



wwPDB EM Validation Summary Report ⓘ

Apr 1, 2025 – 10:23 pm BST

PDB ID : 6YNY / pdb_00006yny
EMDB ID : EMD-10860
Title : Cryo-EM structure of Tetrahymena thermophila mitochondrial ATP synthase
- F1Fo composite dimer model
Authors : Kock Flygaard, R.; Muhleip, A.; Amunts, A.
Deposited on : 2020-04-14
Resolution : 2.70 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:

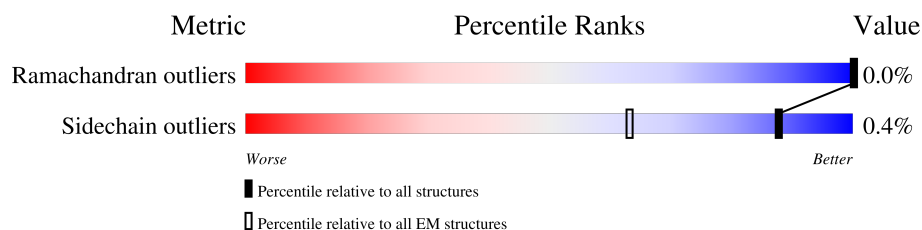
EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 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.

















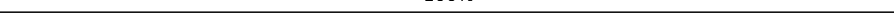
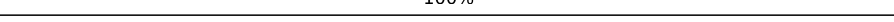




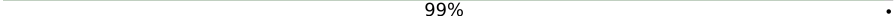
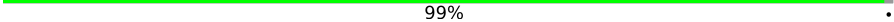



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	446	97% .
1	a	446	97% .
2	B	381	34% 93% 7%
2	b	381	33% 93% 7%
3	D	234	17% 88% 12%
3	d	234	16% 88% 12%
4	F	204	98% .
4	f	204	98% .
5	I	209	99% .






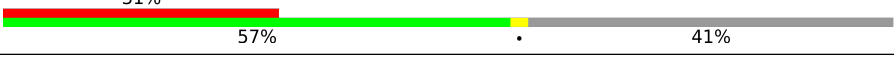

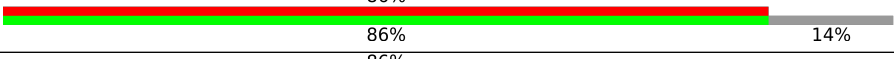

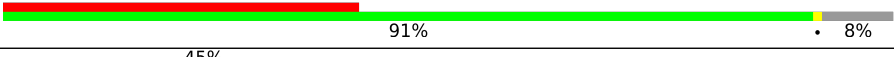
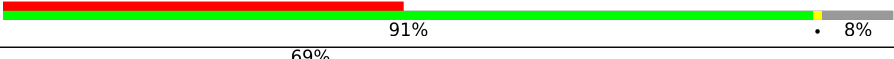
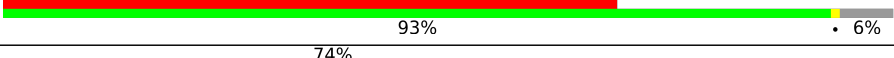
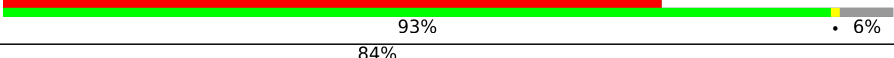
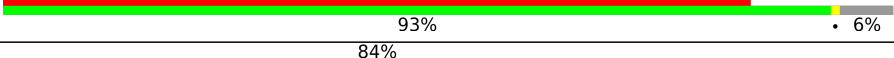
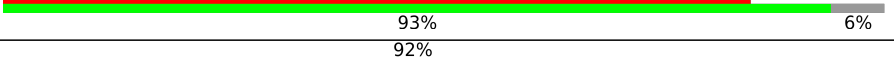
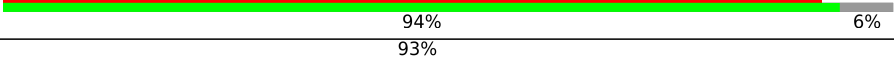
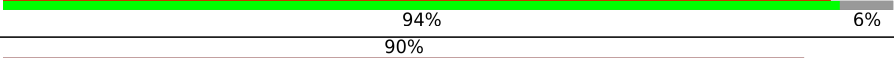
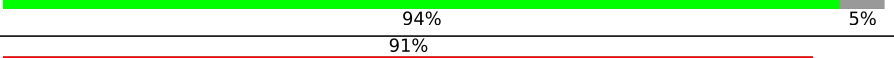
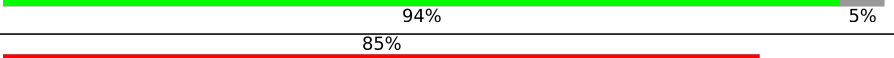
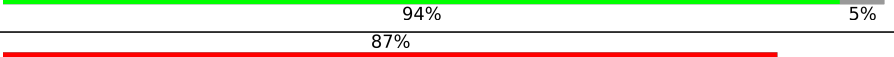
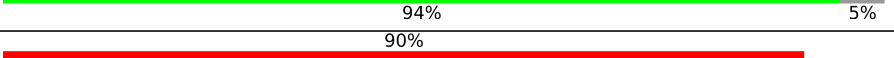
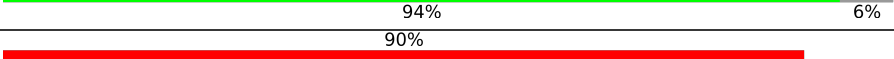
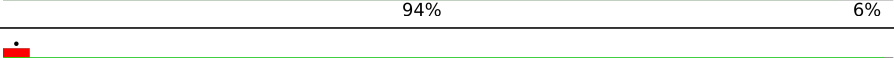
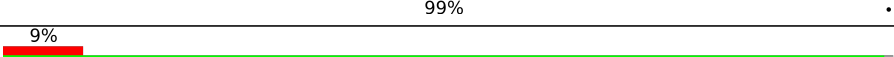
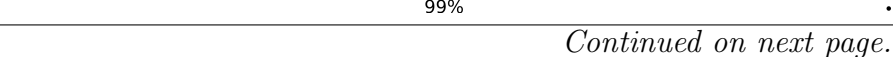
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Mol	Chain	Length	Quality of chain
5	i	209	 100%
6	K	179	 100%
6	k	179	 99%
7	C	100	 95%
7	c	100	 95%
8	G	286	 89%
8	g	286	 89%
9	H	268	 86%
9	h	268	 86%
10	J	273	 98%
10	j	273	 99%
11	L	247	 99%
11	l	247	 99%
12	M	221	 100%
12	m	221	 100%
13	N	179	 66%
13	n	179	 66%
14	O	154	 64%
14	o	154	 64%
15	P	152	 99%
15	p	152	 99%
16	Q	152	 71%
16	q	152	 71%
17	R	149	 93%
17	r	149	 97%

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Mol	Chain	Length	Quality of chain
18	S	145	
18	s	145	
19	E	480	
19	e	480	
20	i1	108	
20	i2	108	
21	t	460	
22	G1	219	
22	G2	219	
23	g1	299	
23	g2	299	
24	A1	546	
24	A2	546	
24	B1	546	
24	B2	546	
24	C1	546	
24	C2	546	
25	D1	497	
25	D2	497	
25	E1	497	
25	E2	497	
25	F1	497	
25	F2	497	
26	H1	76	
26	H2	76	

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Mol	Chain	Length	Quality of chain
26	I1	76	
26	I2	76	
26	J1	76	
26	J2	76	
26	K1	76	
26	K2	76	
26	L1	76	
26	L2	76	
26	M1	76	
26	M2	76	
26	N1	76	
26	N2	76	
26	O1	76	
26	O2	76	
26	P1	76	
26	P2	76	
26	Q1	76	
26	Q2	76	
27	d1	158	
27	d2	158	
28	e1	71	
28	e2	71	

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 285933 atoms, of which 143905 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 subunit a.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	a	433	Total	C	H	N	O	S	0	0
			7155	2453	3527	526	633	16		
1	A	433	Total	C	H	N	O	S	0	0
			7157	2453	3529	526	633	16		

- Molecule 2 is a protein called subunit b.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	b	354	Total	C	H	N	O	S	0	0
			5726	1845	2851	487	531	12		
2	B	354	Total	C	H	N	O	S	0	0
			5724	1845	2849	487	531	12		

- Molecule 3 is a protein called subunit d.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	d	206	Total	C	H	N	O	S	0	0
			3274	1065	1598	274	332	5		
3	D	206	Total	C	H	N	O	S	0	0
			3274	1065	1598	274	332	5		

- Molecule 4 is a protein called subunit f.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	f	200	Total	C	H	N	O	S	0	0
			3373	1095	1691	299	278	10		
4	F	200	Total	C	H	N	O	S	0	0
			3374	1095	1692	299	278	10		

- Molecule 5 is a protein called subunit i/j.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	i	209	Total	C	H	N	O	S	0	0
			3462	1121	1742	304	285	10		
5	I	209	Total	C	H	N	O	S	0	0
			3460	1121	1740	304	285	10		

- Molecule 6 is a protein called subunit k.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	k	179	Total	C	H	N	O	S	0	0
			2902	939	1429	257	266	11		
6	K	179	Total	C	H	N	O	S	0	0
			2903	939	1430	257	266	11		

- Molecule 7 is a protein called subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	c	96	Total	C	H	N	O	S	0	0
			1671	565	830	131	143	2		
7	C	96	Total	C	H	N	O	S	0	0
			1671	565	830	131	143	2		

- Molecule 8 is a protein called ATPTT3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	g	256	Total	C	H	N	O	S	0	0
			4338	1474	2118	348	388	10		
8	G	256	Total	C	H	N	O	S	0	0
			4338	1474	2118	348	388	10		

- Molecule 9 is a protein called ATPTT4.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	h	231	Total	C	H	N	O	S	0	0
			3836	1236	1883	361	350	6		
9	H	231	Total	C	H	N	O	S	0	0
			3836	1236	1883	361	350	6		

- Molecule 10 is a protein called ATPTT5.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	j	269	Total	C	H	N	O	S	0	0
			4346	1381	2147	406	404	8		

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Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	269	Total	C	H	N	O	S	0	0
			4346	1381	2147	406	404	8		

- Molecule 11 is a protein called ATPTT6.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	I	246	Total	C	H	N	O	S	0	0
			4070	1344	1999	360	361	6		
11	L	246	Total	C	H	N	O	S	0	0
			4070	1344	1999	360	361	6		

- Molecule 12 is a protein called ATPTT7.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	m	221	Total	C	H	N	O	S	0	0
			3696	1205	1835	313	336	7		
12	M	221	Total	C	H	N	O	S	0	0
			3696	1205	1835	313	336	7		

- Molecule 13 is a protein called ATPTT8.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	n	119	Total	C	H	N	O	S	0	0
			1960	655	962	164	173	6		
13	N	119	Total	C	H	N	O	S	0	0
			1960	655	962	164	173	6		

- Molecule 14 is a protein called ATPTT9.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	o	99	Total	C	H	N	O	S	0	0
			1599	507	794	145	147	6		
14	O	99	Total	C	H	N	O	S	0	0
			1599	507	794	145	147	6		

- Molecule 15 is a protein called ATPTT10.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	p	150	Total	C	H	N	O	S	0	0
			2413	788	1196	204	224	1		
15	P	150	Total	C	H	N	O	S	0	0
			2413	788	1196	204	224	1		

- Molecule 16 is a protein called ATPTT11.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	q	108	Total	C	H	N	O	S	0	0
			1749	556	874	149	169	1		
16	Q	108	Total	C	H	N	O	S	0	0
			1749	556	874	149	169	1		

- Molecule 17 is a protein called ATPTT12.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	r	145	Total	C	H	N	O	S	0	0
			2373	776	1180	201	212	4		
17	R	140	Total	C	H	N	O	S	0	0
			2288	750	1134	194	206	4		

- Molecule 18 is a protein called ATPTT13.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	s	124	Total	C	H	N	O	S	0	0
			2025	648	1009	174	189	5		
18	S	125	Total	C	H	N	O	S	0	0
			2039	652	1016	175	191	5		

- Molecule 19 is a protein called ATPTT1.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	e	417	Total	C	H	N	O	S	0	0
			6681	2171	3286	602	614	8		
19	E	417	Total	C	H	N	O	S	0	0
			6681	2171	3286	602	614	8		

- Molecule 20 is a protein called Inhibitor of F1 (IF1).

