



wwPDB EM Validation Summary Report ⓘ

Dec 12, 2022 – 02:43 am GMT

PDB ID : 6TMK
EMDB ID : EMD-10524
Title : Cryo-EM structure of Toxoplasma gondii mitochondrial ATP synthase dimer, composite model
Authors : Muhleip, A.; Kock Flygaard, R.; Amunts, A.
Deposited on : 2019-12-04
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

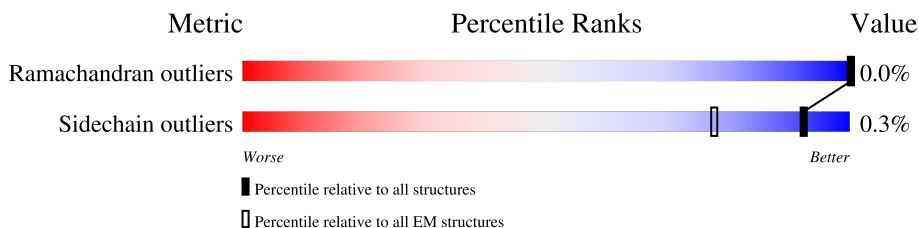
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.90 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.



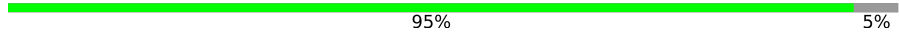








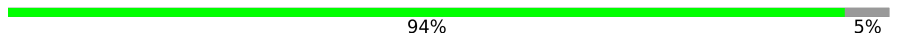
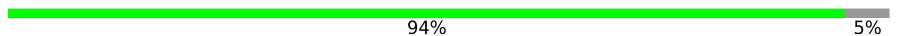


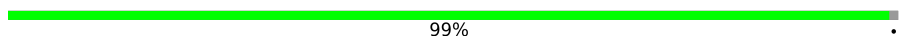



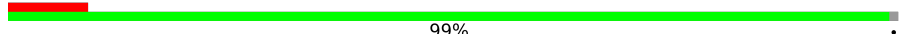
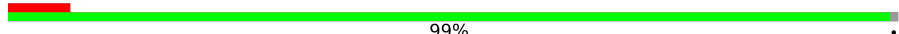


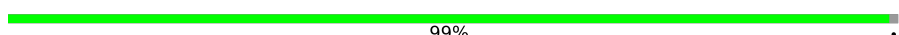
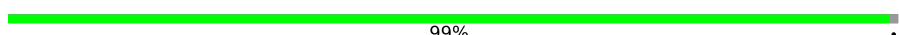
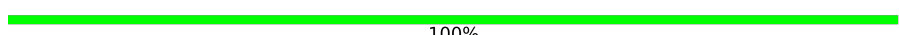
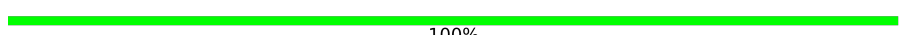
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	Q	134	98% ..
1	q	134	99% .
2	I	236	38% 62%
2	i	236	38% 62%
3	T	133	69% 31%
3	t	133	69% 31%
4	G	252	44% 56%
4	g	252	44% 56%
5	O	157	95% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	o	157	 95% 5%
6	K	224	 52% 48%
6	k	224	 52% 48%
7	J	229	 76% 23%
7	j	229	 76% 23%
8	S	128	 74% 26%
8	s	128	 74% 26%
9	U	126	 75% 25%
9	u	126	 75% 25%
10	H	239	 94% 5%
10	h	239	 94% 5%
11	E	325	 43% 57%
11	e	325	 43% 57%
12	X	83	 99%
12	x	83	 99%
13	B	571	 18% 85% 15%
13	b	571	 12% 85% 15%
14	R	134	 9% 99%
14	r	134	 7% 99%
15	P	138	 78% 22%
15	p	138	 78% 22%
16	V	111	 99%
16	v	111	 99%
17	L	208	 100%
17	l	208	 100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
18	C	398	31% 69%
18	c	398	31% 69%
19	D	310	82% 18%
19	d	310	82% 18%
20	M	205	47% 53%
20	m	205	47% 53%
21	N	166	96% ..
21	n	166	96% ..
22	F	267	70% 30%
22	f	267	70% 30%
23	W	106	91% . 8%
23	w	106	91% . 8%
24	A	536	5% 87% 13%
24	a	536	6% 87% 13%
25	i1	145	28% 72%
25	i2	145	28% 72%
26	A1	565	38% 90% 9%
26	A2	565	51% 90% 9%
26	C1	565	16% 90% 10%
26	C2	565	15% 90% 10%
26	E1	565	33% 90% 10%
26	E2	565	42% 90% 10%
27	B1	560	16% 84% . 14%
27	B2	560	21% 85% 14%
27	D1	560	19% 85% 15%







Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	D2	560	23% 85% 15%
27	F1	560	45% 84% 15%
27	F2	560	52% 84% 15%
28	g1	314	6% 87% 13%
28	g2	314	5% 87% 13%
29	d1	183	15% 78% 22%
29	d2	183	8% 78% 22%
30	e1	73	89% 11%
30	e2	73	89% 11%
31	G1	252	39% 71% 29%
31	G2	252	47% 71% 29%
32	H1	166	40% 57%
32	H2	166	43% 57%
32	I1	166	5% 42% 57%
32	I2	166	42% 57%
32	J1	166	6% 43% 57%
32	J2	166	43% 57%
32	K1	166	8% 42% 57%
32	K2	166	43% 57%
32	L1	166	42% 57%
32	L2	166	5% 42% 57%
32	M1	166	42% 57%
32	M2	166	5% 43% 57%
32	N1	166	43% 57%
32	N2	166	43% 57%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
32	O1	166	 43% 57%
32	O2	166	 43% 57%
32	P1	166	 43% 57%
32	P2	166	 43% 57%
32	Q1	166	 42% 57%
32	Q2	166	 43% 57%

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 266834 atoms, of which 134048 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 ATPTG11.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	q	133	Total	C	H	N	O	S	0	0
			2119	674	1044	194	202	5		
1	Q	133	Total	C	H	N	O	S	0	0
			2119	674	1044	194	202	5		

- Molecule 2 is a protein called ATPTG7.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	i	90	Total	C	H	N	O	S	0	0
			1386	433	678	136	129	10		
2	I	90	Total	C	H	N	O	S	0	0
			1386	433	678	136	129	10		

- Molecule 3 is a protein called ATPTG14.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	t	92	Total	C	H	N	O	S	0	0
			1439	463	716	127	129	4		
3	T	92	Total	C	H	N	O	S	0	0
			1439	463	716	127	129	4		

- Molecule 4 is a protein called ATPTG5.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	g	112	Total	C	H	N	O	S	0	0
			1732	548	856	152	168	8		
4	G	112	Total	C	H	N	O	S	0	0
			1732	548	856	152	168	8		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	51	VAL	PHE	conflict	UNP S7WD71

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
g	73	CYS	SER	conflict	UNP S7WD71
g	110	LYS	GLU	conflict	UNP S7WD71
g	233	THR	MET	conflict	UNP S7WD71
G	51	VAL	PHE	conflict	UNP S7WD71
G	73	CYS	SER	conflict	UNP S7WD71
G	110	LYS	GLU	conflict	UNP S7WD71
G	233	THR	MET	conflict	UNP S7WD71

- Molecule 5 is a protein called subunit k.

Mol	Chain	Residues	Atoms					AltConf	Trace	
5	o	149	Total	C	H	N	O	S	0	0
			2415	786	1195	210	219	5		
5	O	149	Total	C	H	N	O	S	0	0
			2415	786	1195	210	219	5		

- Molecule 6 is a protein called subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace	
6	k	117	Total	C	H	N	O	S	0	0
			1904	645	952	145	155	7		
6	K	117	Total	C	H	N	O	S	0	0
			1904	645	952	145	155	7		

- Molecule 7 is a protein called subunit i/j.

Mol	Chain	Residues	Atoms					AltConf	Trace	
7	j	176	Total	C	H	N	O	S	0	0
			2981	1003	1469	261	244	4		
7	J	176	Total	C	H	N	O	S	0	0
			2981	1003	1469	261	244	4		

- Molecule 8 is a protein called ATPTG13.

Mol	Chain	Residues	Atoms					AltConf	Trace	
8	s	95	Total	C	H	N	O	S	0	0
			1570	526	770	130	142	2		
8	S	95	Total	C	H	N	O	S	0	0
			1570	526	770	130	142	2		

- Molecule 9 is a protein called ATPTG15.

Mol	Chain	Residues	Atoms					AltConf	Trace	
9	u	94	Total	C	H	N	O	S	0	0
			1492	482	741	132	133	4		
9	U	94	Total	C	H	N	O	S	0	0
			1492	482	741	132	133	4		

- Molecule 10 is a protein called ATPTG6.

Mol	Chain	Residues	Atoms					AltConf	Trace	
10	h	226	Total	C	H	N	O	S	0	0
			3589	1157	1741	334	348	9		
10	H	226	Total	C	H	N	O	S	0	0
			3589	1157	1741	334	348	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	89	ASN	HIS	conflict	UNP A0A125YLR08
H	89	ASN	HIS	conflict	UNP A0A125YLR08

- Molecule 11 is a protein called ATPTG3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
11	e	140	Total	C	H	N	O	S	0	0
			2179	719	1064	187	204	5		
11	E	140	Total	C	H	N	O	S	0	0
			2179	719	1064	187	204	5		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	?	-	LYS	deletion	UNP A0A125YLR0
e	63	PRO	SER	conflict	UNP A0A125YLR0
e	99	LEU	PRO	conflict	UNP A0A125YLR0
e	312	ALA	THR	conflict	UNP A0A125YLR0
E	?	-	LYS	deletion	UNP A0A125YLR0
E	63	PRO	SER	conflict	UNP A0A125YLR0
E	99	LEU	PRO	conflict	UNP A0A125YLR0
E	312	ALA	THR	conflict	UNP A0A125YLR0

- Molecule 12 is a protein called ATPTG17.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	x	82	1298	420	639	116	120	3	0	0
12	X	82	1298	420	639	116	120	3	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	77	TRP	-	expression tag	UNP S7W180
x	78	MET	-	expression tag	UNP S7W180
x	79	PHE	-	expression tag	UNP S7W180
x	80	GLY	-	expression tag	UNP S7W180
x	81	ASN	-	expression tag	UNP S7W180
x	82	SER	-	expression tag	UNP S7W180
x	83	TYR	-	expression tag	UNP S7W180
X	77	TRP	-	expression tag	UNP S7W180
X	78	MET	-	expression tag	UNP S7W180
X	79	PHE	-	expression tag	UNP S7W180
X	80	GLY	-	expression tag	UNP S7W180
X	81	ASN	-	expression tag	UNP S7W180
X	82	SER	-	expression tag	UNP S7W180
X	83	TYR	-	expression tag	UNP S7W180

- Molecule 13 is a protein called subunit b.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
13	b	484	7841	2525	3909	652	740	15	0	0
13	B	484	7841	2525	3909	652	740	15	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	48	LEU	SER	conflict	UNP S7V2T0
b	472	THR	ALA	conflict	UNP S7V2T0
B	48	LEU	SER	conflict	UNP S7V2T0
B	472	THR	ALA	conflict	UNP S7V2T0

- Molecule 14 is a protein called ATPTG12.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
14	r	133	2144	681	1073	182	202	6	0	0
14	R	133	2144	681	1073	182	202	6	0	0

- Molecule 15 is a protein called ATPTG10.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
15	p	108	1711	553	847	148	157	6	0	0
15	P	108	1711	553	847	148	157	6	0	0

- Molecule 16 is a protein called subunit f.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
16	v	110	1801	590	888	170	148	5	0	0
16	V	110	1801	590	888	170	148	5	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	54	ALA	VAL	conflict	UNP S7UQT7
V	54	ALA	VAL	conflict	UNP S7UQT7

- Molecule 17 is a protein called ATPTG8.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
17	l	207	3273	1013	1647	298	305	10	0	0
17	L	207	3273	1013	1647	298	305	10	0	0

- Molecule 18 is a protein called ATPTG1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
18	c	122	2029	656	999	189	184	1	0	0
18	C	122	2029	656	999	189	184	1	0	0

- Molecule 19 is a protein called ATPTG2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
19	d	255	Total 4056	C 1326	H 1975	N 366	O 381	S 8	0	0
19	D	255	Total 4056	C 1326	H 1975	N 366	O 381	S 8	0	0

- Molecule 20 is a protein called subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
20	m	96	Total 1509	C 501	H 744	N 126	O 131	S 7	0	0
20	M	96	Total 1509	C 501	H 744	N 126	O 131	S 7	0	0

- Molecule 21 is a protein called ATPTG9.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
21	n	160	Total 2449	C 774	H 1202	N 227	O 235	S 11	0	0
21	N	160	Total 2449	C 774	H 1202	N 227	O 235	S 11	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	140	SER	ALA	conflict	UNP A0A125YUZ2
N	140	SER	ALA	conflict	UNP A0A125YUZ2

- Molecule 22 is a protein called ATPTG4.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
22	f	188	Total 2867	C 919	H 1425	N 245	O 274	S 4	0	0
22	F	188	Total 2867	C 919	H 1425	N 245	O 274	S 4	0	0

- Molecule 23 is a protein called ATPTG16.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
23	w	97	Total 1520	C 497	H 760	N 128	O 131	S 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
23	W	97	Total	C	H	N	O	S	0	0
			1520	497	760	128	131	4		

- Molecule 24 is a protein called subunit d.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
24	a	467	Total	C	H	N	O	S	0	0
			7396	2405	3616	656	698	21		
24	A	467	Total	C	H	N	O	S	0	0
			7396	2405	3616	656	698	21		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	351	THR	ALA	conflict	UNP S7V493
A	351	THR	ALA	conflict	UNP S7V493

- Molecule 25 is a protein called Inhibitor of F1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
25	i2	40	Total	C	H	N	O	S	0	0
			660	213	324	56	66	1		
25	i1	40	Total	C	H	N	O	S	0	0
			660	213	324	56	66	1		

- Molecule 26 is a protein called ATP synthase subunit alpha,subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
26	A2	512	Total	C	H	N	O	S	0	0
			7925	2464	4003	688	751	19		
26	E2	507	Total	C	H	N	O	S	0	0
			7848	2441	3962	682	744	19		
26	C2	507	Total	C	H	N	O	S	0	0
			7849	2442	3967	682	739	19		
26	A1	512	Total	C	H	N	O	S	0	0
			7925	2464	4003	688	751	19		
26	E1	507	Total	C	H	N	O	S	0	0
			7848	2441	3962	682	744	19		
26	C1	507	Total	C	H	N	O	S	0	0
			7849	2442	3967	682	739	19		

- Molecule 27 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	B2	479	Total	C	H	N	O	S	0	0
			7314	2293	3676	628	703	14		
27	F2	475	Total	C	H	N	O	S	0	0
			7265	2278	3653	624	696	14		
27	D2	475	Total	C	H	N	O	S	0	0
			7265	2278	3653	624	696	14		
27	B1	479	Total	C	H	N	O	S	0	0
			7314	2293	3676	628	703	14		
27	F1	475	Total	C	H	N	O	S	0	0
			7265	2278	3653	624	696	14		
27	D1	475	Total	C	H	N	O	S	0	0
			7265	2278	3653	624	696	14		

- Molecule 28 is a protein called ATP synthase subunit gamma.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	g2	272	Total	C	H	N	O	S	0	0
			4289	1330	2173	376	394	16		
28	g1	272	Total	C	H	N	O	S	0	0
			4289	1330	2173	376	394	16		

- Molecule 29 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	d2	143	Total	C	H	N	O	S	0	0
			2145	667	1076	181	216	5		
29	d1	143	Total	C	H	N	O	S	0	0
			2145	667	1076	181	216	5		

- Molecule 30 is a protein called ATP synthase subunit epsilon.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	e2	65	Total	C	H	N	O	S	0	0
			1077	337	539	99	98	4		
30	e1	65	Total	C	H	N	O	S	0	0
			1077	337	539	99	98	4		

- Molecule 31 is a protein called Oligomycin sensitivity conferring protein (OSCP).

Mol	Chain	Residues	Atoms						AltConf	Trace
31	G2	180	Total	C	H	N	O	S	0	0
			2901	895	1486	255	261	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O	S		
31	G1	180	2901	895	1486	255	261	4	0	0

- Molecule 32 is a protein called subunit c.

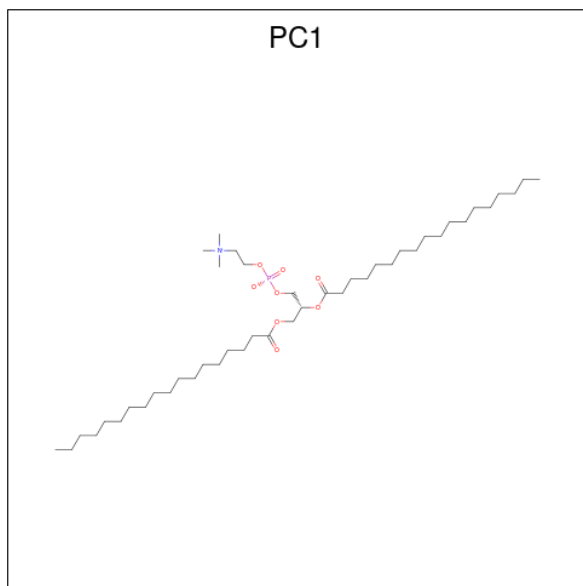
Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O	S		
32	H2	71	1028	328	527	77	92	4	0	0
32	I2	71	1028	328	527	77	92	4	0	0
32	J2	71	1028	328	527	77	92	4	0	0
32	K2	71	1028	328	527	77	92	4	0	0
32	L2	71	1028	328	527	77	92	4	0	0
32	M2	71	1028	328	527	77	92	4	0	0
32	N2	71	1028	328	527	77	92	4	0	0
32	O2	71	1028	328	527	77	92	4	0	0
32	P2	71	1028	328	527	77	92	4	0	0
32	Q2	71	1028	328	527	77	92	4	0	0
32	H1	71	1028	328	527	77	92	4	0	0
32	I1	71	1028	328	527	77	92	4	0	0
32	J1	71	1028	328	527	77	92	4	0	0
32	K1	71	1028	328	527	77	92	4	0	0
32	L1	71	1028	328	527	77	92	4	0	0
32	M1	71	1028	328	527	77	92	4	0	0
32	N1	71	1028	328	527	77	92	4	0	0
32	O1	71	1028	328	527	77	92	4	0	0

Continued on next page...

Continued from previous page...

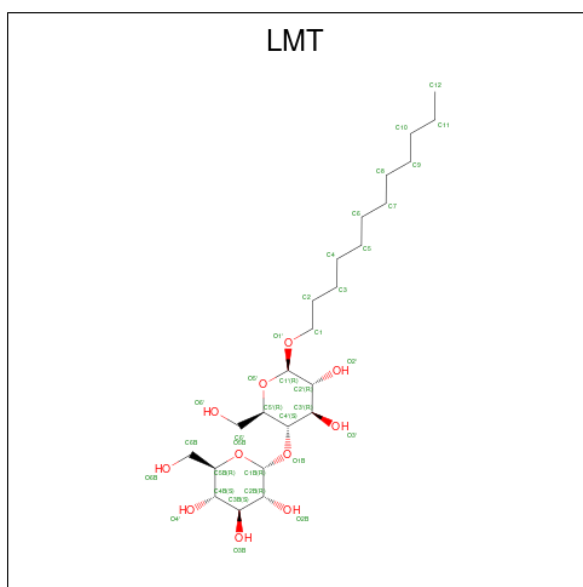
Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
32	P1	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		
32	Q1	71	Total	C	H	N	O	S	0	0
			1028	328	527	77	92	4		

- Molecule 33 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



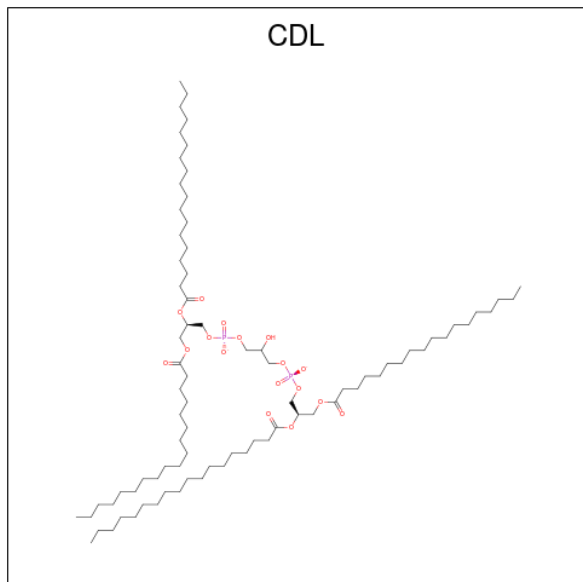
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
33	o	1	Total	C	H	N	O	P	0
			284	88	176	2	16	2	
33	o	1	Total	C	H	N	O	P	0
			284	88	176	2	16	2	
33	v	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
33	O	1	Total	C	H	N	O	P	0
			284	88	176	2	16	2	
33	O	1	Total	C	H	N	O	P	0
			284	88	176	2	16	2	
33	V	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	

- Molecule 34 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
34	o	1	81	24	46	11	0
34	h	1	81	24	46	11	0
34	x	1	81	24	46	11	0
34	c	1	162	48	92	22	0
34	c	1	162	48	92	22	0
34	d	1	162	48	92	22	0
34	d	1	162	48	92	22	0
34	O	1	81	24	46	11	0
34	H	1	81	24	46	11	0
34	X	1	81	24	46	11	0
34	C	1	162	48	92	22	0
34	C	1	162	48	92	22	0
34	D	1	162	48	92	22	0
34	D	1	162	48	92	22	0

- Molecule 35 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



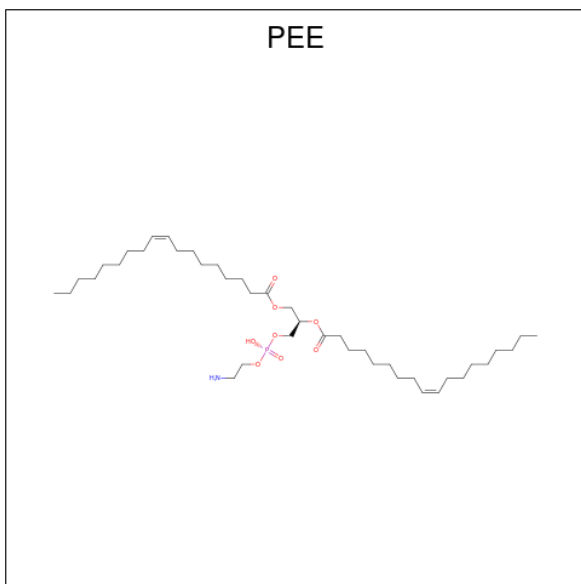
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
35	o	1	256	81	156	17	2	0
35	u	1	256	81	156	17	2	0
35	h	1	256	81	156	17	2	0
35	e	1	256	81	156	17	2	0
35	b	1	512	162	312	34	4	0
35	b	1	512	162	312	34	4	0
35	v	1	256	81	156	17	2	0
35	c	1	256	81	156	17	2	0
35	d	1	256	81	156	17	2	0
35	O	1	256	81	156	17	2	0
35	U	1	256	81	156	17	2	0
35	H	1	256	81	156	17	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
35	E	1	Total 256	C 81	H 156	O 17	P 2	0
35	B	1	Total 512	C 162	H 312	O 34	P 4	0
35	B	1	Total 512	C 162	H 312	O 34	P 4	0
35	V	1	Total 256	C 81	H 156	O 17	P 2	0
35	C	1	Total 256	C 81	H 156	O 17	P 2	0
35	D	1	Total 256	C 81	H 156	O 17	P 2	0

- Molecule 36 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



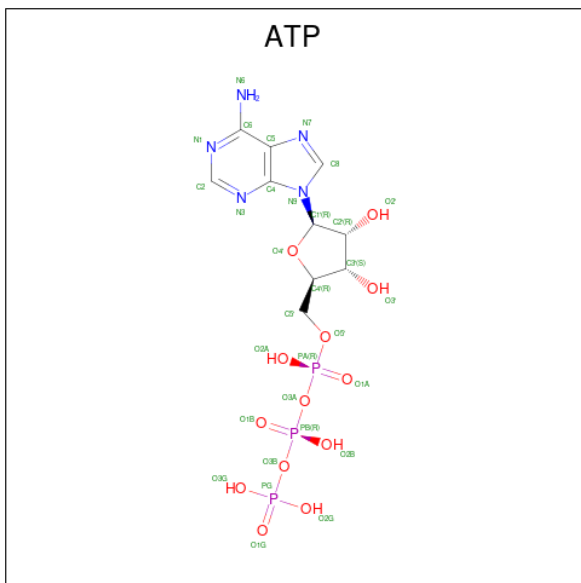
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
36	j	1	Total 266	C 82	H 164	N 2	O 16	P 2	0
36	j	1	Total 266	C 82	H 164	N 2	O 16	P 2	0
36	c	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
36	J	1	Total 266	C 82	H 164	N 2	O 16	P 2	0
36	J	1	Total 266	C 82	H 164	N 2	O 16	P 2	0

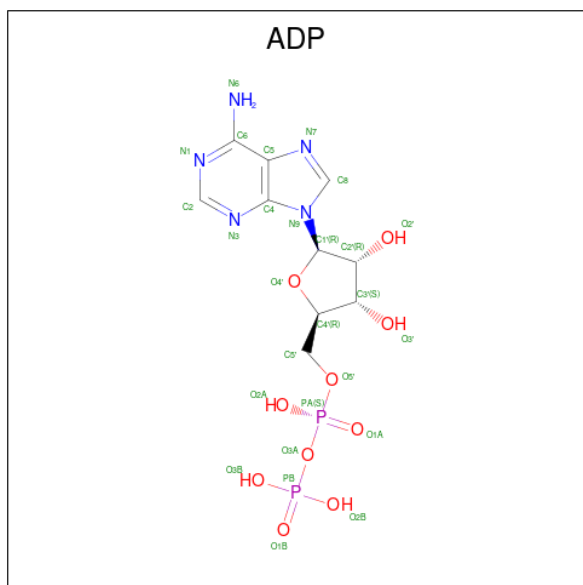
Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
36	C	1	133	41	82	1	8	1	0

- Molecule 37 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



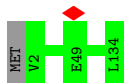


Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
38	B2	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
38	D2	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	
38	B1	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	
38	D1	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	

3 Residue-property plots [i](#)

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

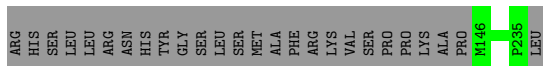
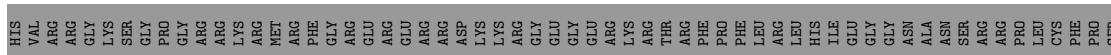
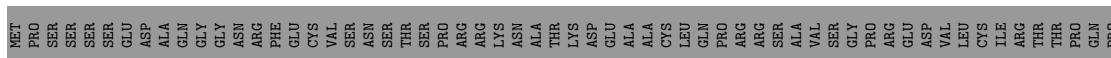
- Molecule 1: ATPTG11



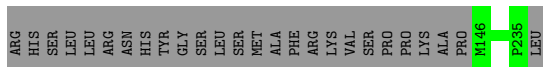
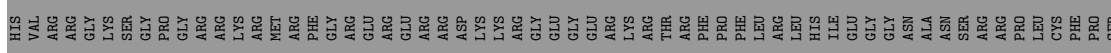
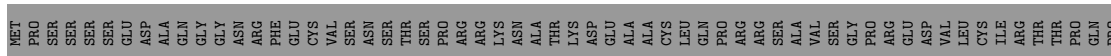
- Molecule 1: ATPTG11

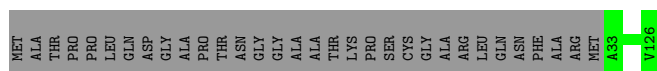


- Molecule 2: ATPTG7

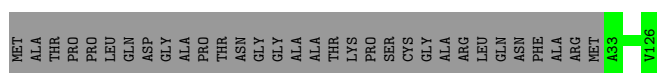
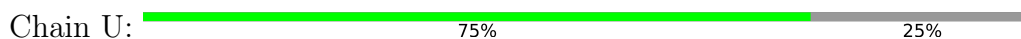


- Molecule 2: ATPTG7

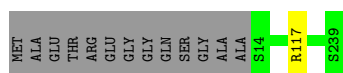




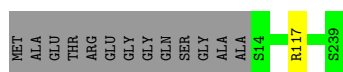
● Molecule 9: ATPTG15



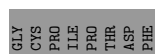
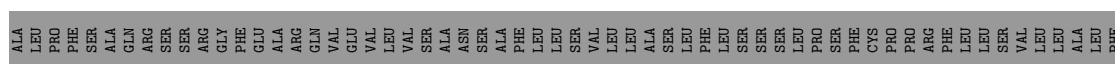
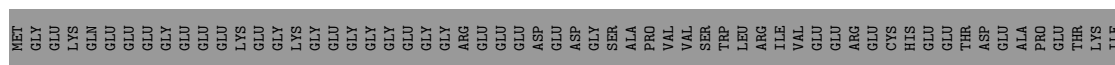
● Molecule 10: ATPTG6



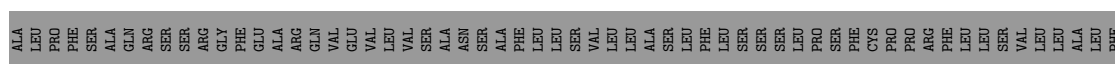
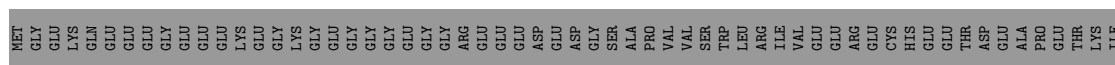
● Molecule 10: ATPTG6



● Molecule 11: ATPTG3

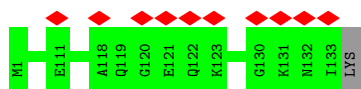


● Molecule 11: ATPTG3

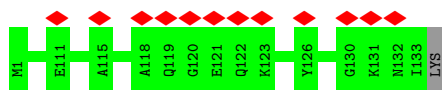




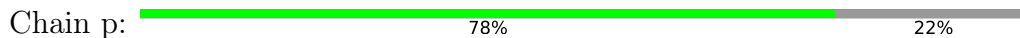
• Molecule 14: ATPTG12



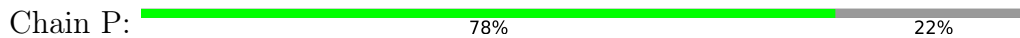
• Molecule 14: ATPTG12



• Molecule 15: ATPTG10



• Molecule 15: ATPTG10



• Molecule 16: subunit f

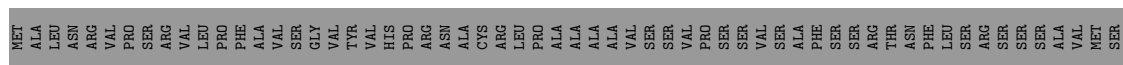


• Molecule 16: subunit f

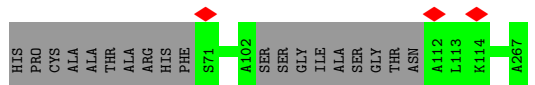
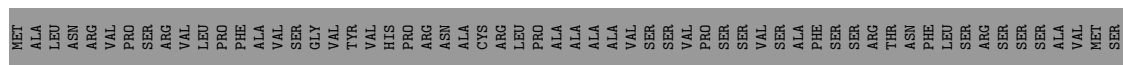


• Molecule 17: ATPTG8

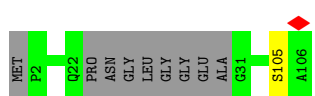
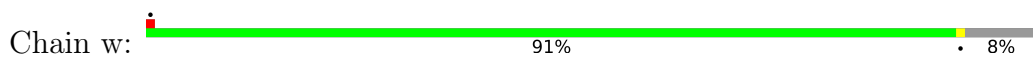




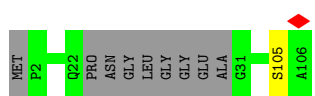
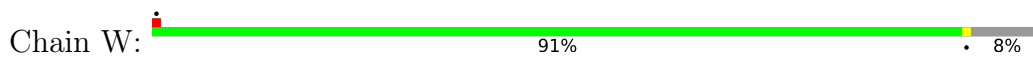
• Molecule 22: ATPTG4



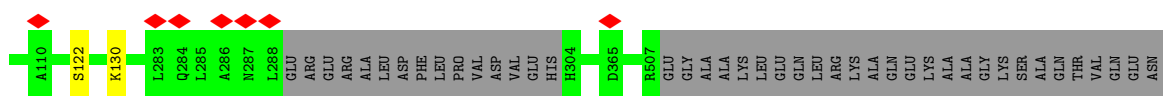
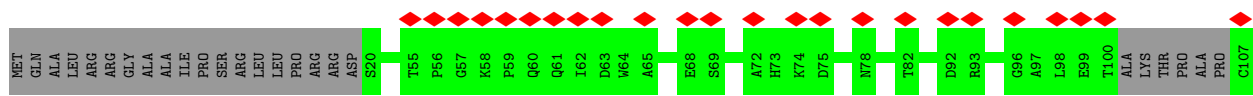
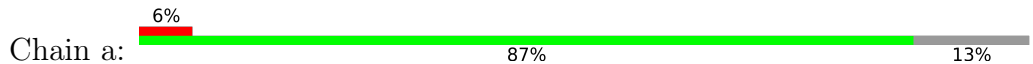
• Molecule 23: ATPTG16



