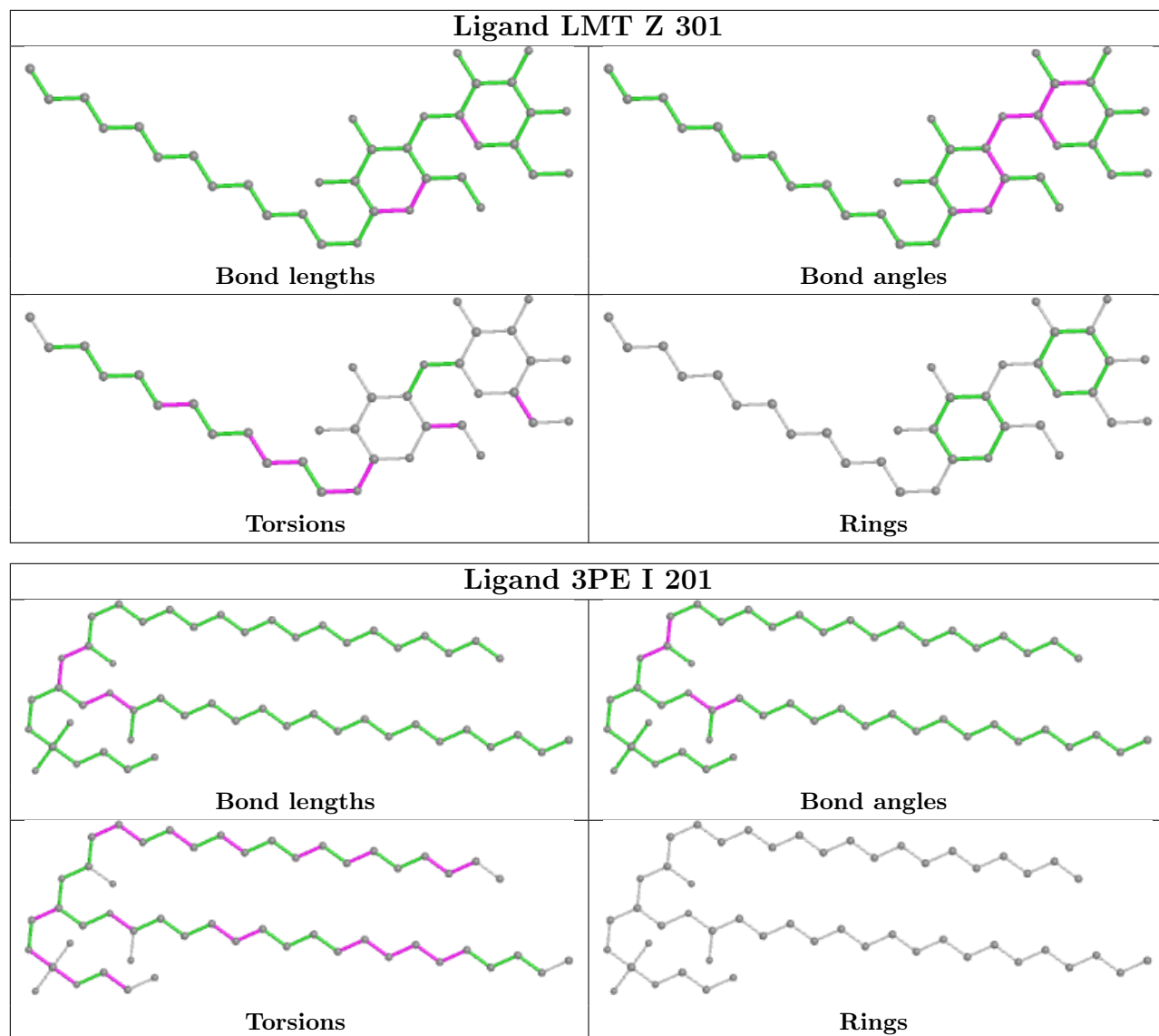


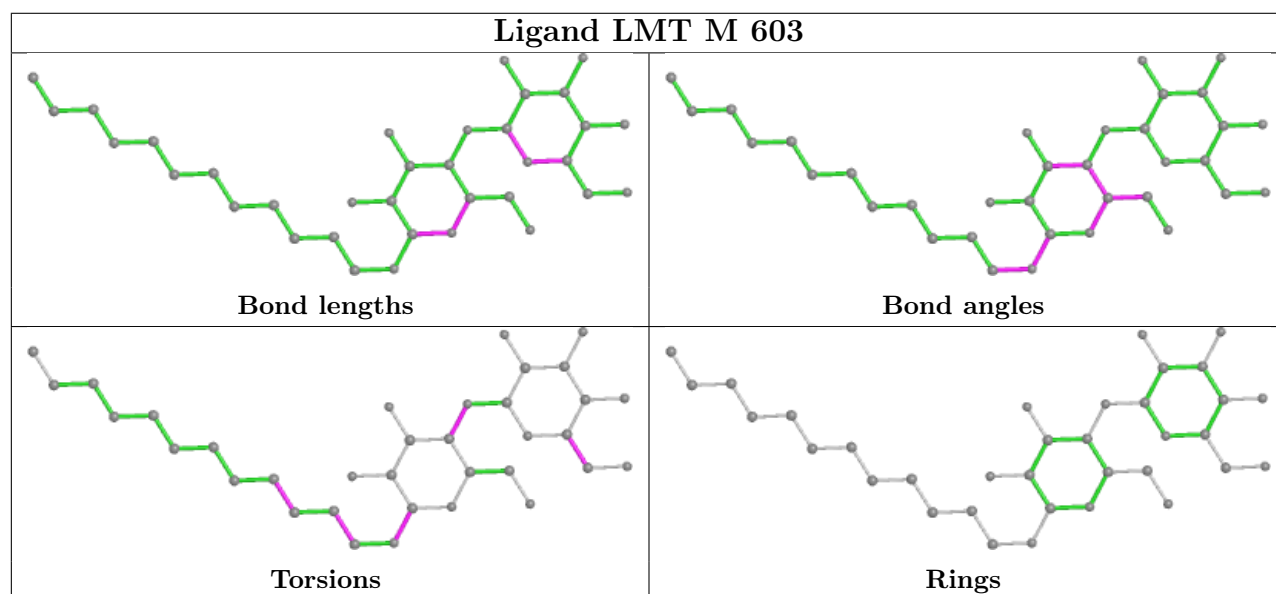