Mol	Chain	Residues	Atoms						AltConf	Trace
20	i2	64	Total	C	H	N	O	S	0	0
			1112	351	556	97	107	1		
20	i1	68	Total	C	H	N	O	S	0	0
			1167	368	582	103	113	1		

- Molecule 21 is a protein called ATPTT2.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	t	365	Total	C	H	N	O	S	0	0
			5889	1925	2876	533	544	11		

- Molecule 22 is a protein called Oligomycin sensitivity-conferring protein (OSCP).

Mol	Chain	Residues	Atoms						AltConf	Trace
22	G1	188	Total	C	H	N	O	S	0	0
			3000	942	1515	252	287	4		
22	G2	188	Total	C	H	N	O	S	0	0
			3000	942	1515	252	287	4		

- Molecule 23 is a protein called subunit gamma.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	g1	275	Total	C	H	N	O	S	0	0
			4332	1343	2206	373	400	10		
23	g2	275	Total	C	H	N	O	S	0	0
			4332	1343	2206	373	400	10		

- Molecule 24 is a protein called subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	C1	513	Total	C	H	N	O	S	0	0
			7980	2481	4058	685	739	17		
24	B1	511	Total	C	H	N	O	S	0	0
			7934	2469	4030	681	737	17		
24	A1	512	Total	C	H	N	O	S	0	0
			7946	2472	4037	682	738	17		
24	C2	513	Total	C	H	N	O	S	0	0
			7980	2481	4058	685	739	17		
24	B2	511	Total	C	H	N	O	S	0	0
			7934	2469	4030	681	737	17		
24	A2	512	Total	C	H	N	O	S	0	0
			7946	2472	4037	682	738	17		

- Molecule 25 is a protein called subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	D1	470	Total	C	H	N	O	S	0	0
			7135	2243	3581	612	688	11		
25	F1	469	Total	C	H	N	O	S	0	0
			7113	2237	3568	610	687	11		

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Mol	Chain	Residues	Atoms						AltConf	Trace
25	E1	470	Total	C	H	N	O	S	0	0
			7135	2243	3581	612	688	11		
25	D2	470	Total	C	H	N	O	S	0	0
			7135	2243	3581	612	688	11		
25	F2	469	Total	C	H	N	O	S	0	0
			7113	2237	3568	610	687	11		
25	E2	470	Total	C	H	N	O	S	0	0
			7135	2243	3581	612	688	11		

- Molecule 26 is a protein called subunit c.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	P1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	O1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	N1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	M1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	L1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	K1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	J1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	I1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	H1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	Q1	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	P2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	O2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	N2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	M2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0
26	L2	75	Total 1148	C 377	H 587	N 84	O 94	S 6	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
26	K2	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	J2	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	I2	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	H2	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		
26	Q2	75	Total	C	H	N	O	S	0	0
			1148	377	587	84	94	6		

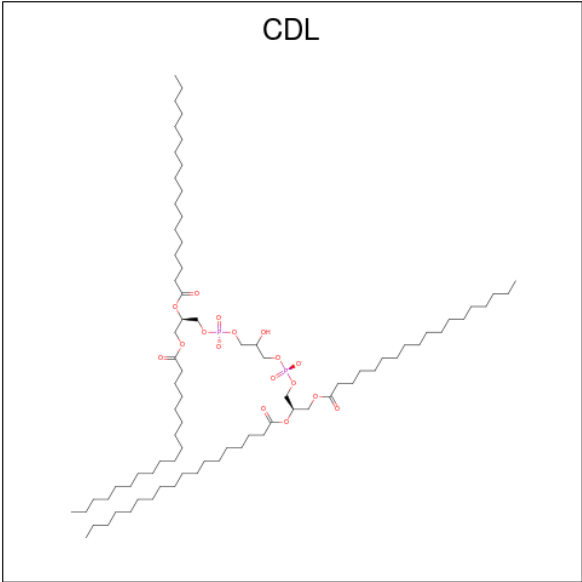
- Molecule 27 is a protein called subunit delta.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	d1	134	Total	C	H	N	O	S	0	0
			2144	674	1082	185	200	3		
27	d2	134	Total	C	H	N	O	S	0	0
			2144	674	1082	185	200	3		

- Molecule 28 is a protein called subunit epsilon.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	e1	68	Total	C	H	N	O	S	0	0
			1096	347	559	94	95	1		
28	e2	68	Total	C	H	N	O	S	0	0
			1096	347	559	94	95	1		

- Molecule 29 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



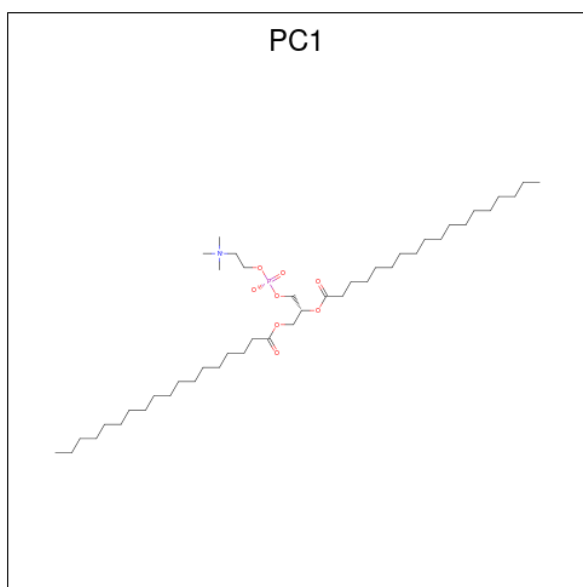
Mol	Chain	Residues	Atoms					AltConf
29	a	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	a	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	b	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	f	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	f	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	f	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	i	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	k	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	k	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	j	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	j	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	l	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	l	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	p	1	Total	C	H	O	P	0
			256	81	156	17	2	

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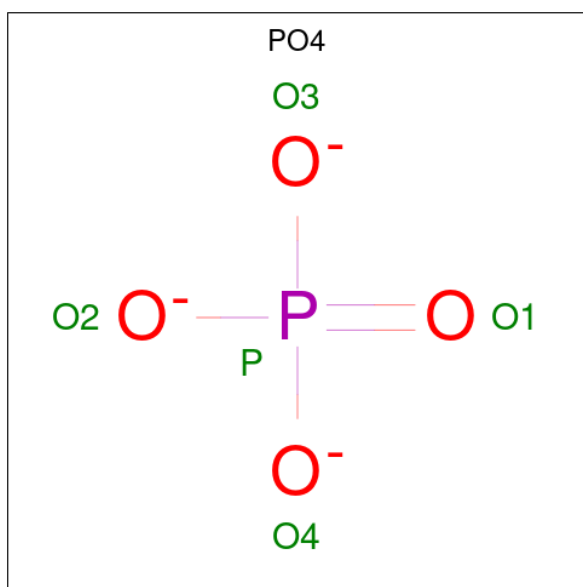
Mol	Chain	Residues	Atoms					AltConf
29	r	1	Total 256	C 81	H 156	O 17	P 2	0
29	A	1	Total 256	C 81	H 156	O 17	P 2	0
29	B	1	Total 256	C 81	H 156	O 17	P 2	0
29	B	1	Total 256	C 81	H 156	O 17	P 2	0
29	B	1	Total 256	C 81	H 156	O 17	P 2	0
29	B	1	Total 256	C 81	H 156	O 17	P 2	0
29	F	1	Total 256	C 81	H 156	O 17	P 2	0
29	I	1	Total 256	C 81	H 156	O 17	P 2	0
29	I	1	Total 256	C 81	H 156	O 17	P 2	0
29	K	1	Total 256	C 81	H 156	O 17	P 2	0
29	K	1	Total 256	C 81	H 156	O 17	P 2	0
29	J	1	Total 256	C 81	H 156	O 17	P 2	0
29	J	1	Total 256	C 81	H 156	O 17	P 2	0
29	L	1	Total 256	C 81	H 156	O 17	P 2	0
29	L	1	Total 256	C 81	H 156	O 17	P 2	0
29	P	1	Total 256	C 81	H 156	O 17	P 2	0

- Molecule 30 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



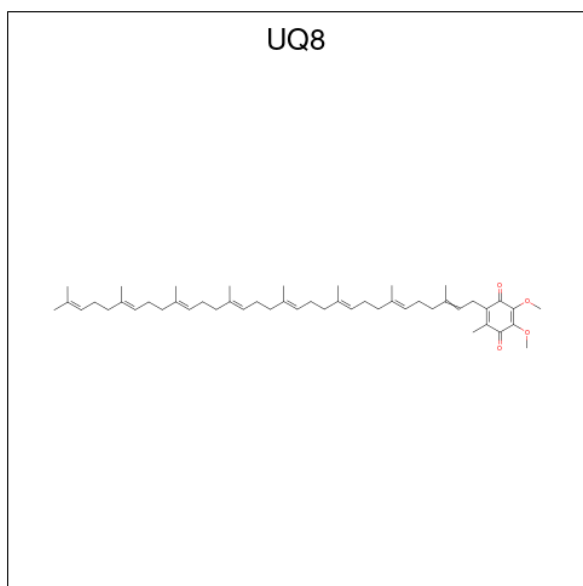
Mol	Chain	Residues	Atoms						AltConf
30	d	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	g	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	g	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	D	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	G	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	G	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	

- Molecule 31 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



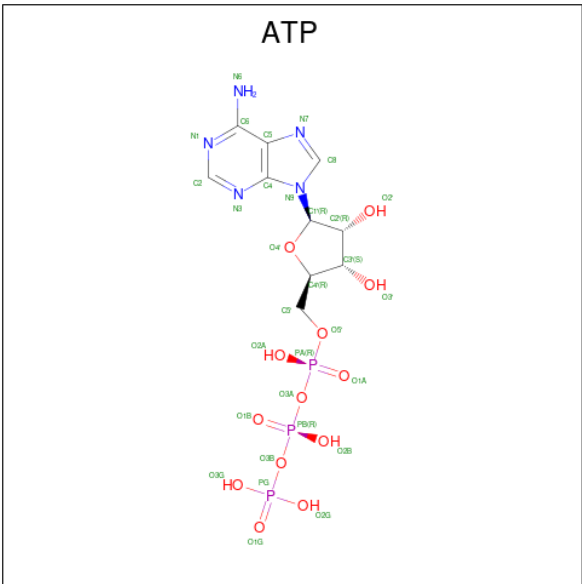
Mol	Chain	Residues	Atoms			AltConf
31	f	1	Total	O	P	0
			5	4	1	
31	F	1	Total	O	P	0
			5	4	1	

- Molecule 32 is Ubiquinone-8 (CCD ID: UQ8) (formula: $C_{49}H_{74}O_4$).