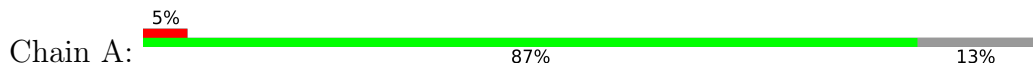
• Molecule 23: ATPTG16

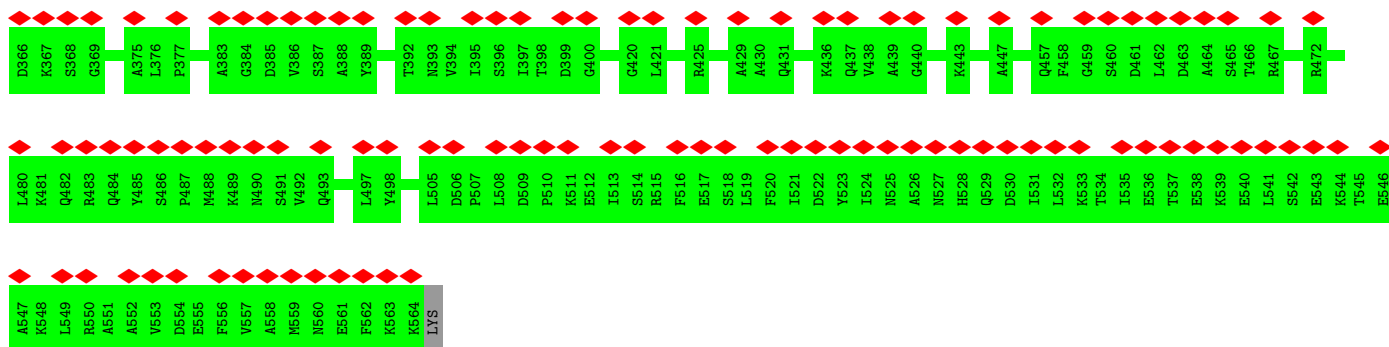


• Molecule 24: subunit d

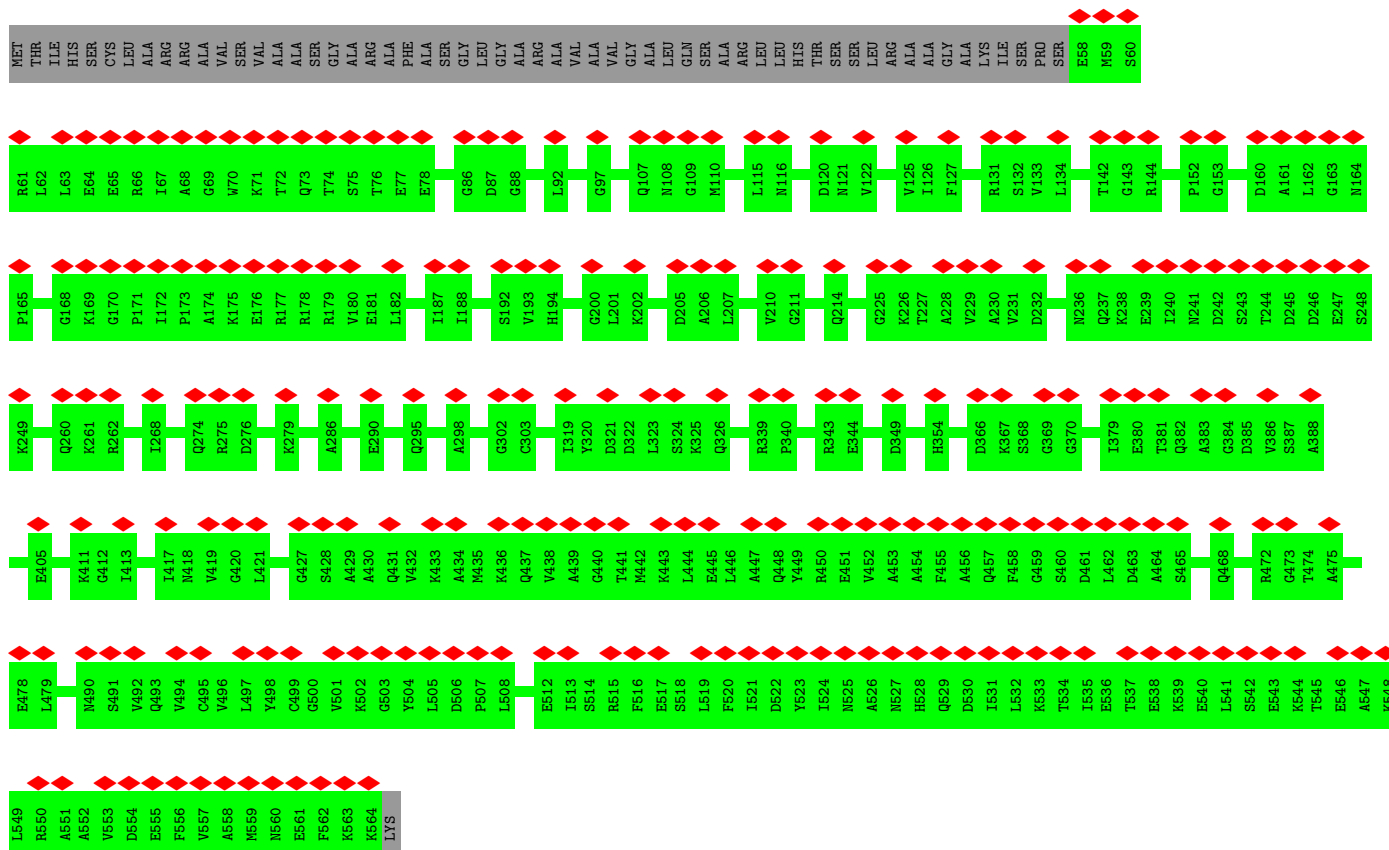
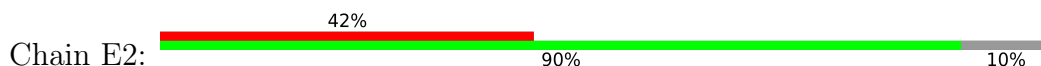


• Molecule 24: subunit d

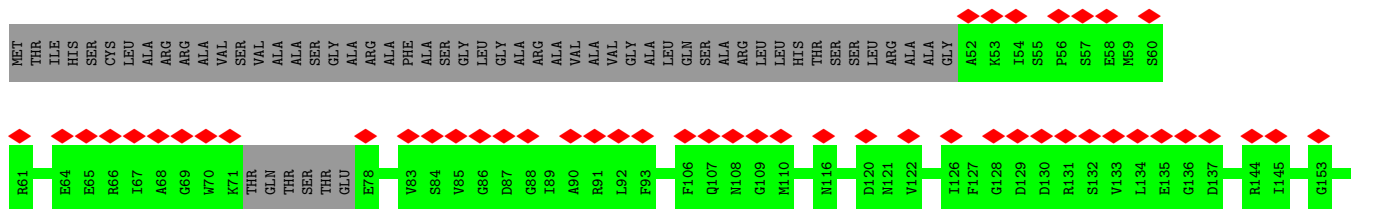
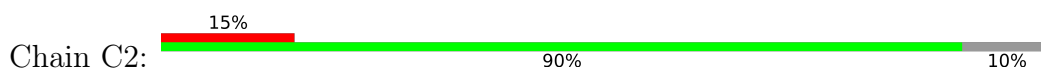


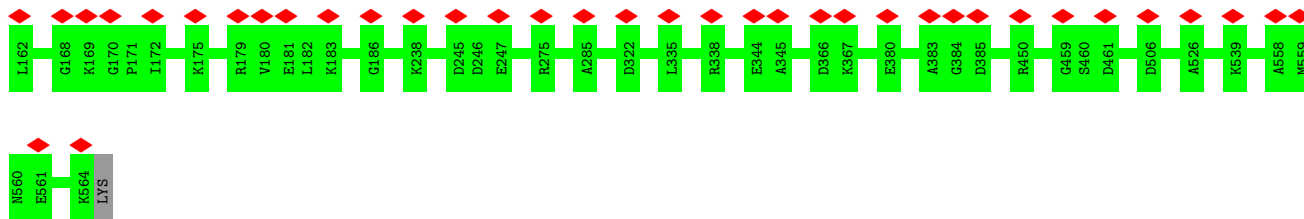


• Molecule 26: ATP synthase subunit alpha,subunit alpha

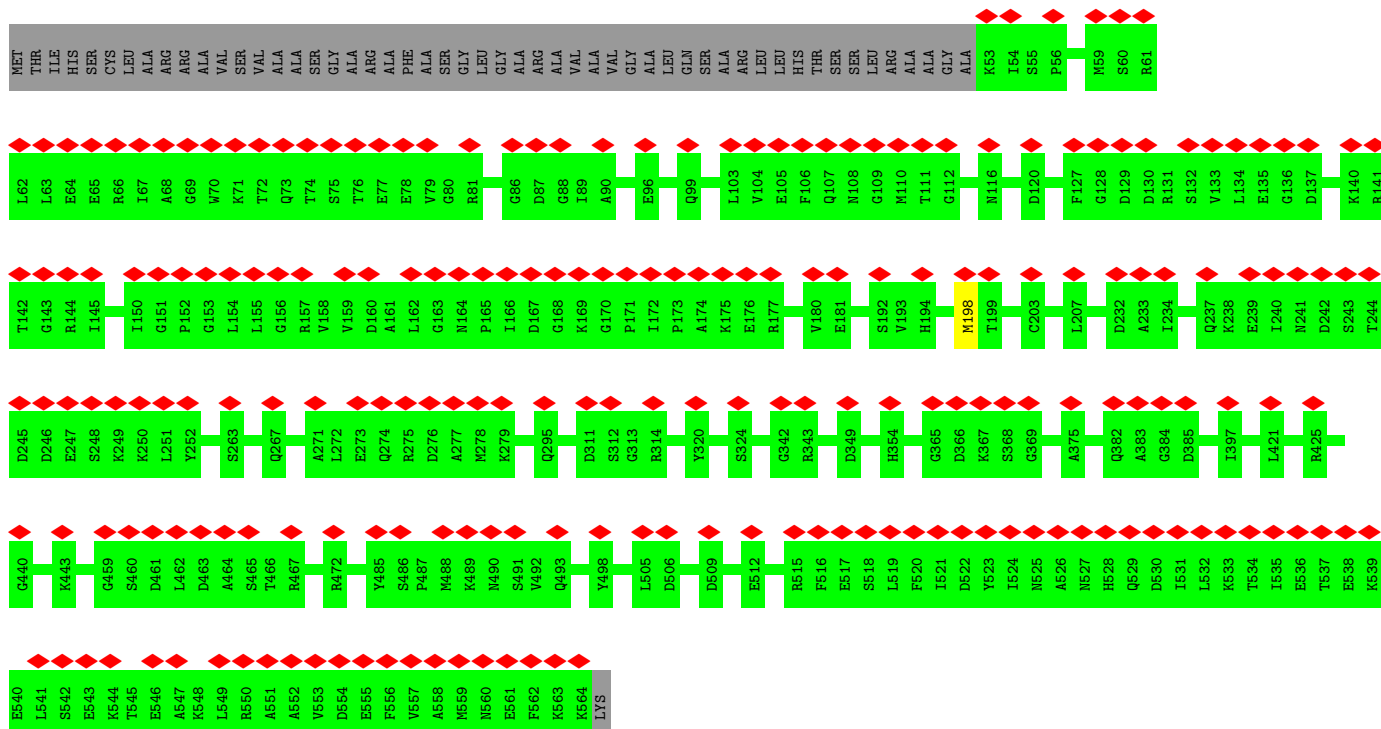
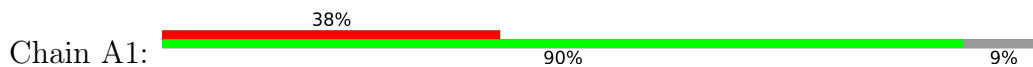


• Molecule 26: ATP synthase subunit alpha,subunit alpha

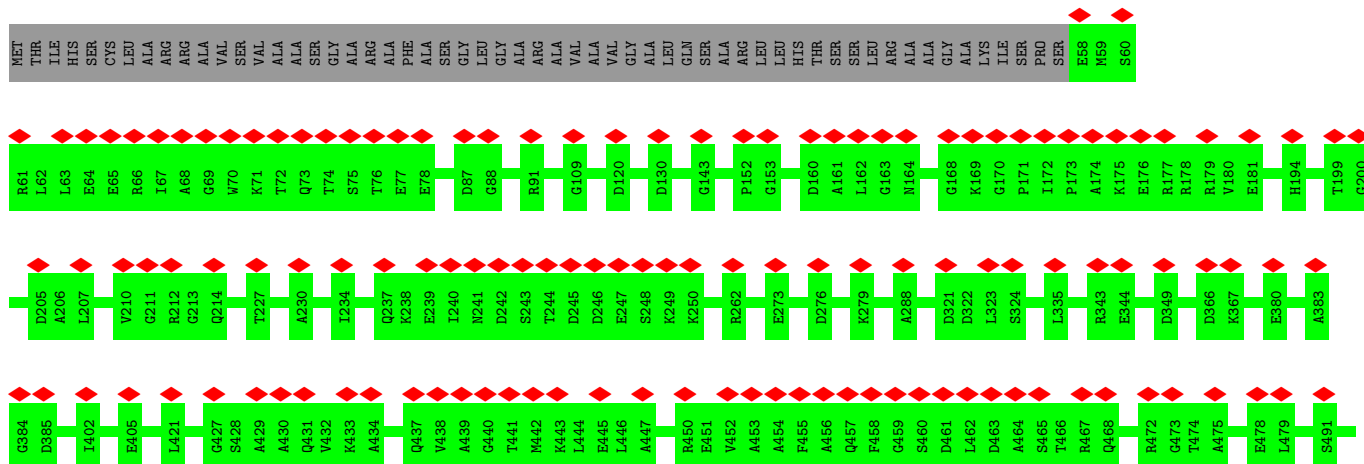
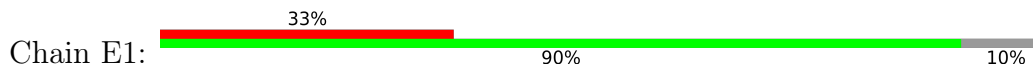




• Molecule 26: ATP synthase subunit alpha,subunit alpha

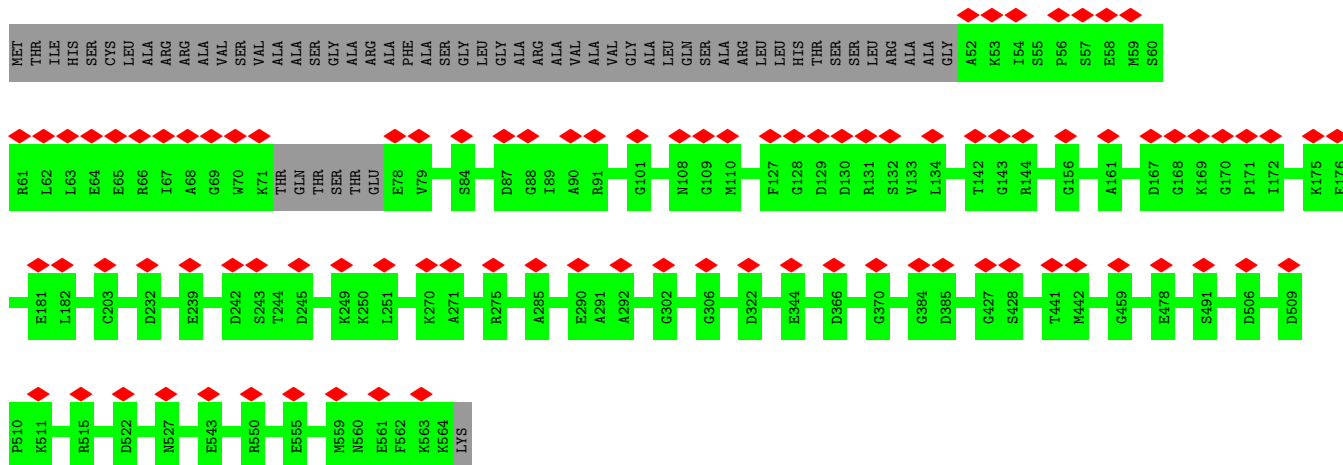
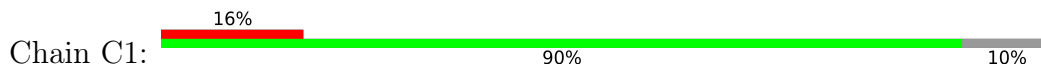


• Molecule 26: ATP synthase subunit alpha,subunit alpha

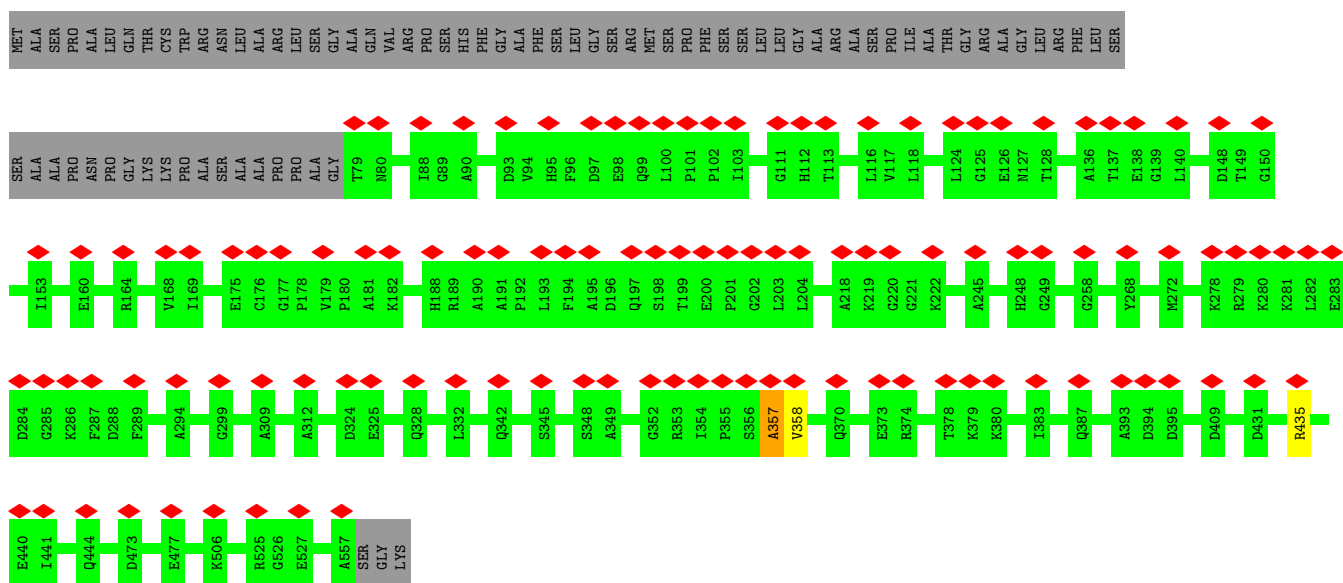
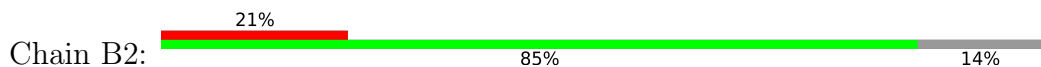




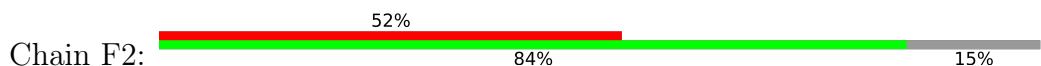
• Molecule 26: ATP synthase subunit alpha,subunit alpha

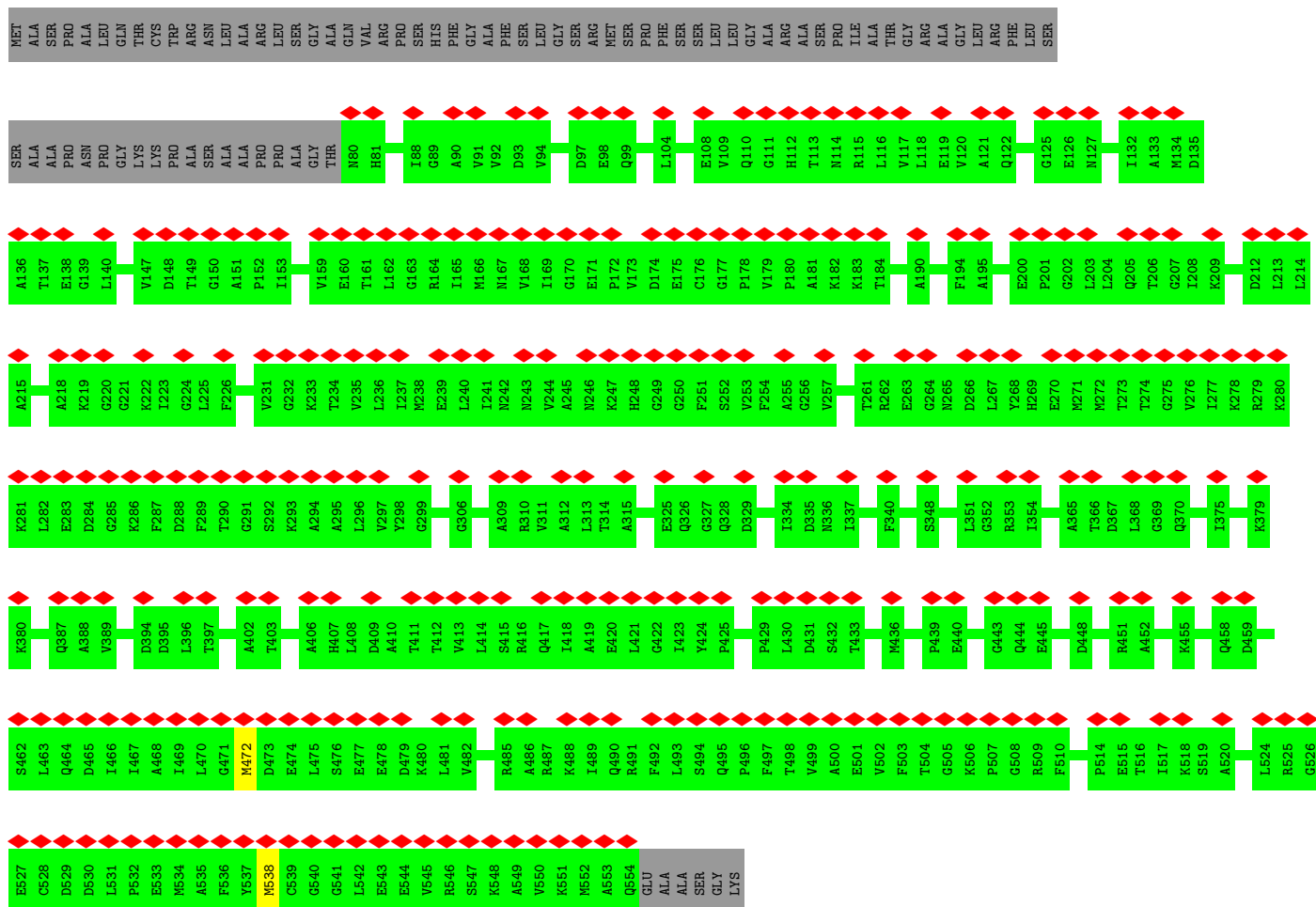


• Molecule 27: ATP synthase subunit beta

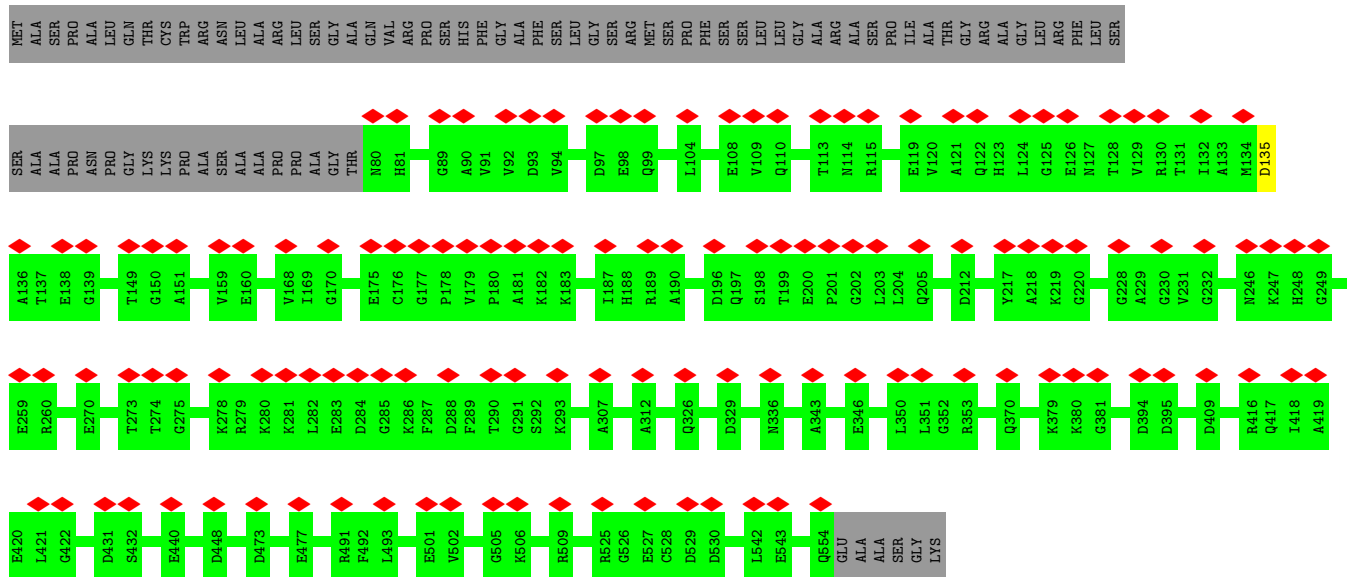
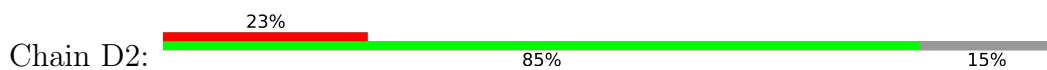


• Molecule 27: ATP synthase subunit beta

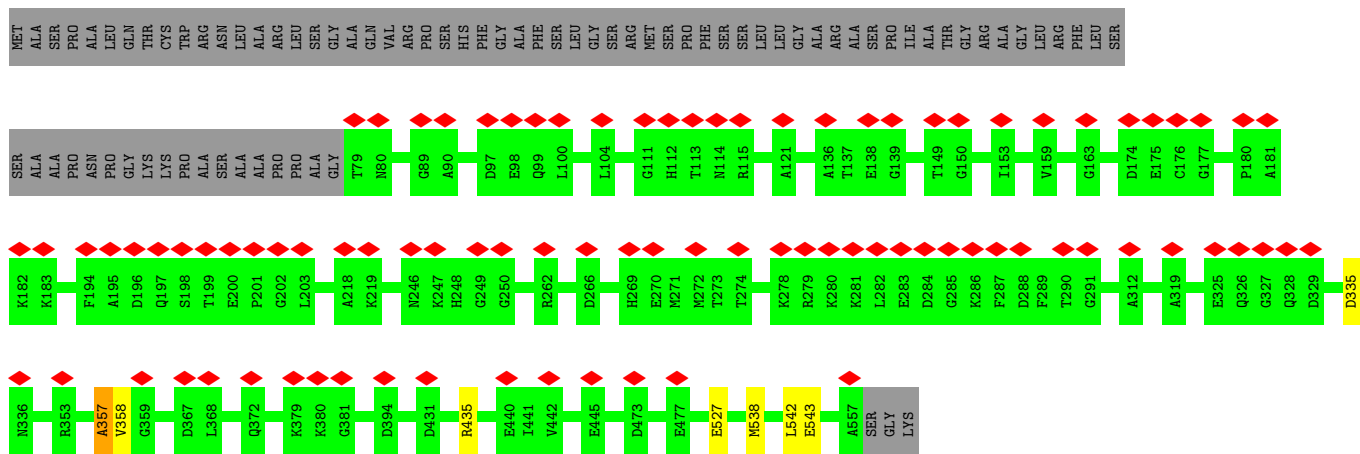
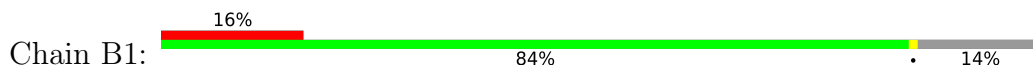




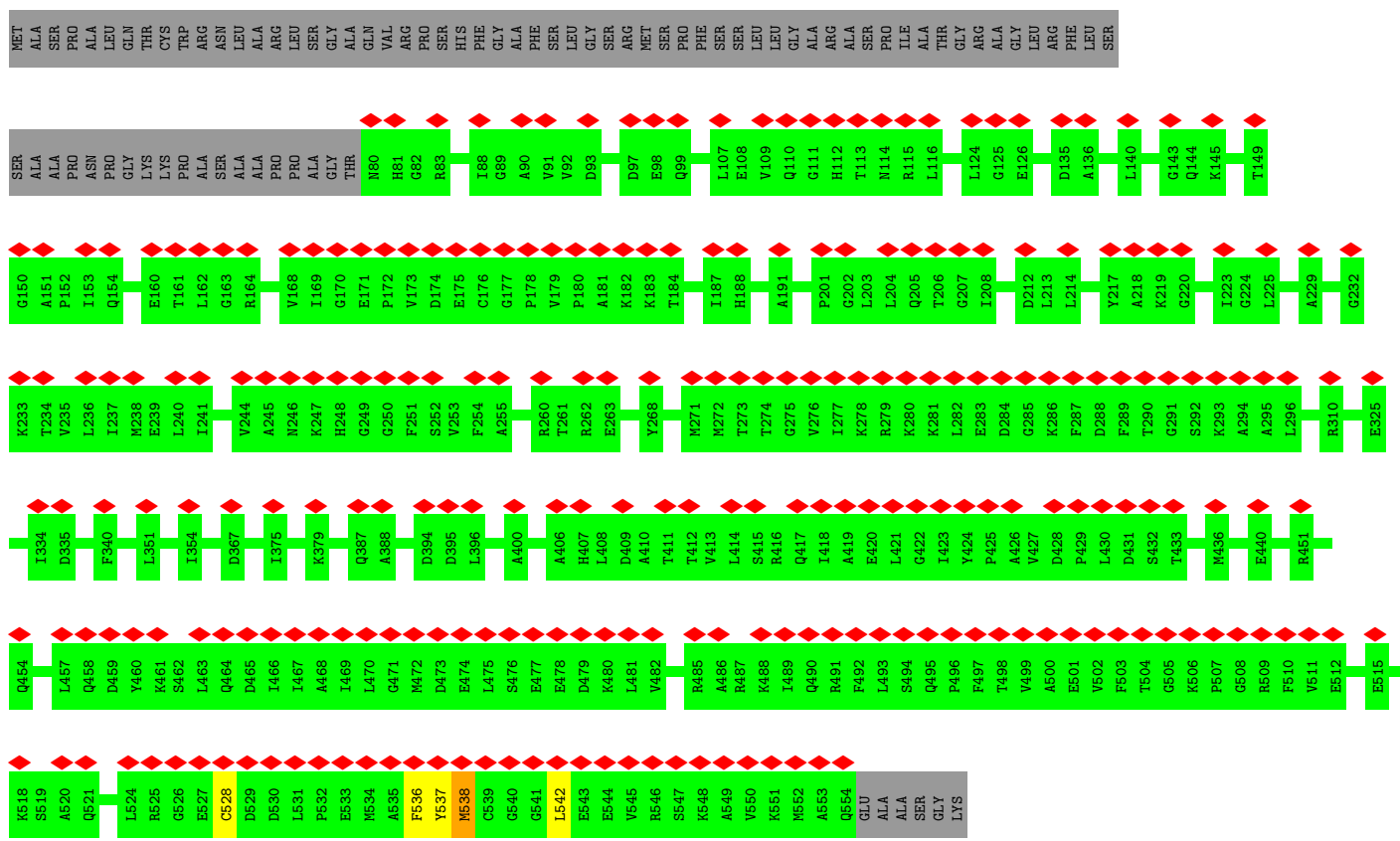
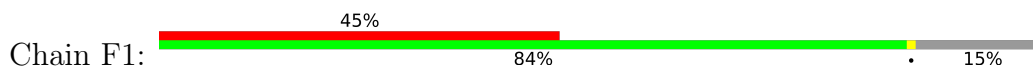
• Molecule 27: ATP synthase subunit beta



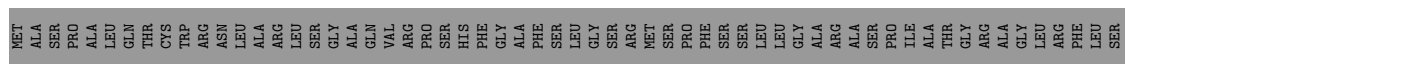
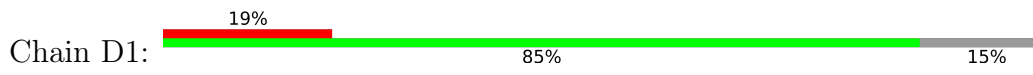
• Molecule 27: ATP synthase subunit beta