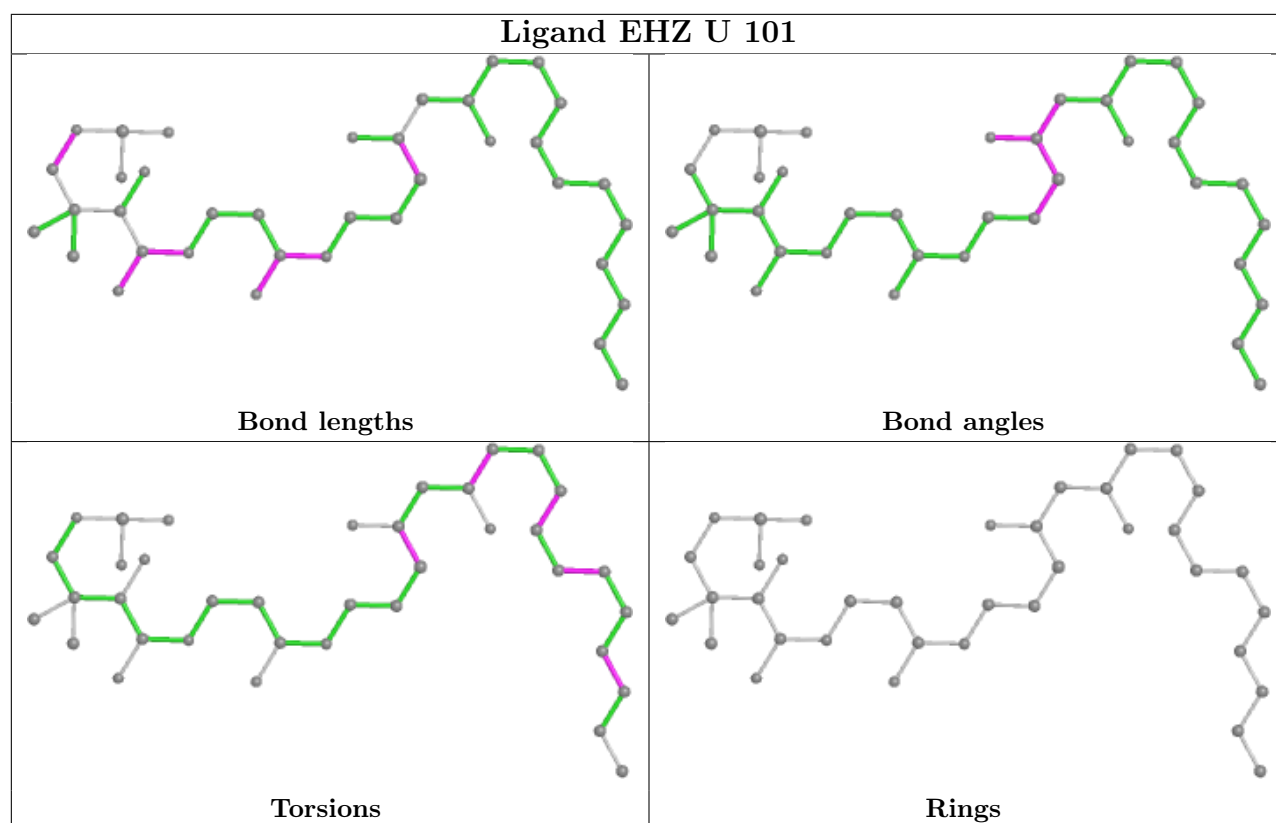