Mol	Chain	Residues	Atoms				AltConf
32	i	1	Total	C	H	O	0
			127	49	74	4	
32	I	1	Total	C	H	O	0
			127	49	74	4	

- Molecule 33 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms						AltConf
33	g	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	G	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	C1	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	B1	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	A1	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	C2	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	B2	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
33	A2	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	

- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

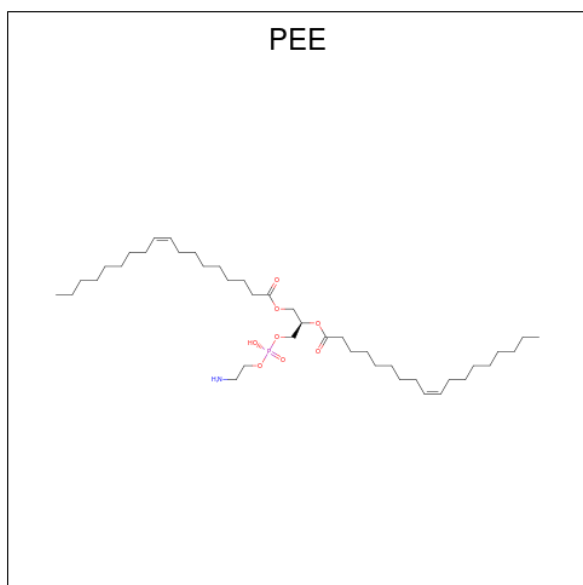
Mol	Chain	Residues	Atoms		AltConf
34	g	1	Total	Mg	0
			1	1	
34	G	1	Total	Mg	0
			1	1	
34	C1	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
34	D1	1	Total	Mg	0
			1	1	
34	B1	1	Total	Mg	0
			1	1	
34	A1	1	Total	Mg	0
			1	1	
34	E1	1	Total	Mg	0
			1	1	
34	C2	1	Total	Mg	0
			1	1	
34	D2	1	Total	Mg	0
			1	1	
34	B2	1	Total	Mg	0
			1	1	
34	A2	1	Total	Mg	0
			1	1	
34	E2	1	Total	Mg	0
			1	1	

- Molecule 35 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



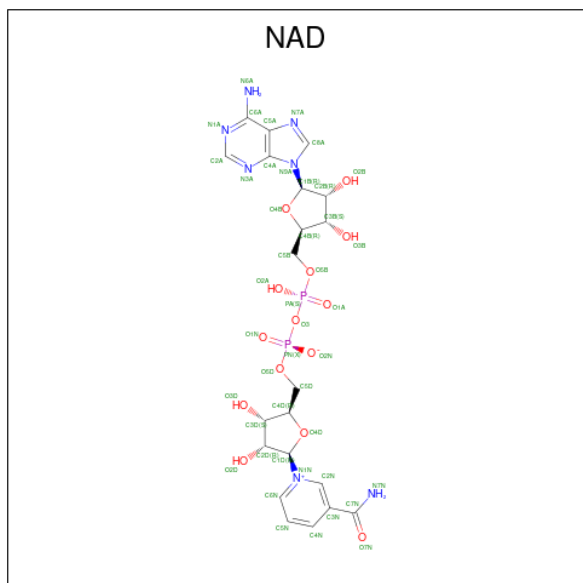
Mol	Chain	Residues	Atoms					AltConf	
35	m	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
35	A	1	Total	C	H	N	O	P	0
			123	38	75	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf	
35	J	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
35	L	1	Total	C	H	N	O	P	0
			123	38	75	1	8	1	

- Molecule 36 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).





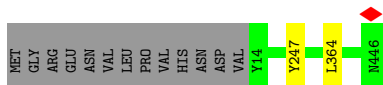
Mol	Chain	Residues	Atoms						AltConf
37	D1	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	
37	B1	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	
37	D2	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	
37	B2	1	Total	C	H	N	O	P	0
			38	10	11	5	10	2	

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.

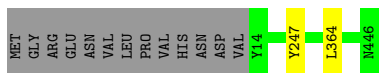
- Molecule 1: subunit a

Chain a:  97%

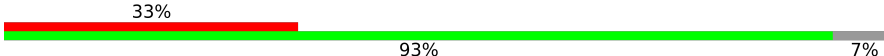


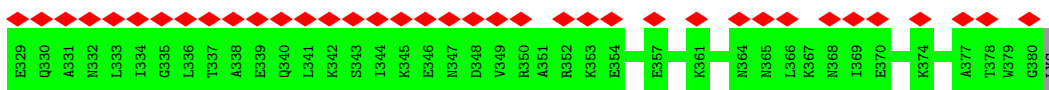
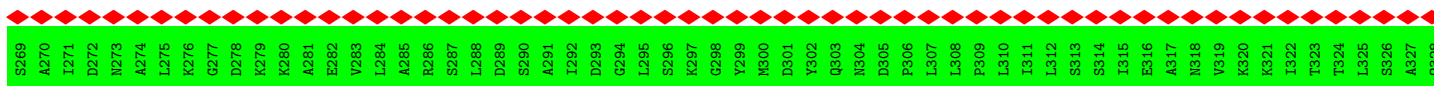
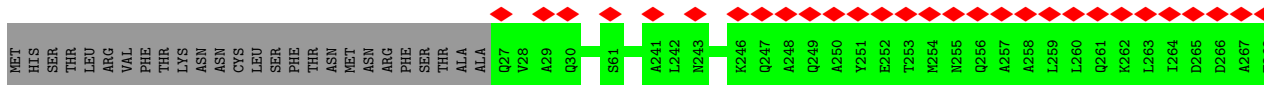
- Molecule 1: subunit a

Chain A:  97%

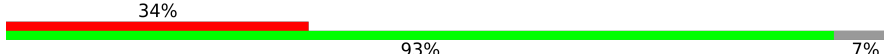


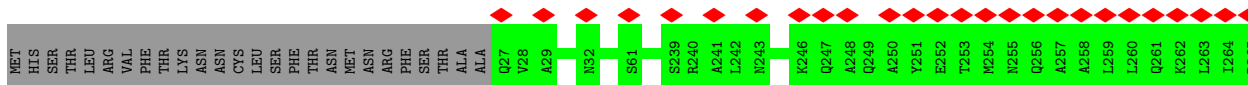
- Molecule 2: subunit b

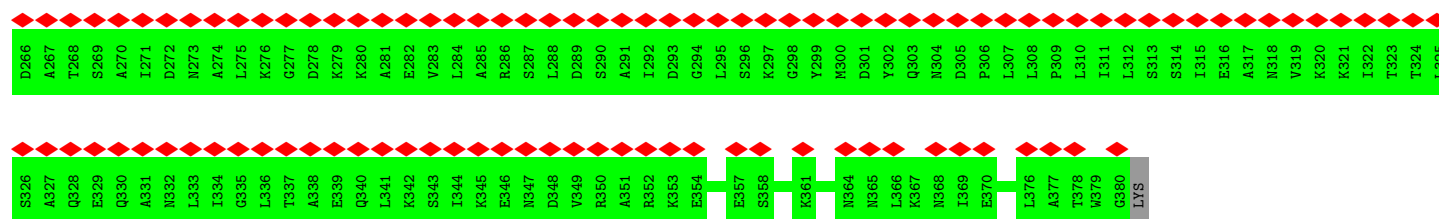
Chain b:  33% 93% 7%



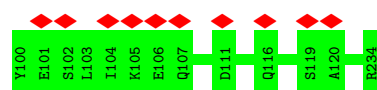
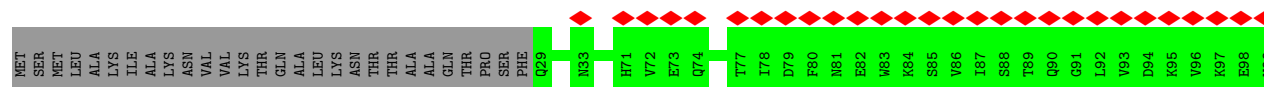
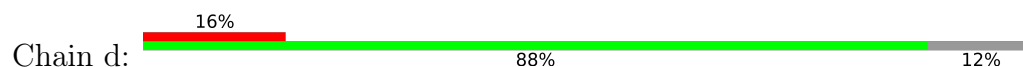
- Molecule 2: subunit b

Chain B:  34% 93% 7%

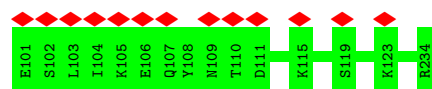
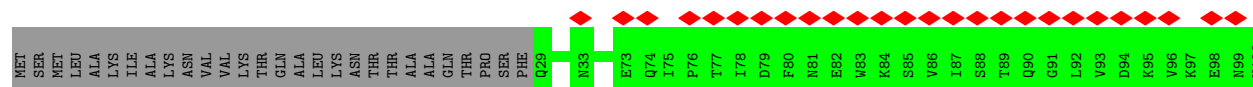
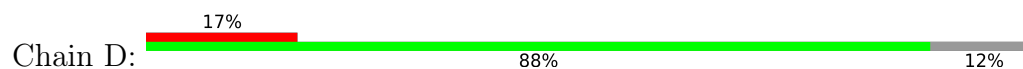




- Molecule 3: subunit d



- Molecule 3: subunit d



- Molecule 4: subunit f



- Molecule 4: subunit f



- Molecule 5: subunit i/j



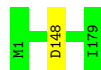
- Molecule 5: subunit i/j

Chain I:  99%



- Molecule 6: subunit k

Chain k:  99%



- Molecule 6: subunit k

Chain K:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: subunit 8

Chain c:  95%




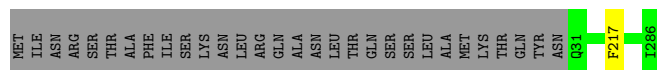
- Molecule 7: subunit 8

Chain C:  95%




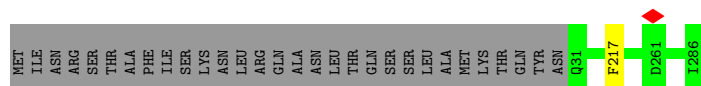
- Molecule 8: ATPPT3

Chain g:  89%




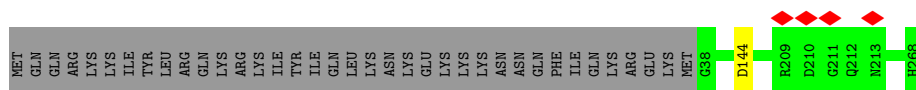
- Molecule 8: ATPPT3

Chain G:  89%

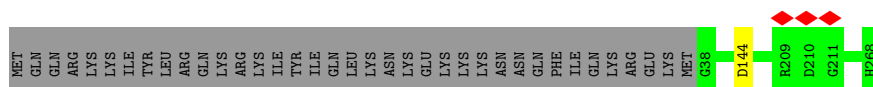
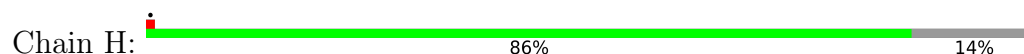


- Molecule 9: ATPPT4

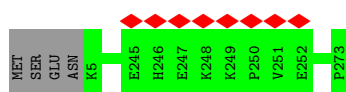
Chain h:  86%



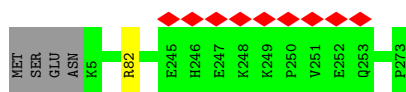
• Molecule 9: ATPTT4



• Molecule 10: ATPTT5



• Molecule 10: ATPTT5



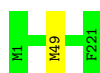
• Molecule 11: ATPTT6



• Molecule 11: ATPTT6



• Molecule 12: ATPTT7



• Molecule 12: ATPTT7



- Molecule 13: ATPTT8

MET	GLU	GLY	PHE	ILE	GLN	ASN	LYS	ARG	LYS	LYS	GLU	GLU	GLU	GLU	GLU	SER	LYS	LYS	GLU	GLU	GLU	GLU	GLN	LEU	ASN	LYS	GLN	GLN	GLN	LYS	LYS	ASP	GLN	LYS	ARG	LYS	LYS	Tyr	LEU	Tyr	GLN	GLN	ARG	LYS	LYS	GLU	MET
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