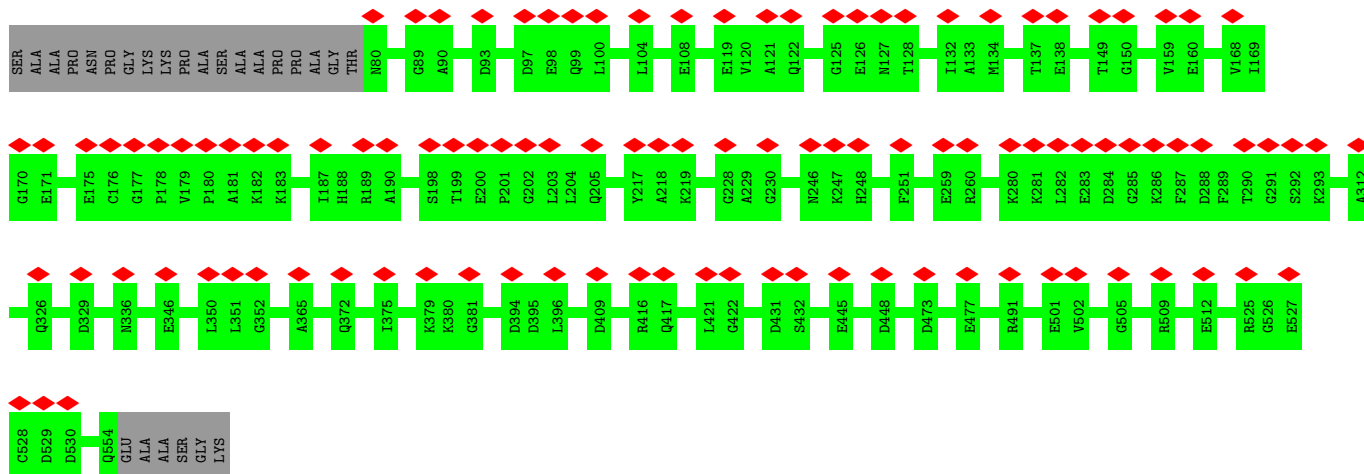


• Molecule 27: ATP synthase subunit beta

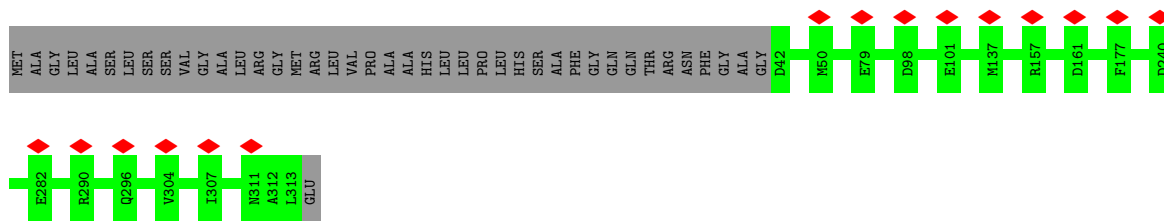
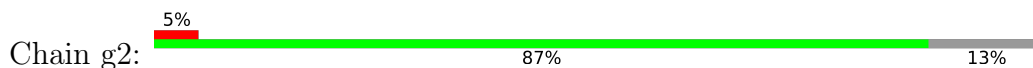


• Molecule 27: ATP synthase subunit beta

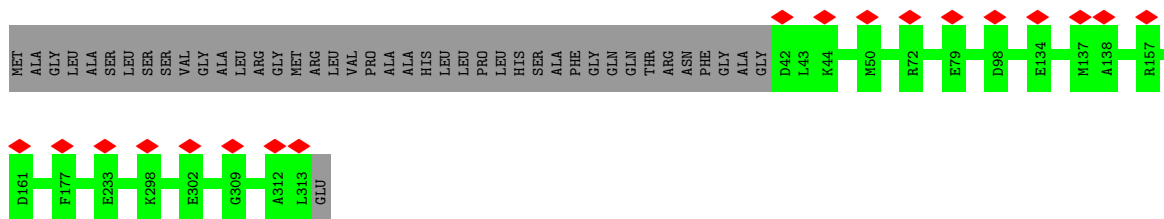
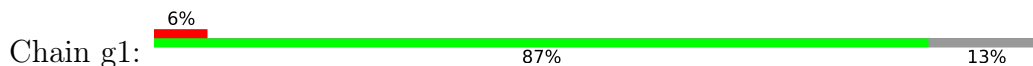




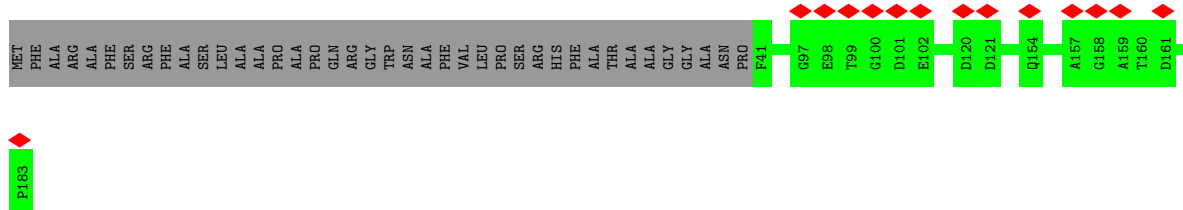
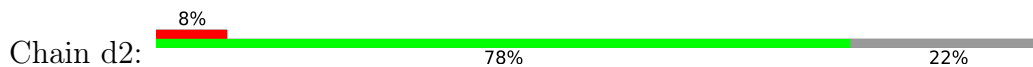
- Molecule 28: ATP synthase subunit gamma



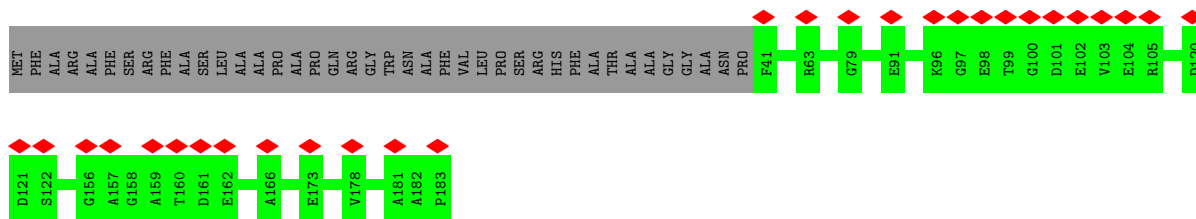
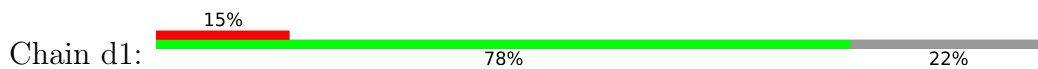
- Molecule 28: ATP synthase subunit gamma



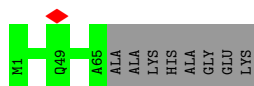
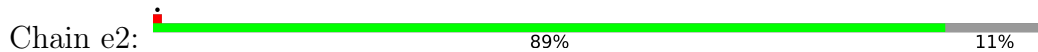
- Molecule 29: ATP synthase subunit delta



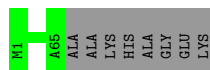
- Molecule 29: ATP synthase subunit delta



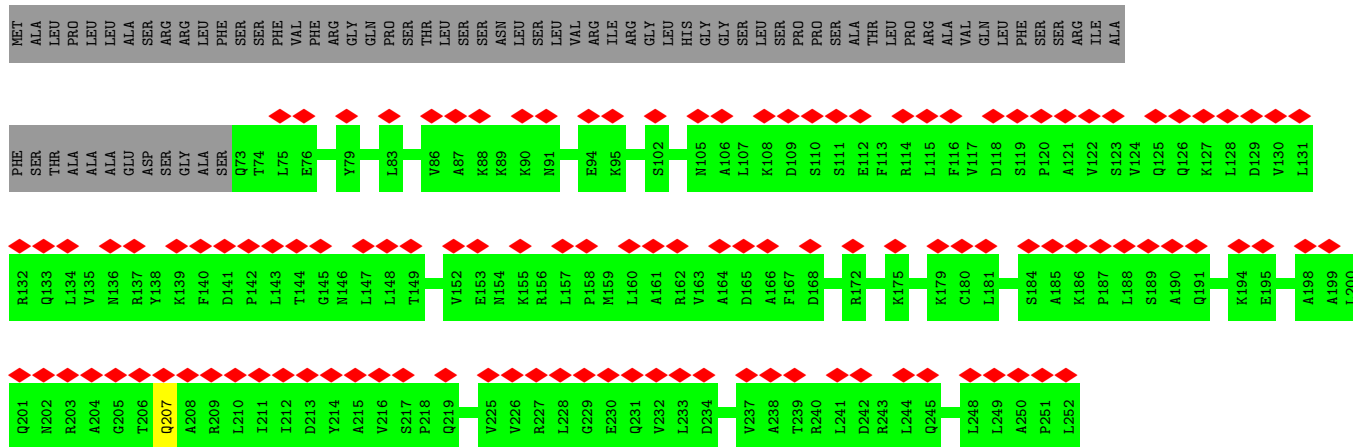
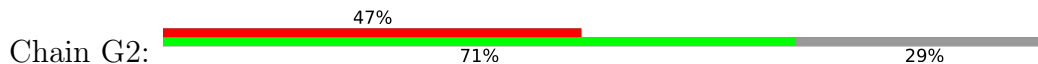
● Molecule 30: ATP synthase subunit epsilon



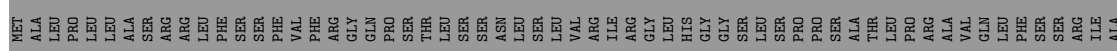
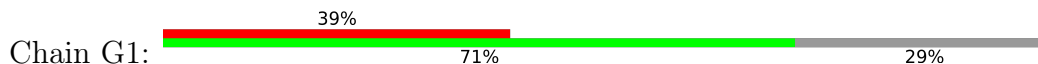
● Molecule 30: ATP synthase subunit epsilon

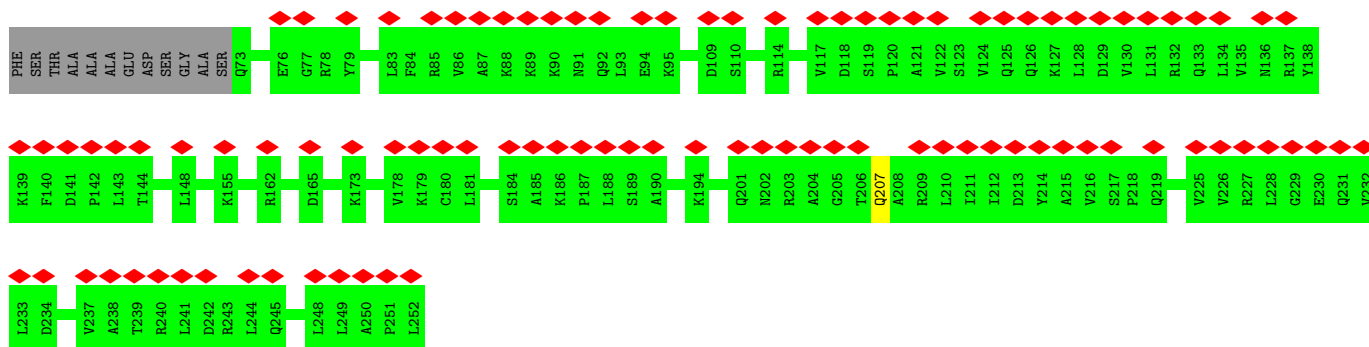


● Molecule 31: Oligomycin sensitivity conferring protein (OSCP)

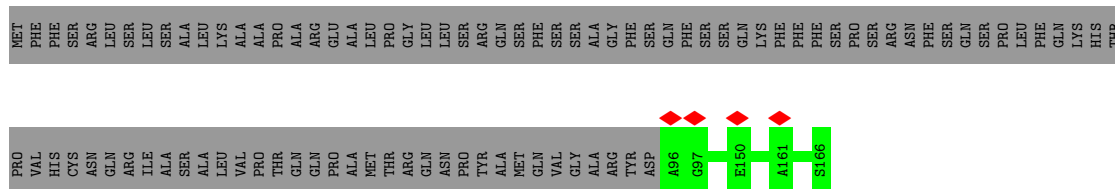


● Molecule 31: Oligomycin sensitivity conferring protein (OSCP)

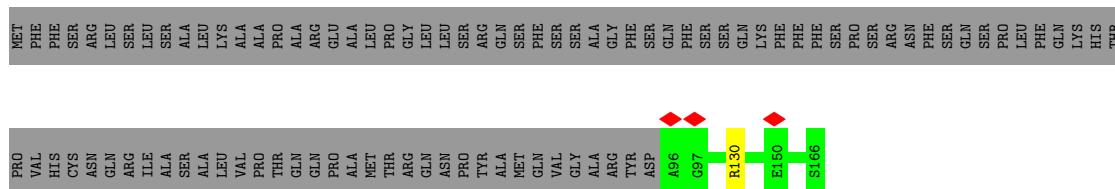




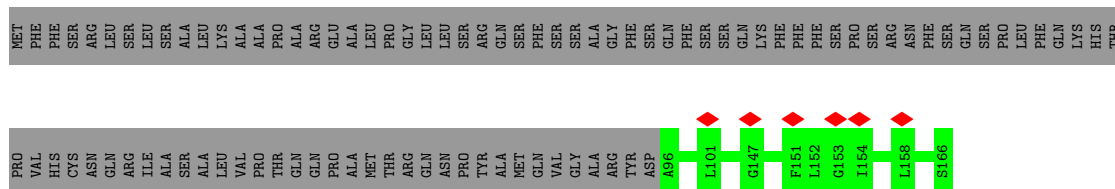
• Molecule 32: subunit c



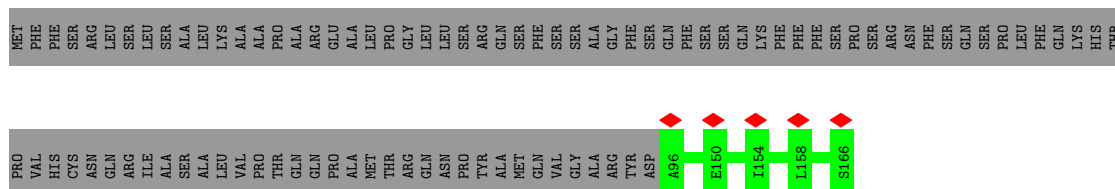
• Molecule 32: subunit c



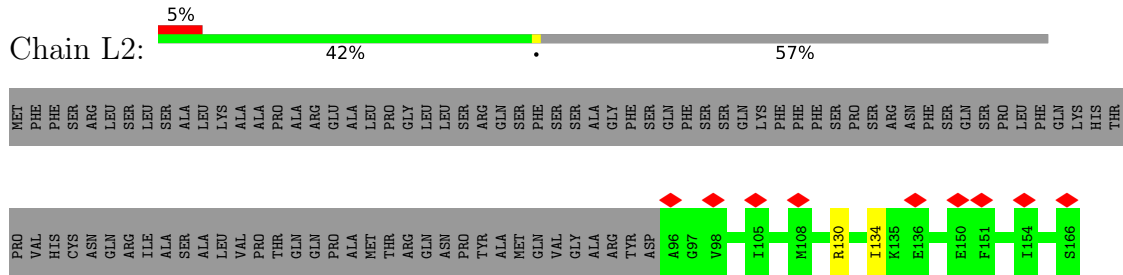
• Molecule 32: subunit c



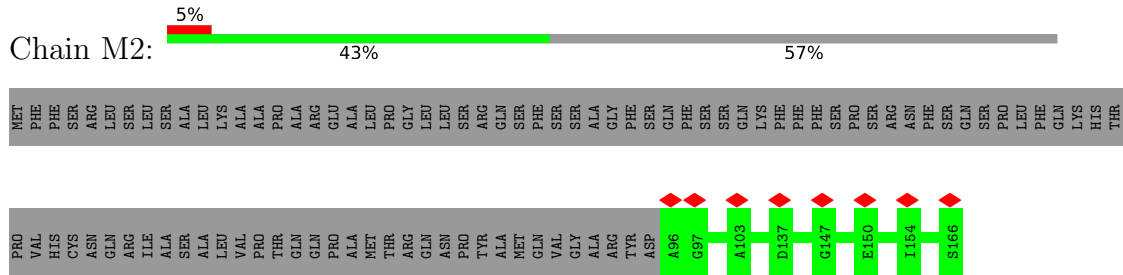
• Molecule 32: subunit c



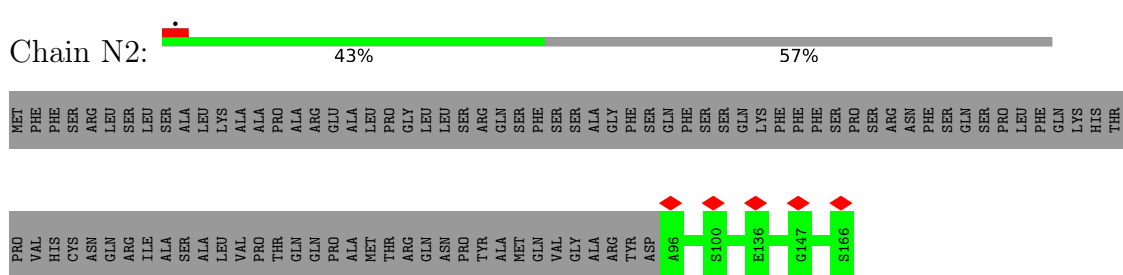
Molecule 32: subunit c



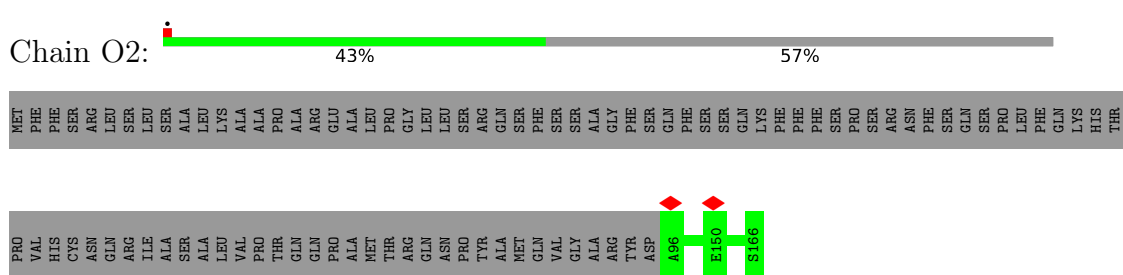
Molecule 32: subunit c



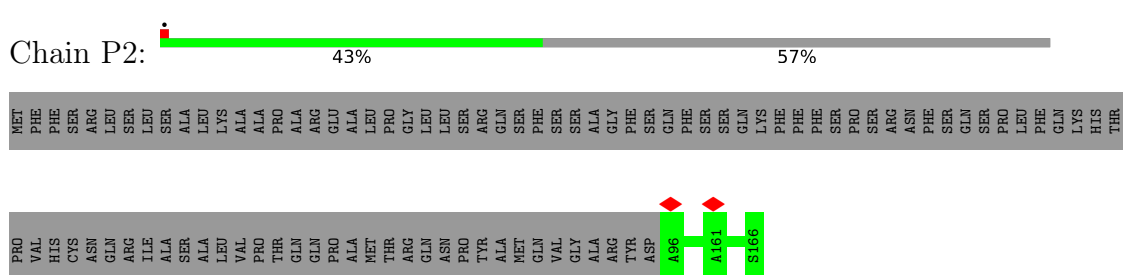
Molecule 32: subunit c



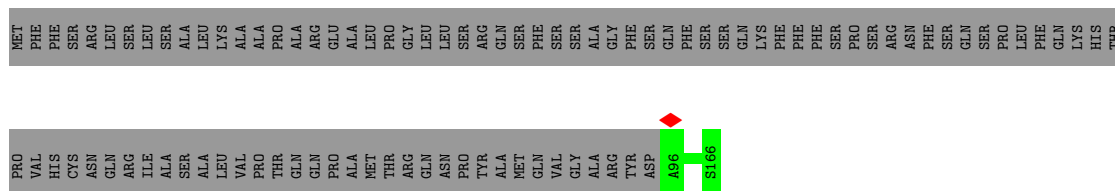
Molecule 32: subunit c



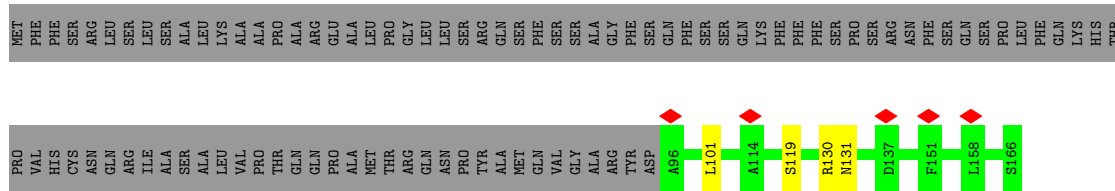
Molecule 32: subunit c



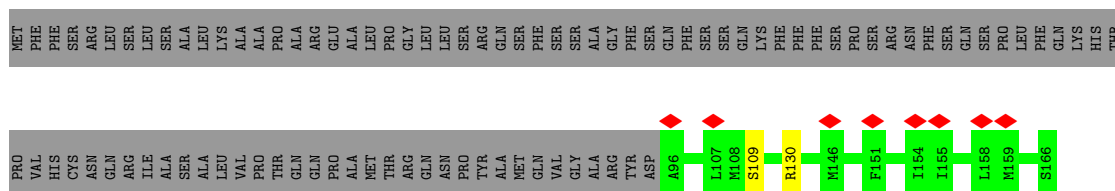
Molecule 32: subunit c



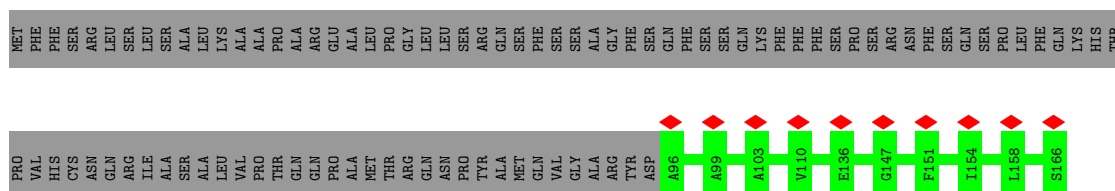
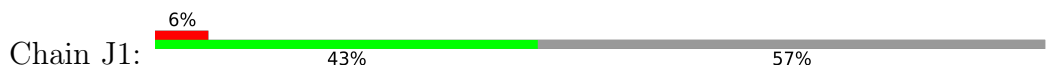
• Molecule 32: subunit c



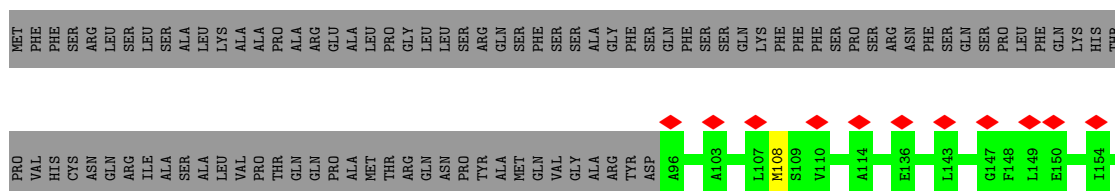
• Molecule 32: subunit c



• Molecule 32: subunit c



• Molecule 32: subunit c



• Molecule 32: subunit c



MET	PHE	PHE	ARG	LEU	SER	LEU	SER	ALA	LEU	LYS	ALA	ALA	PRO	PRO	ALA	ALA	ARG	GLU	PRO	ALA	LEU	PRO	GLY	LEU	LEU	SER	ARG	GLN	PHE	SER	SER	ALA	ALA	GLY	PHE	ASP	GLN	PHE	SER	SER	GLN	LYS	PHE	PHE	PHE	PRO	ARG	ASN	PHE	GLN	LEU	GLN	LYS	HIS	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

PRO	VAL	HIS	CYS	ASN	GLN	ARG	ILE	ALA	SER	LEU	VAL	VAL	PRO	THR	GLN	GLN	PRO	GLU	ALA	ALA	MET	THR	THR	GLY	LEU	LEU	ASN	TYR	ALA	GLN	PHE	VAL	GLY	ALA	ARG	TYR	ASP	A96	M146	E150	F151	I154	A161	S166
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------

• Molecule 32: subunit c



MET	PHE	PHE	ARG	LEU	SER	LEU	SER	ALA	LEU	LYS	ALA	ALA	PRO	PRO	ALA	ALA	ARG	GLU	PRO	ALA	LEU	PRO	GLY	LEU	LEU	SER	ARG	GLN	PHE	SER	SER	ALA	ALA	GLY	PHE	ASP	GLN	PHE	SER	SER	GLN	LYS	PHE	PHE	PHE	PRO	ARG	ASN	PHE	GLN	LEU	GLN	LYS	HIS	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

PRO	VAL	HIS	CYS	ASN	GLN	ARG	ILE	ALA	SER	LEU	VAL	VAL	PRO	THR	GLN	GLN	PRO	GLU	ALA	ALA	MET	THR	THR	GLY	LEU	LEU	ASN	TYR	ALA	GLN	PHE	VAL	GLY	ALA	ARG	TYR	ASP	A96	T128	E150	S166
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------

• Molecule 32: subunit c



MET	PHE	PHE	ARG	LEU	SER	LEU	SER	ALA	LEU	LYS	ALA	ALA	PRO	PRO	ALA	ALA	ARG	GLU	PRO	ALA	LEU	PRO	GLY	LEU	LEU	SER	ARG	GLN	PHE	SER	SER	ALA	ALA	GLY	PHE	ASP	GLN	PHE	SER	SER	GLN	LYS	PHE	PHE	PHE	PRO	ARG	ASN	PHE	GLN	LEU	GLN	LYS	HIS	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

PRO	VAL	HIS	CYS	ASN	GLN	ARG	ILE	ALA	SER	LEU	VAL	VAL	PRO	THR	GLN	GLN	PRO	GLU	ALA	ALA	MET	THR	THR	GLY	LEU	LEU	ASN	TYR	ALA	GLN	PHE	VAL	GLY	ALA	ARG	TYR	ASP	A96	E150	T154	S166
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------

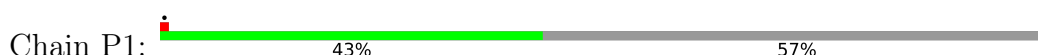
• Molecule 32: subunit c



MET	PHE	PHE	ARG	LEU	SER	LEU	SER	ALA	LEU	LYS	ALA	ALA	PRO	PRO	ALA	ALA	ARG	GLU	PRO	ALA	LEU	PRO	GLY	LEU	LEU	SER	ARG	GLN	PHE	SER	SER	ALA	ALA	GLY	PHE	ASP	GLN	PHE	SER	SER	GLN	LYS	PHE	PHE	PHE	PRO	ARG	ASN	PHE	GLN	LEU	GLN	LYS	HIS	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

PRO	VAL	HIS	CYS	ASN	GLN	ARG	ILE	ALA	SER	LEU	VAL	VAL	PRO	THR	GLN	GLN	PRO	GLU	ALA	ALA	MET	THR	THR	GLY	LEU	LEU	ASN	TYR	ALA	GLN	PHE	VAL	GLY	ALA	ARG	TYR	ASP	A96	E150	S166
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------

• Molecule 32: subunit c



MET	PHE	PHE	ARG	LEU	SER	LEU	SER	ALA	LEU	LYS	ALA	ALA	PRO	PRO	ALA	ALA	ARG	GLU	PRO	ALA	LEU	PRO	GLY	LEU	LEU	SER	ARG	GLN	PHE	SER	SER	ALA	ALA	GLY	PHE	ASP	GLN	PHE	SER	SER	GLN	LYS	PHE	PHE	PHE	PRO	ARG	ASN	PHE	GLN	LEU	GLN	LYS	HIS	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

PRO	VAL	HIS	CYS	ASN	GLN	ARG	ILE	ALA	SER	LEU	VAL	VAL	PRO	THR	GLN	GLN	PRO	GLU	ALA	ALA	MET	THR	THR	GLY	LEU	LEU	ASN	TYR	ALA	GLN	PHE	VAL	GLY	ALA	ARG	TYR	ASP	A96	H	S166
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	---	------

• Molecule 32: subunit c



MET PHE PHE PHE SER ARG LEU SER LEU SER ALA LEU LYS ALA ALA PRO ARG GLU ALA LEU PRO GLY GLN LEU LEU SER ARG GLN PHE SER SER ALA GLN TYR ASP

PRO VAL HIS CYS ASN GLN ARG ILE ALA SER LEU VAL PRO THR GLN GLN PRO MET THR ARG GLN ASN PRO TYR ALA MET THR ARG GLN ASN PRO TYR ALA MET THR ARG GLN ALA ARG TYR ASP
A96 R130 E136 D137 S166

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	101505	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	165000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.375	Depositor
Minimum map value	-0.174	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.024	Depositor
Map size (Å)	464.8, 464.8, 464.8	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PC1, CDL, ADP, ATP, LMT, PEE

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	Q	0.32	0/1103	0.43	0/1496
1	q	0.31	0/1103	0.43	0/1496
2	I	0.34	0/719	0.42	0/962
2	i	0.34	0/719	0.42	0/962
3	T	0.32	0/741	0.45	0/1007
3	t	0.32	0/741	0.44	0/1007
4	G	0.34	0/896	0.43	0/1216
4	g	0.34	0/896	0.44	0/1216
5	O	0.41	0/1250	0.46	0/1682
5	o	0.41	0/1250	0.45	0/1682
6	K	0.37	0/981	0.42	0/1321
6	k	0.37	0/981	0.42	0/1321
7	J	0.48	0/1573	0.47	0/2137
7	j	0.48	0/1573	0.47	0/2137
8	S	0.38	0/826	0.44	0/1119
8	s	0.38	0/826	0.44	0/1119
9	U	0.44	0/770	0.45	0/1040
9	u	0.44	0/770	0.46	0/1040
10	H	0.43	0/1902	0.44	0/2575
10	h	0.43	0/1902	0.44	0/2575
11	E	0.42	0/1154	0.45	0/1572
11	e	0.42	0/1154	0.45	0/1572
12	X	0.36	0/678	0.42	0/923
12	x	0.36	0/678	0.42	0/923
13	B	0.35	0/4016	0.43	0/5422
13	b	0.35	0/4016	0.43	0/5422
14	R	0.34	0/1092	0.44	0/1470
14	r	0.34	0/1092	0.46	0/1470
15	P	0.36	0/888	0.39	0/1202
15	p	0.36	0/888	0.40	0/1202
16	V	0.44	0/944	0.47	0/1280
16	v	0.44	0/944	0.47	0/1280

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	L	0.38	0/1651	0.45	0/2227
17	l	0.38	0/1651	0.45	0/2227
18	C	0.42	0/1057	0.46	0/1428
18	c	0.41	0/1057	0.46	0/1428
19	D	0.41	0/2143	0.46	0/2912
19	d	0.41	0/2143	0.46	0/2912
20	M	0.41	0/789	0.45	0/1065
20	m	0.40	0/789	0.45	0/1065
21	N	0.34	0/1280	0.42	0/1734
21	n	0.34	0/1280	0.42	0/1734
22	F	0.35	0/1475	0.44	0/2009
22	f	0.35	0/1475	0.44	0/2009
23	W	0.41	0/784	0.48	0/1064
23	w	0.41	0/784	0.48	0/1064
24	A	0.32	0/3883	0.40	0/5262
24	a	0.32	0/3883	0.40	0/5262
25	i1	0.27	0/343	0.38	0/459
25	i2	0.27	0/343	0.37	0/459
26	A1	0.25	0/3979	0.44	0/5372
26	A2	0.25	0/3979	0.44	0/5372
26	C1	0.25	0/3938	0.44	0/5314
26	C2	0.25	0/3938	0.43	0/5314
26	E1	0.24	0/3942	0.43	0/5322
26	E2	0.24	0/3942	0.43	0/5322
27	B1	0.26	0/3698	0.46	0/5016
27	B2	0.26	0/3698	0.45	0/5016
27	D1	0.25	0/3672	0.44	0/4980
27	D2	0.25	0/3672	0.44	0/4980
27	F1	0.25	0/3672	0.47	1/4980 (0.0%)
27	F2	0.25	0/3672	0.45	0/4980
28	g1	0.26	0/2145	0.40	0/2890
28	g2	0.26	0/2145	0.41	0/2890
29	d1	0.25	0/1083	0.43	0/1466
29	d2	0.26	0/1083	0.44	0/1466
30	e1	0.29	0/547	0.43	0/733
30	e2	0.28	0/547	0.42	0/733
31	G1	0.25	0/1431	0.44	0/1929
31	G2	0.24	0/1431	0.43	0/1929
32	H1	0.30	0/507	0.55	0/686
32	H2	0.27	0/507	0.41	0/686
32	I1	0.30	0/507	0.47	0/686
32	I2	0.26	0/507	0.41	0/686
32	J1	0.29	0/507	0.44	0/686

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	J2	0.27	0/507	0.42	0/686
32	K1	0.28	0/507	0.46	0/686
32	K2	0.26	0/507	0.40	0/686
32	L1	0.29	0/507	0.47	0/686
32	L2	0.28	0/507	0.55	0/686
32	M1	0.28	0/507	0.43	0/686
32	M2	0.26	0/507	0.40	0/686
32	N1	0.27	0/507	0.41	0/686
32	N2	0.26	0/507	0.40	0/686
32	O1	0.28	0/507	0.41	0/686
32	O2	0.28	0/507	0.41	0/686
32	P1	0.31	0/507	0.46	0/686
32	P2	0.30	0/507	0.46	0/686
32	Q1	0.29	0/507	0.46	0/686
32	Q2	0.28	0/507	0.42	0/686
All	All	0.32	0/132230	0.44	1/178892 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	J	0	1
7	j	0	1
26	A1	0	1
26	A2	0	1
27	B1	0	1
27	B2	0	1
27	F1	1	0
All	All	1	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	F1	538	MET	N-CA-CB	6.08	121.55	110.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	F1	538	MET	CA

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	A1	198	MET	Peptide
26	A2	198	MET	Peptide
27	B2	357	ALA	Peptide
7	J	89	PHE	Peptide
7	j	89	PHE	Peptide