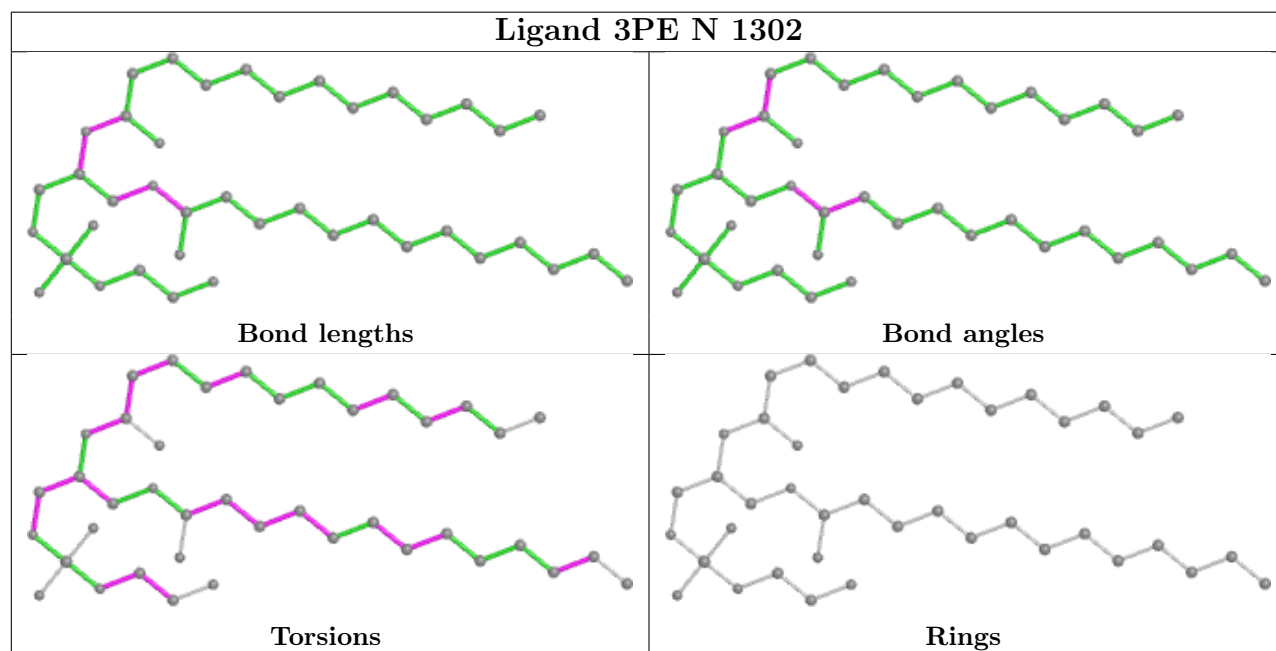
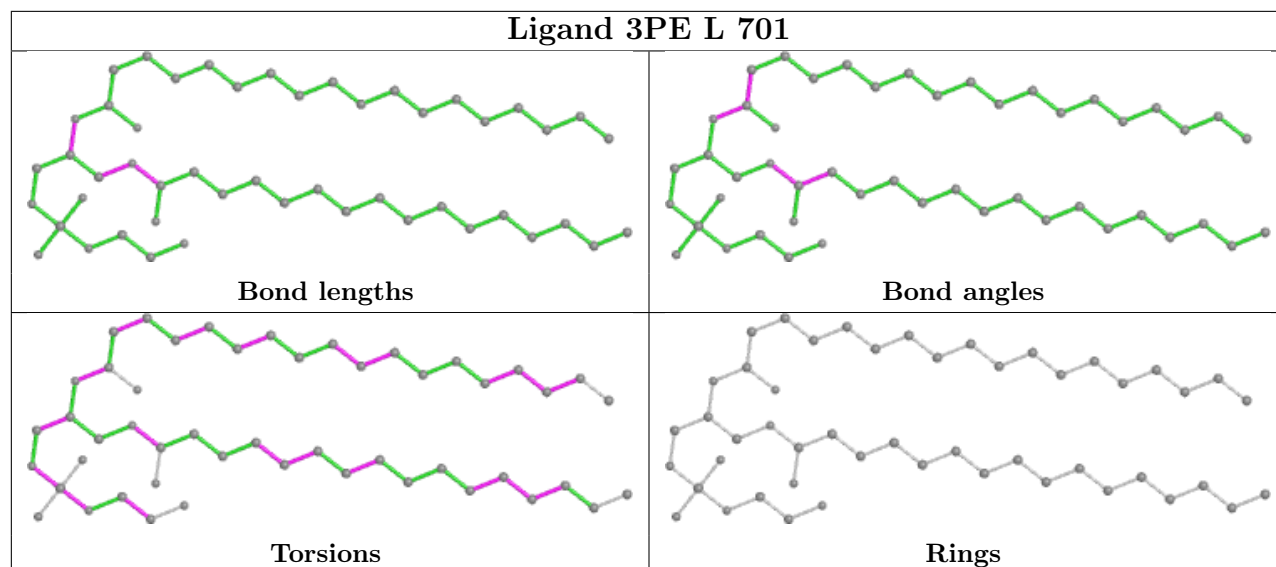