- Molecule 13: ATPPT8

MET	GLU	GLY	PHE	ILE	GLN	ASN	LYS	ARG	LYS	LYS	GLU	GLU	GLU	GLU	SER	LYS	GLY	GLN	ASN	GLN	LEU	ASN	LYS	GLN	GLN	GLU	GLU	LYS	TYR	GLN	GLN	LYS	LYS	ASP	GLN	LYS	ARG	LYS	LYS	TYR	TYR	LEU	TYR	GLN	GLN	ARG	LYS	GLU	MET
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



- Molecule 14: ATPTT9

MET	LYS	GLN	LYS	ILE	ASN	LYS	LYS	LEU	LEU	LYS	ASN	LYS	GLY	VAL	GLN	ASP	LYS	TYR	LYS	TYR	LEU	SER	LYS	LEU	ILE	LEU	LEU	ASP	GLN	GLU	ILE	LYS	ARG	LYS	ASN	LYS	LYS	LYS	GLU	LYS	ASN	LYS	ILE	LEU	LEU	GLU	GLU	P65	K153	ASN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	-----

- Molecule 14: ATPTT9

MET	LYS	GLN	LYS	ILE	ASN	LYS	LEU	LEU	LYS	ASN	GLY	VAL	GLN	ASP	LYS	TYR	LYS	TYR	LEU	SER	LYS	LEU	ILE	LEU	LEU	ASP	GLN	GLU	ILE	LYS	GLY	LYS	ASN	LYS	GLU	LYS	ARG	LYS	LYS	GLU	GLU	LYS	ASN	LYS	LEU	ILE	LEU	LEU	GLU	GLU	ASN	MET
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

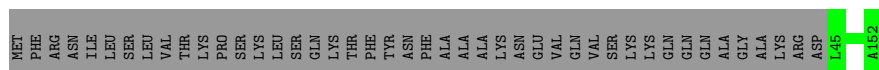
- Molecule 15: ATPTT10

Diagram illustrating a protein segment with residues MET, S2, K64, H151, and ASN. A red diamond is positioned above the K64 residue.

- Molecule 15: ATPTT10

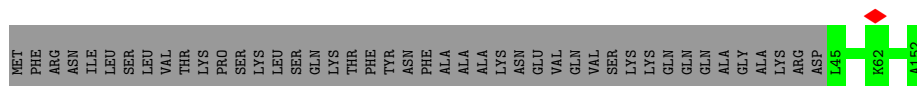
- Molecule 16: ATPTT11

Chain q:  71% 29%



- Molecule 16: ATPTT11

Chain Q:  71% 29%



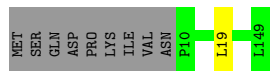
- Molecule 17: ATPTT12

Chain r:  97% ..




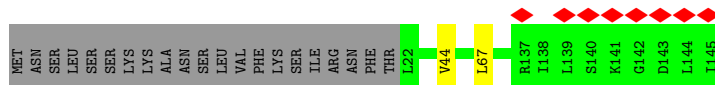
- Molecule 17: ATPTT12

Chain R:  93% • 6%




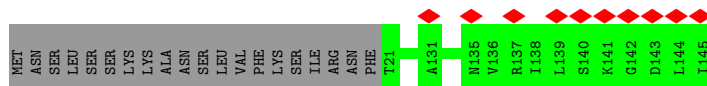
- Molecule 18: ATPTT13

Chain s:  6% 84% • 14%




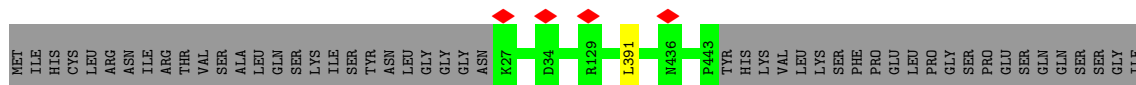
- Molecule 18: ATPTT13

Chain S:  7% 86% 14%




- Molecule 19: ATPTT1

Chain e:  87% 13%



SER
LYS
TYR
PHE
PRO
THR
LYS
THR
GLU
ASN
LYS
LYS
ALA
HIS

• Molecule 19: ATPTT1

Chain E:  86% 13%

MET ILE HIS CYS ILE LEU PRO THR LYS ASN ILE ARG THR THR VAL SER LEU GLN SER LYS ILE SER TYR ASN GLN GLY GLY ASN K27 D34 K57 E118 W350 L391 R439 F443

SER
SER
GLY
ILE
SER
LYS
TYR
PHE
PRO
THR
LYS
THR
GLU
ASN
LYS
ALA
HIS

• Molecule 20: Inhibitor of F1 (IF1)

Chain i2:  31% 57% 41%

MET ASN ARG SER VAL ILE ALA LYS ASN THR ILE GLN THR TYR ARG ALA PHE PHE T28 R29 E30 E31 E32 D35 K36 R37 T38 K39 K43 V44 Y45 F46 D47 Q48 E49 D50 R51 K52 A53 M54 K55 R56 L57 L58 E59 K60 L61 N62 T63

THR SER LYS PHE VAL GLU ASP SER GLU TYR LEU ALA PRO GLN ASN L79 E82 N91 D102 G106 LYS ASN

• Molecule 20: Inhibitor of F1 (IF1)

Chain i1:  25% 63% 37%

MET ASN ARG SER VAL ILE ALA LYS ASN THR ILE GLN THR TYR ARG ALA PHE PHE T28 R29 E30 E31 E32 W33 L34 D35 K36 R37 Y45 F46 D47 Q48 E49 D50 R51 K52 A53 M54 K55 R56 L57 L58 E59 K60 N62 T63 THR SER LYS

PHE VAL GLU ASP SER GLU TYR LEU A75 H89 D102 G106 LYS ASN


• Molecule 21: ATPTT2

Chain t:  79% 21%

MET LYS MET GLU TYR LEU GLN SER GLU TYR GLU LYS ASP ALA ILE ASN LYS GLN ILE HIS LYS GLU LYS GLU LYS GLN VAL PHE THR LYS ARG THR LYS VAL PHE CYS LEU TRP GLY ALA GLN PRO ALA TYR ASN PHE S94 E135 T140 R158 A288 K289 T290 Q291 M458 GLU GLN

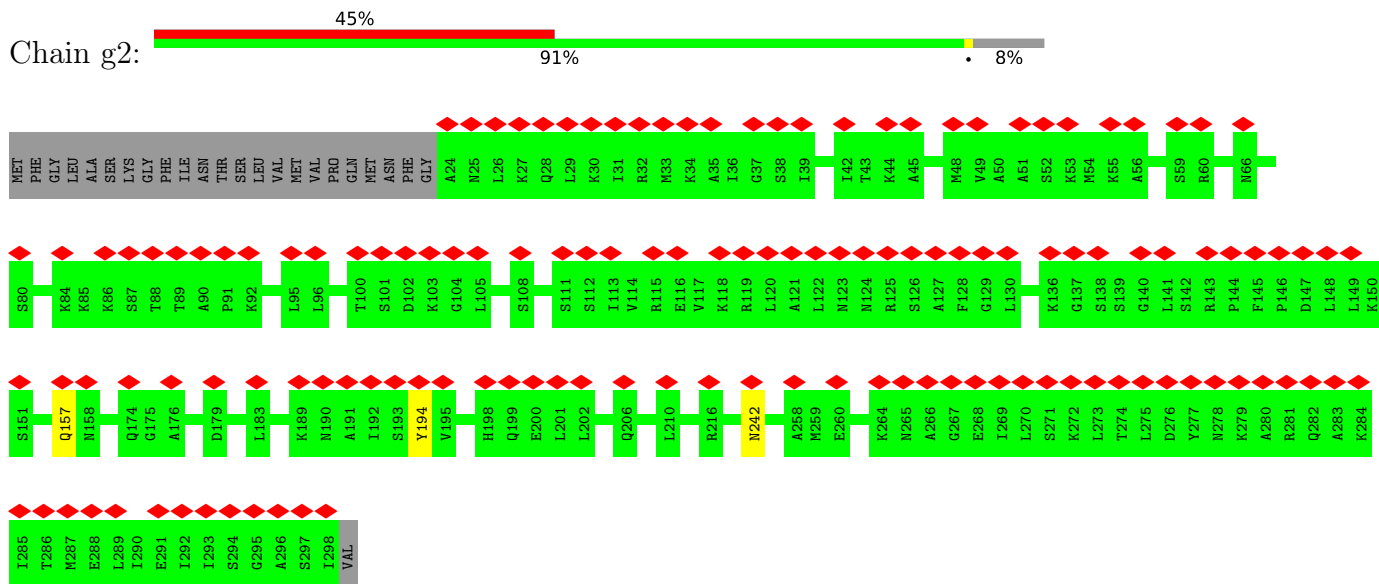
ILE GLN LYS LYS GLN ARG LYS TYR GLY ARG MET ILE ASN THR ARG LYS VAL PHE CYS LEU TRP GLY ALA GLN PRO ALA TYR ASN PHE S94 E135 T140 R158 A288 K289 T290 Q291 M458 GLU GLN

• Molecule 22: Oligomycin sensitivity-conferring protein (OSCP)

Chain G1:  86% 86% 14%

- Molecule 23: subunit gamma

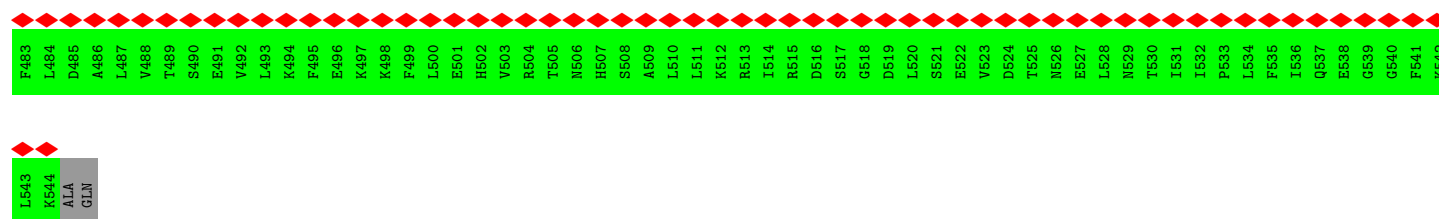
Chain g2:



- Molecule 24: subunit alpha

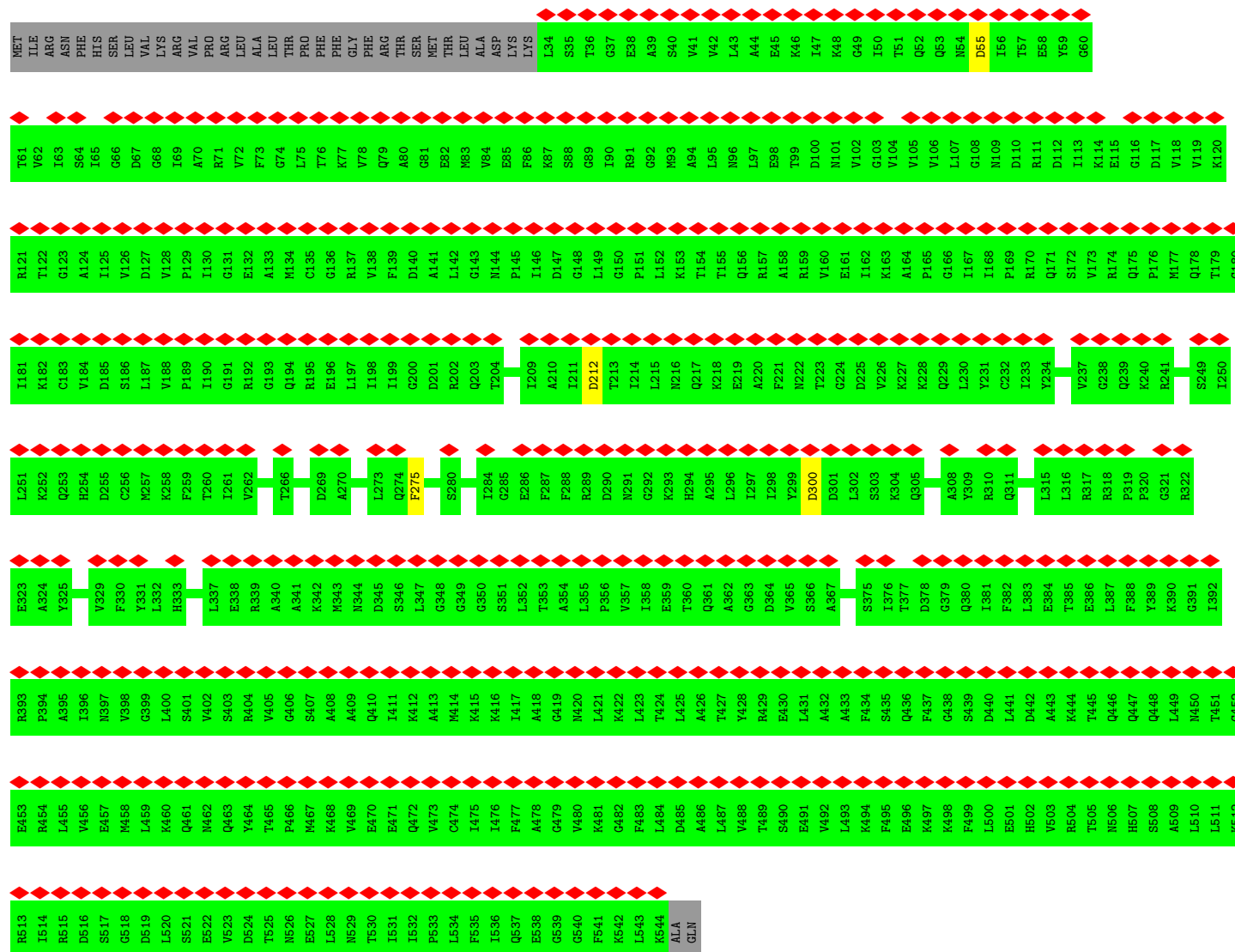
Chain C1:





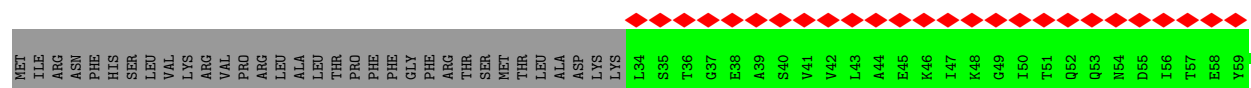
• Molecule 24: subunit alpha

Chain B1: 84% 93% 6%

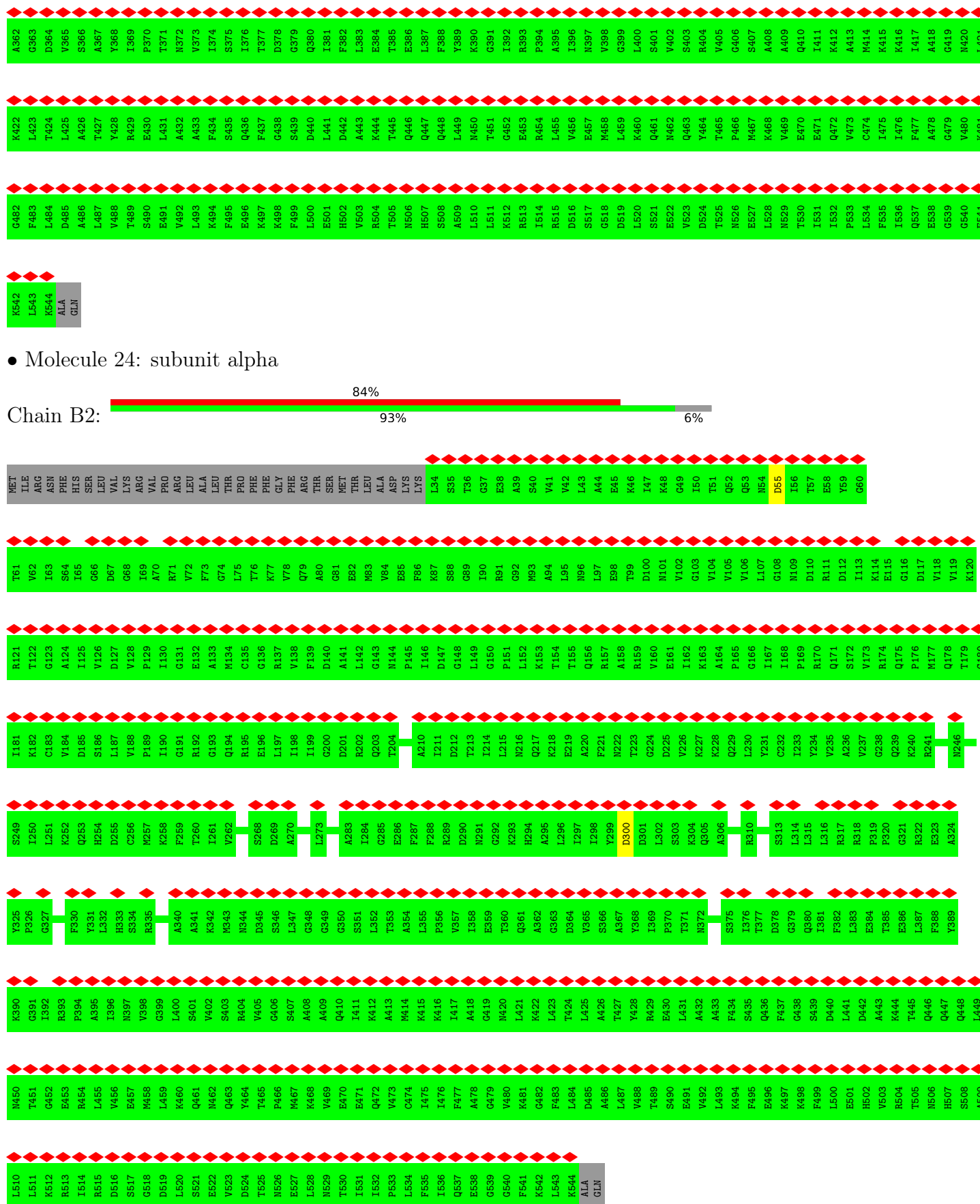


• Molecule 24: subunit alpha

Chain A1: 69% 93% 6%



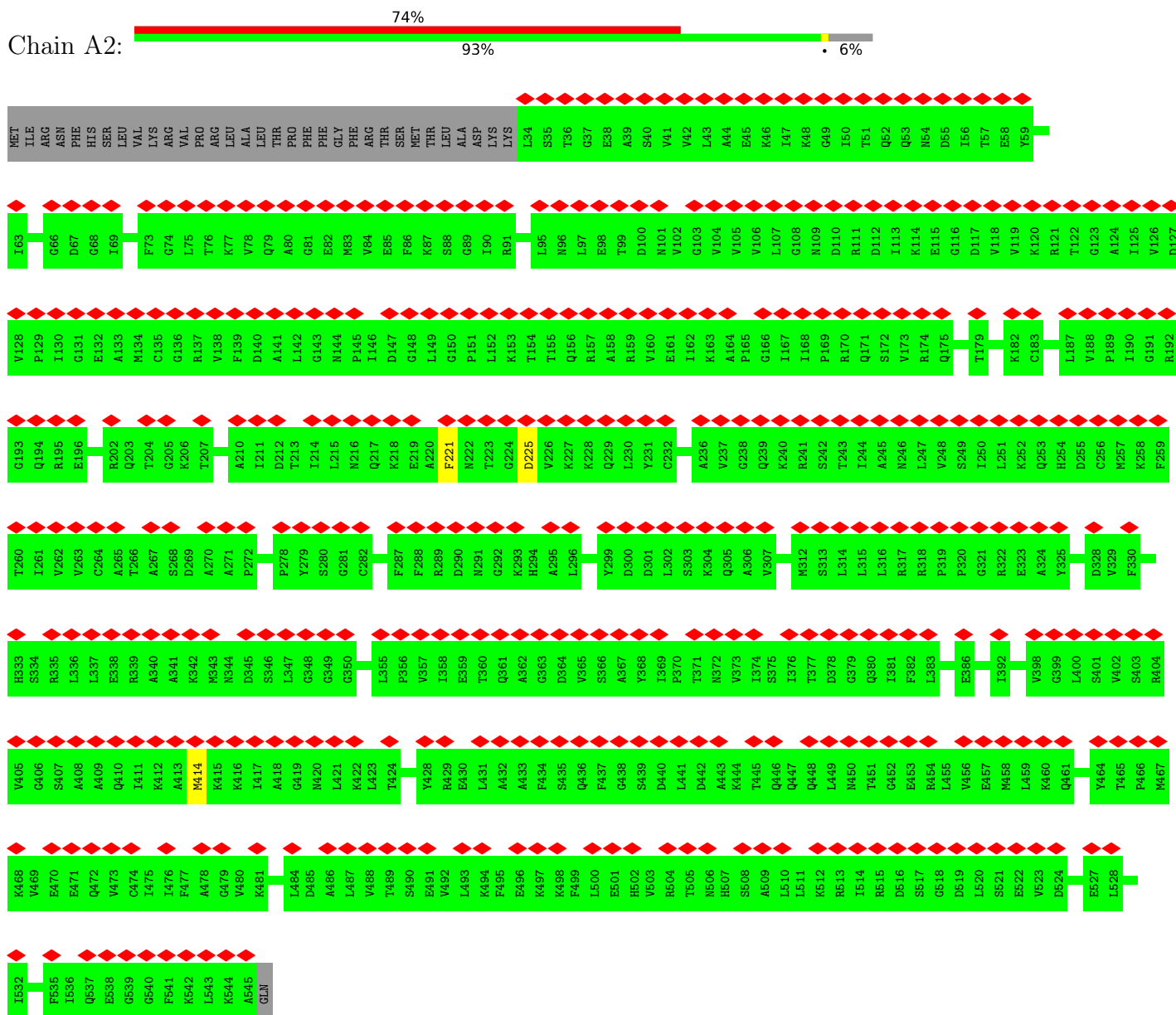




• Molecule 24: subunit alpha

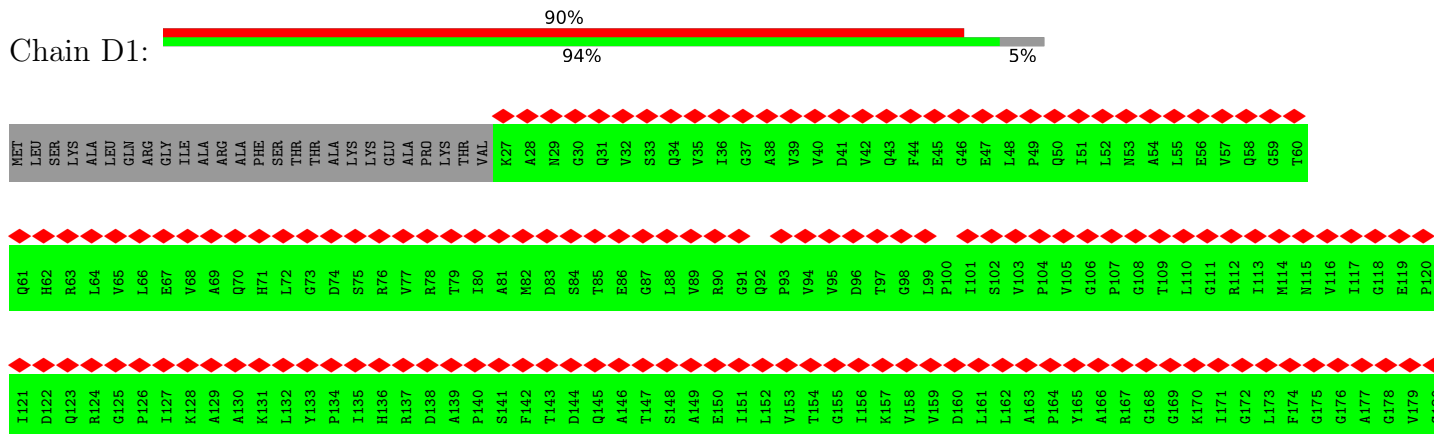
- Molecule 24: subunit alpha

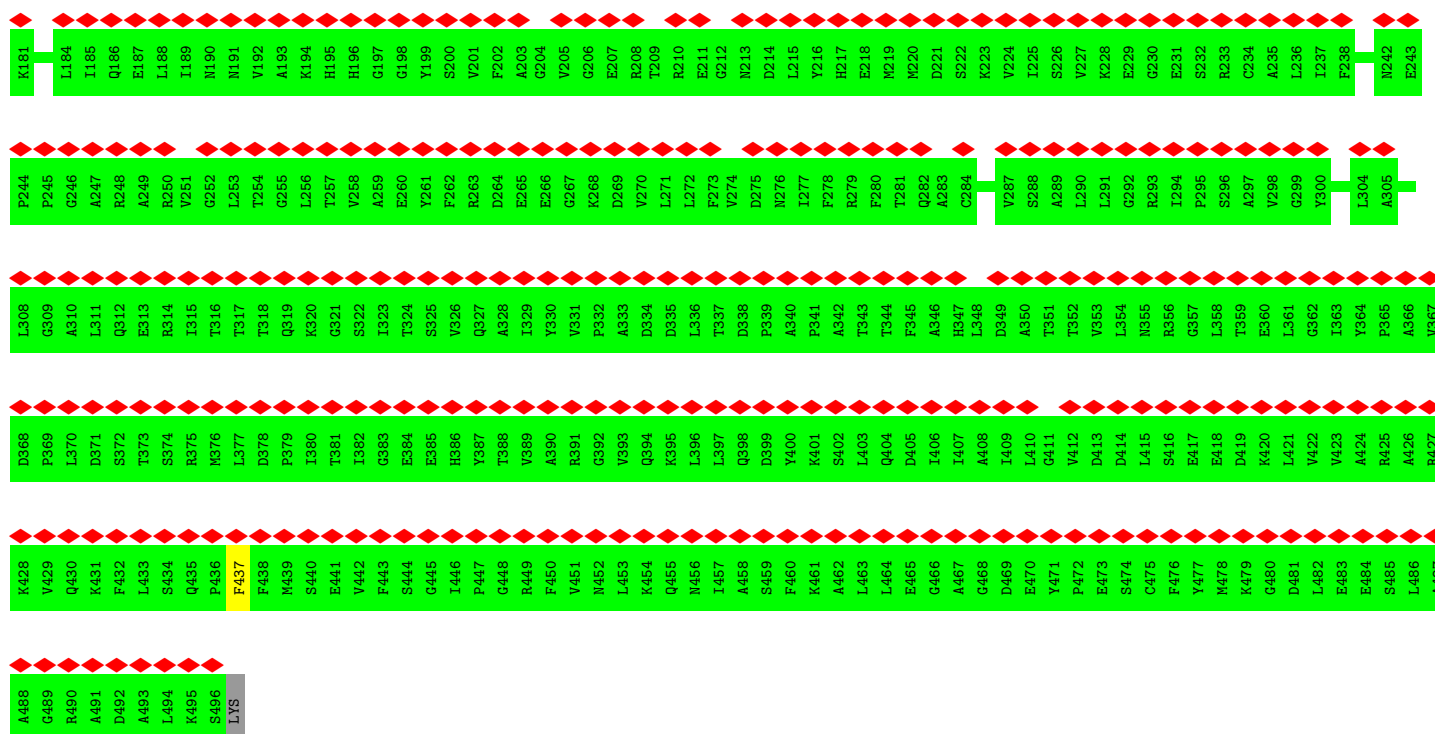
Chain A2:



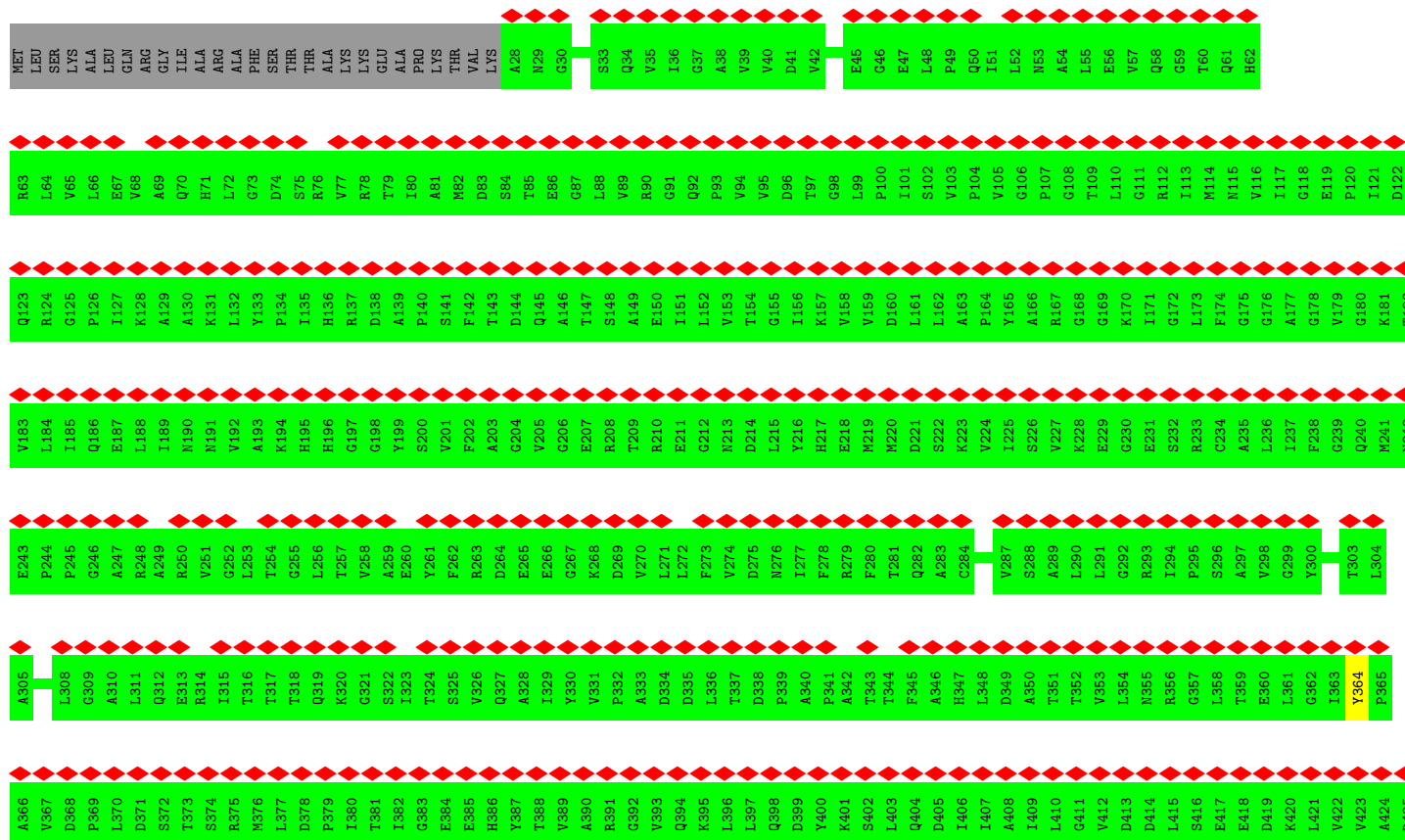
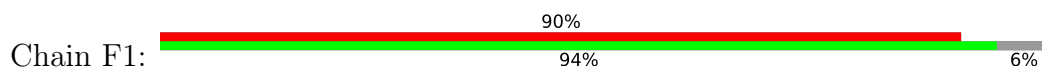
- Molecule 25: subunit beta

Chain D1:





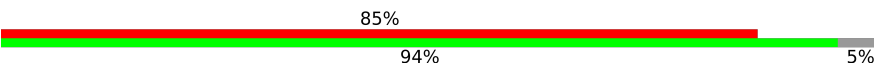
● Molecule 25: subunit beta



A426 R427 K428 V429 K431 F432 L433 S434 Q435 P436 F437 F438 M439 S440 E441 V442 F443 S444 G445 I446 P447 G448 R449 F450 V451 N452 L453 K454 Q455 N456 I457 A458 S459 F460 K461 A462 L463 L464 E465 G466 A467 G468 D469 E470 Y471 P472 E473 S474 F475 F476 Y477 M478 K479 G480 D481 L482 E483 E484 S485

L486 A487 A488 G489 R490 K491 D492 A493 L494 K495 S496
 LYS

• Molecule 25: subunit beta

Chain E1: 

MET LEU SER LYS ALA LEU GLN ARG GLY ILE ALA ARG ALA PHE SER THR THR ALA LYS LYS GLU ALA PRO LYS THR VAL K27 A28 N29 G30 Q31 V32 S33 Q34 V35 I36 G37 A38 V39 V40 D41 V42 Q43 F44 E45 G46 E47 L48 P49 Q50 I51 N53 A54 L55 E56 V57 Q58 G59 T60

Q61 H62 R63 L64 V65 L66 E67 V68 A69 Q70 H71 L72 L73 Q73 D74 S75 R76 V77 R78 T79 I80 M82 D83 S84 T85 E86 G87 L88 V89 G91 Q92 Q93 V94 V95 D96 T97 G98 L99 P100 S102 V103 P104 V105 G106 P107 G108 T109 L110 G111 R112 I113 M114 N115 V116 G118 E119 P120

I121 D122 Q123 R124 G125 P126 I127 K128 A129 A130 K131 L132 Y133 P134 I135 H136 R137 D138 A139 P140 S141 F142 T143 D144 Q145 T147 S148 A149 I151 L152 V153 G155 I156 K157 V158 V159 D160 K223 L162 A163 P164 V165 A166 R167 G169 K170 I171 G172 L173 F174 G175 A177 G178 V179 G180

K181 T182 V183 L184 I185 Q186 E187 L188 I189 N191 V192 A193 K194 H195 H196 G197 G198 Y199 S200 V201 F202 A203 E207 R208 T209 R210 G212 N213 D214 L215 Y216 H217 E218 M219 M220 S222 K223 V224 I225 S226 V227 K228 E229 G230 E231 S232 R233 C234 A235 L236 I237 F238 N242 E243 P244