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	Q	131/134 (98%)	125 (95%)	6 (5%)	0	100	100
1	q	131/134 (98%)	126 (96%)	5 (4%)	0	100	100
2	I	88/236 (37%)	85 (97%)	3 (3%)	0	100	100
2	i	88/236 (37%)	85 (97%)	3 (3%)	0	100	100
3	T	90/133 (68%)	87 (97%)	3 (3%)	0	100	100
3	t	90/133 (68%)	87 (97%)	3 (3%)	0	100	100
4	G	110/252 (44%)	102 (93%)	8 (7%)	0	100	100
4	g	110/252 (44%)	102 (93%)	8 (7%)	0	100	100
5	O	147/157 (94%)	141 (96%)	6 (4%)	0	100	100
5	o	147/157 (94%)	141 (96%)	6 (4%)	0	100	100
6	K	115/224 (51%)	112 (97%)	3 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	k	115/224 (51%)	111 (96%)	4 (4%)	0	100	100
7	J	174/229 (76%)	166 (95%)	8 (5%)	0	100	100
7	j	174/229 (76%)	166 (95%)	8 (5%)	0	100	100
8	S	93/128 (73%)	92 (99%)	1 (1%)	0	100	100
8	s	93/128 (73%)	92 (99%)	1 (1%)	0	100	100
9	U	92/126 (73%)	90 (98%)	2 (2%)	0	100	100
9	u	92/126 (73%)	90 (98%)	2 (2%)	0	100	100
10	H	224/239 (94%)	216 (96%)	8 (4%)	0	100	100
10	h	224/239 (94%)	214 (96%)	10 (4%)	0	100	100
11	E	138/325 (42%)	135 (98%)	3 (2%)	0	100	100
11	e	138/325 (42%)	135 (98%)	3 (2%)	0	100	100
12	X	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
12	x	80/83 (96%)	76 (95%)	4 (5%)	0	100	100
13	B	480/571 (84%)	466 (97%)	14 (3%)	0	100	100
13	b	480/571 (84%)	465 (97%)	15 (3%)	0	100	100
14	R	131/134 (98%)	122 (93%)	9 (7%)	0	100	100
14	r	131/134 (98%)	124 (95%)	7 (5%)	0	100	100
15	P	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
15	p	106/138 (77%)	104 (98%)	2 (2%)	0	100	100
16	V	108/111 (97%)	108 (100%)	0	0	100	100
16	v	108/111 (97%)	108 (100%)	0	0	100	100
17	L	205/208 (99%)	201 (98%)	4 (2%)	0	100	100
17	l	205/208 (99%)	201 (98%)	4 (2%)	0	100	100
18	C	120/398 (30%)	114 (95%)	6 (5%)	0	100	100
18	c	120/398 (30%)	114 (95%)	6 (5%)	0	100	100
19	D	251/310 (81%)	246 (98%)	5 (2%)	0	100	100
19	d	251/310 (81%)	246 (98%)	5 (2%)	0	100	100
20	M	94/205 (46%)	91 (97%)	3 (3%)	0	100	100
20	m	94/205 (46%)	91 (97%)	3 (3%)	0	100	100
21	N	158/166 (95%)	156 (99%)	2 (1%)	0	100	100
21	n	158/166 (95%)	156 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	F	184/267 (69%)	173 (94%)	11 (6%)	0	100	100
22	f	184/267 (69%)	173 (94%)	11 (6%)	0	100	100
23	W	93/106 (88%)	87 (94%)	6 (6%)	0	100	100
23	w	93/106 (88%)	88 (95%)	5 (5%)	0	100	100
24	A	461/536 (86%)	445 (96%)	16 (4%)	0	100	100
24	a	461/536 (86%)	445 (96%)	16 (4%)	0	100	100
25	i1	38/145 (26%)	38 (100%)	0	0	100	100
25	i2	38/145 (26%)	38 (100%)	0	0	100	100
26	A1	510/565 (90%)	488 (96%)	22 (4%)	0	100	100
26	A2	510/565 (90%)	489 (96%)	21 (4%)	0	100	100
26	C1	503/565 (89%)	487 (97%)	16 (3%)	0	100	100
26	C2	503/565 (89%)	485 (96%)	18 (4%)	0	100	100
26	E1	505/565 (89%)	482 (95%)	23 (5%)	0	100	100
26	E2	505/565 (89%)	485 (96%)	20 (4%)	0	100	100
27	B1	477/560 (85%)	453 (95%)	22 (5%)	2 (0%)	34	66
27	B2	477/560 (85%)	454 (95%)	21 (4%)	2 (0%)	34	66
27	D1	473/560 (84%)	455 (96%)	18 (4%)	0	100	100
27	D2	473/560 (84%)	452 (96%)	21 (4%)	0	100	100
27	F1	473/560 (84%)	455 (96%)	18 (4%)	0	100	100
27	F2	473/560 (84%)	455 (96%)	18 (4%)	0	100	100
28	g1	270/314 (86%)	260 (96%)	10 (4%)	0	100	100
28	g2	270/314 (86%)	260 (96%)	10 (4%)	0	100	100
29	d1	141/183 (77%)	136 (96%)	5 (4%)	0	100	100
29	d2	141/183 (77%)	137 (97%)	4 (3%)	0	100	100
30	e1	63/73 (86%)	59 (94%)	4 (6%)	0	100	100
30	e2	63/73 (86%)	59 (94%)	4 (6%)	0	100	100
31	G1	178/252 (71%)	159 (89%)	19 (11%)	0	100	100
31	G2	178/252 (71%)	159 (89%)	19 (11%)	0	100	100
32	H1	69/166 (42%)	69 (100%)	0	0	100	100
32	H2	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	I1	69/166 (42%)	68 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	I2	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	J1	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	J2	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	K1	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	K2	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	L1	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	L2	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
32	M1	69/166 (42%)	63 (91%)	6 (9%)	0	100	100
32	M2	69/166 (42%)	64 (93%)	5 (7%)	0	100	100
32	N1	69/166 (42%)	69 (100%)	0	0	100	100
32	N2	69/166 (42%)	69 (100%)	0	0	100	100
32	O1	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	O2	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
32	P1	69/166 (42%)	66 (96%)	3 (4%)	0	100	100
32	P2	69/166 (42%)	66 (96%)	3 (4%)	0	100	100
32	Q1	69/166 (42%)	69 (100%)	0	0	100	100
32	Q2	69/166 (42%)	68 (99%)	1 (1%)	0	100	100
All	All	16388/22836 (72%)	15771 (96%)	613 (4%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
27	B1	358	VAL
27	B2	357	ALA
27	B2	358	VAL
27	B1	357	ALA

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	119/120 (99%)	117 (98%)	2 (2%)	60	86
1	q	119/120 (99%)	119 (100%)	0	100	100
2	I	71/197 (36%)	71 (100%)	0	100	100
2	i	71/197 (36%)	71 (100%)	0	100	100
3	T	77/106 (73%)	77 (100%)	0	100	100
3	t	77/106 (73%)	77 (100%)	0	100	100
4	G	93/214 (44%)	93 (100%)	0	100	100
4	g	93/214 (44%)	93 (100%)	0	100	100
5	O	127/129 (98%)	127 (100%)	0	100	100
5	o	127/129 (98%)	127 (100%)	0	100	100
6	K	100/175 (57%)	100 (100%)	0	100	100
6	k	100/175 (57%)	100 (100%)	0	100	100
7	J	160/195 (82%)	160 (100%)	0	100	100
7	j	160/195 (82%)	160 (100%)	0	100	100
8	S	86/113 (76%)	86 (100%)	0	100	100
8	s	86/113 (76%)	86 (100%)	0	100	100
9	U	76/98 (78%)	76 (100%)	0	100	100
9	u	76/98 (78%)	76 (100%)	0	100	100
10	H	197/204 (97%)	196 (100%)	1 (0%)	88	96
10	h	197/204 (97%)	196 (100%)	1 (0%)	88	96
11	E	118/258 (46%)	118 (100%)	0	100	100
11	e	118/258 (46%)	118 (100%)	0	100	100
12	X	70/71 (99%)	70 (100%)	0	100	100
12	x	70/71 (99%)	70 (100%)	0	100	100
13	B	428/491 (87%)	427 (100%)	1 (0%)	93	98
13	b	428/491 (87%)	427 (100%)	1 (0%)	93	98
14	R	116/117 (99%)	116 (100%)	0	100	100
14	r	116/117 (99%)	116 (100%)	0	100	100
15	P	91/113 (80%)	91 (100%)	0	100	100
15	p	91/113 (80%)	91 (100%)	0	100	100
16	V	86/87 (99%)	86 (100%)	0	100	100
16	v	86/87 (99%)	86 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	L	177/178 (99%)	177 (100%)	0	100	100
17	l	177/178 (99%)	177 (100%)	0	100	100
18	C	107/338 (32%)	107 (100%)	0	100	100
18	c	107/338 (32%)	107 (100%)	0	100	100
19	D	218/259 (84%)	218 (100%)	0	100	100
19	d	218/259 (84%)	217 (100%)	1 (0%)	88	96
20	M	77/156 (49%)	77 (100%)	0	100	100
20	m	77/156 (49%)	77 (100%)	0	100	100
21	N	138/144 (96%)	137 (99%)	1 (1%)	84	95
21	n	138/144 (96%)	137 (99%)	1 (1%)	84	95
22	F	155/218 (71%)	155 (100%)	0	100	100
22	f	155/218 (71%)	155 (100%)	0	100	100
23	W	84/89 (94%)	83 (99%)	1 (1%)	71	91
23	w	84/89 (94%)	83 (99%)	1 (1%)	71	91
24	A	392/447 (88%)	391 (100%)	1 (0%)	92	98
24	a	392/447 (88%)	390 (100%)	2 (0%)	88	96
25	i1	37/125 (30%)	37 (100%)	0	100	100
25	i2	37/125 (30%)	37 (100%)	0	100	100
26	A1	421/454 (93%)	421 (100%)	0	100	100
26	A2	421/454 (93%)	421 (100%)	0	100	100
26	C1	415/454 (91%)	415 (100%)	0	100	100
26	C2	415/454 (91%)	415 (100%)	0	100	100
26	E1	416/454 (92%)	416 (100%)	0	100	100
26	E2	416/454 (92%)	416 (100%)	0	100	100
27	B1	390/447 (87%)	384 (98%)	6 (2%)	65	87
27	B2	390/447 (87%)	389 (100%)	1 (0%)	92	98
27	D1	388/447 (87%)	388 (100%)	0	100	100
27	D2	388/447 (87%)	387 (100%)	1 (0%)	92	98
27	F1	388/447 (87%)	383 (99%)	5 (1%)	69	90
27	F2	388/447 (87%)	386 (100%)	2 (0%)	88	96
28	g1	228/257 (89%)	228 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	g2	228/257 (89%)	228 (100%)	0	100	100
29	d1	118/144 (82%)	118 (100%)	0	100	100
29	d2	118/144 (82%)	118 (100%)	0	100	100
30	e1	57/61 (93%)	57 (100%)	0	100	100
30	e2	57/61 (93%)	57 (100%)	0	100	100
31	G1	154/212 (73%)	153 (99%)	1 (1%)	86	96
31	G2	154/212 (73%)	153 (99%)	1 (1%)	86	96
32	H1	52/133 (39%)	48 (92%)	4 (8%)	13	35
32	H2	52/133 (39%)	52 (100%)	0	100	100
32	I1	52/133 (39%)	50 (96%)	2 (4%)	33	67
32	I2	52/133 (39%)	51 (98%)	1 (2%)	57	84
32	J1	52/133 (39%)	52 (100%)	0	100	100
32	J2	52/133 (39%)	52 (100%)	0	100	100
32	K1	52/133 (39%)	51 (98%)	1 (2%)	57	84
32	K2	52/133 (39%)	52 (100%)	0	100	100
32	L1	52/133 (39%)	51 (98%)	1 (2%)	57	84
32	L2	52/133 (39%)	50 (96%)	2 (4%)	33	67
32	M1	52/133 (39%)	51 (98%)	1 (2%)	57	84
32	M2	52/133 (39%)	52 (100%)	0	100	100
32	N1	52/133 (39%)	52 (100%)	0	100	100
32	N2	52/133 (39%)	52 (100%)	0	100	100
32	O1	52/133 (39%)	52 (100%)	0	100	100
32	O2	52/133 (39%)	52 (100%)	0	100	100
32	P1	52/133 (39%)	52 (100%)	0	100	100
32	P2	52/133 (39%)	52 (100%)	0	100	100
32	Q1	52/133 (39%)	51 (98%)	1 (2%)	57	84
32	Q2	52/133 (39%)	52 (100%)	0	100	100
All	All	13790/18698 (74%)	13746 (100%)	44 (0%)	92	98

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	F1	528	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	H1	119	SER
27	F1	536	PHE
27	F1	542	LEU
32	H1	131	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
32	N2	115	GLN
27	B1	80	ASN
26	C1	490	ASN
27	B1	99	GLN
24	A	321	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

54 ligands 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
35	CDL	h	302	-	99,99,99	0.87	6 (6%)	105,111,111	0.98	4 (3%)
35	CDL	c	401	-	99,99,99	0.88	6 (6%)	105,111,111	0.91	4 (3%)
34	LMT	H	301	-	36,36,36	1.13	2 (5%)	47,47,47	1.03	2 (4%)
34	LMT	d	401	-	36,36,36	1.15	2 (5%)	47,47,47	0.90	1 (2%)
34	LMT	C	404	-	36,36,36	1.11	2 (5%)	47,47,47	1.14	3 (6%)
37	ATP	C1	601	-	26,33,33	4.78	9 (34%)	31,52,52	2.52	9 (29%)
35	CDL	e	401	-	99,99,99	0.88	8 (8%)	105,111,111	1.01	4 (3%)
33	PC1	O	204	5	53,53,53	0.95	4 (7%)	59,61,61	1.04	2 (3%)
35	CDL	u	201	-	99,99,99	0.88	7 (7%)	105,111,111	1.01	4 (3%)
35	CDL	B	602	-	99,99,99	0.88	8 (8%)	105,111,111	0.98	4 (3%)
35	CDL	E	401	-	99,99,99	0.88	8 (8%)	105,111,111	1.01	4 (3%)
37	ATP	E1	601	-	26,33,33	4.81	8 (30%)	31,52,52	2.49	8 (25%)
33	PC1	O	201	-	53,53,53	0.96	3 (5%)	59,61,61	1.05	3 (5%)
37	ATP	A2	601	-	26,33,33	4.80	7 (26%)	31,52,52	2.49	8 (25%)
37	ATP	C2	601	-	26,33,33	4.82	8 (30%)	31,52,52	2.47	8 (25%)
36	PEE	C	403	-	50,50,50	1.15	5 (10%)	53,55,55	1.00	2 (3%)
34	LMT	X	101	-	36,36,36	1.16	2 (5%)	47,47,47	1.03	3 (6%)
34	LMT	C	402	-	36,36,36	1.10	2 (5%)	47,47,47	1.00	1 (2%)
35	CDL	V	202	-	99,99,99	0.88	7 (7%)	105,111,111	0.97	4 (3%)
33	PC1	V	201	-	53,53,53	0.99	3 (5%)	59,61,61	0.98	2 (3%)
33	PC1	v	201	-	53,53,53	0.99	3 (5%)	59,61,61	0.99	2 (3%)
35	CDL	v	202	-	99,99,99	0.88	7 (7%)	105,111,111	0.98	4 (3%)
34	LMT	d	403	-	36,36,36	1.12	2 (5%)	47,47,47	0.85	1 (2%)
34	LMT	O	202	-	36,36,36	1.12	2 (5%)	47,47,47	0.94	1 (2%)
36	PEE	J	302	-	50,50,50	1.14	6 (12%)	53,55,55	1.15	3 (5%)
35	CDL	B	601	-	99,99,99	0.87	7 (7%)	105,111,111	1.00	3 (2%)
33	PC1	o	201	-	53,53,53	0.96	4 (7%)	59,61,61	1.04	3 (5%)
35	CDL	d	402	-	99,99,99	0.88	8 (8%)	105,111,111	1.02	3 (2%)
36	PEE	c	403	-	50,50,50	1.15	5 (10%)	53,55,55	1.01	2 (3%)
34	LMT	D	403	-	36,36,36	1.11	2 (5%)	47,47,47	0.89	1 (2%)
34	LMT	h	301	-	36,36,36	1.13	2 (5%)	47,47,47	1.03	2 (4%)
35	CDL	C	401	-	99,99,99	0.88	6 (6%)	105,111,111	0.85	3 (2%)
38	ADP	B1	601	-	24,29,29	3.67	9 (37%)	29,45,45	3.44	6 (20%)
35	CDL	b	601	-	99,99,99	0.87	8 (8%)	105,111,111	1.00	4 (3%)
34	LMT	x	101	-	36,36,36	1.16	2 (5%)	47,47,47	1.03	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	ADP	D2	601	-	24,29,29	3.68	9 (37%)	29,45,45	3.46	6 (20%)
38	ADP	D1	601	-	24,29,29	3.69	8 (33%)	29,45,45	3.58	7 (24%)
33	PC1	o	204	5	53,53,53	0.96	4 (7%)	59,61,61	1.04	2 (3%)
35	CDL	b	602	-	99,99,99	0.88	8 (8%)	105,111,111	0.98	4 (3%)
35	CDL	U	201	-	99,99,99	0.88	7 (7%)	105,111,111	1.00	4 (3%)
34	LMT	c	404	-	36,36,36	1.11	2 (5%)	47,47,47	1.07	2 (4%)
37	ATP	E2	601	-	26,33,33	4.80	8 (30%)	31,52,52	2.47	9 (29%)
34	LMT	D	401	-	36,36,36	1.15	2 (5%)	47,47,47	0.86	1 (2%)
36	PEE	j	301	-	50,50,50	1.12	6 (12%)	53,55,55	1.08	3 (5%)
35	CDL	D	402	-	99,99,99	0.88	8 (8%)	105,111,111	1.02	3 (2%)
38	ADP	B2	601	-	24,29,29	3.67	9 (37%)	29,45,45	3.70	8 (27%)
37	ATP	A1	601	-	26,33,33	4.81	7 (26%)	31,52,52	2.43	8 (25%)
34	LMT	c	402	-	36,36,36	1.10	2 (5%)	47,47,47	1.01	1 (2%)
35	CDL	H	302	-	99,99,99	0.87	7 (7%)	105,111,111	0.98	4 (3%)
34	LMT	o	202	-	36,36,36	1.12	2 (5%)	47,47,47	0.91	1 (2%)
35	CDL	O	203	-	99,99,99	0.88	7 (7%)	105,111,111	1.00	5 (4%)
35	CDL	o	203	-	99,99,99	0.88	7 (7%)	105,111,111	1.00	5 (4%)
36	PEE	J	301	-	50,50,50	1.12	6 (12%)	53,55,55	1.07	3 (5%)
36	PEE	j	302	-	50,50,50	1.14	6 (12%)	53,55,55	1.08	3 (5%)

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
35	CDL	h	302	-	-	45/110/110/110	-
35	CDL	c	401	-	-	64/110/110/110	-
34	LMT	H	301	-	-	9/21/61/61	0/2/2/2
34	LMT	d	401	-	-	9/21/61/61	0/2/2/2
34	LMT	C	404	-	-	7/21/61/61	0/2/2/2
37	ATP	C1	601	-	-	5/18/38/38	0/3/3/3
35	CDL	e	401	-	-	49/110/110/110	-
33	PC1	O	204	5	-	25/57/57/57	-
35	CDL	u	201	-	-	37/110/110/110	-
35	CDL	B	602	-	-	48/110/110/110	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	CDL	E	401	-	-	49/110/110/110	-
37	ATP	E1	601	-	-	3/18/38/38	0/3/3/3
33	PC1	O	201	-	-	22/57/57/57	-
37	ATP	A2	601	-	-	0/18/38/38	0/3/3/3
37	ATP	C2	601	-	-	4/18/38/38	0/3/3/3
36	PEE	C	403	-	-	22/54/54/54	-
34	LMT	X	101	-	-	12/21/61/61	0/2/2/2
34	LMT	C	402	-	-	8/21/61/61	0/2/2/2
35	CDL	V	202	-	-	39/110/110/110	-
33	PC1	V	201	-	-	31/57/57/57	-
33	PC1	v	201	-	-	31/57/57/57	-
35	CDL	v	202	-	-	40/110/110/110	-
34	LMT	d	403	-	-	5/21/61/61	0/2/2/2
34	LMT	O	202	-	-	4/21/61/61	0/2/2/2
36	PEE	J	302	-	-	19/54/54/54	-
35	CDL	B	601	-	-	39/110/110/110	-
33	PC1	o	201	-	-	23/57/57/57	-
35	CDL	d	402	-	-	45/110/110/110	-
36	PEE	c	403	-	-	22/54/54/54	-
34	LMT	D	403	-	-	5/21/61/61	0/2/2/2
34	LMT	h	301	-	-	9/21/61/61	0/2/2/2
35	CDL	C	401	-	-	60/110/110/110	-
38	ADP	B1	601	-	-	4/12/32/32	0/3/3/3
35	CDL	b	601	-	-	39/110/110/110	-
34	LMT	x	101	-	-	12/21/61/61	0/2/2/2
38	ADP	D2	601	-	-	2/12/32/32	0/3/3/3
38	ADP	D1	601	-	-	0/12/32/32	0/3/3/3
33	PC1	o	204	5	-	25/57/57/57	-
35	CDL	b	602	-	-	50/110/110/110	-
35	CDL	U	201	-	-	38/110/110/110	-
34	LMT	c	404	-	-	7/21/61/61	0/2/2/2
37	ATP	E2	601	-	-	3/18/38/38	0/3/3/3
34	LMT	D	401	-	-	11/21/61/61	0/2/2/2
36	PEE	j	301	-	-	22/54/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	CDL	D	402	-	-	46/110/110/110	-
38	ADP	B2	601	-	-	4/12/32/32	0/3/3/3
37	ATP	A1	601	-	-	0/18/38/38	0/3/3/3
34	LMT	c	402	-	-	8/21/61/61	0/2/2/2
35	CDL	H	302	-	-	45/110/110/110	-
34	LMT	o	202	-	-	4/21/61/61	0/2/2/2
35	CDL	O	203	-	-	40/110/110/110	-
35	CDL	o	203	-	-	40/110/110/110	-
36	PEE	J	301	-	-	22/54/54/54	-
36	PEE	j	302	-	-	20/54/54/54	-

The worst 5 of 295 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	C2	601	ATP	C2'-C1'	-17.47	1.27	1.53
37	A2	601	ATP	C2'-C1'	-17.41	1.27	1.53
37	A1	601	ATP	C2'-C1'	-17.40	1.27	1.53
37	E1	601	ATP	C2'-C1'	-17.34	1.27	1.53
37	E2	601	ATP	C2'-C1'	-17.33	1.27	1.53

The worst 5 of 200 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	B2	601	ADP	C1'-N9-C4	15.61	154.07	126.64
38	D1	601	ADP	C1'-N9-C4	14.69	152.45	126.64
38	D2	601	ADP	C1'-N9-C4	14.02	151.28	126.64
38	B1	601	ADP	C1'-N9-C4	13.90	151.06	126.64
37	E1	601	ATP	C5-C6-N6	7.56	131.84	120.35

There are no chirality outliers.

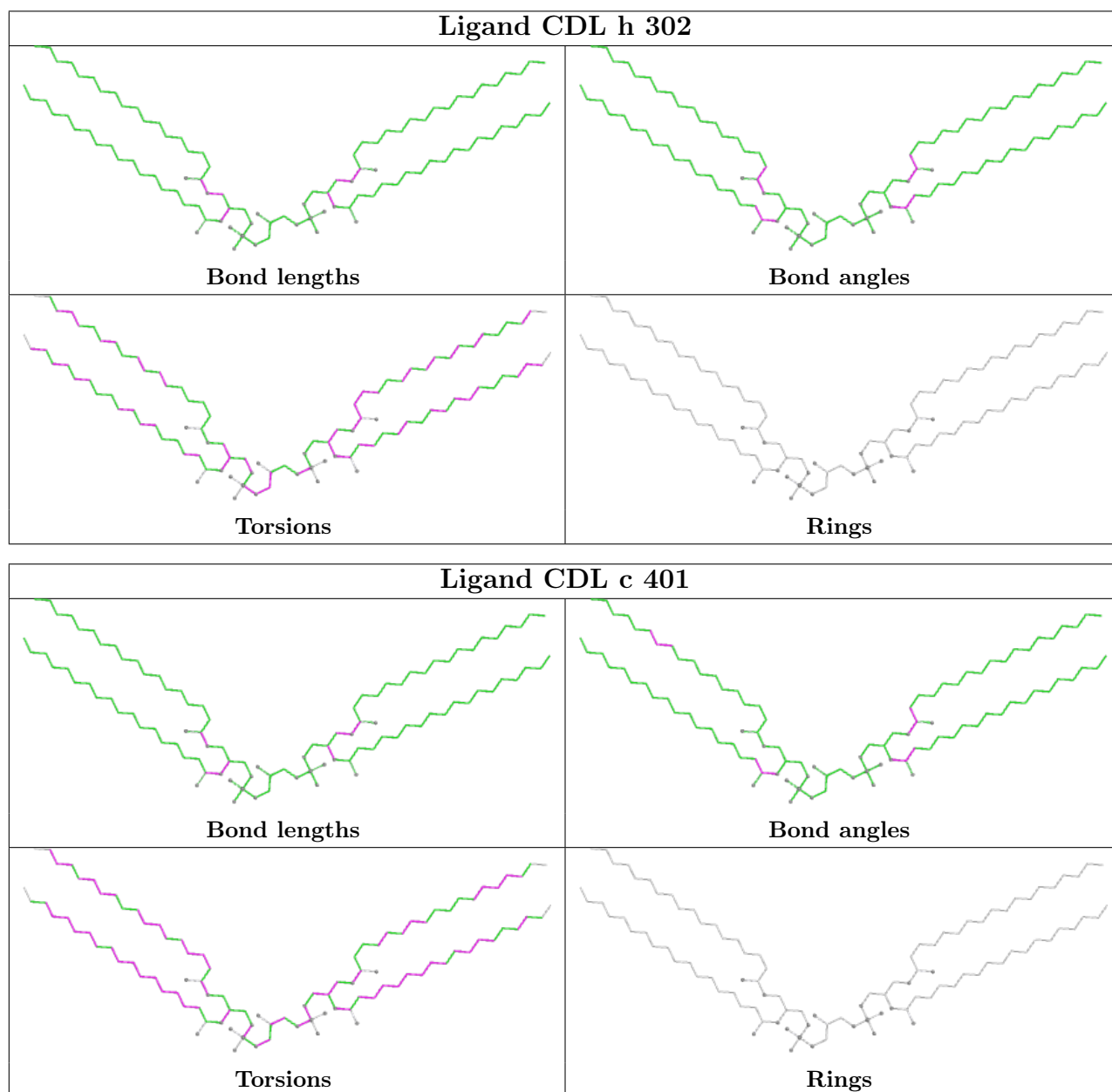
5 of 1232 torsion outliers are listed below:

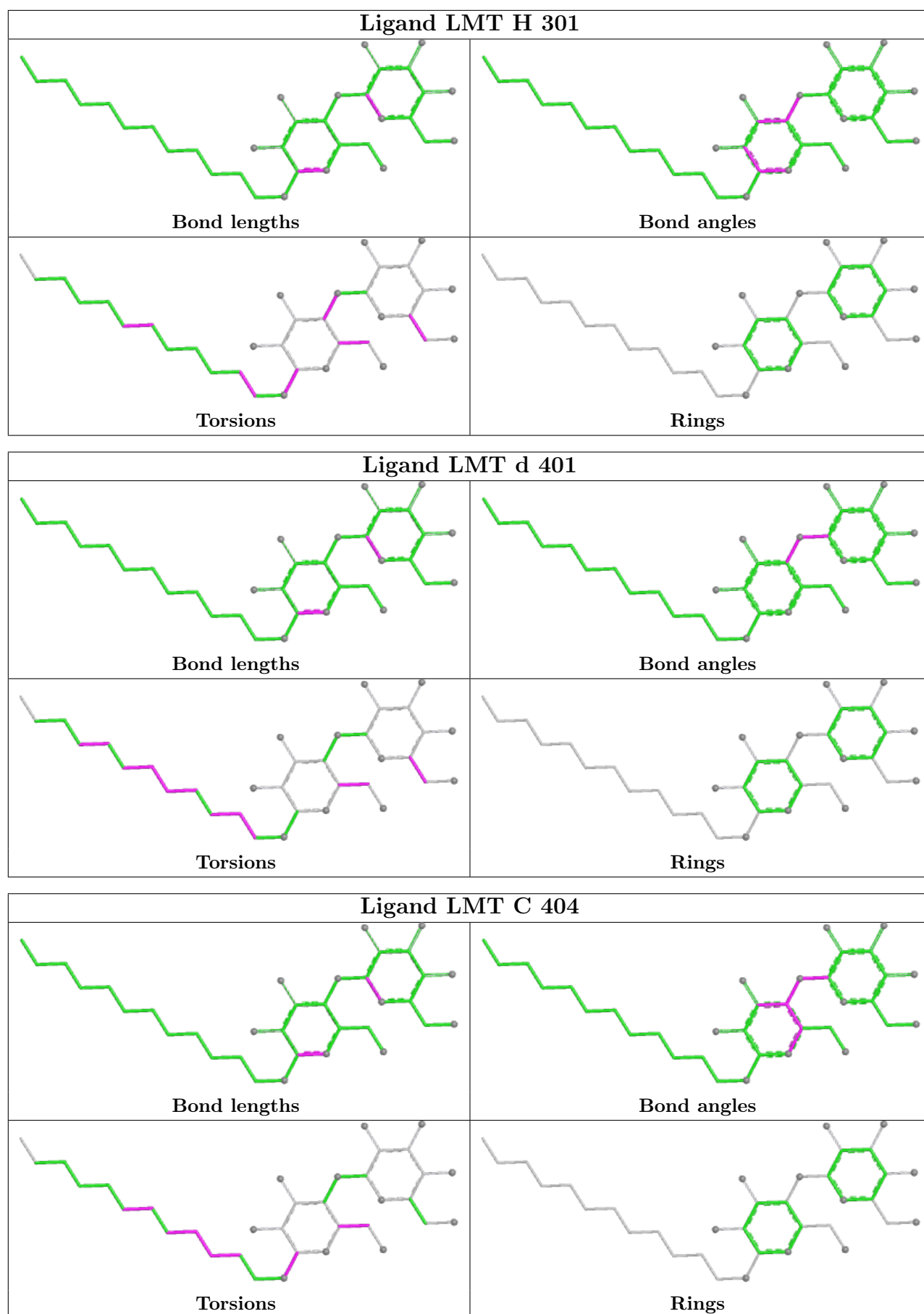
Mol	Chain	Res	Type	Atoms
33	o	201	PC1	C1-O11-P-O14
33	o	201	PC1	O13-C11-C12-N
33	o	201	PC1	C22-C21-O21-C2
33	o	204	PC1	C11-O13-P-O14
33	o	204	PC1	C22-C21-O21-C2

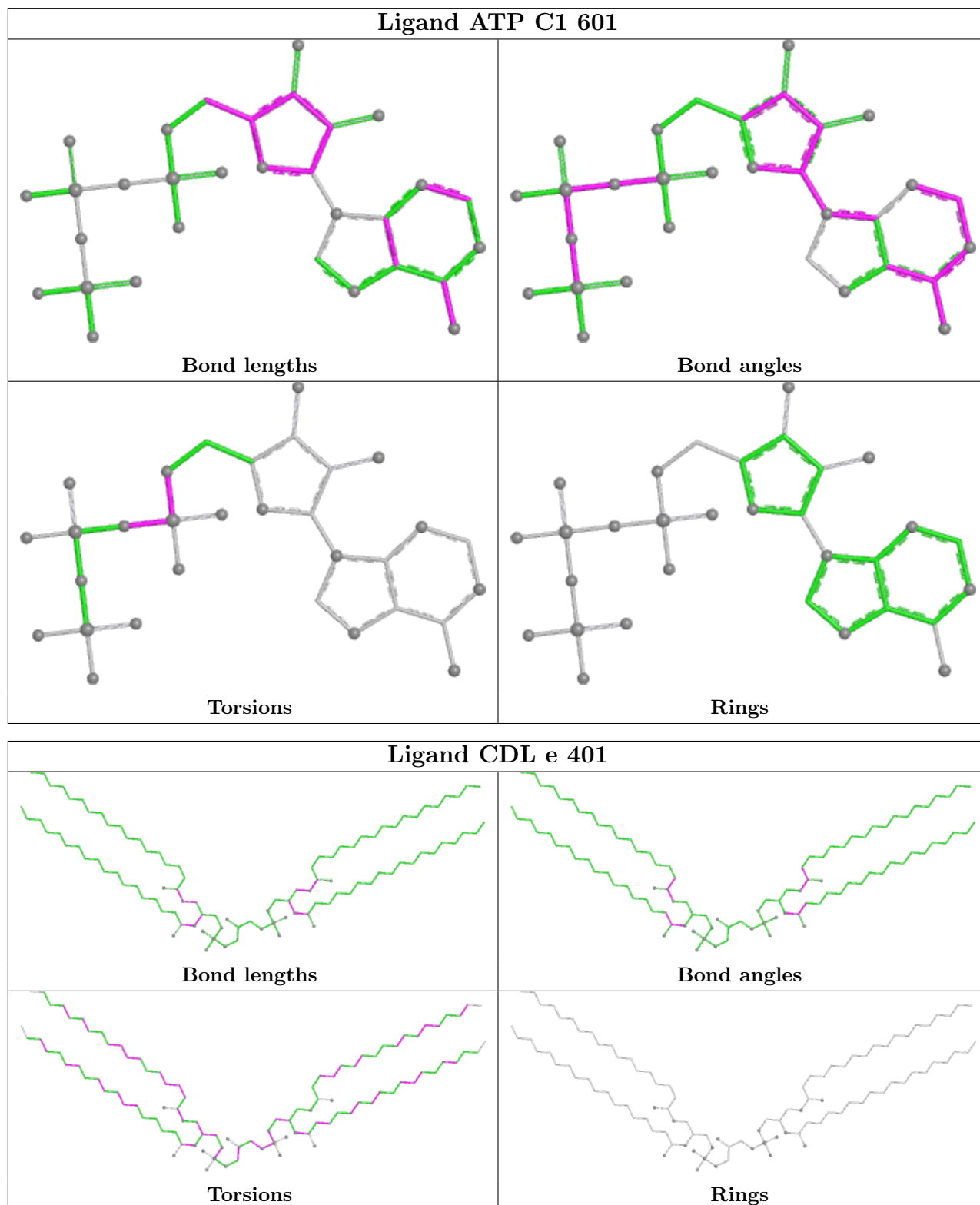
There are no ring outliers.