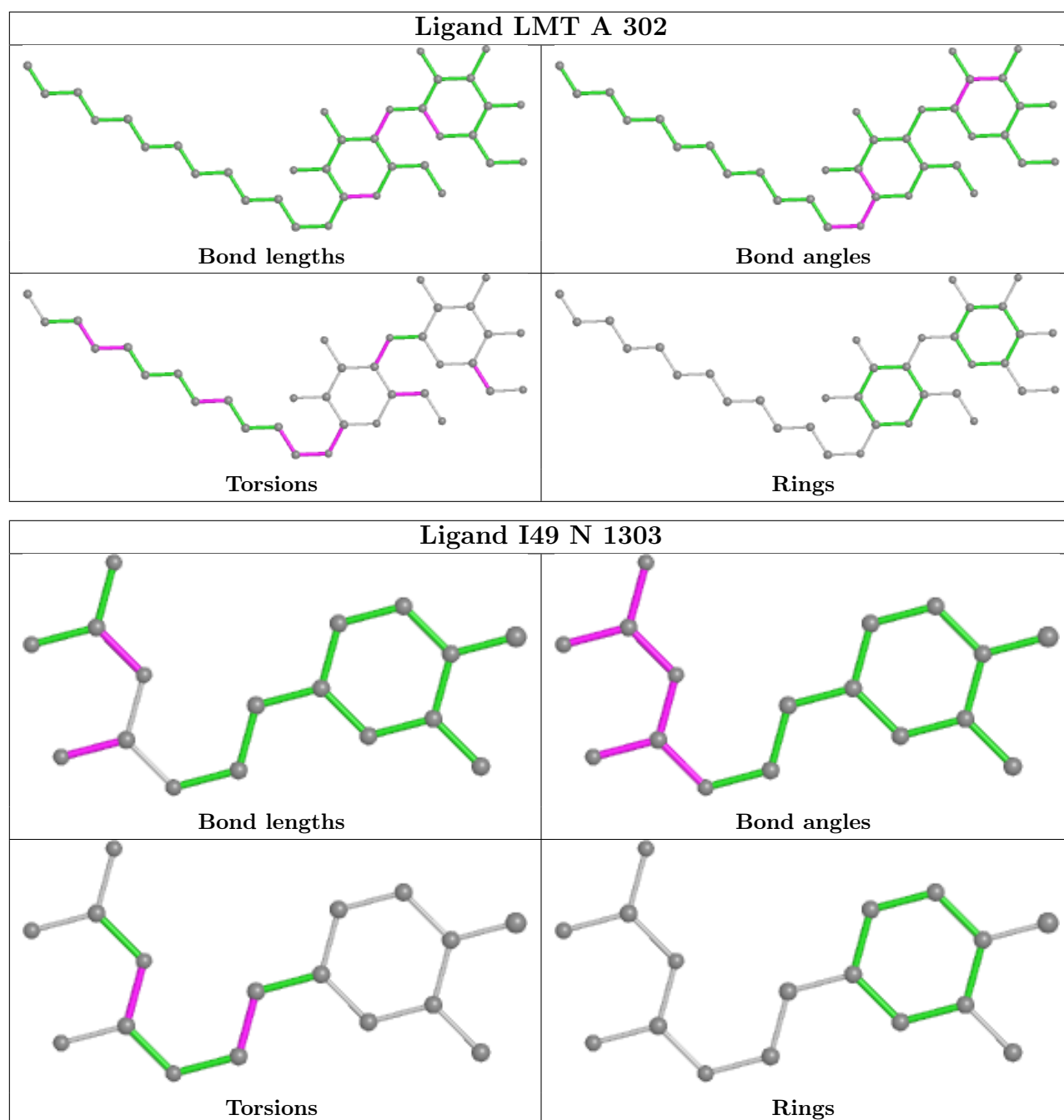












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

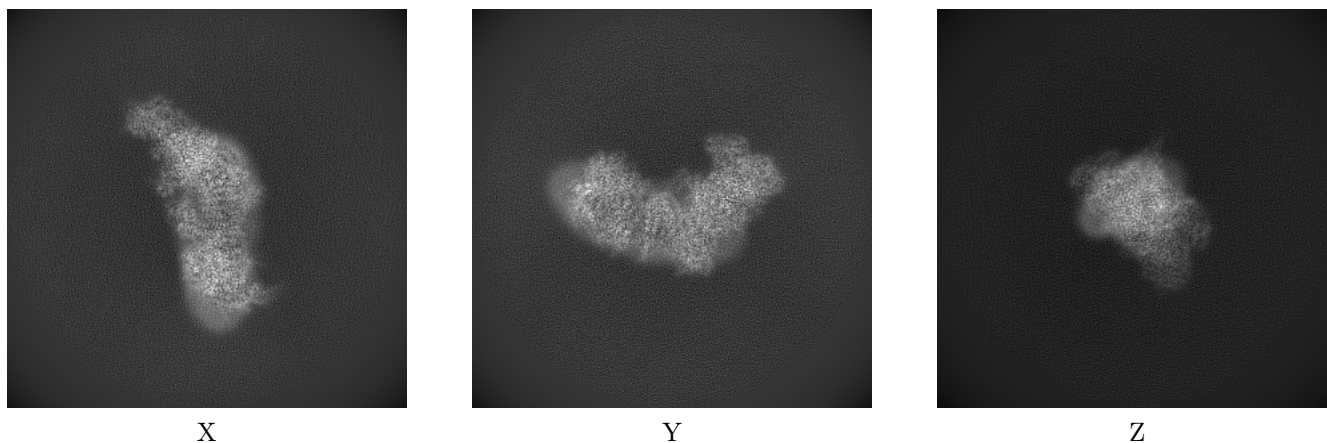
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14266. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

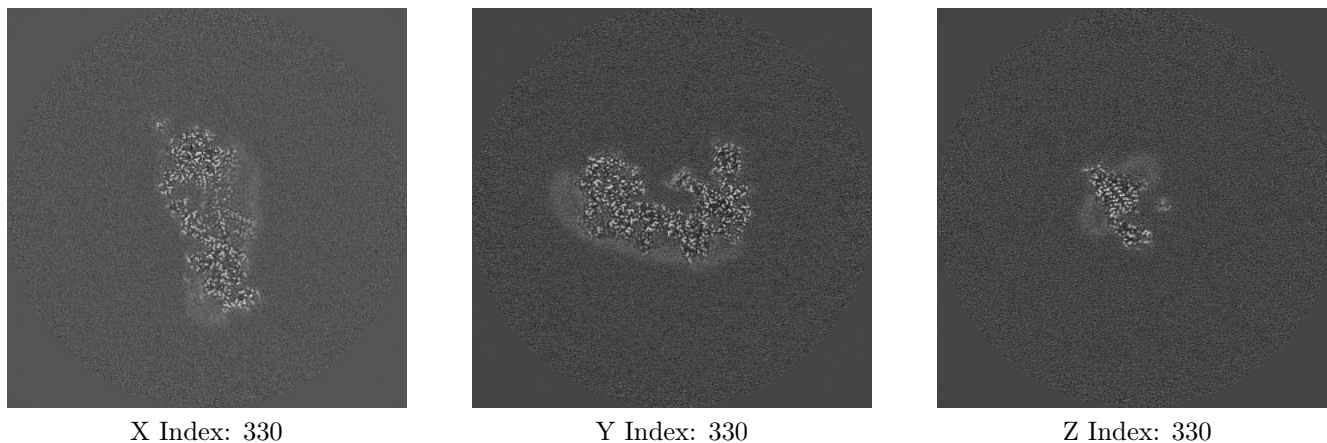
6.1.1 Primary map



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

6.2 Central slices [i](#)

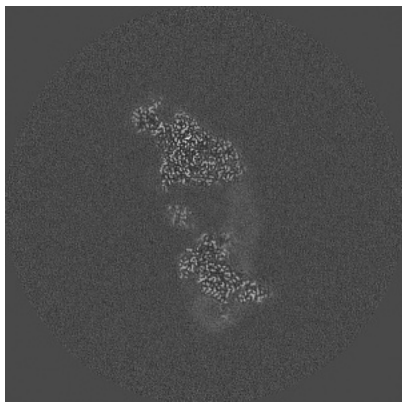
6.2.1 Primary map



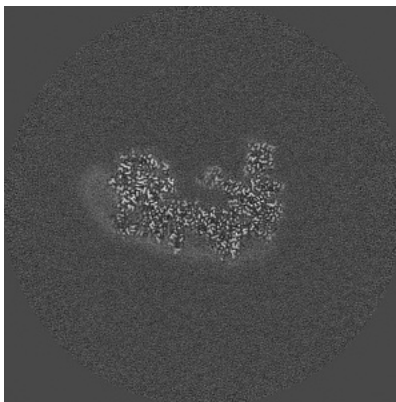
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