P245 G246 A247 R248 A249 R250 V251 G252 L253 T254 G255 L256 T257 V258 A259 E260 Y261 F262 R263 D264 E265 E266 G267 D269 V270 L271 L272 F273 V274 D276 I277 F278 R279 F280 T281 Q282 E286 A289 L290 L291 G292 R293 I294 P295 S296 A297 V298 G299 L304 A305 T306 D307 L308 G309 A310

L311 Q312 E313 R314 I315 T316 T317 T318 Q319 K320 G321 S322 I323 T324 S325 V326 Q327 Y330 V331 P332 A333 D334 D335 L336 T337 P338 D339 A340 P341 A342 T343 T344 F345 A346 H347 L348 D349 A350 T351 T352 V353 L354 N355 R356 G357 L358 T359 E360 L361 G362 I363 Y364 P365 A366 V367 P368 L370 D371

S372 T373 S374 R375 M376 L377 D378 P379 I380 T381 I382 G383 E384 E385 H386 A390 R391 G392 V393 Q394 L397 Q398 S399 Y400 S402 K401 L403 A404 D405 I406 A408 I409 L410 G411 V412 D413 D414 L415 S416 E417 A418 D419 K420 L421 V422 V423 A424 A426 R427 K428 V429 K431 F432 L433 S434

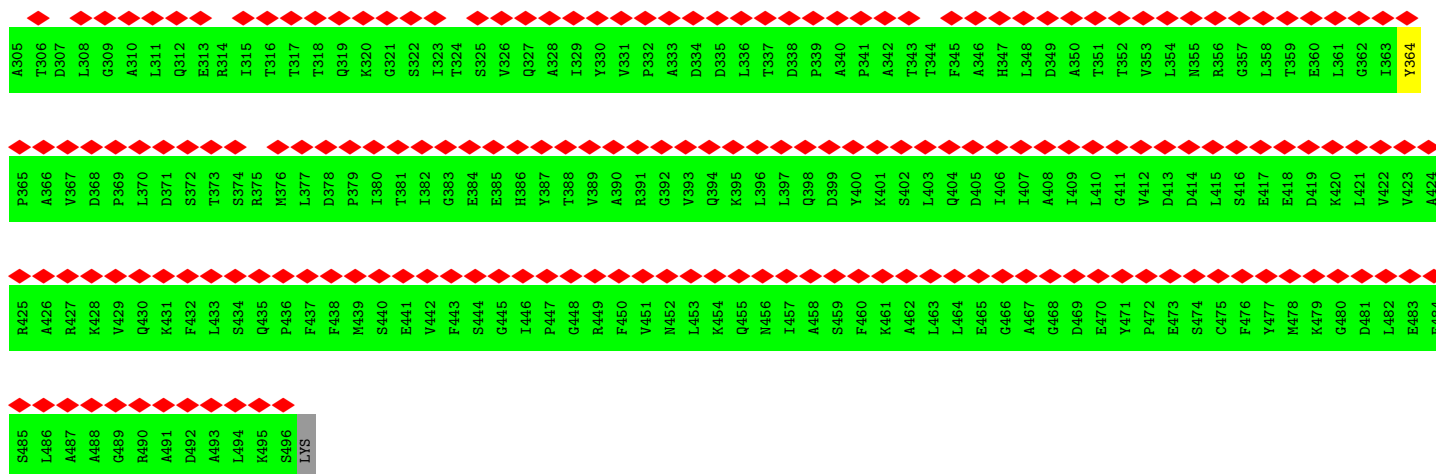
Q435 P436 F437 F438 M439 S440 E441 V442 F443 S444 G445 I446 P447 G448 R449 F450 V451 N452 L453 K454 Q455 N456 I457 A458 S459 F460 K461 A462 L463 L464 E465 G466 A467 G468 D469 E470 Y471 P472 E473 S474 F475 F476 Y477 M478 K479 G480 D481 L482 E483 E484 S485 L486 A487 A488 G489 R490 K491 D492 A493 L494

K495 S496
 LYS

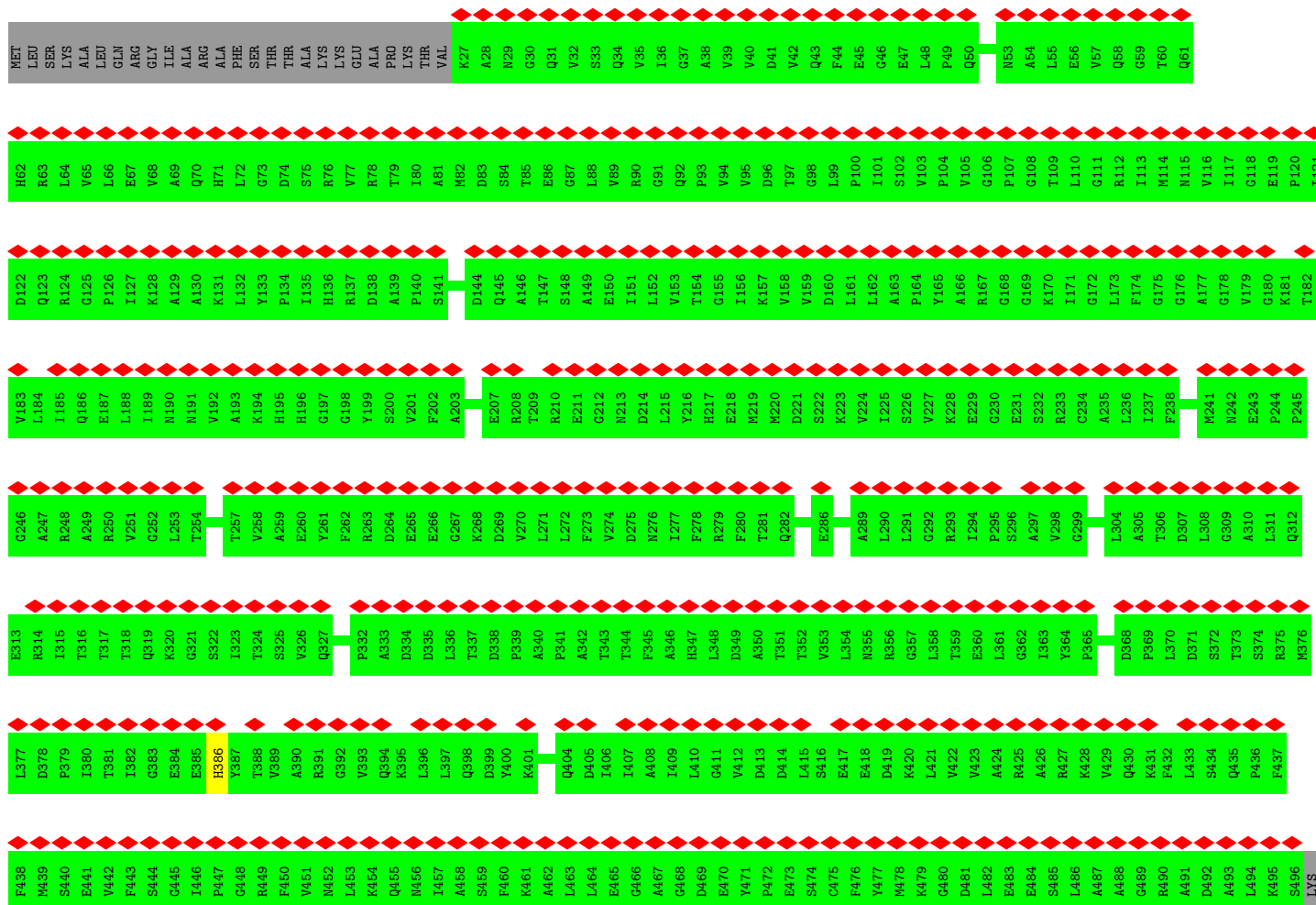
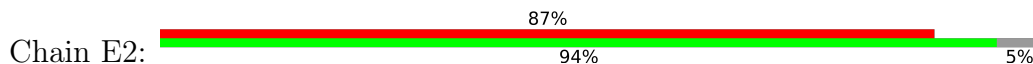
• Molecule 25: subunit beta

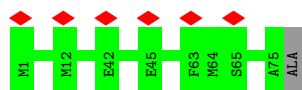
Chain D2: 

MET LEU SER LYS ALA LEU GLN ARG GLY ILE ALA ARG ALA PHE SER THR THR ALA LYS LYS GLU ALA PRO LYS THR VAL K27 A28 N29 G30 Q31 V32 S33 Q34 V35 I36 G37 A38 V39 V40 D41 V42 Q43 F44 E45 G46 E47 L48 P49 Q50 I51 N53 A54 L55 E56 V57 Q58 G59 T60