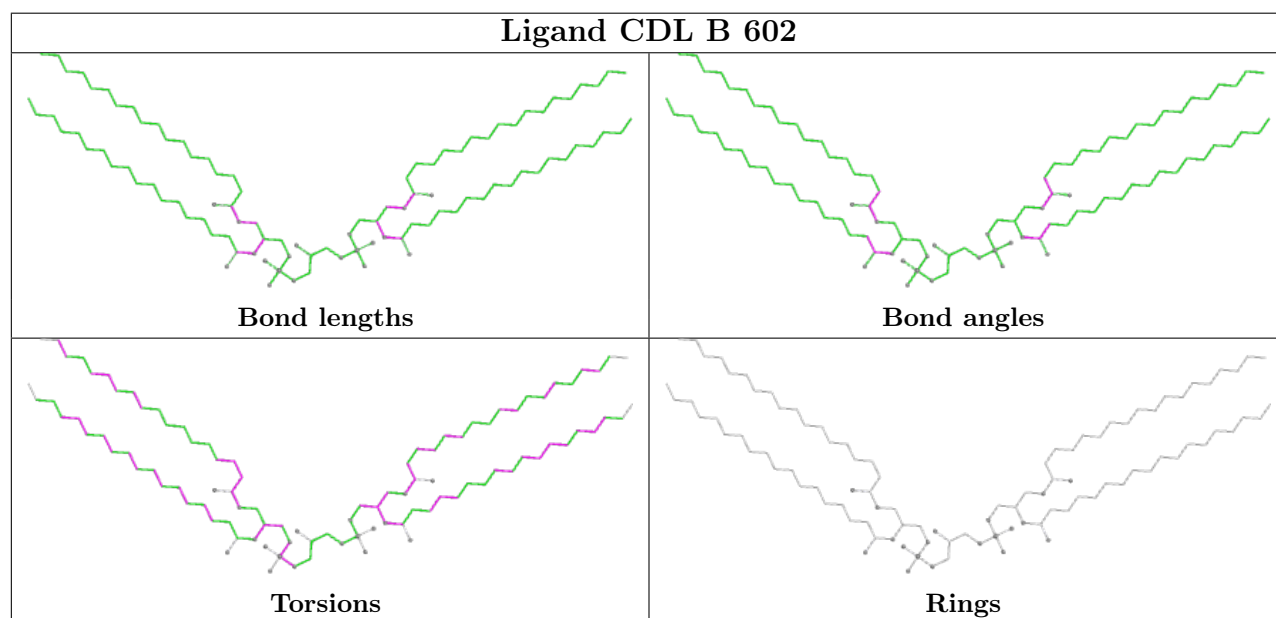
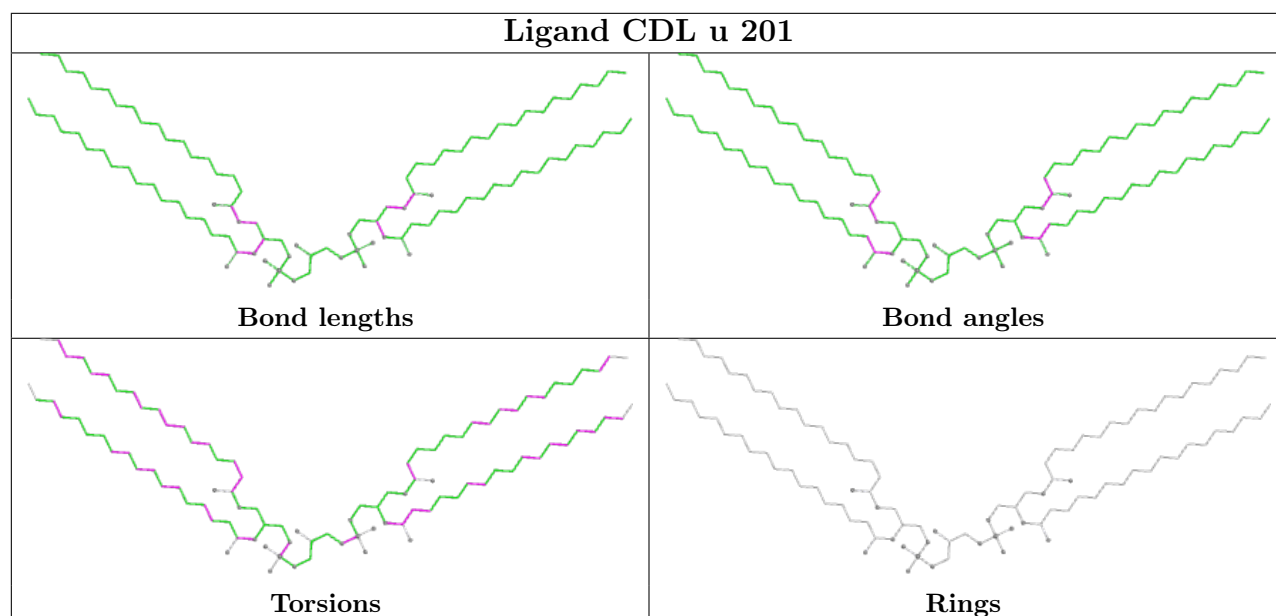
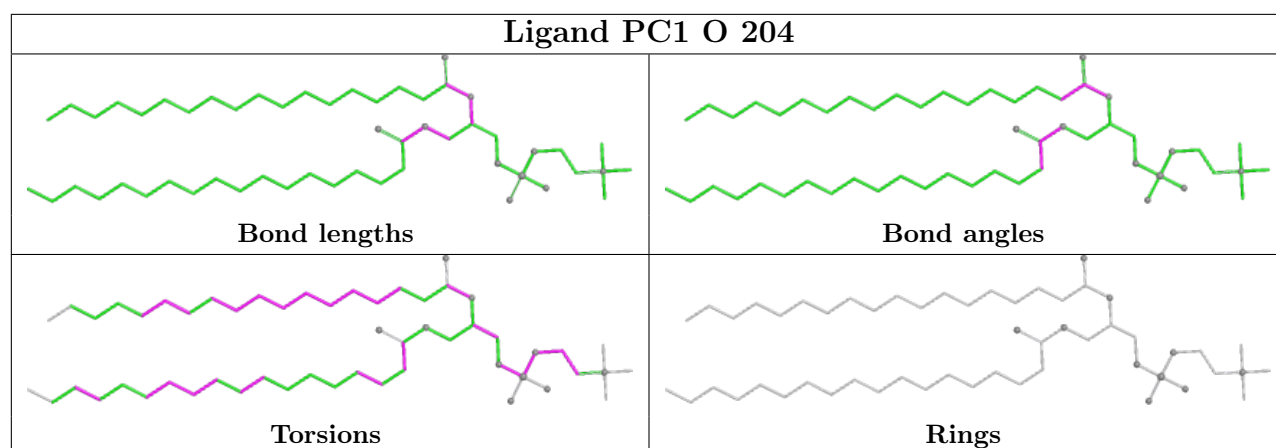
No monomer is involved in short contacts.

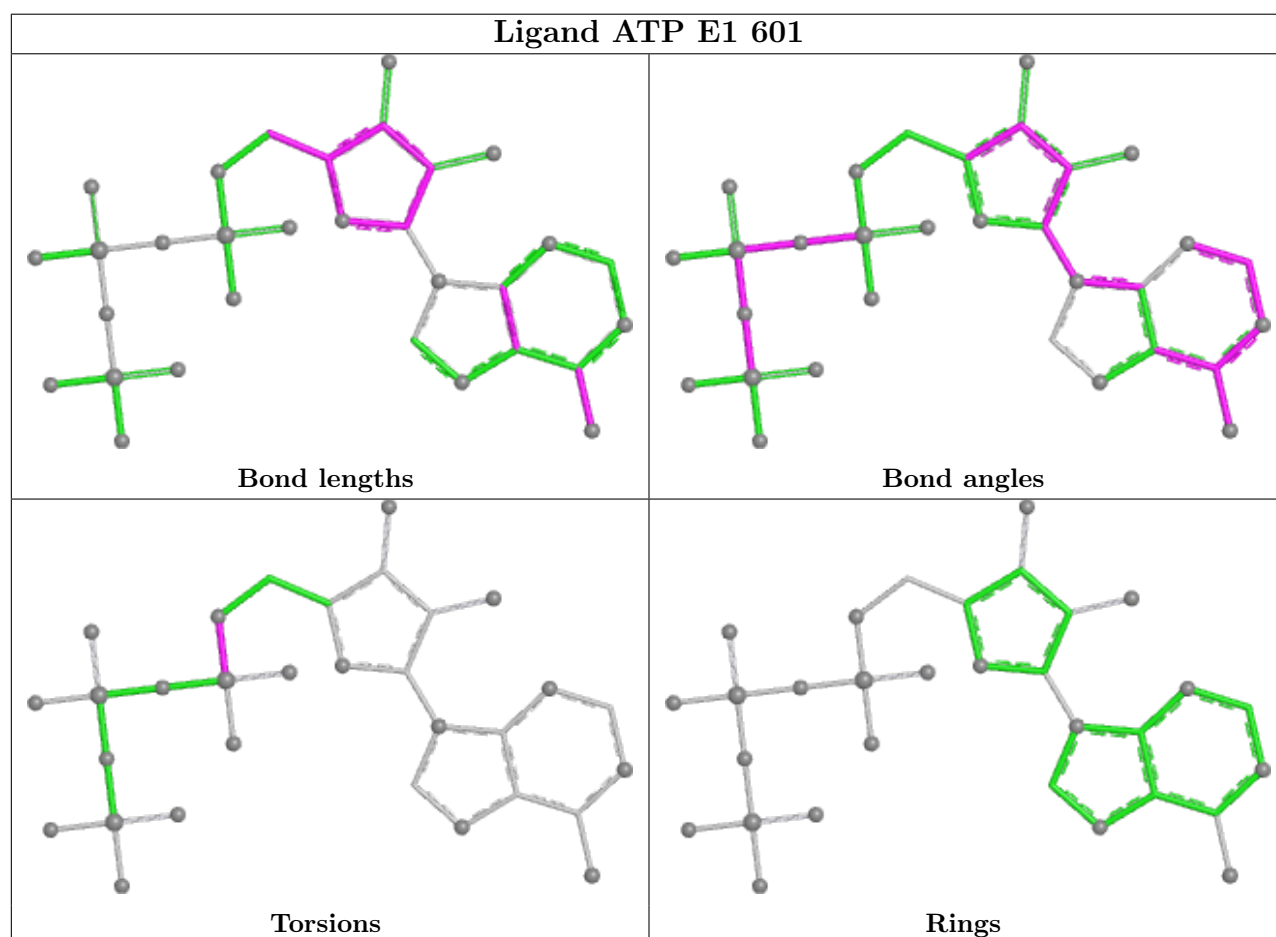
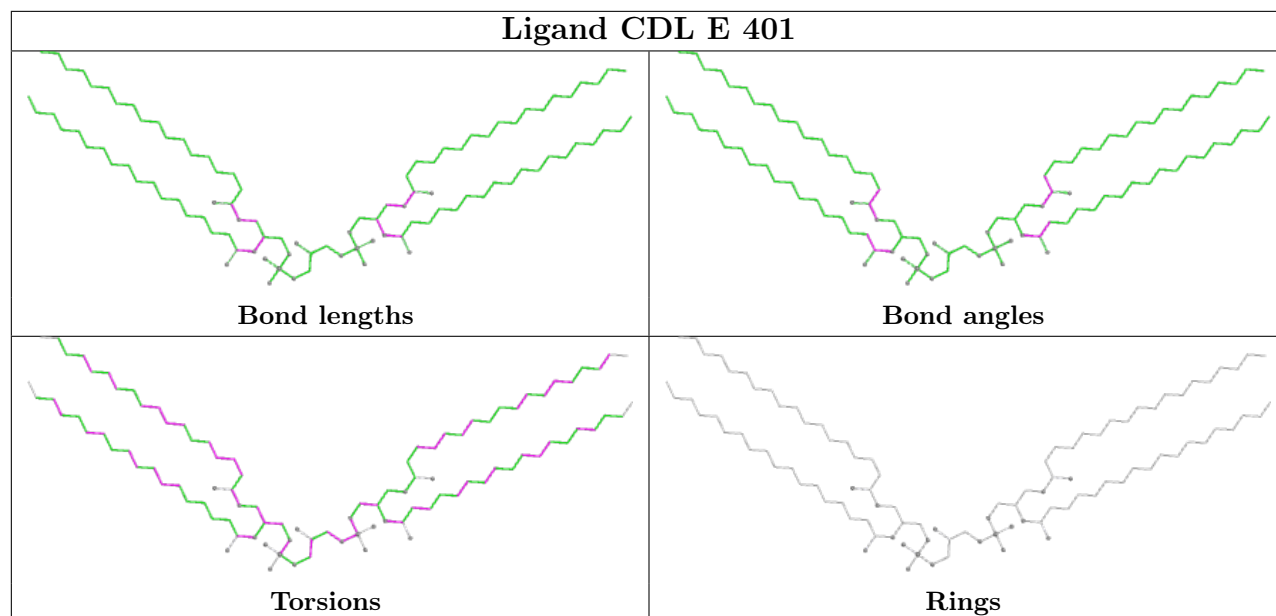
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

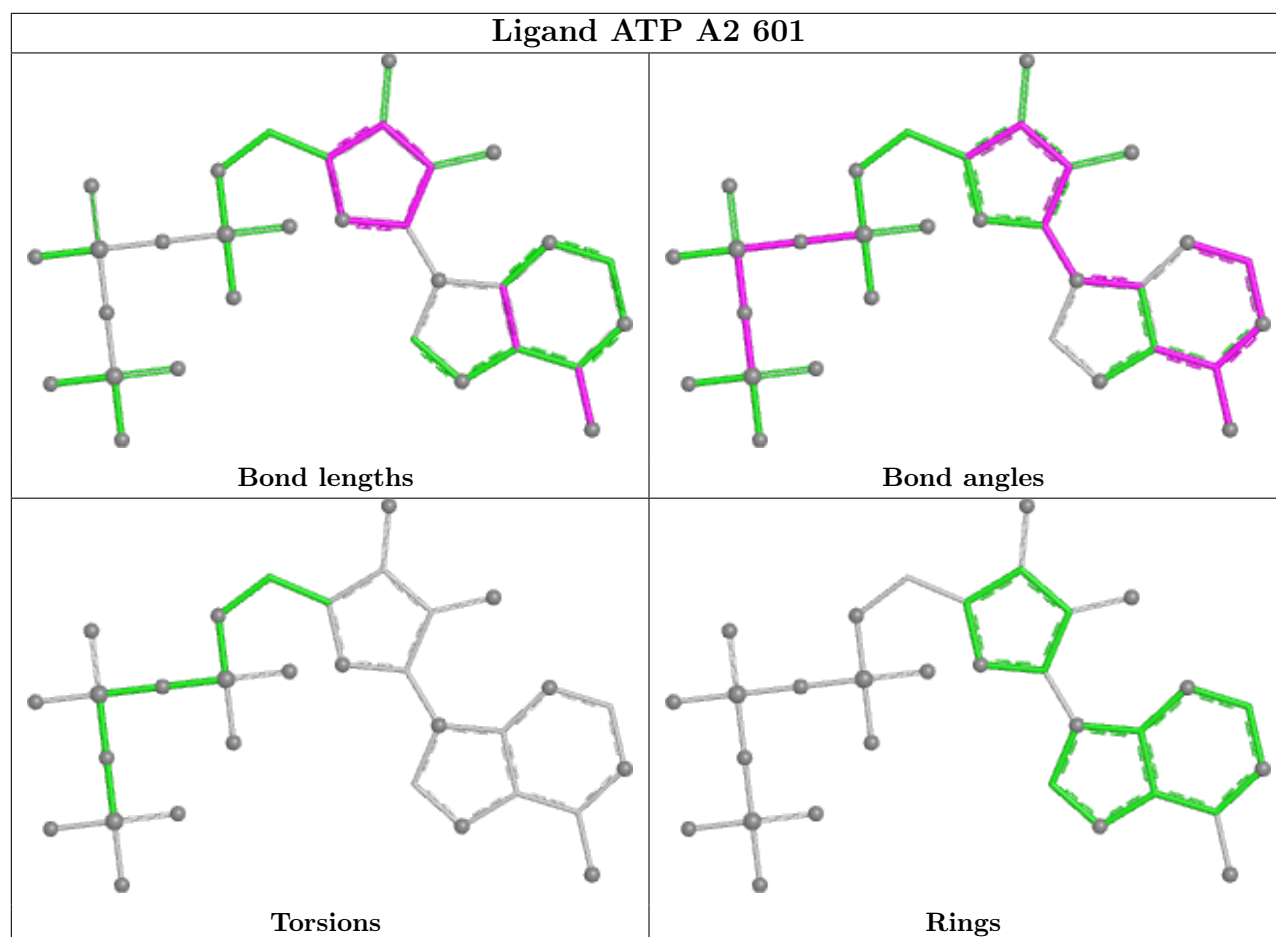
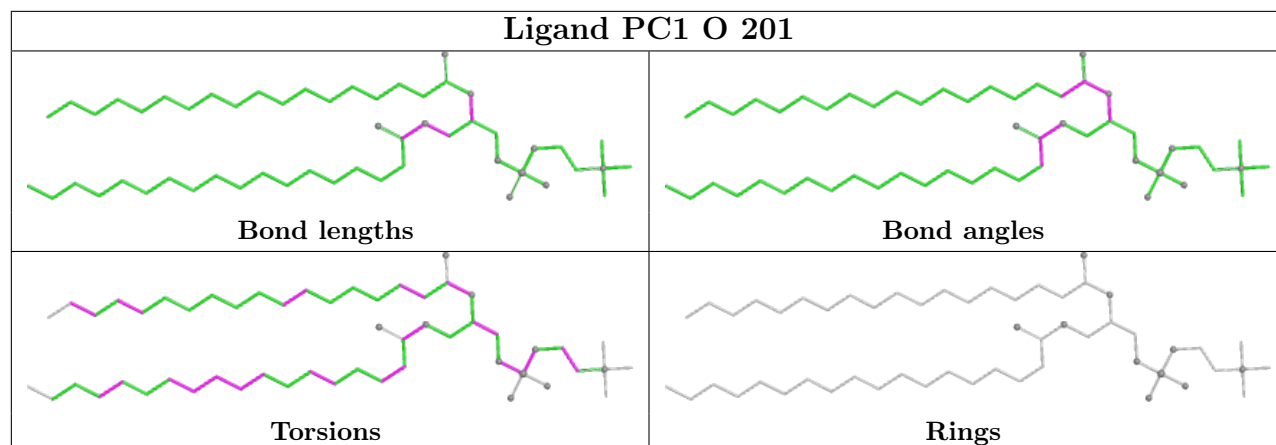


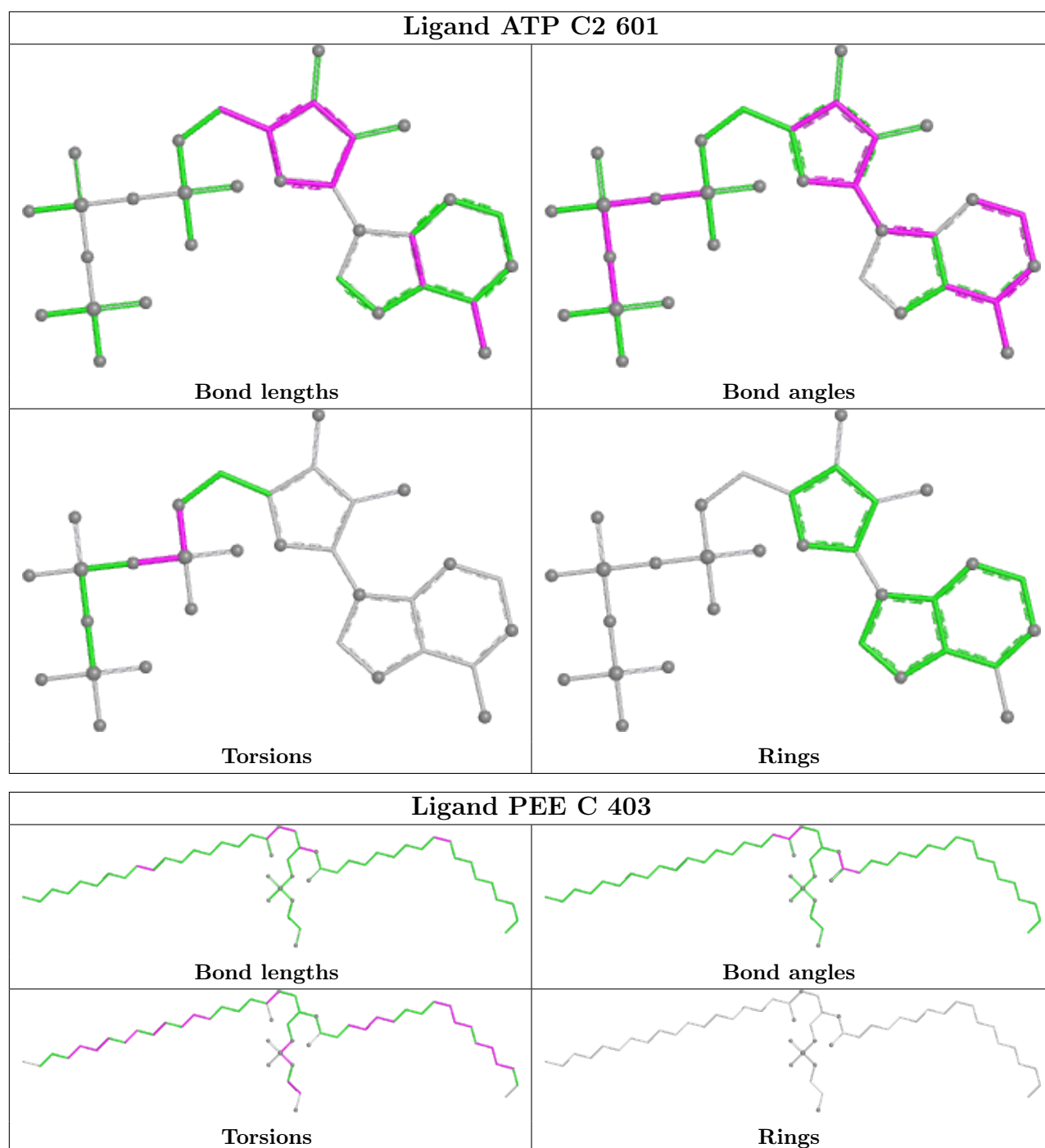


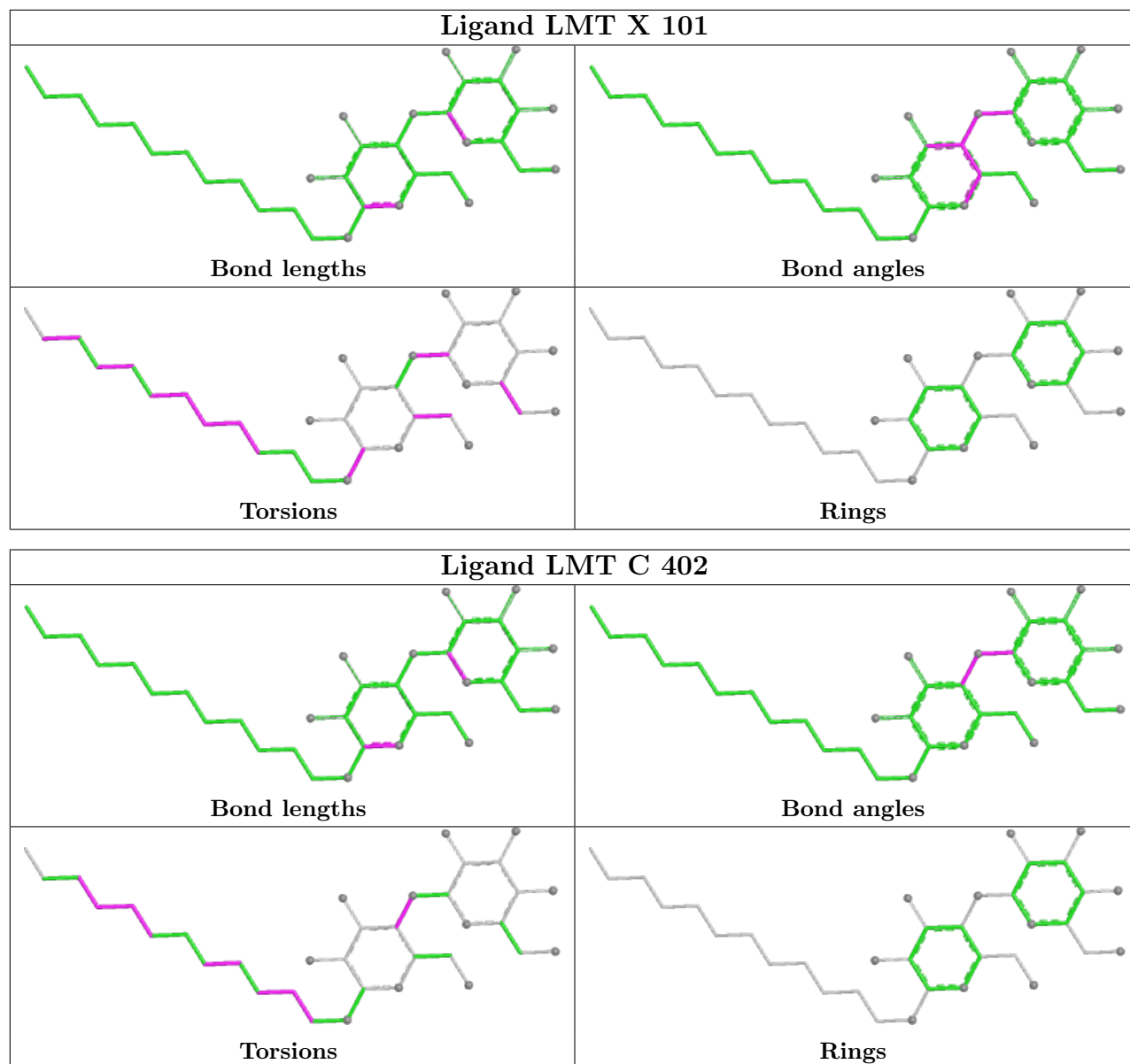


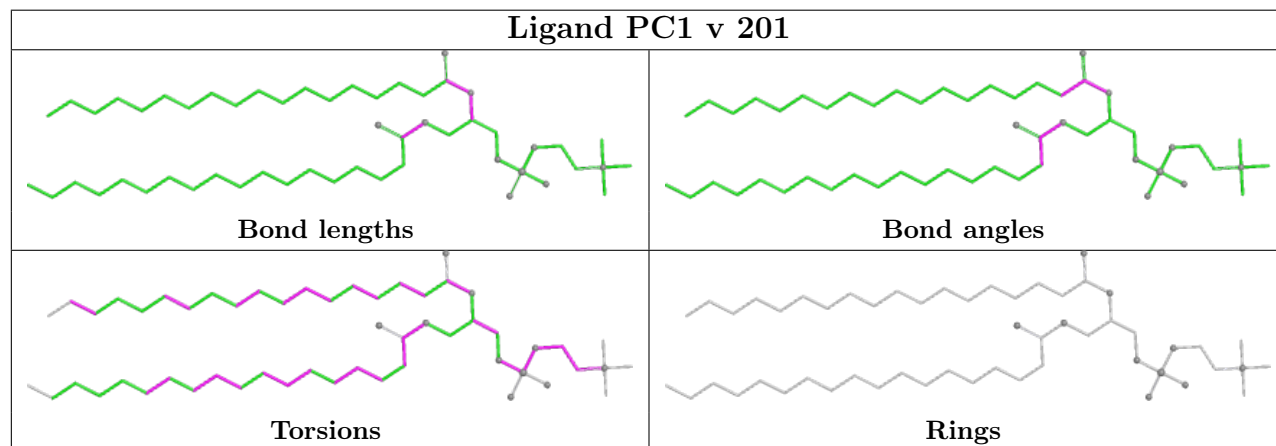
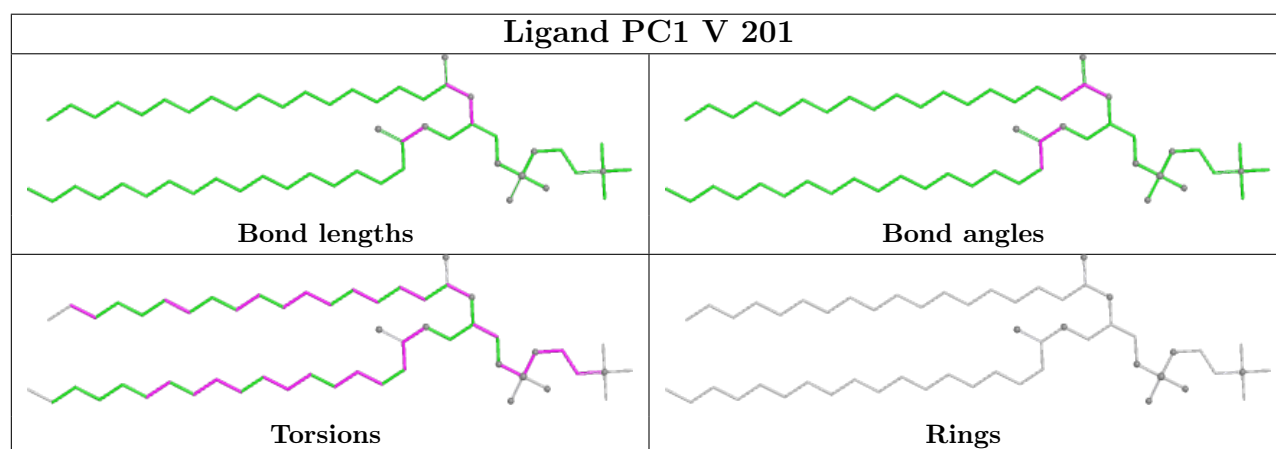
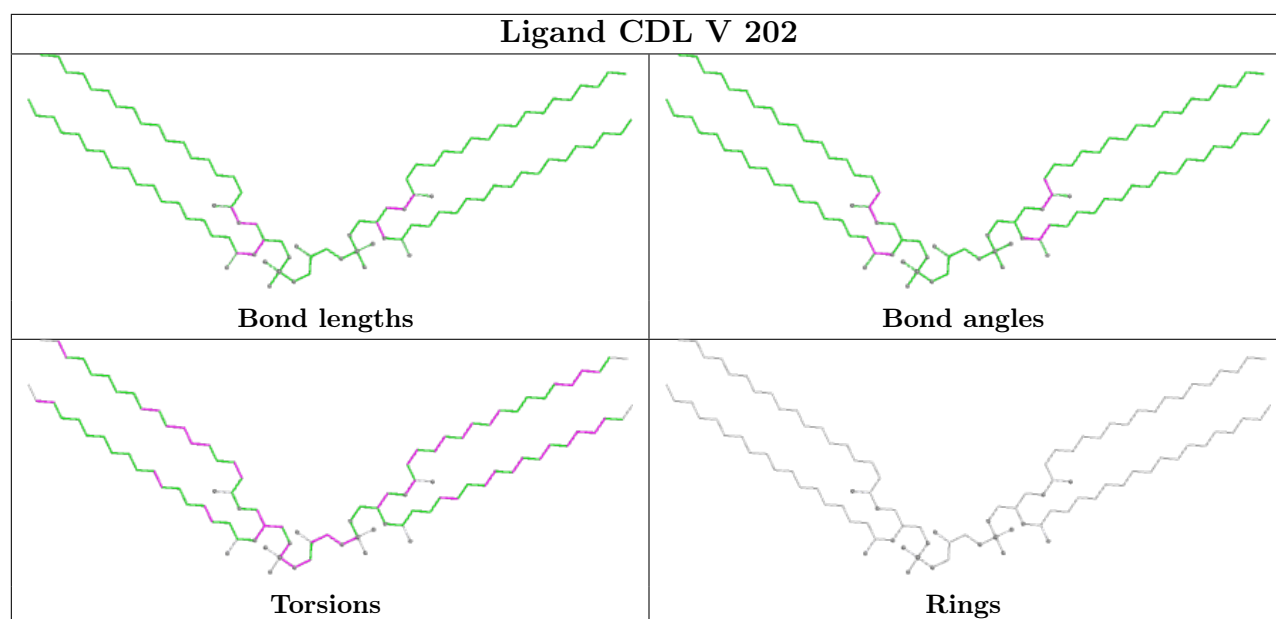