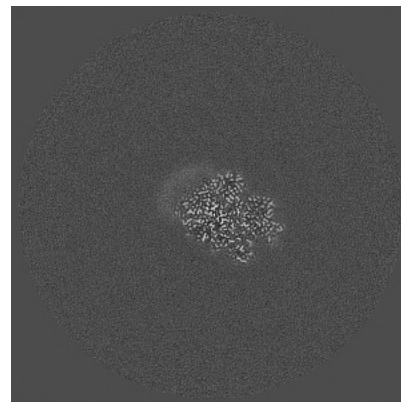
6.3.1 Primary map



X Index: 354



Y Index: 332



Z Index: 421

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

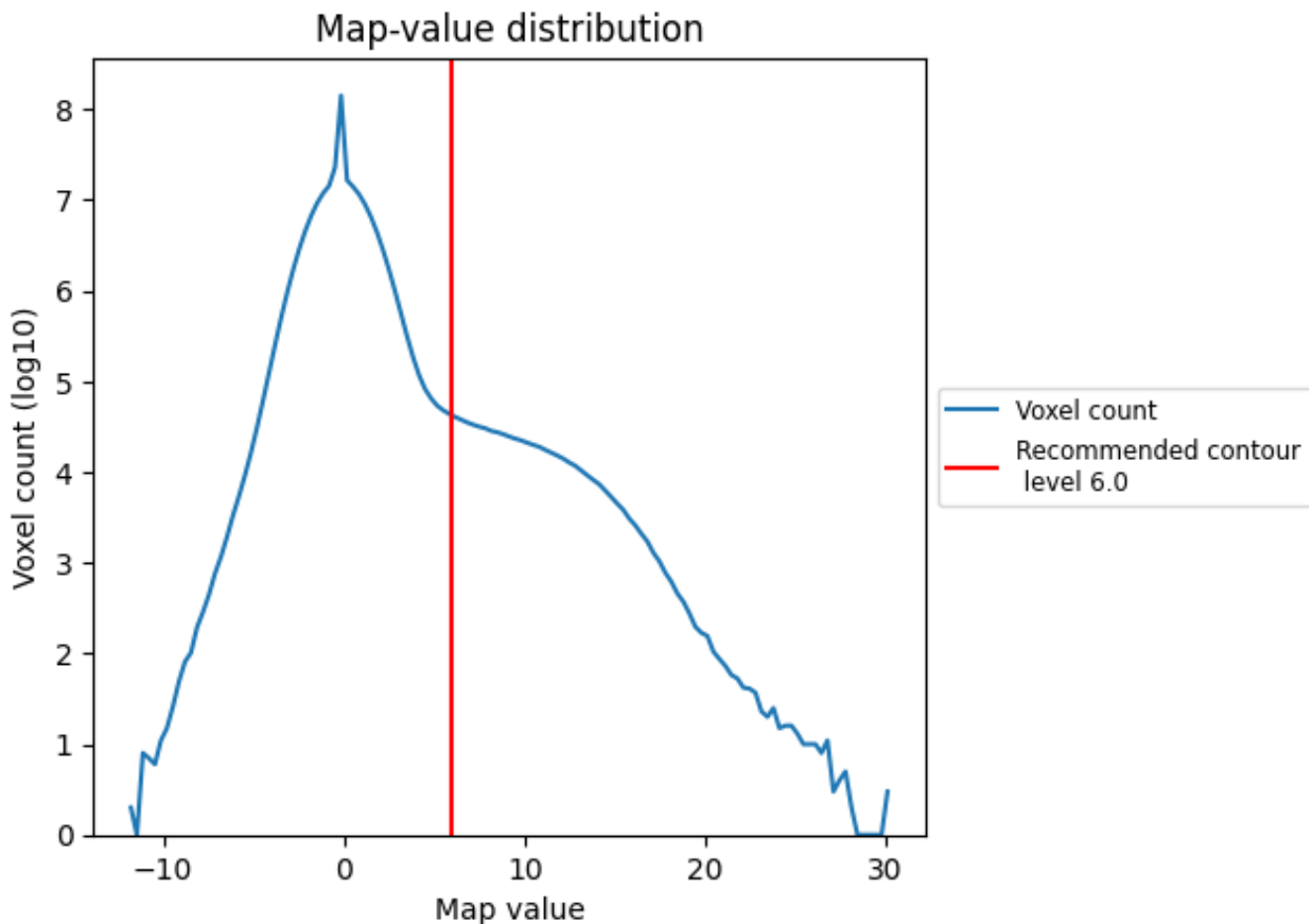
6.5 Mask visualisation

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

7 Map analysis [i](#)

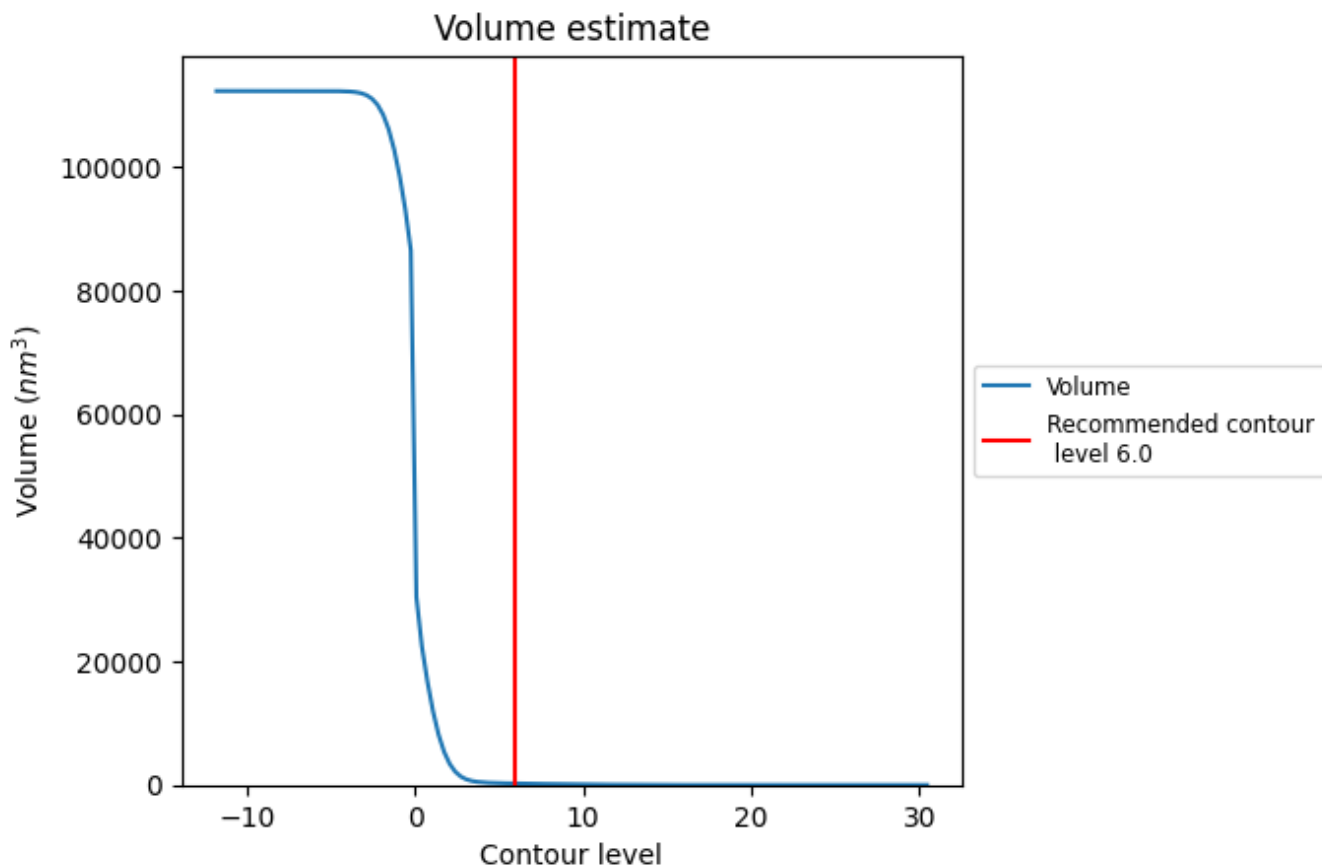
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

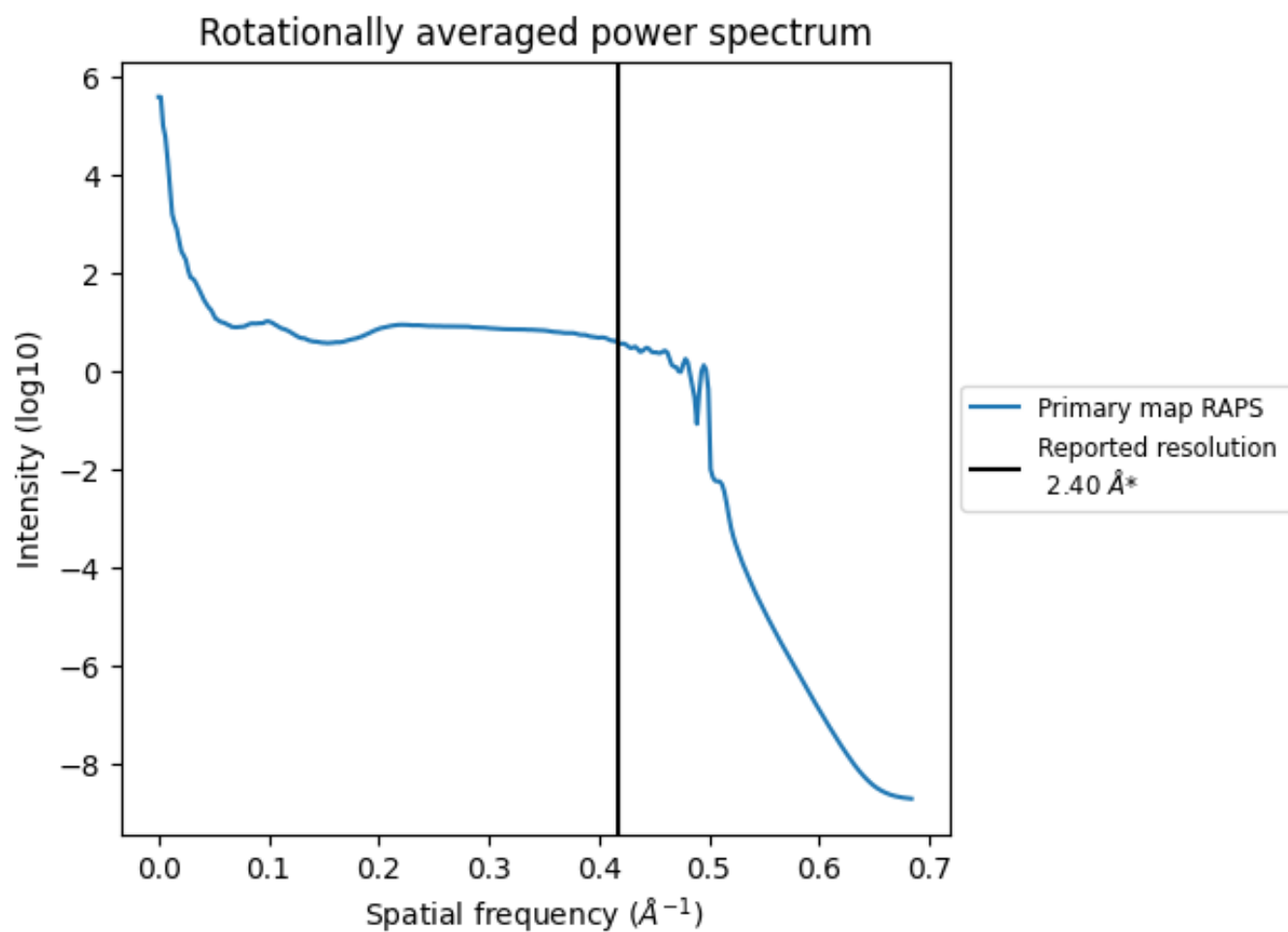
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 235 nm^3 ; this corresponds to an approximate mass of 212 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 0.417\AA^{-1}