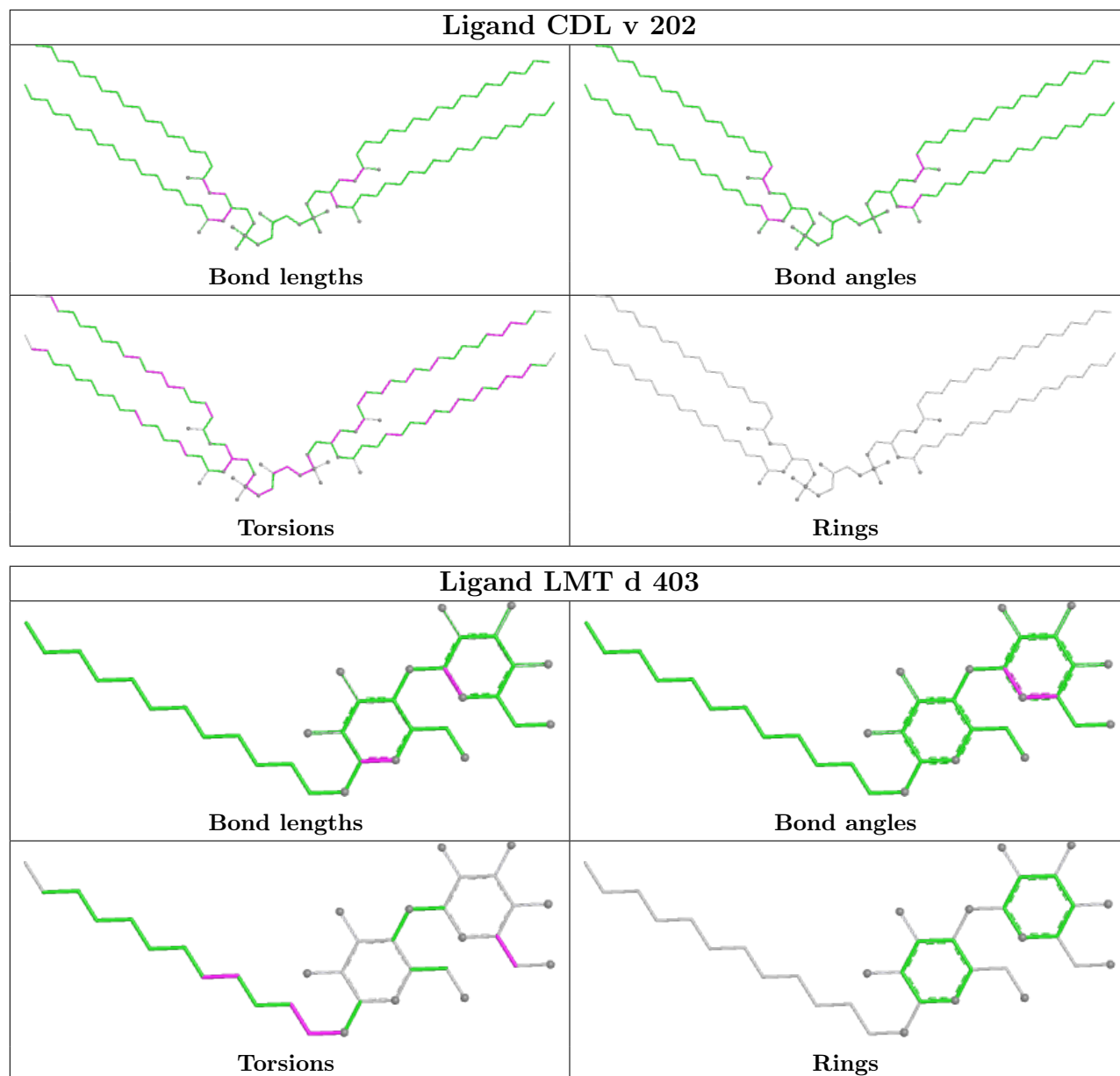


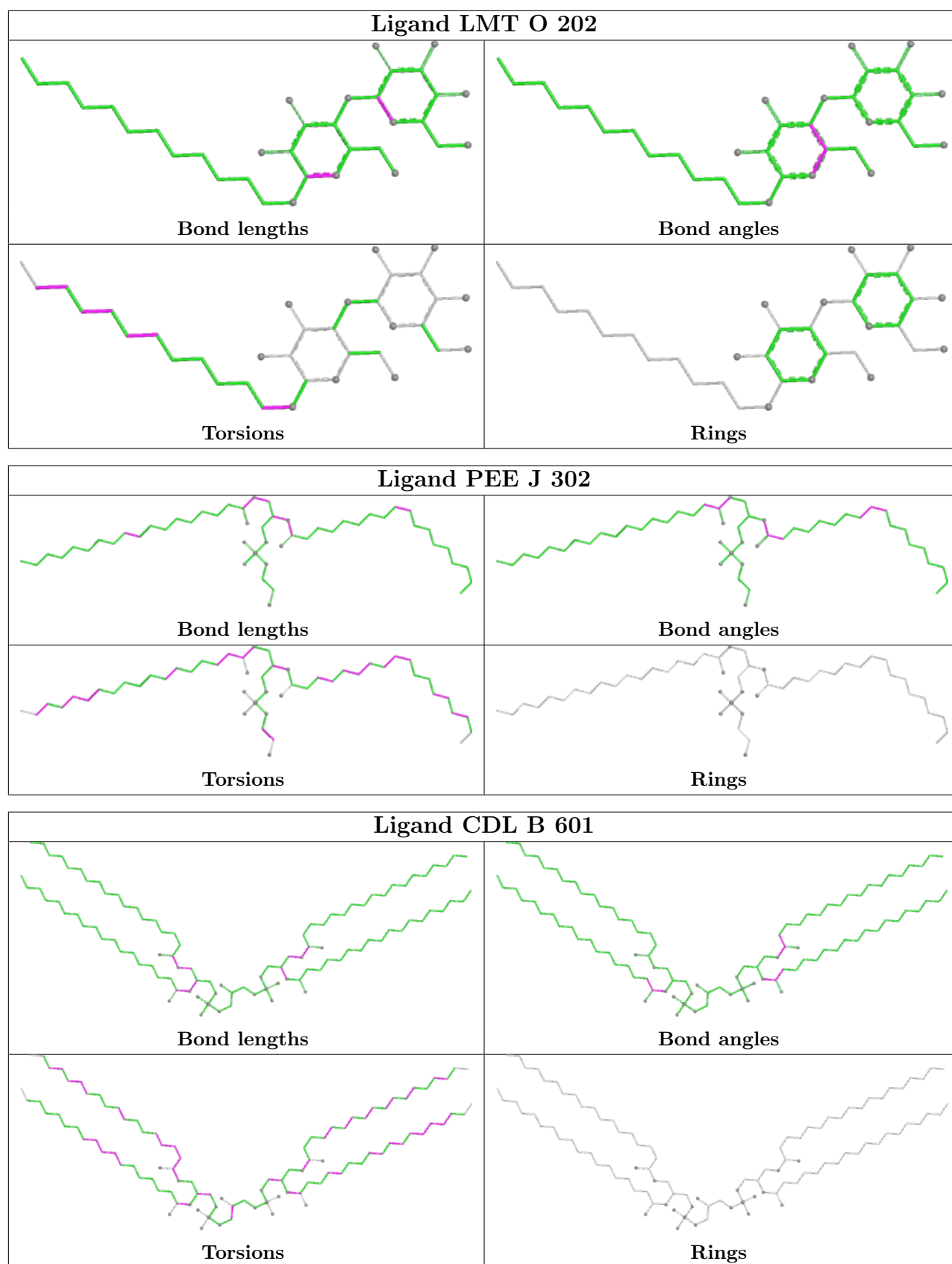


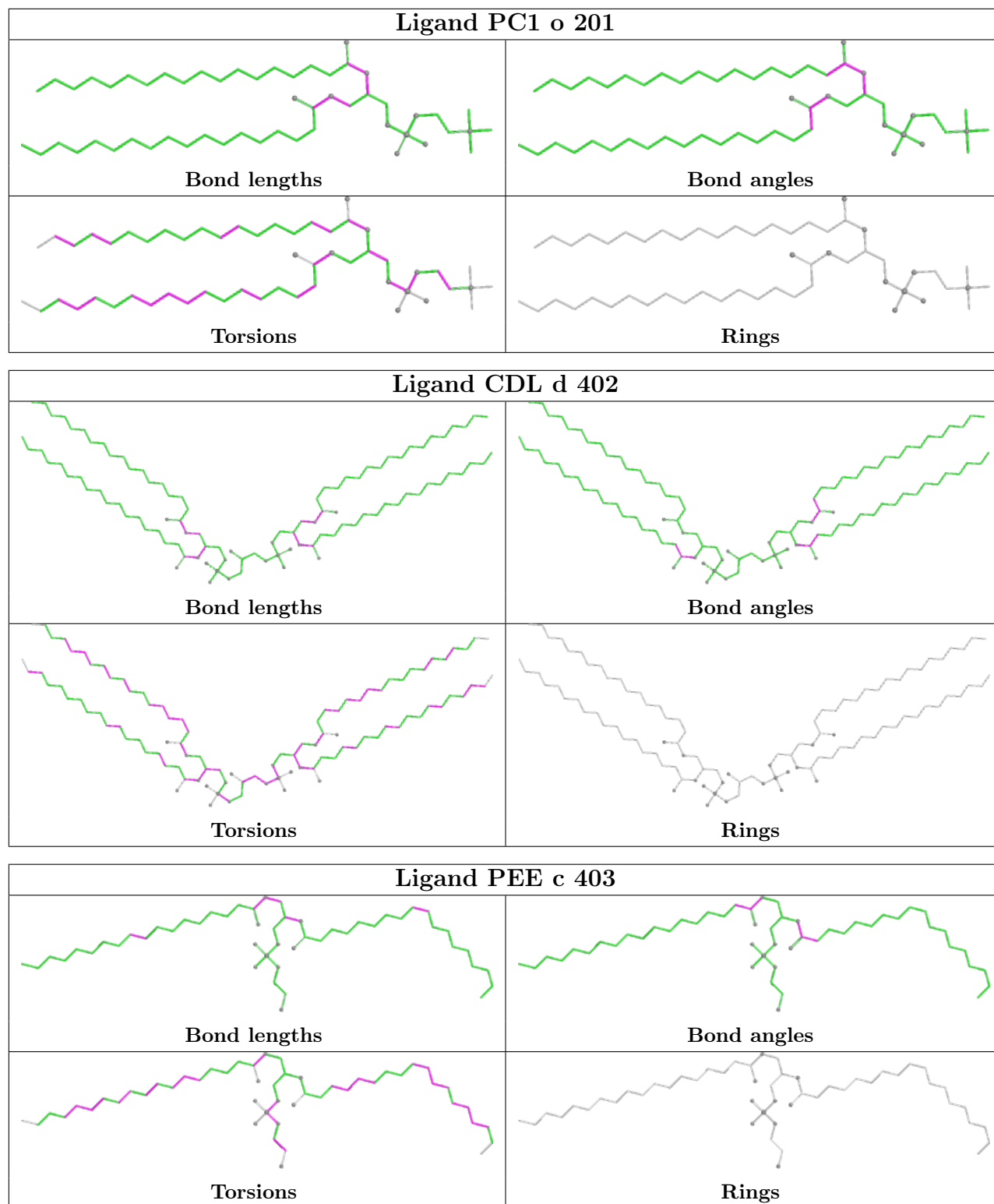


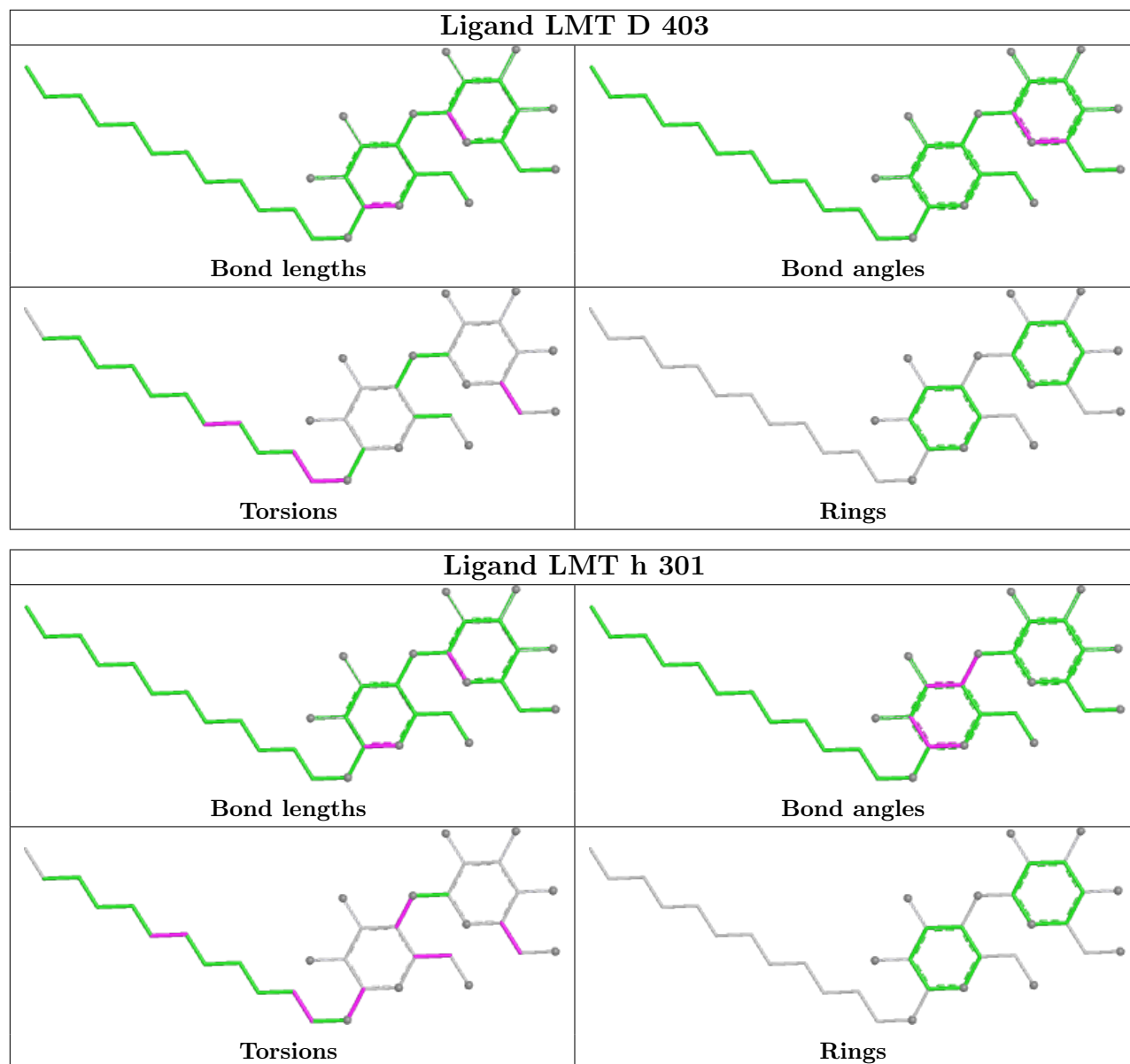


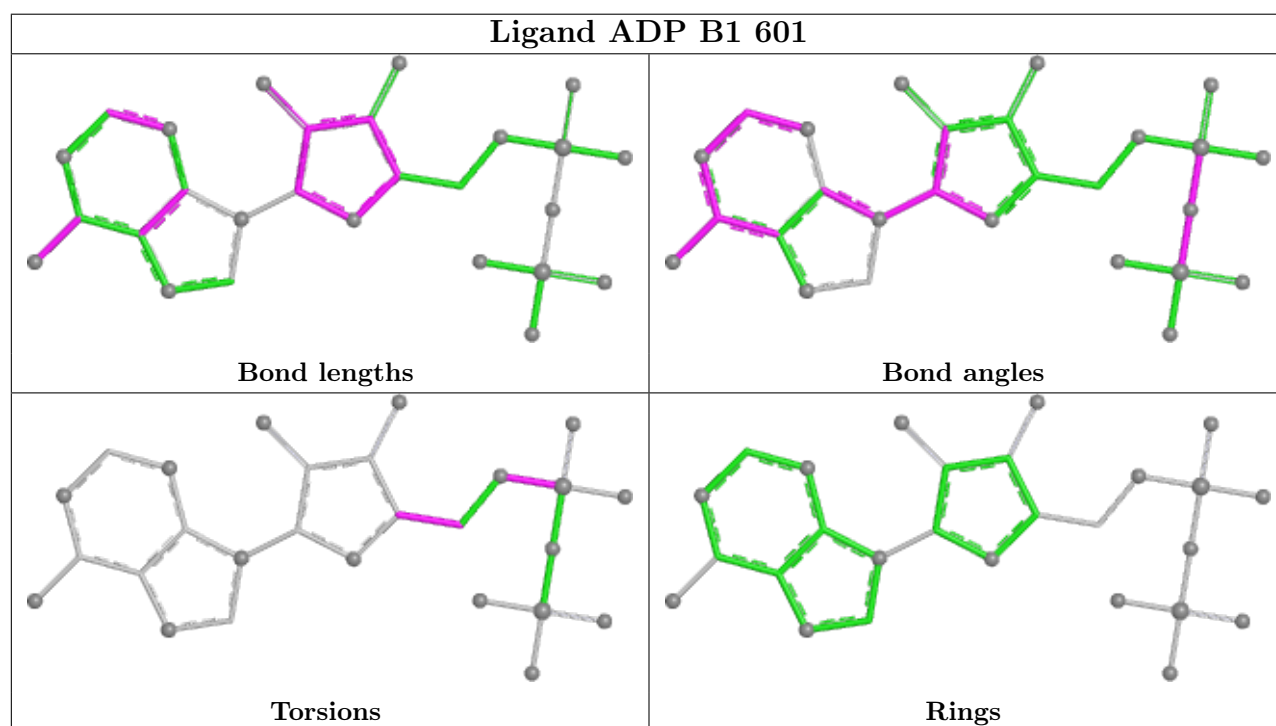
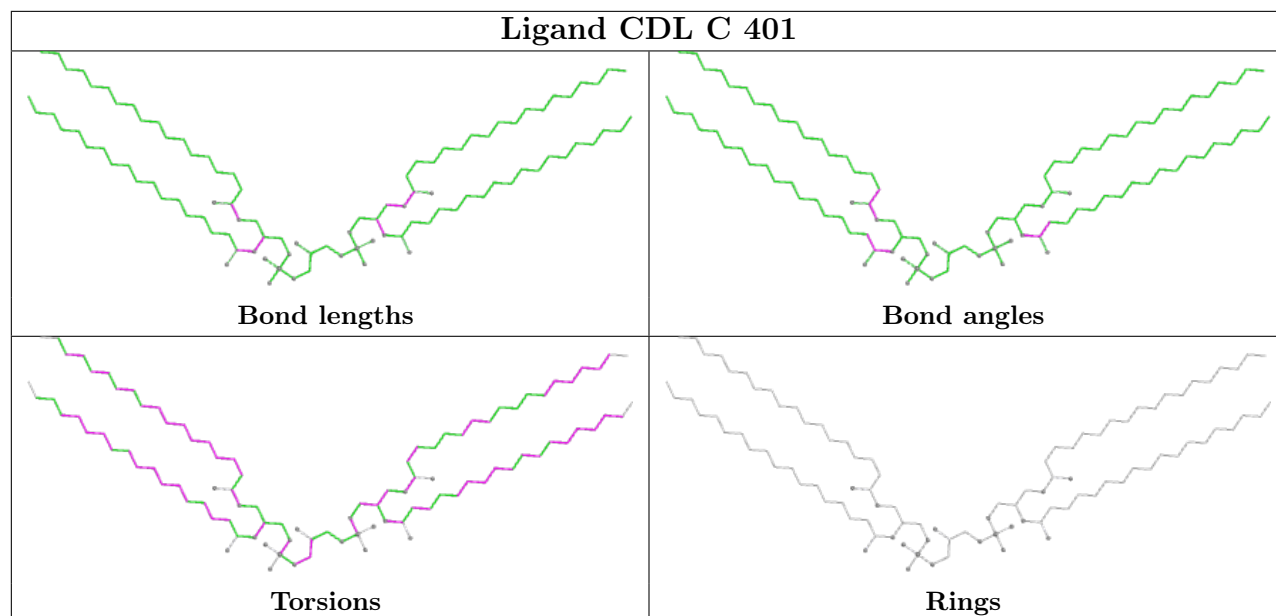


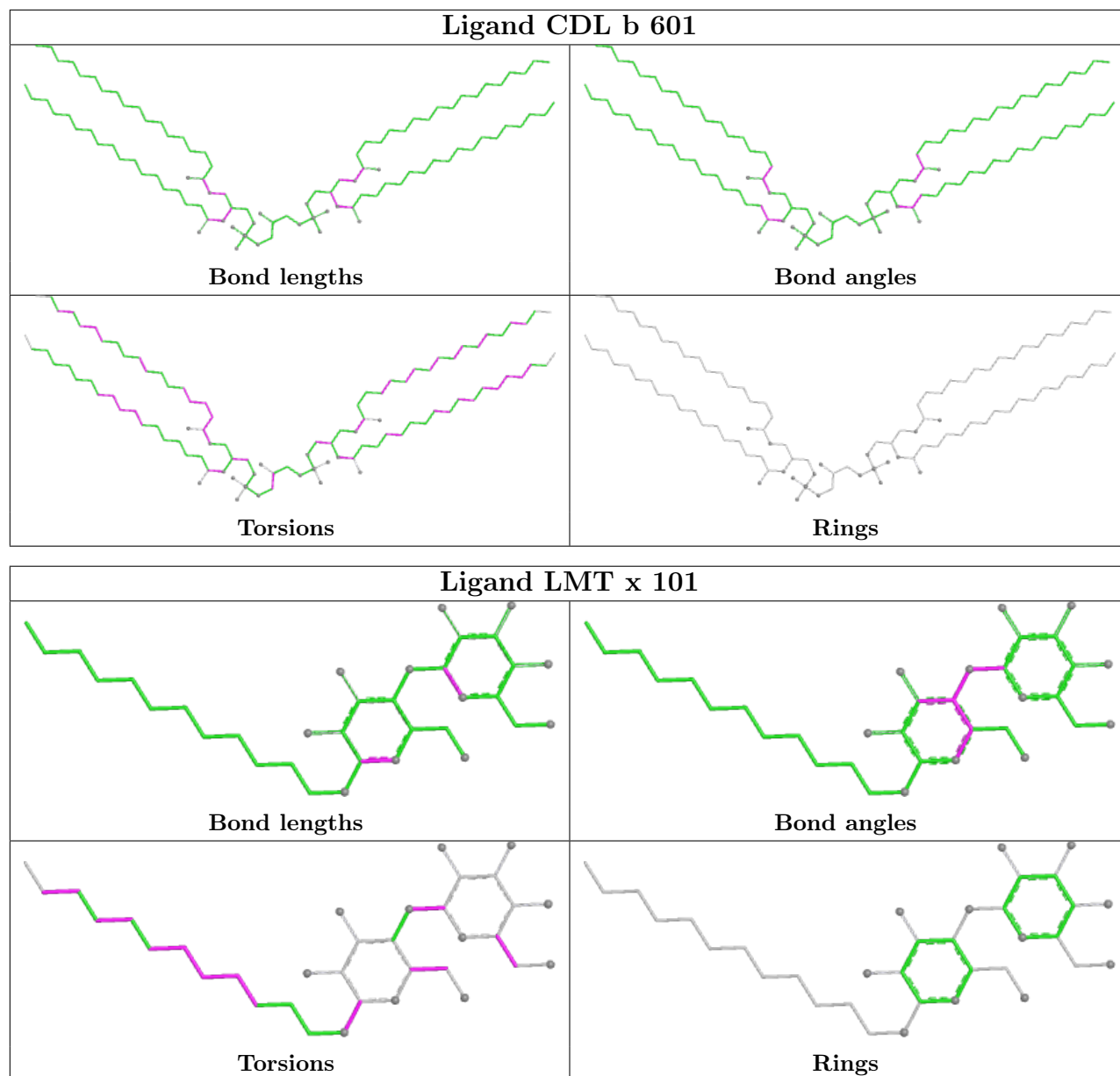


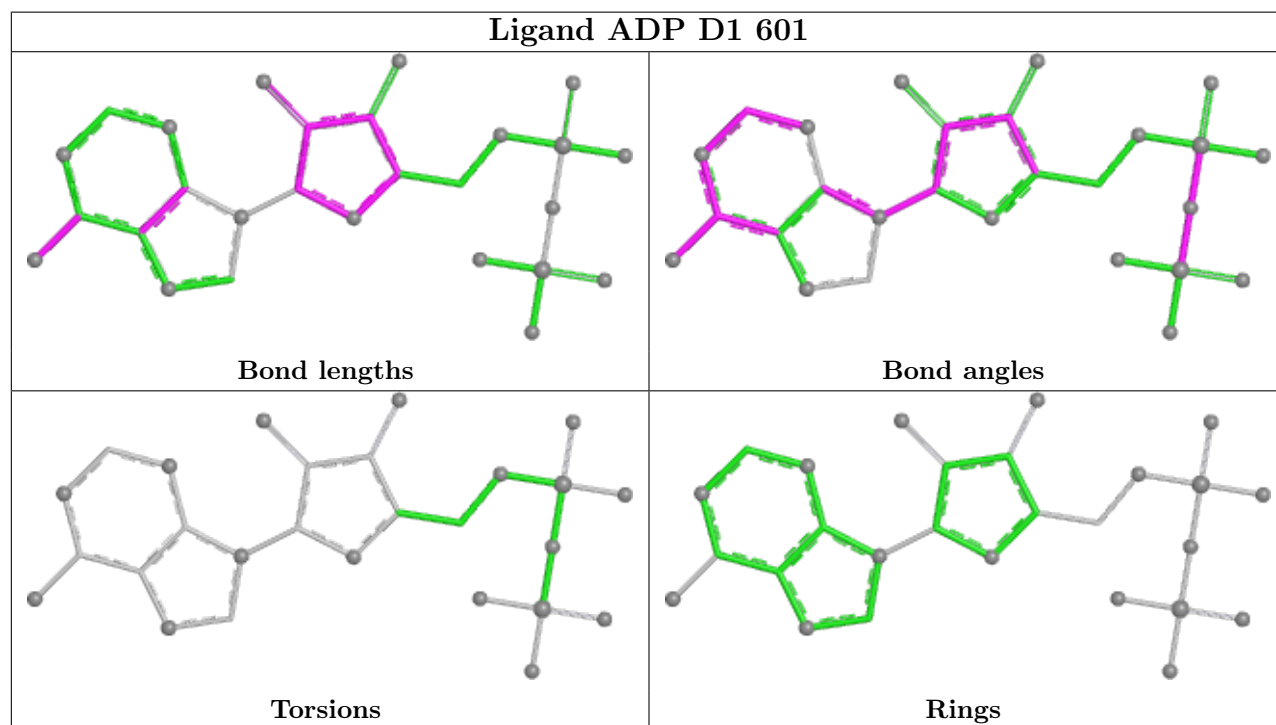
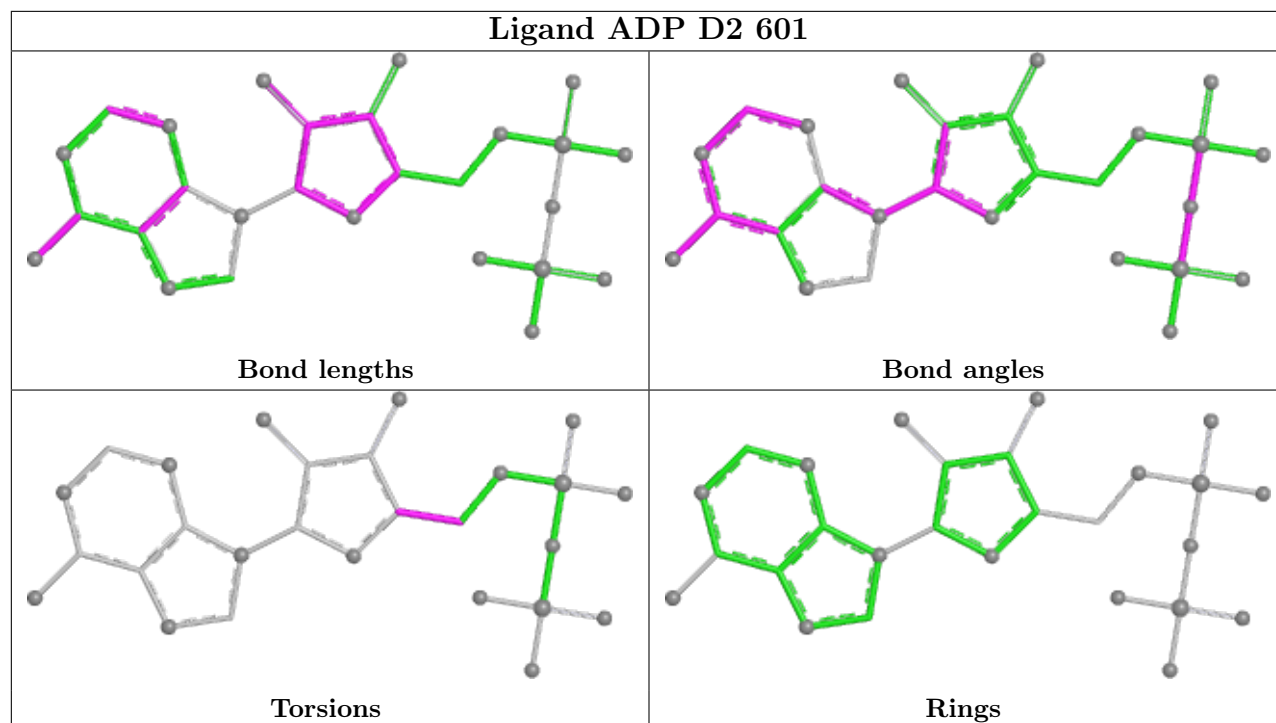


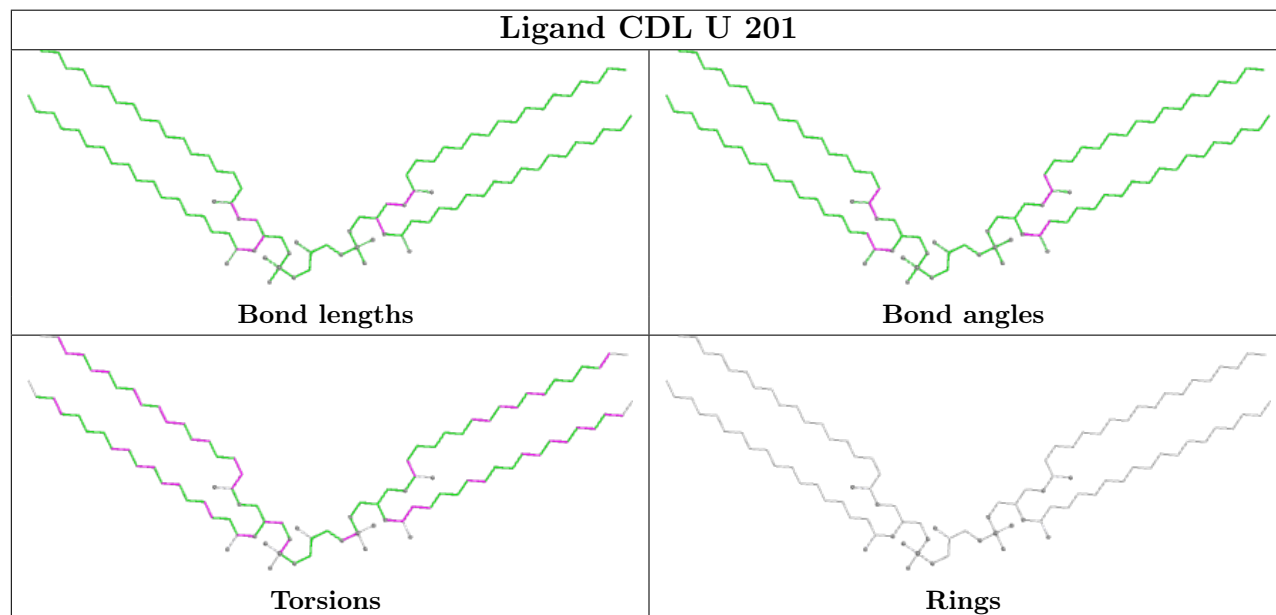
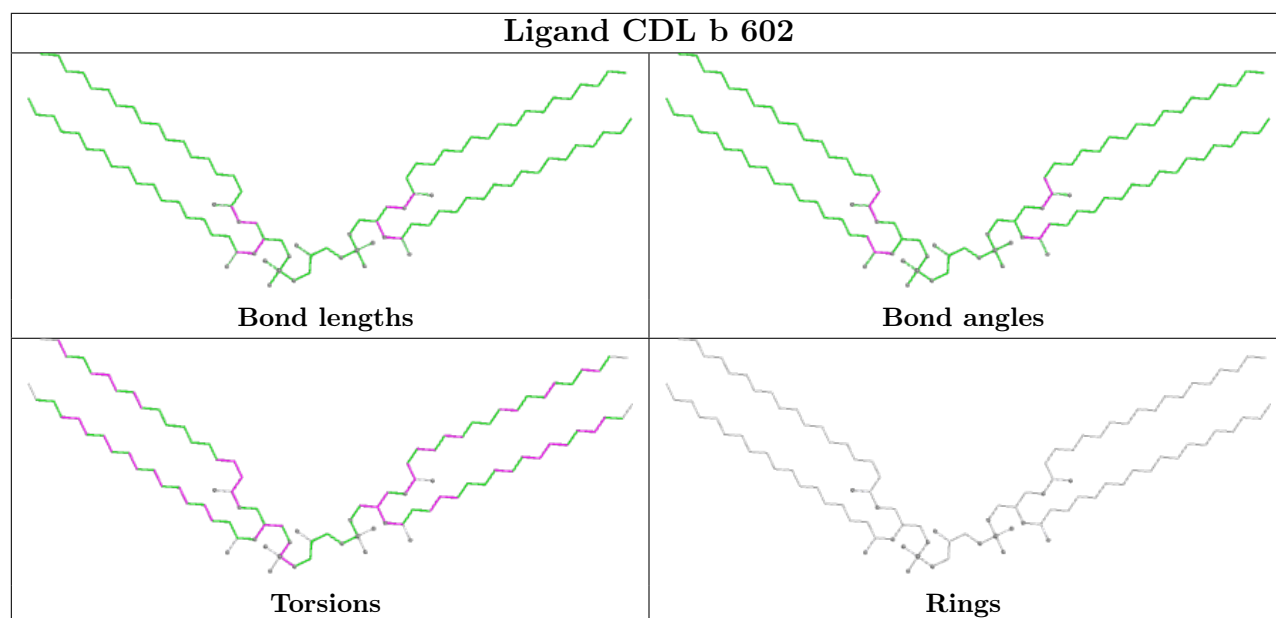
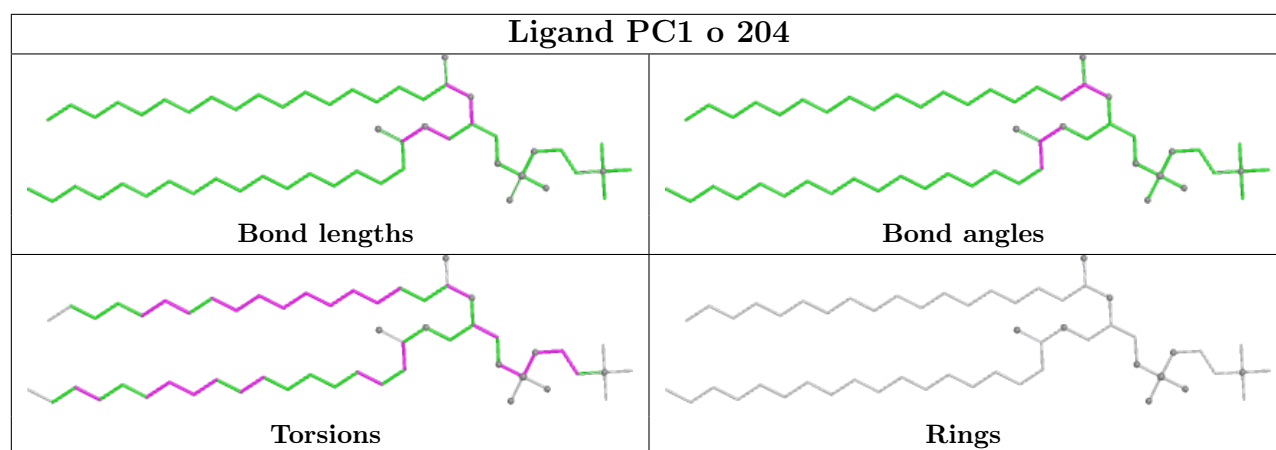