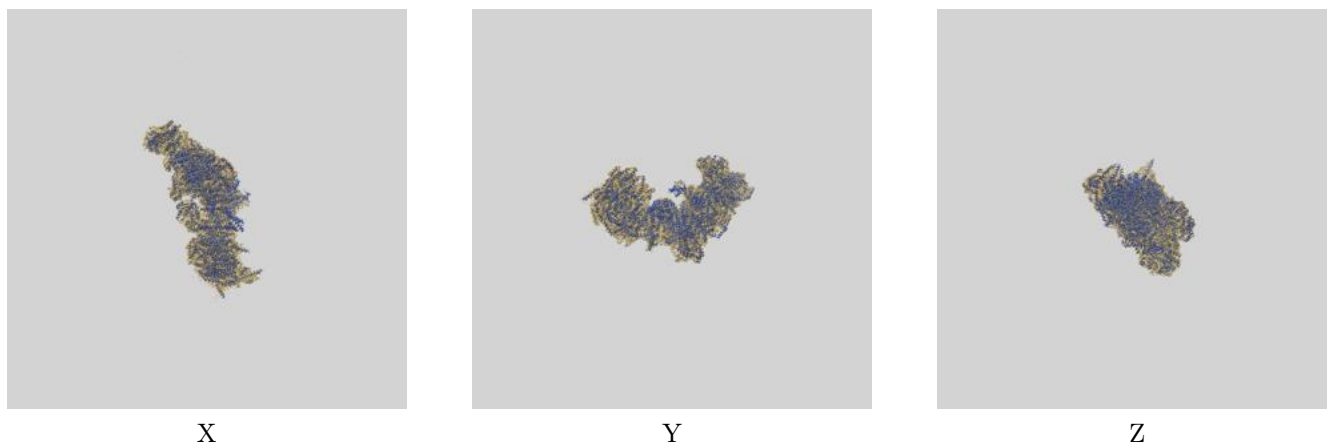
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

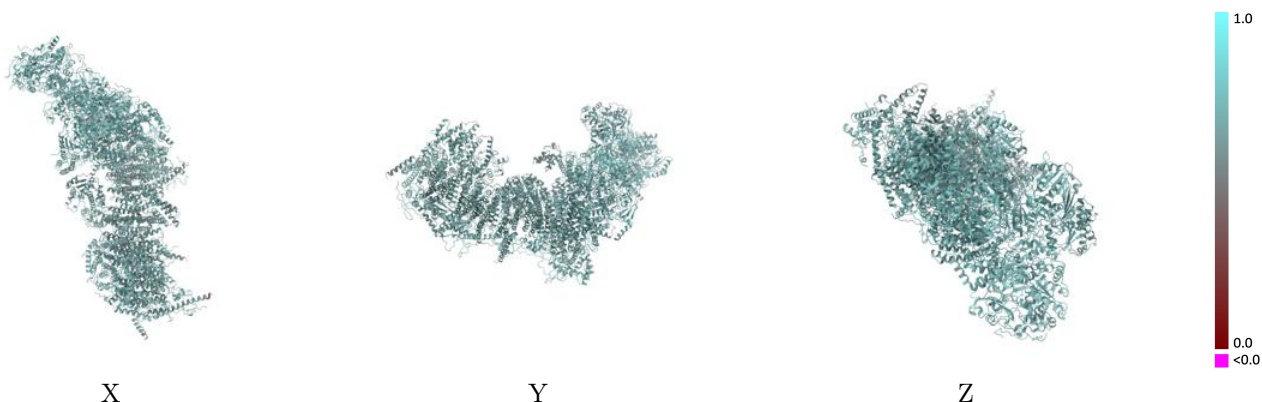
This section contains information regarding the fit between EMDB map EMD-14266 and PDB model 7R44. Per-residue inclusion information can be found in section 3 on page 23.

9.1 Map-model overlay [i](#)



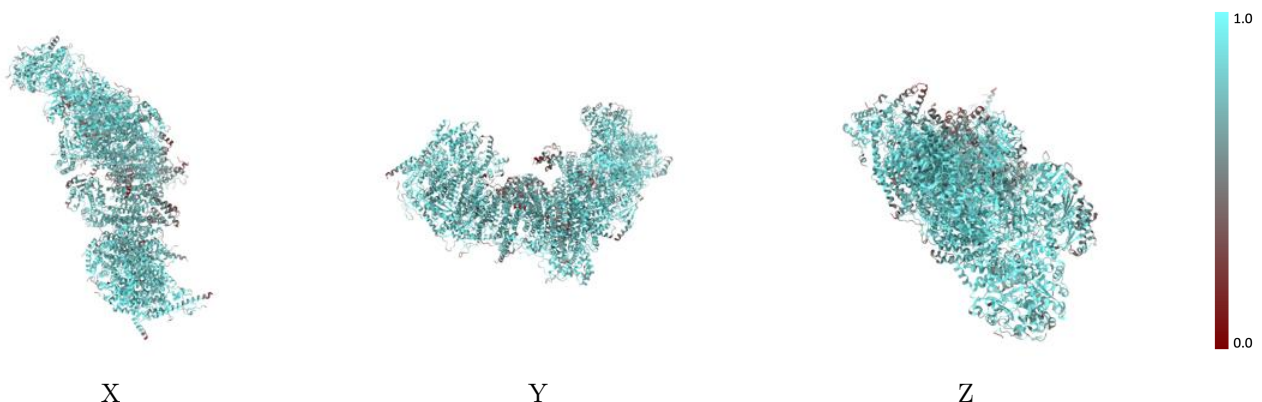
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



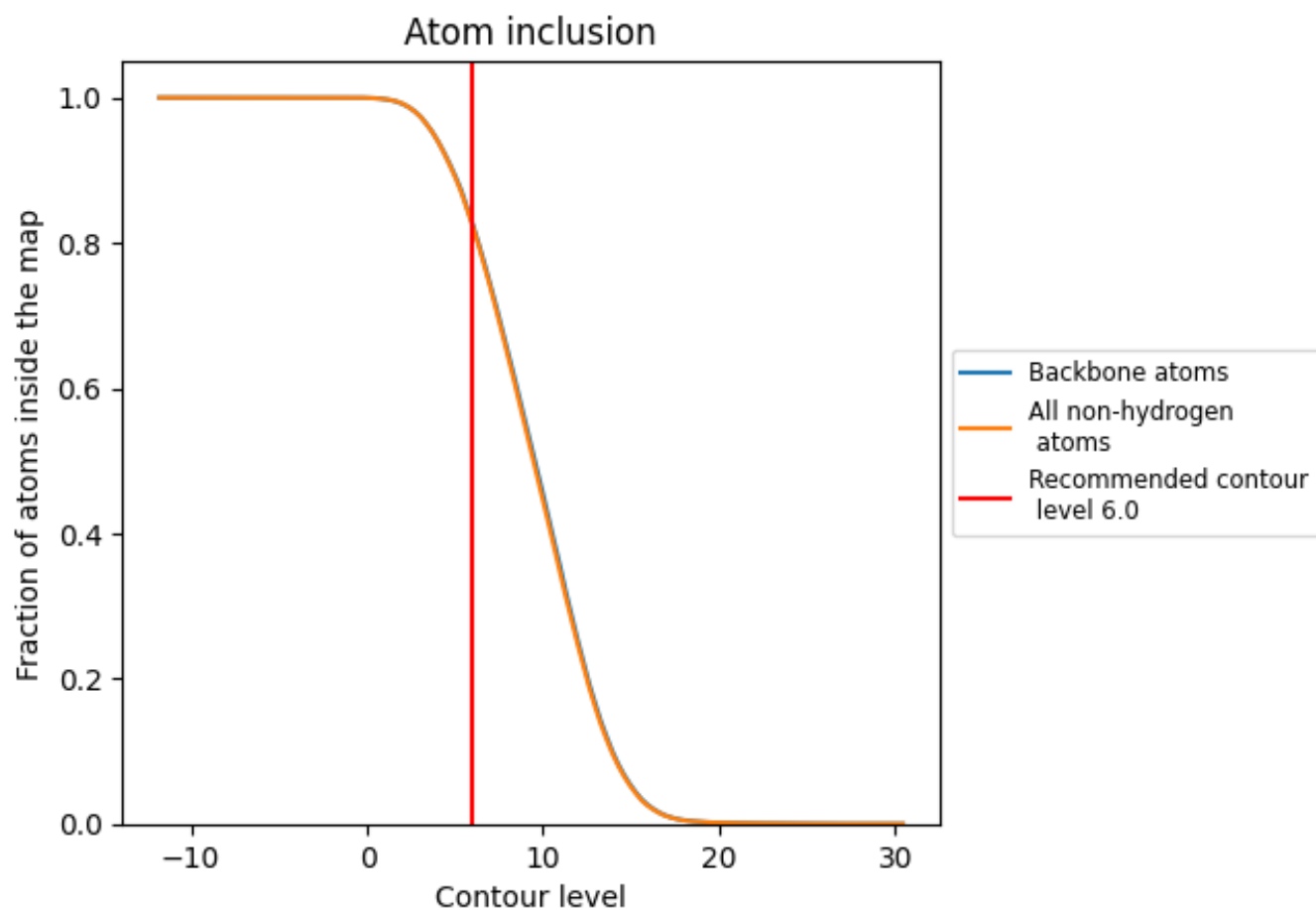
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6.0).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 82% 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 (6.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8240	 0.6740
A	 0.8014	 0.6780
B	 0.8984	 0.7130
C	 0.9301	 0.7160
D	 0.9034	 0.7120
E	 0.8109	 0.6700
F	 0.8501	 0.6840
G	 0.8591	 0.6910
H	 0.9160	 0.7000
I	 0.9284	 0.7170
J	 0.7795	 0.6650
K	 0.8358	 0.6880
L	 0.8535	 0.6600
M	 0.8836	 0.6800
N	 0.9094	 0.6940
O	 0.7873	 0.6560
P	 0.7931	 0.6810
Q	 0.8570	 0.7030
R	 0.8387	 0.6890
S	 0.7205	 0.6580
T	 0.4503	 0.5760
U	 0.8591	 0.6510
V	 0.7969	 0.6830
W	 0.7951	 0.6810
X	 0.7809	 0.6520
Y	 0.5005	 0.6180
Z	 0.7515	 0.6580
a	 0.7744	 0.6690
b	 0.7237	 0.6390
c	 0.6591	 0.6390
d	 0.7900	 0.6640
e	 0.7115	 0.6450
f	 0.6872	 0.6400
g	 0.7718	 0.6460
h	 0.8131	 0.6680



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.7723	 0.6280
j	 0.8265	 0.6320
k	 0.7477	 0.6170
l	 0.8396	 0.6500
m	 0.7718	 0.6360
n	 0.8672	 0.6590
o	 0.8292	 0.6310
p	 0.8287	 0.6520
q	 0.8209	 0.6900
r	 0.7951	 0.6920
s	 0.7849	 0.6750