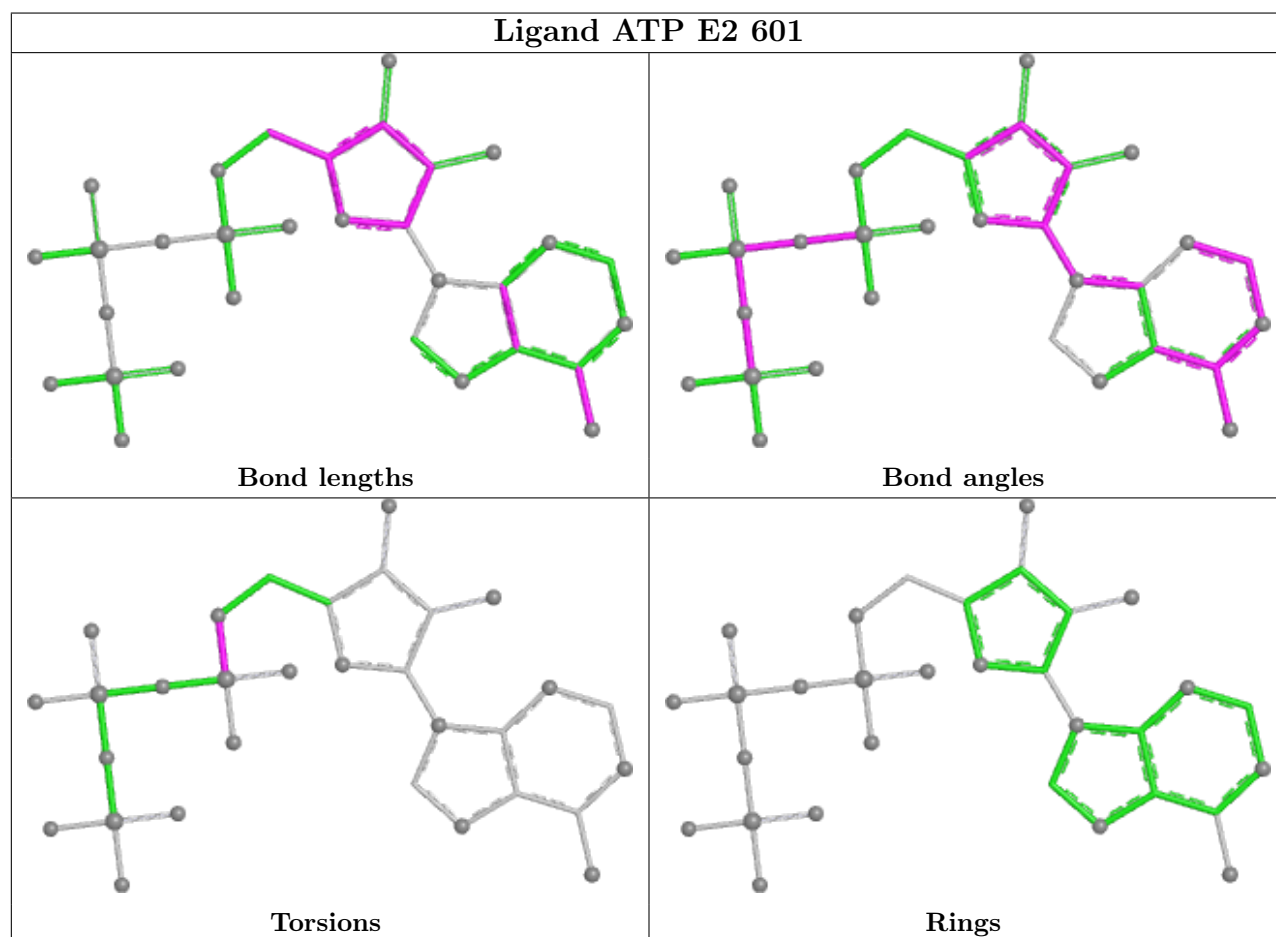
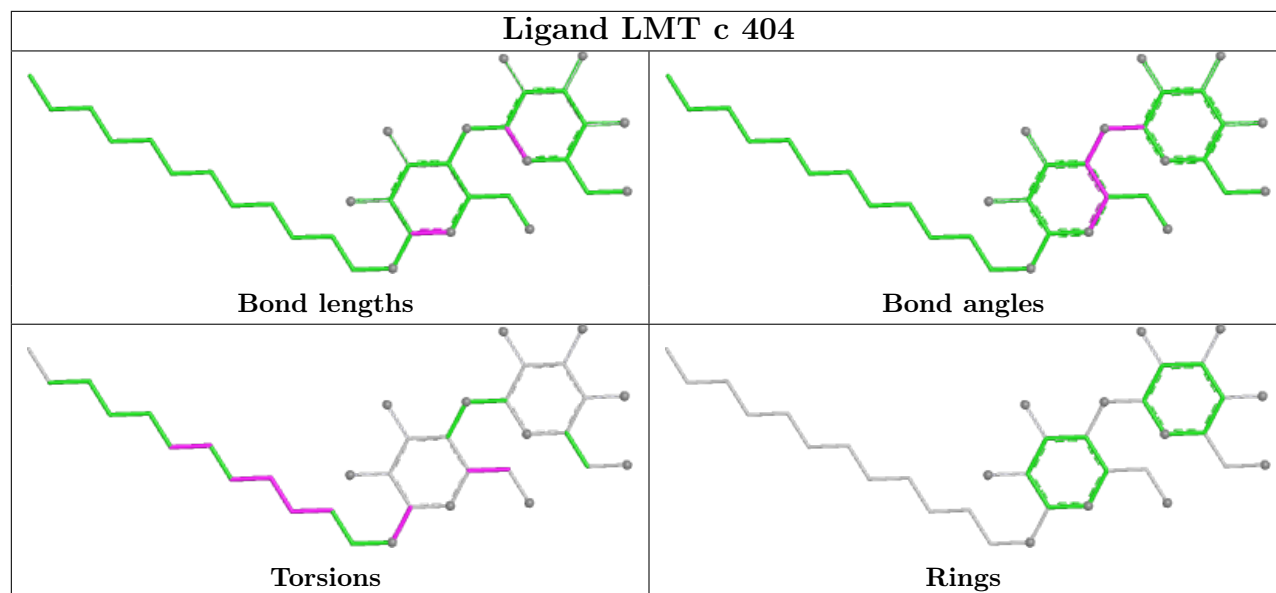


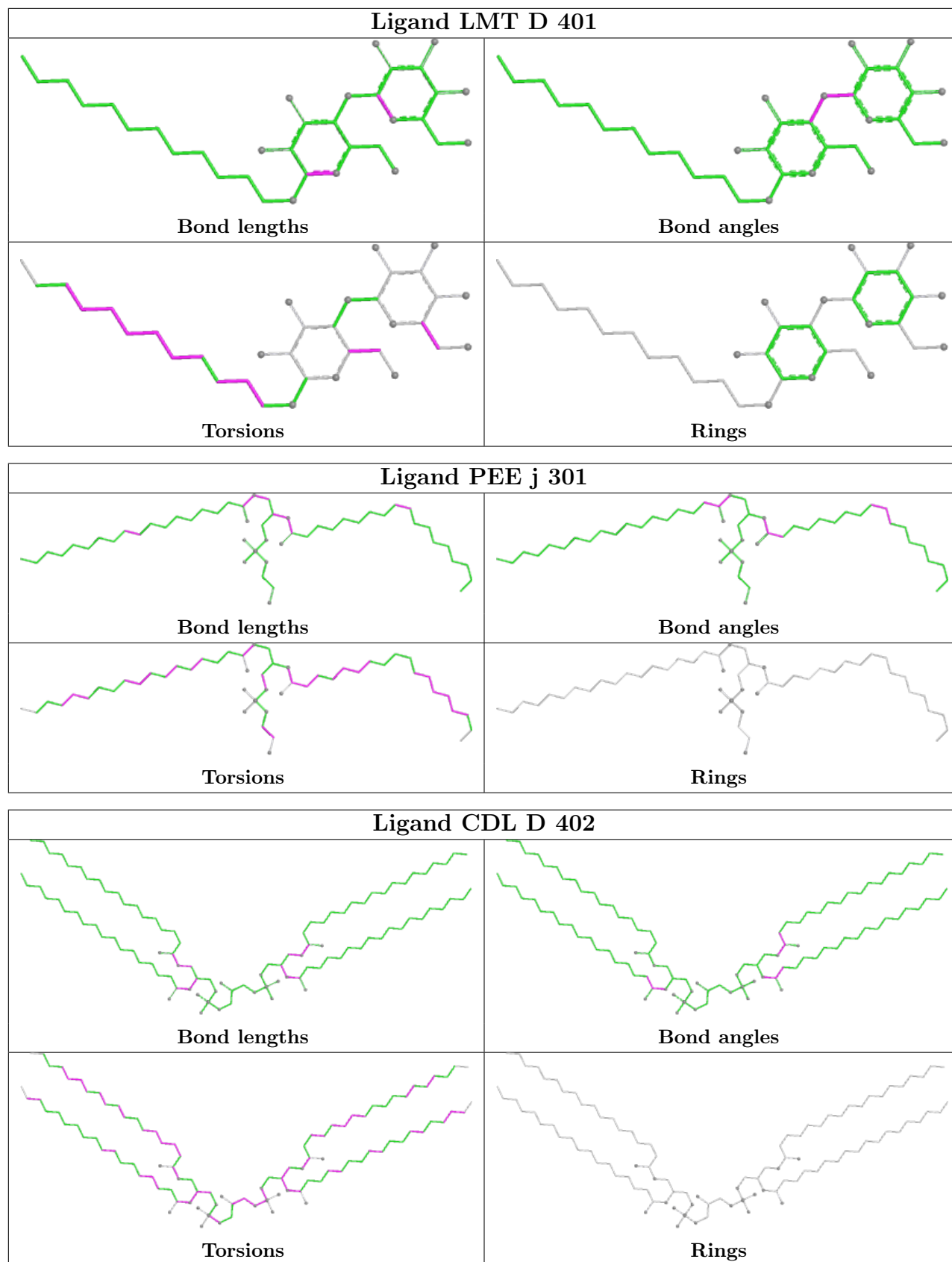


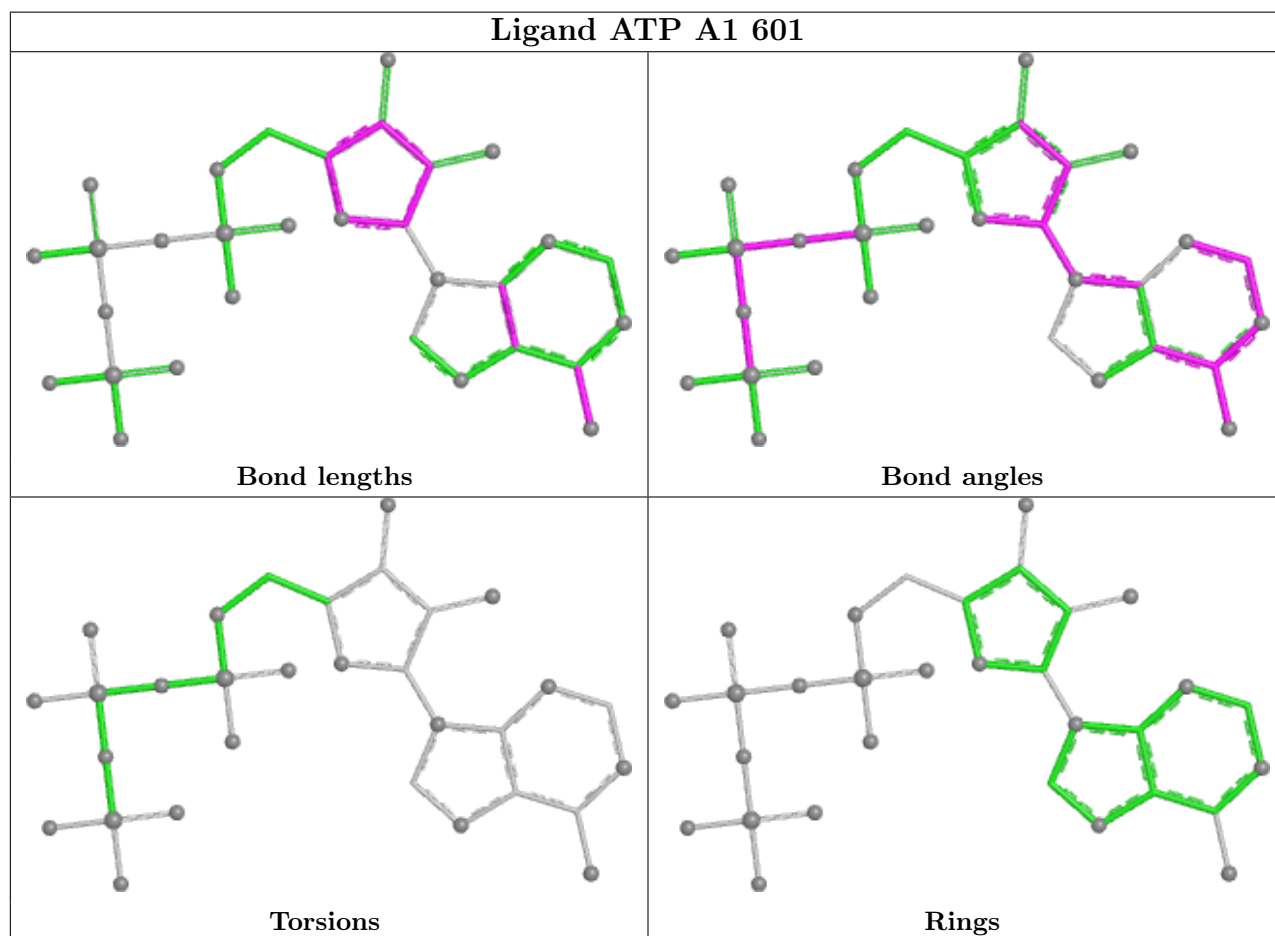
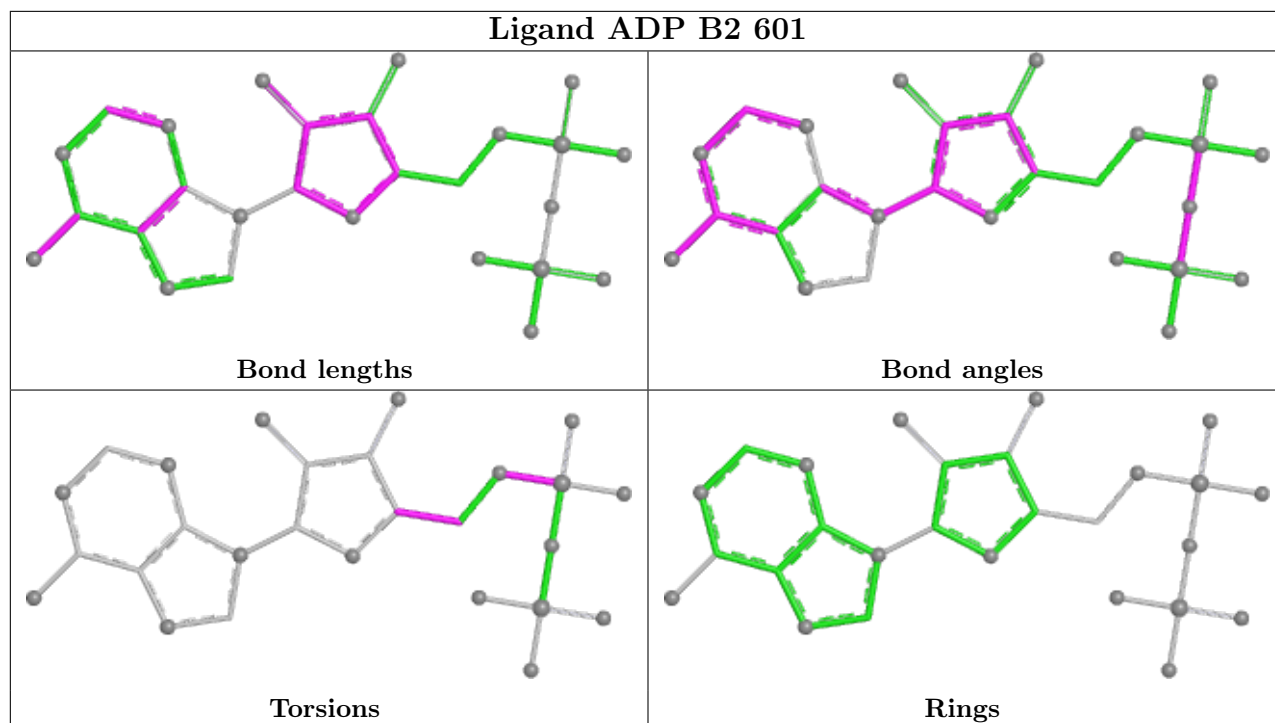


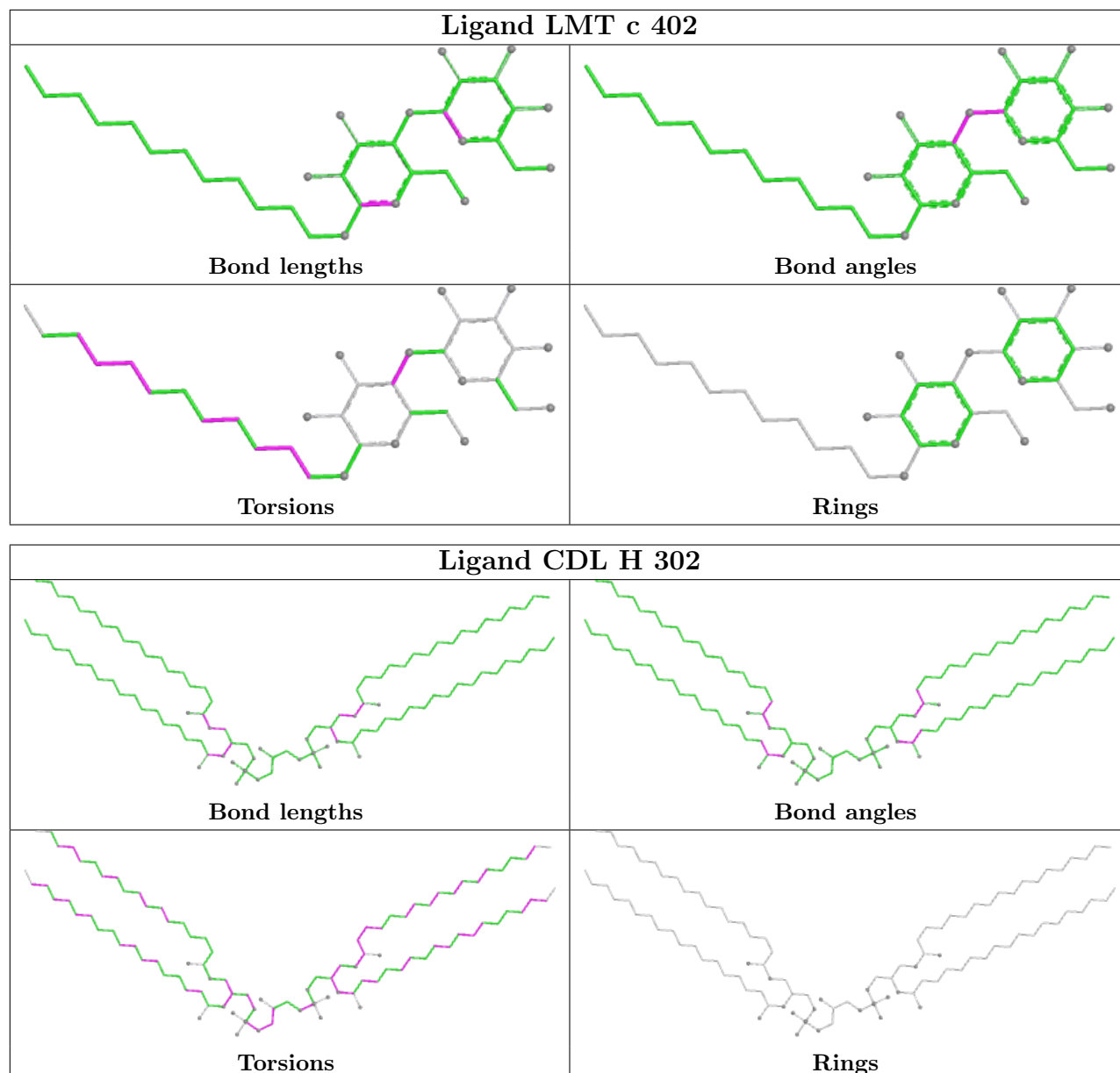


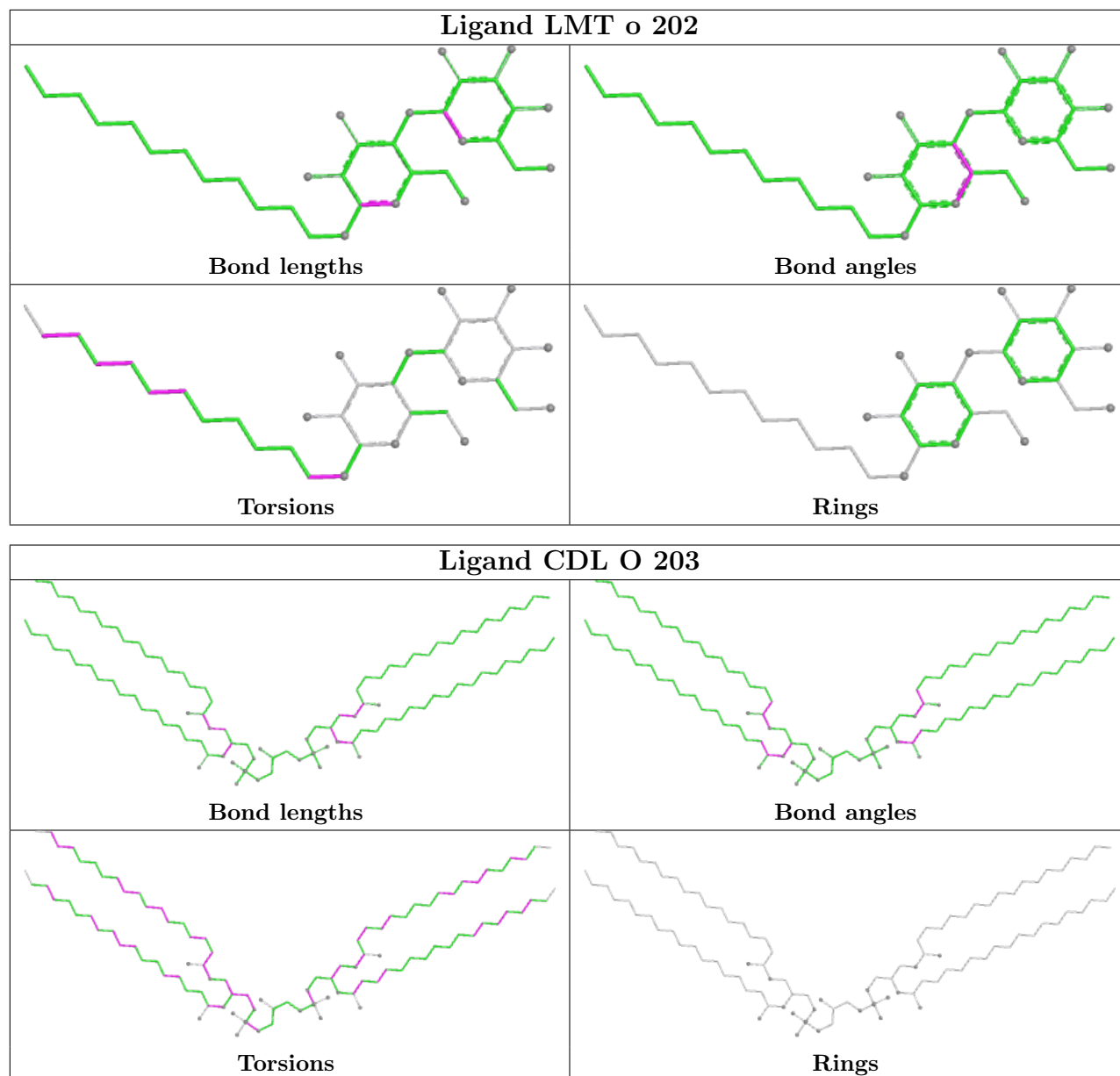


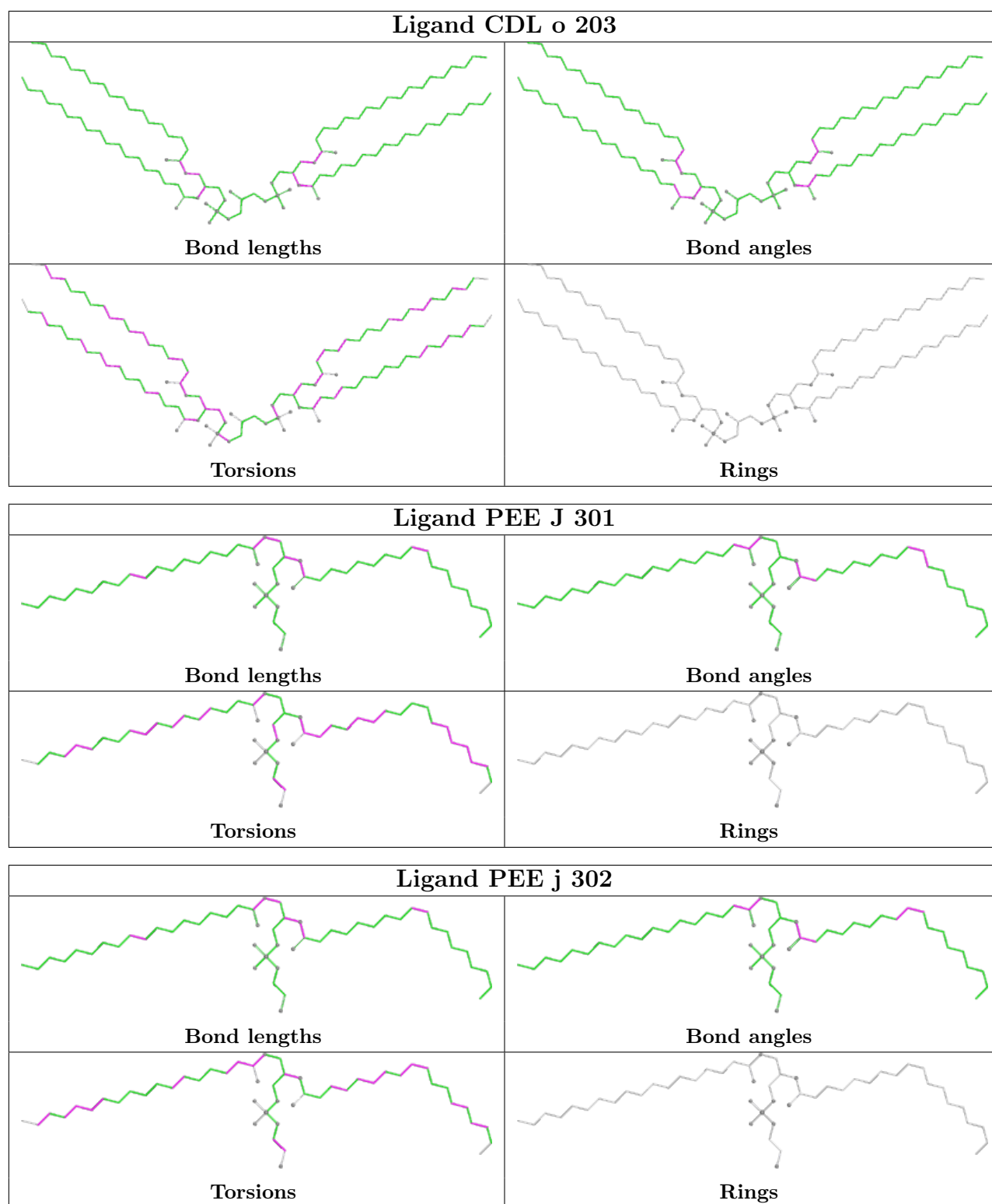












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

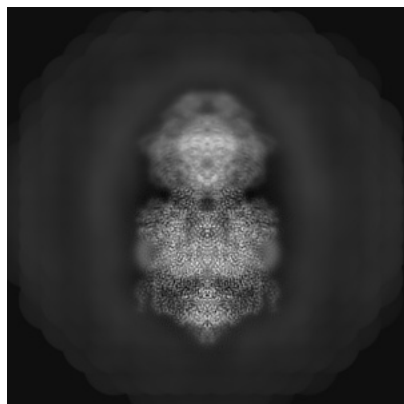
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10524. These allow visual inspection of the internal detail of the map and identification of artifacts.

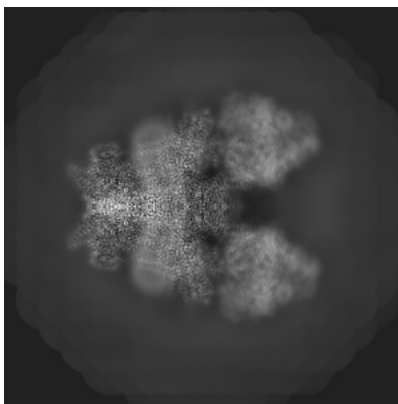
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

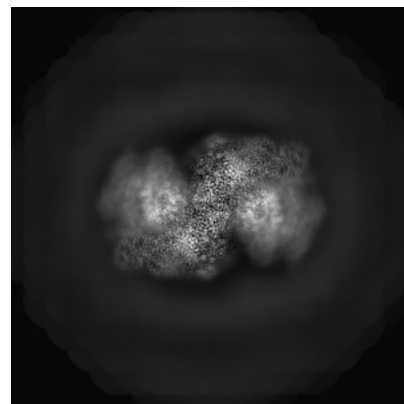
6.1.1 Primary map



X

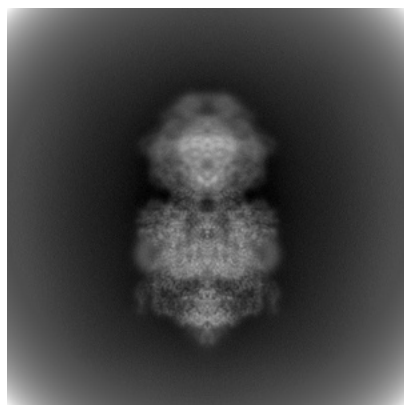


Y

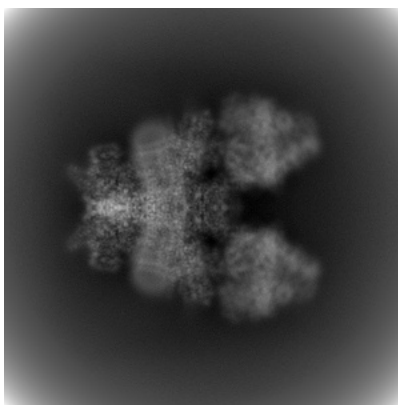


Z

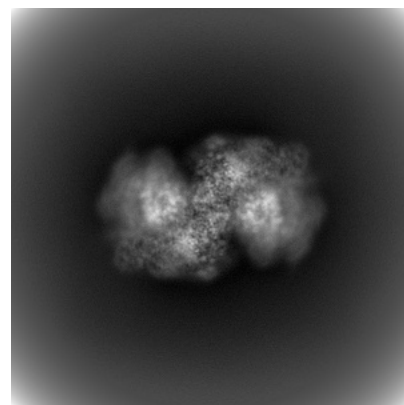
6.1.2 Raw map



X



Y

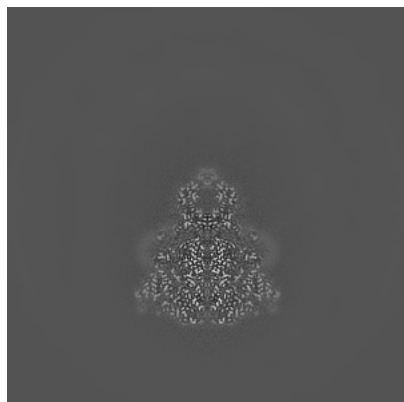


Z

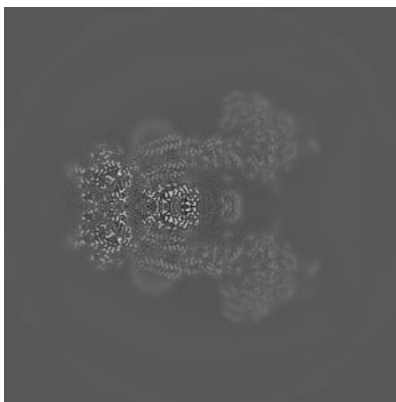
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 280

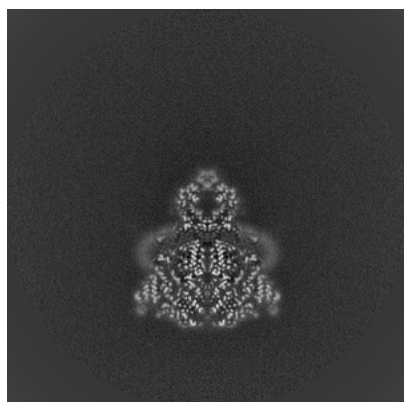


Y Index: 280

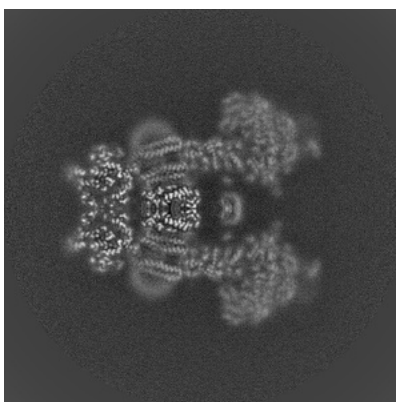


Z Index: 280

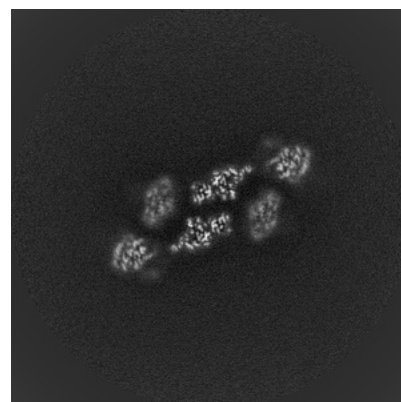
6.2.2 Raw map



X Index: 280



Y Index: 280

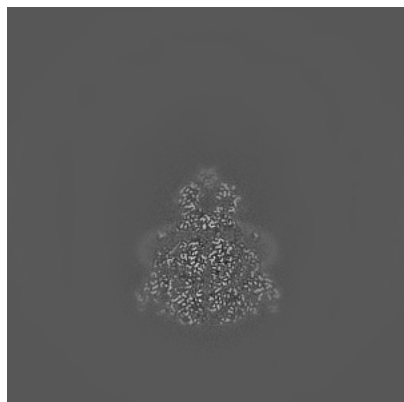


Z Index: 280

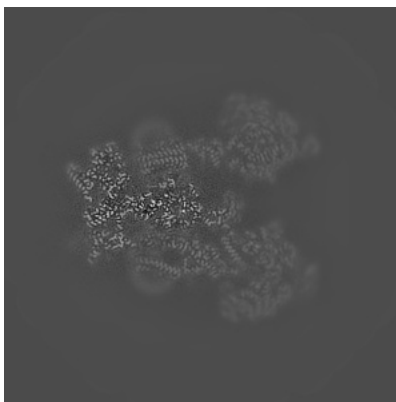
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

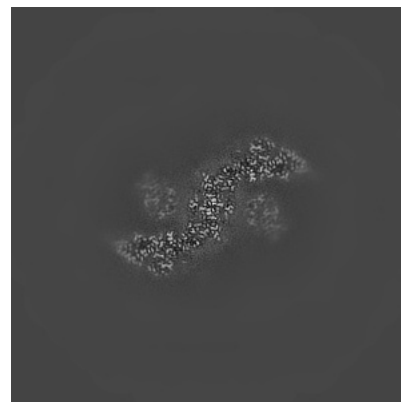
6.3.1 Primary map



X Index: 282

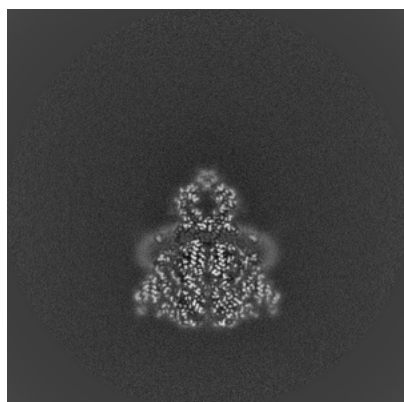


Y Index: 289

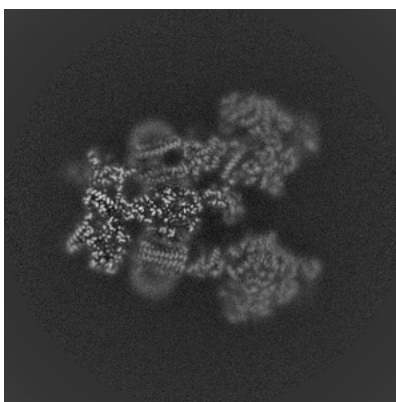


Z Index: 253

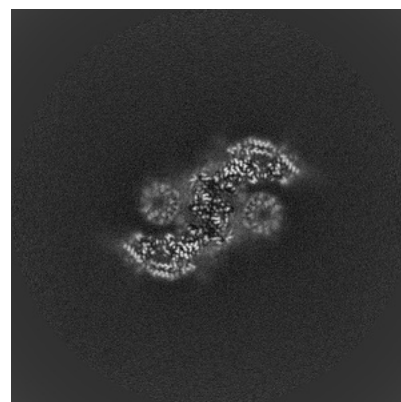
6.3.2 Raw map



X Index: 279



Y Index: 271



Z Index: 248

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

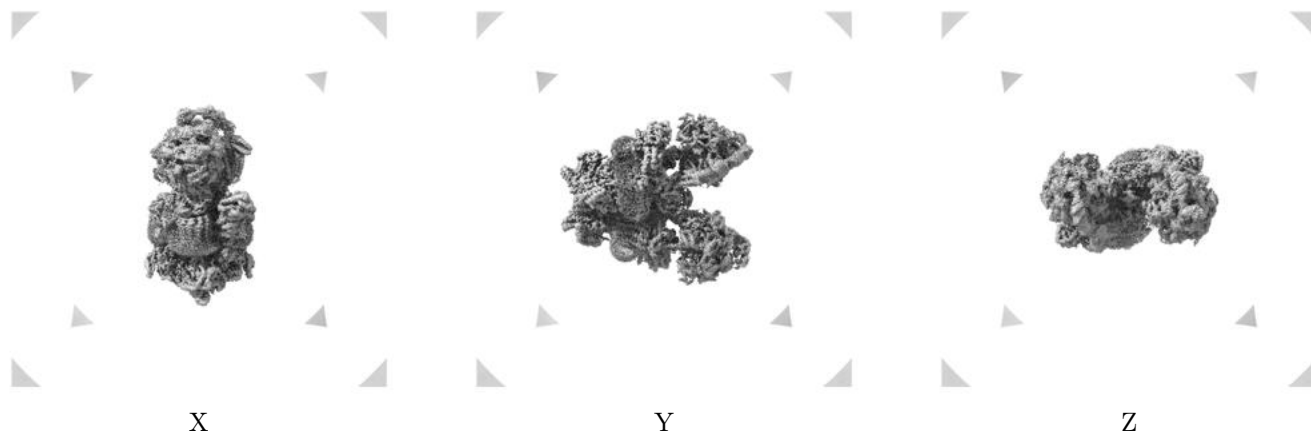
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.024. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

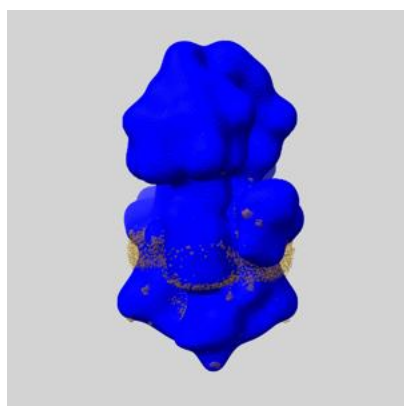
6.5 Mask visualisation [i](#)

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

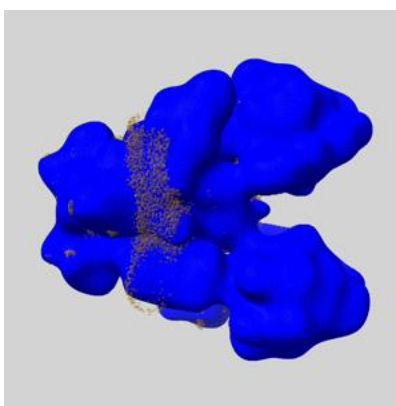
A mask typically either:

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

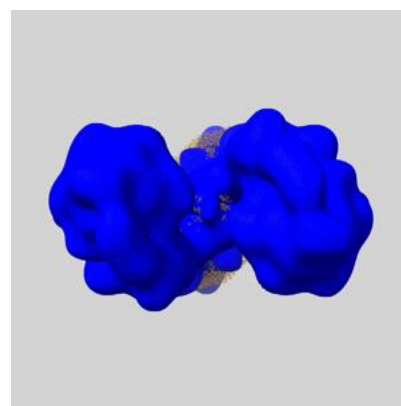
6.5.1 emd_10524_msk_1.map [i](#)



X



Y

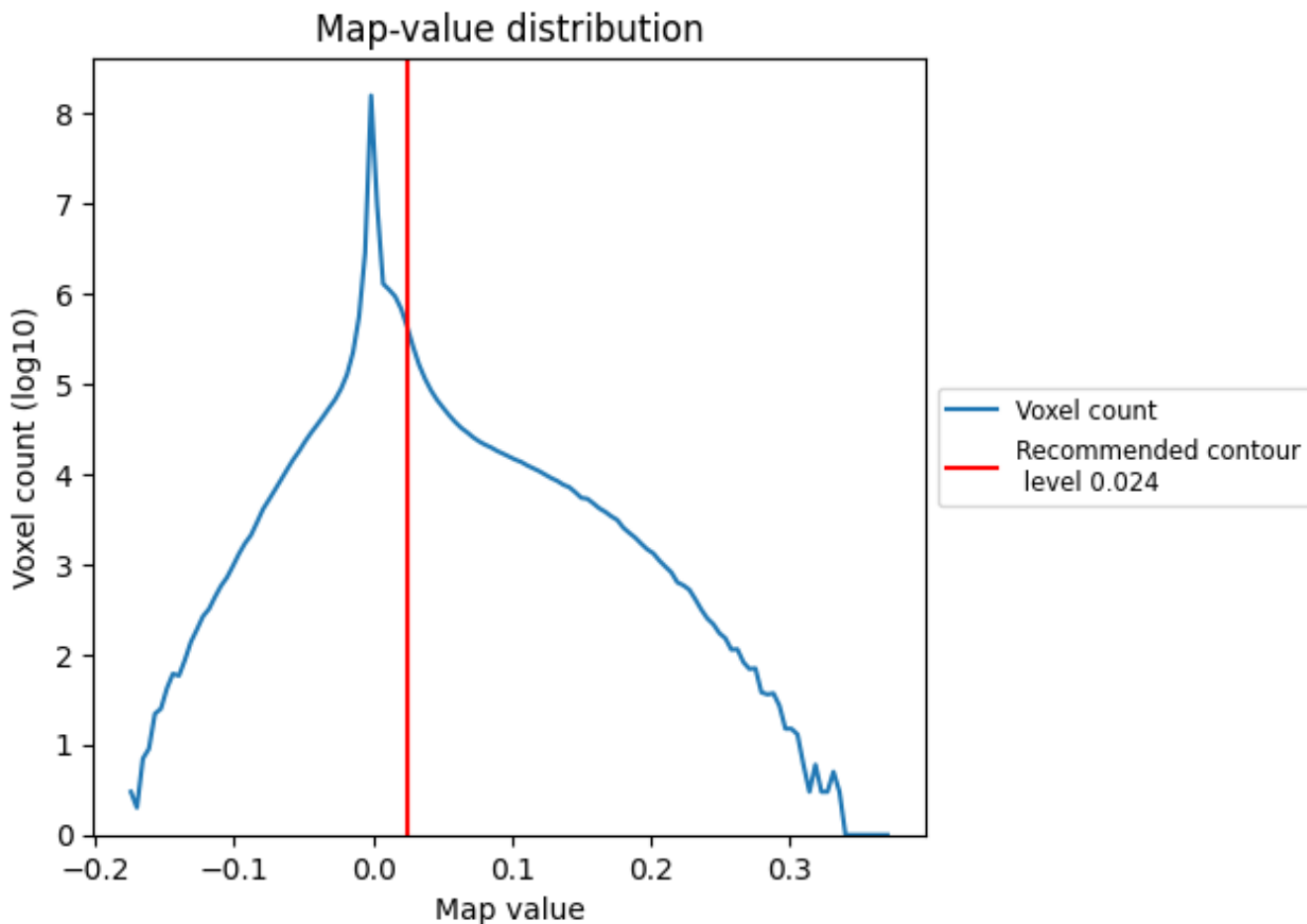


Z

7 Map analysis [i](#)

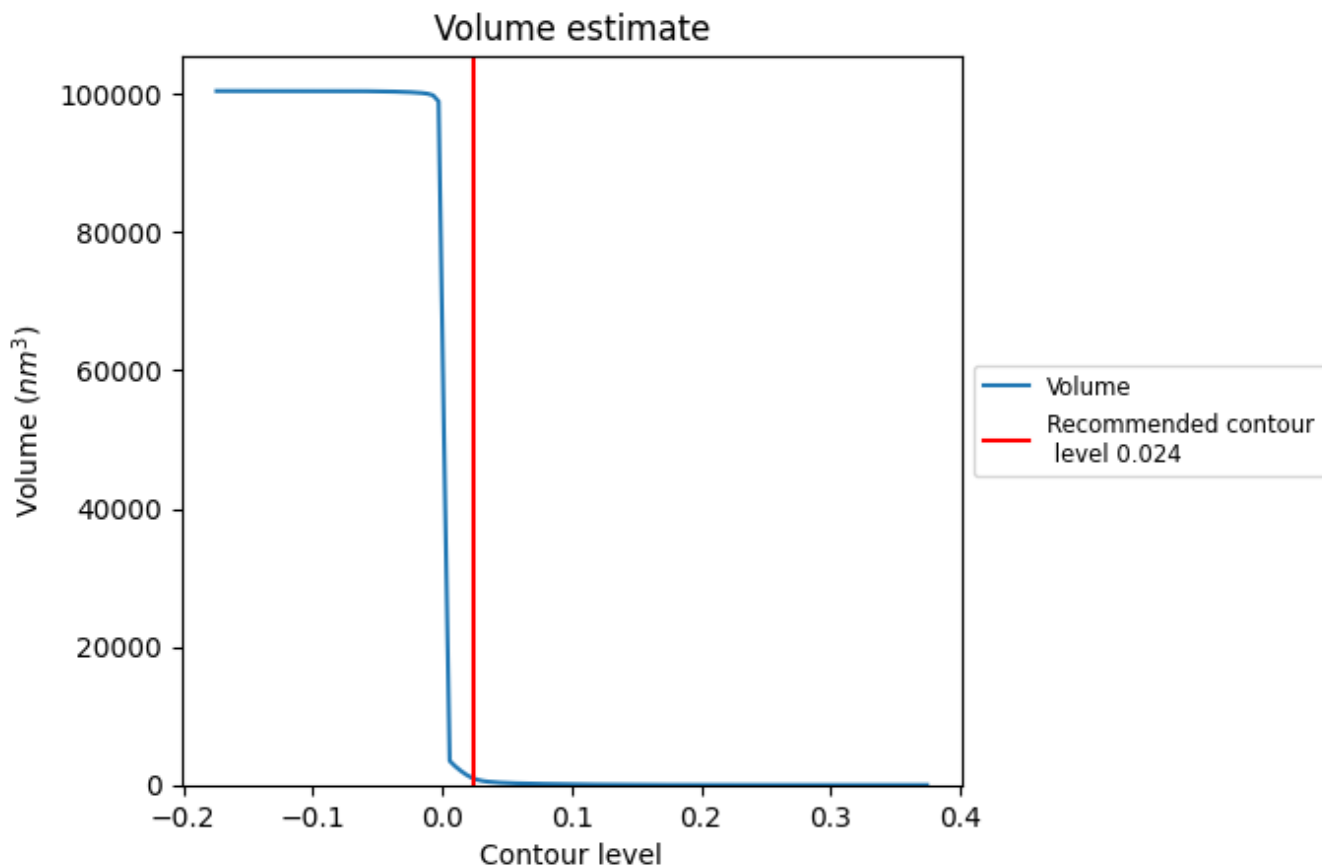
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

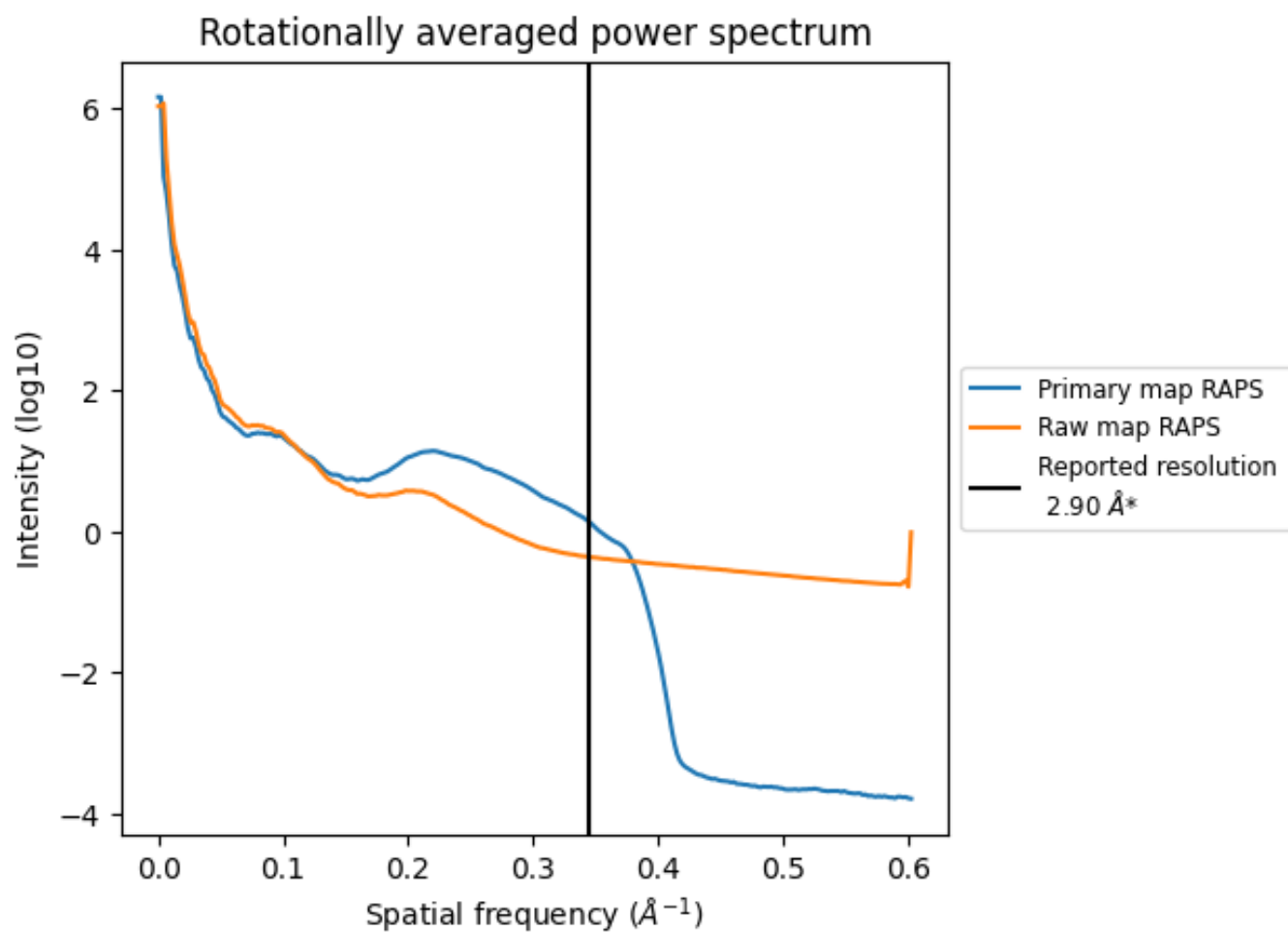
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 964 nm³; this corresponds to an approximate mass of 871 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

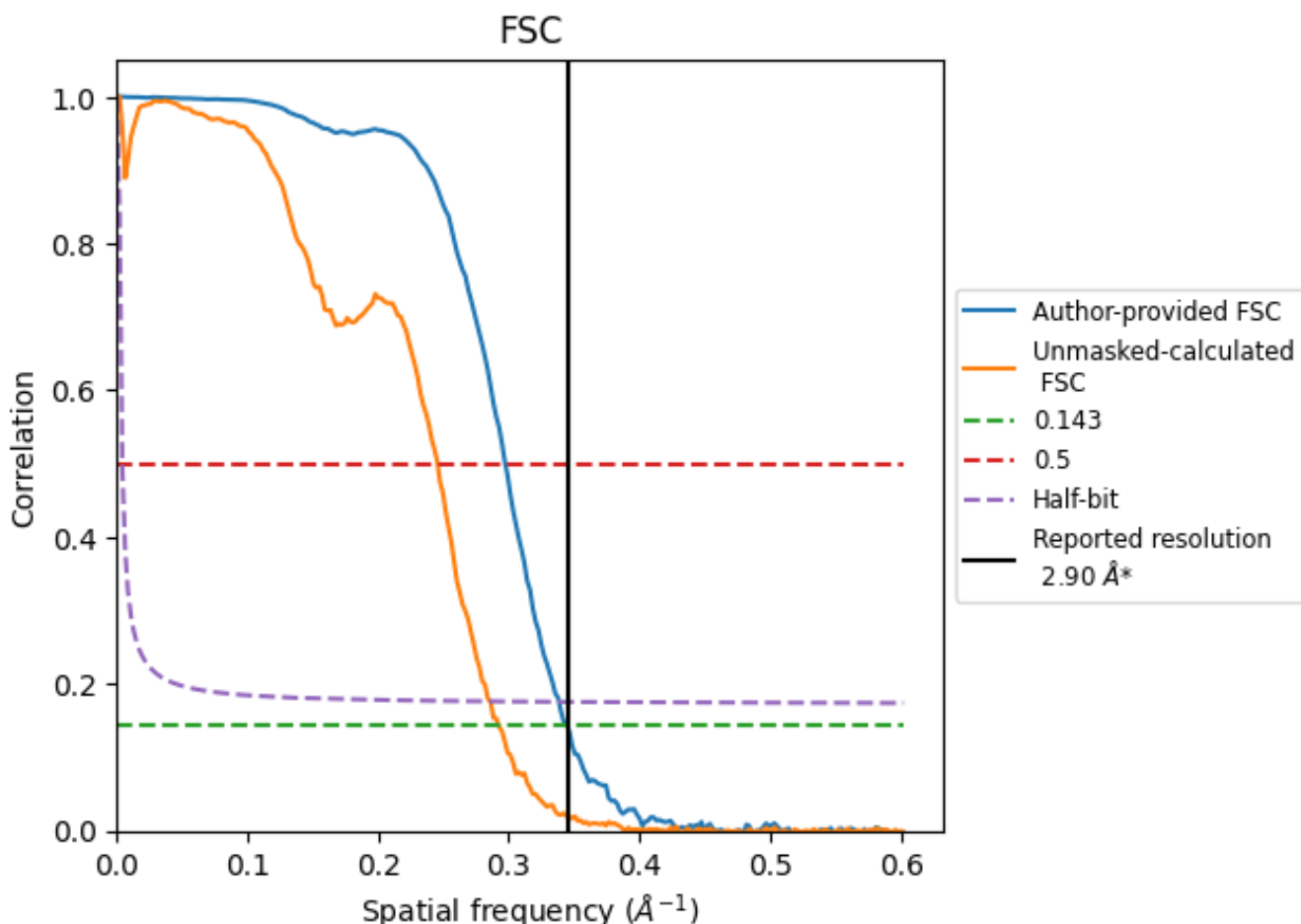


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

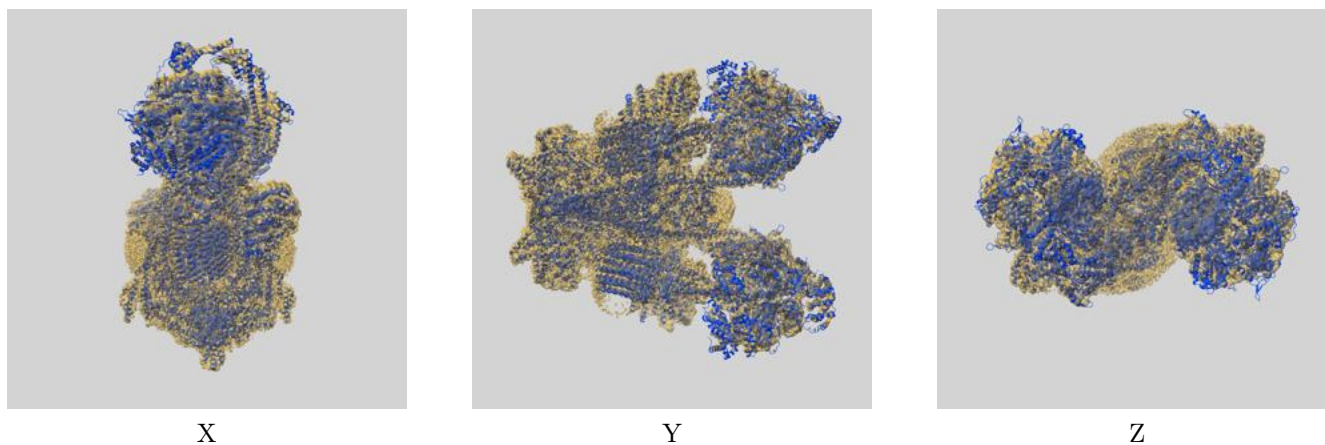
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.36	2.96
Unmasked-calculated*	3.42	4.07	3.50

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.42 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10524 and PDB model 6TMK. Per-residue inclusion information can be found in section [3](#) on page [22](#).

9.1 Map-model overlay [i](#)

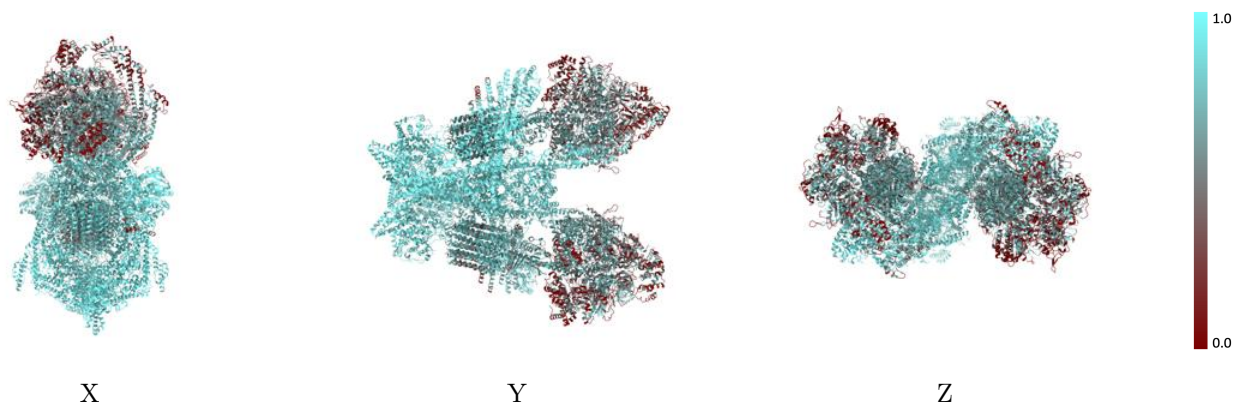


The images above show the 3D surface view of the map at the recommended contour level 0.024 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

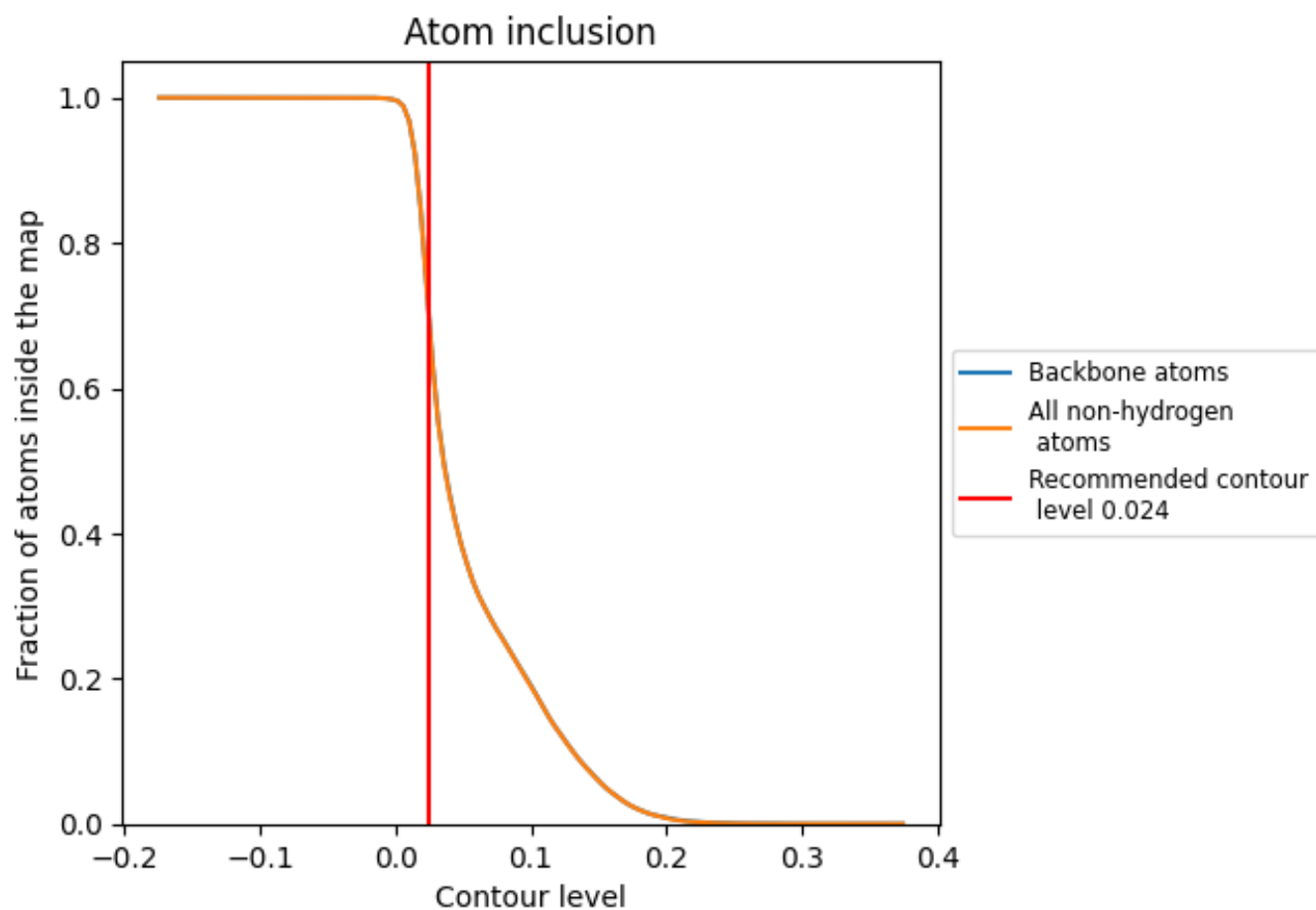
This section was not generated.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.024).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.7151
A	0.8470
A1	0.4344
A2	0.3703
B	0.7263
B1	0.6197
B2	0.5914
C	0.8435
C1	0.6151
C2	0.6099
D	0.9319
D1	0.5764
D2	0.5552
E	0.9328
E1	0.4687
E2	0.4098
F	0.9182
F1	0.3654
F2	0.3170
G	0.9404
G1	0.3517
G2	0.2880
H	0.9411
H1	0.7042
H2	0.7445
I	0.9048
I1	0.6660
I2	0.7123
J	0.9651
J1	0.6559
J2	0.7143
K	0.8898
K1	0.6901
K2	0.7203
L	0.9445

















Continued on next page...

Continued from previous page...

Chain	Atom inclusion
L1	0.7123
L2	0.6761
M	0.9561
M1	0.7525
M2	0.6841
N	0.9059
N1	0.7505
N2	0.7304
O	0.8925
O1	0.8068
O2	0.7787
P	0.9444
P1	0.8008
P2	0.7887
Q	0.8813
Q1	0.7867
Q2	0.7827
R	0.8224
S	0.9242
T	0.9237
U	0.8829
V	0.9486
W	0.9518
X	0.9424
a	0.8357
b	0.7519
c	0.8336
d	0.9328
d1	0.6059
d2	0.6999
e	0.9320
e1	0.7471
e2	0.7605
f	0.9196
g	0.9380
g1	0.7295
g2	0.7305
h	0.9417
i	0.9034
i1	0.7204
i2	0.7295
j	0.9651

Continued on next page...

Continued from previous page...

Chain	Atom inclusion
k	 0.8930
l	 0.9439
m	 0.9601
n	 0.9067
o	 0.8925
p	 0.9456
q	 0.8622
r	 0.8300
s	 0.9229
t	 0.9181
u	 0.8853
v	 0.9467
w	 0.9558
x	 0.9409