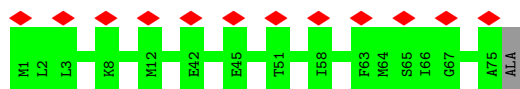


• Molecule 25: subunit beta

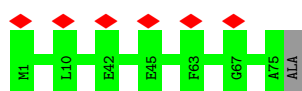




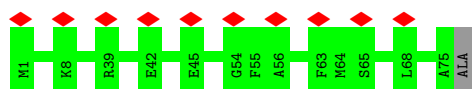
- Molecule 26: subunit c



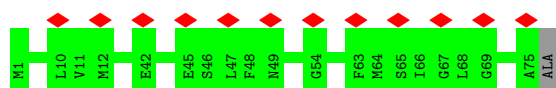
- Molecule 26: subunit c



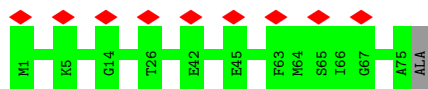
- Molecule 26: subunit c



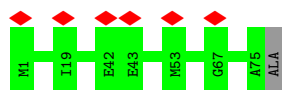
- Molecule 26: subunit c



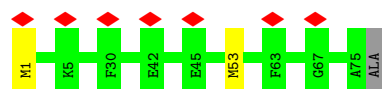
- Molecule 26: subunit c



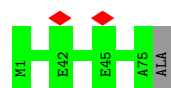
- Molecule 26: subunit c



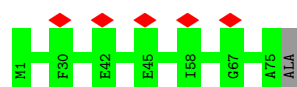
- Molecule 26: subunit c



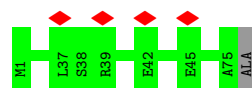
- Molecule 26: subunit c



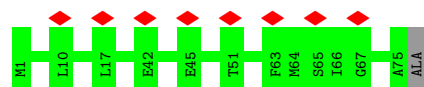
- Molecule 26: subunit c



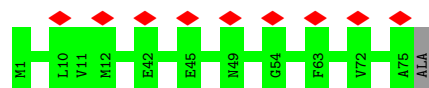
- Molecule 26: subunit c



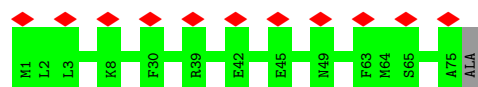
- Molecule 26: subunit c



- Molecule 26: subunit c

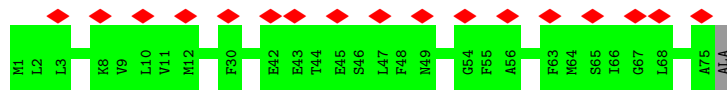


- Molecule 26: subunit c



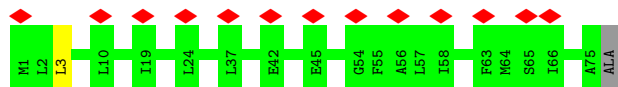
● Molecule 26: subunit c

Chain L2:  22% 99%



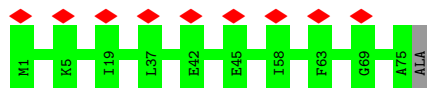
● Molecule 26: subunit c

Chain K2:  17% 97%



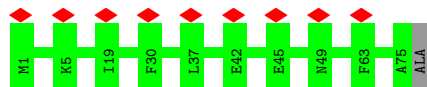
● Molecule 26: subunit c

Chain J2:  12% 99%



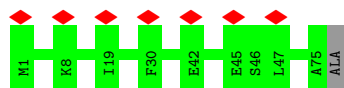
● Molecule 26: subunit c

Chain I2:  12% 99%



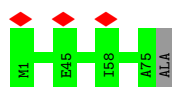
● Molecule 26: subunit c

Chain H2:  9% 99%




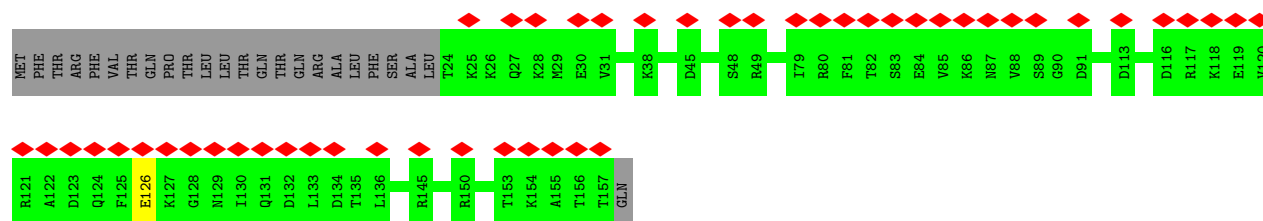
● Molecule 26: subunit c

Chain Q2:  1% 99%

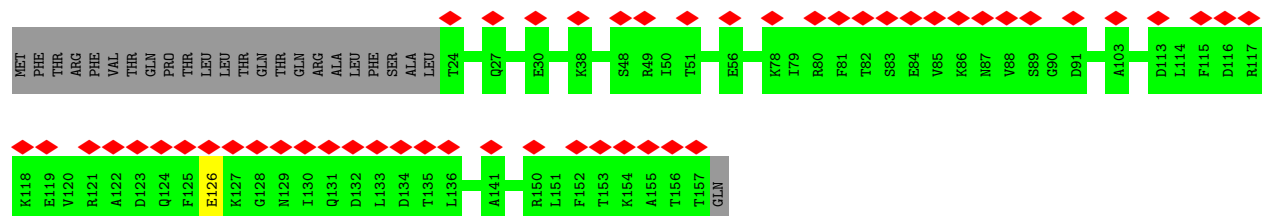
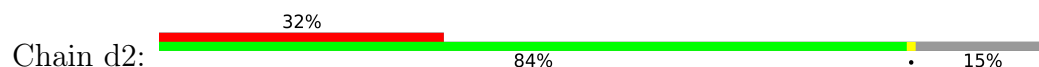


● Molecule 27: subunit delta

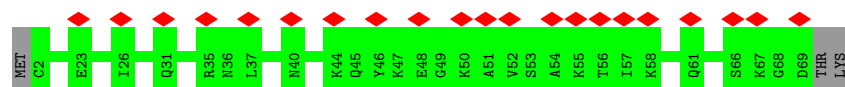
Chain d1:  31% 84% 15%



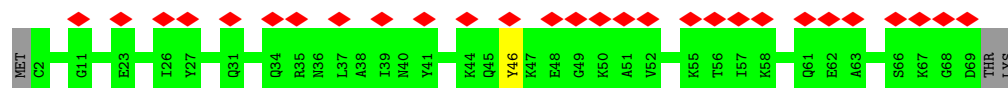
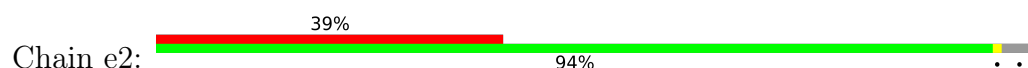
- Molecule 27: subunit delta



- Molecule 28: subunit epsilon



- Molecule 28: subunit epsilon



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	61157	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 ($e^-/\text{\AA}^2$)	30.9	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	0.155	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	498.0, 498.0, 498.0	wwPDB
Map dimensions	600, 600, 600	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: UQ8, ADP, NAD, PO4, PEE, MG, PC1, CDL, ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.36	0/3752	0.39	0/5109
1	a	0.36	0/3752	0.39	0/5109
2	B	0.30	0/2940	0.37	0/3969
2	b	0.30	0/2940	0.36	0/3969
3	D	0.30	0/1715	0.38	0/2321
3	d	0.30	0/1715	0.38	0/2321
4	F	0.36	0/1733	0.41	0/2327
4	f	0.35	0/1733	0.41	0/2327
5	I	0.35	0/1771	0.40	0/2394
5	i	0.35	0/1771	0.40	0/2394
6	K	0.31	0/1508	0.39	0/2024
6	k	0.31	0/1508	0.39	0/2024
7	C	0.35	0/866	0.40	0/1176
7	c	0.35	0/866	0.40	0/1176
8	G	0.36	0/2302	0.42	0/3115
8	g	0.36	0/2302	0.41	0/3115
9	H	0.33	0/2006	0.40	0/2704
9	h	0.33	0/2006	0.40	0/2704
10	J	0.34	0/2256	0.41	0/3069
10	j	0.34	0/2256	0.41	0/3069
11	L	0.35	0/2140	0.40	0/2903
11	l	0.35	0/2140	0.40	0/2903
12	M	0.36	0/1912	0.38	0/2598
12	m	0.35	0/1912	0.38	0/2598
13	N	0.37	0/1030	0.41	0/1393
13	n	0.37	0/1030	0.42	0/1393
14	O	0.31	0/821	0.40	0/1104
14	o	0.30	0/821	0.41	0/1104
15	P	0.29	0/1249	0.38	0/1695
15	p	0.29	0/1249	0.38	0/1695
16	Q	0.31	0/888	0.40	0/1200
16	q	0.32	0/888	0.40	0/1200

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	R	0.35	0/1185	0.39	0/1594
17	r	0.35	0/1225	0.39	0/1649
18	S	0.32	0/1044	0.42	0/1414
18	s	0.33	0/1037	0.42	0/1404
19	E	0.28	0/3492	0.41	0/4720
19	e	0.28	0/3492	0.40	0/4720
20	i1	0.23	0/593	0.34	0/795
20	i2	0.28	0/563	0.36	0/753
21	t	0.33	0/3103	0.40	0/4200
22	G1	0.24	0/1507	0.37	0/2027
22	G2	0.24	0/1507	0.37	0/2027
23	g1	0.24	0/2156	0.38	0/2900
23	g2	0.24	0/2156	0.38	0/2900
24	A1	0.24	0/3961	0.40	0/5346
24	A2	0.24	0/3961	0.40	0/5346
24	B1	0.24	0/3956	0.40	0/5339
24	B2	0.24	0/3956	0.40	0/5339
24	C1	0.24	0/3974	0.40	0/5361
24	C2	0.24	0/3974	0.40	0/5361
25	D1	0.24	0/3613	0.39	0/4900
25	D2	0.24	0/3613	0.39	0/4900
25	E1	0.24	0/3613	0.40	0/4900
25	E2	0.24	0/3613	0.40	0/4900
25	F1	0.24	0/3604	0.40	0/4889
25	F2	0.24	0/3604	0.40	0/4889
26	H1	0.28	0/572	0.36	0/771
26	H2	0.28	0/572	0.37	0/771
26	I1	0.27	0/572	0.36	0/771
26	I2	0.28	0/572	0.41	0/771
26	J1	0.27	0/572	0.36	0/771
26	J2	0.27	0/572	0.36	0/771
26	K1	0.27	0/572	0.36	0/771
26	K2	0.27	0/572	0.36	0/771
26	L1	0.27	0/572	0.36	0/771
26	L2	0.27	0/572	0.35	0/771
26	M1	0.27	0/572	0.35	0/771
26	M2	0.27	0/572	0.36	0/771
26	N1	0.27	0/572	0.35	0/771
26	N2	0.26	0/572	0.35	0/771
26	O1	0.27	0/572	0.35	0/771
26	O2	0.27	0/572	0.35	0/771
26	P1	0.27	0/572	0.35	0/771
26	P2	0.27	0/572	0.35	0/771

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
26	Q1	0.27	0/572	0.35	0/771
26	Q2	0.27	0/572	0.35	0/771
27	d1	0.25	0/1081	0.45	0/1459
27	d2	0.25	0/1081	0.45	0/1459
28	e1	0.25	0/547	0.41	0/735
28	e2	0.25	0/547	0.42	0/735
All	All	0.29	0/140976	0.39	0/190583

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
25	F1	0	1
25	F2	0	1
28	e2	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	F1	364	TYR	Peptide
25	F2	364	TYR	Peptide
28	e2	46	TYR	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	A	431/446 (97%)	426 (99%)	5 (1%)	0	100	100
1	a	431/446 (97%)	422 (98%)	9 (2%)	0	100	100
2	B	352/381 (92%)	341 (97%)	11 (3%)	0	100	100
2	b	352/381 (92%)	339 (96%)	13 (4%)	0	100	100
3	D	204/234 (87%)	199 (98%)	5 (2%)	0	100	100
3	d	204/234 (87%)	198 (97%)	6 (3%)	0	100	100
4	F	198/204 (97%)	197 (100%)	1 (0%)	0	100	100
4	f	198/204 (97%)	196 (99%)	2 (1%)	0	100	100
5	I	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
5	i	207/209 (99%)	202 (98%)	5 (2%)	0	100	100
6	K	177/179 (99%)	166 (94%)	11 (6%)	0	100	100
6	k	177/179 (99%)	169 (96%)	8 (4%)	0	100	100
7	C	94/100 (94%)	90 (96%)	4 (4%)	0	100	100
7	c	94/100 (94%)	90 (96%)	4 (4%)	0	100	100
8	G	254/286 (89%)	246 (97%)	8 (3%)	0	100	100
8	g	254/286 (89%)	244 (96%)	10 (4%)	0	100	100
9	H	229/268 (85%)	225 (98%)	4 (2%)	0	100	100
9	h	229/268 (85%)	226 (99%)	3 (1%)	0	100	100
10	J	267/273 (98%)	261 (98%)	6 (2%)	0	100	100
10	j	267/273 (98%)	262 (98%)	5 (2%)	0	100	100
11	L	244/247 (99%)	239 (98%)	5 (2%)	0	100	100
11	l	244/247 (99%)	241 (99%)	3 (1%)	0	100	100
12	M	219/221 (99%)	219 (100%)	0	0	100	100
12	m	219/221 (99%)	217 (99%)	2 (1%)	0	100	100
13	N	117/179 (65%)	114 (97%)	3 (3%)	0	100	100
13	n	117/179 (65%)	115 (98%)	2 (2%)	0	100	100
14	O	97/154 (63%)	95 (98%)	2 (2%)	0	100	100
14	o	97/154 (63%)	96 (99%)	1 (1%)	0	100	100
15	P	148/152 (97%)	140 (95%)	8 (5%)	0	100	100
15	p	148/152 (97%)	138 (93%)	10 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	Q	106/152 (70%)	105 (99%)	1 (1%)	0	100	100
16	q	106/152 (70%)	105 (99%)	1 (1%)	0	100	100
17	R	138/149 (93%)	136 (99%)	2 (1%)	0	100	100
17	r	143/149 (96%)	142 (99%)	1 (1%)	0	100	100
18	S	123/145 (85%)	119 (97%)	4 (3%)	0	100	100
18	s	122/145 (84%)	122 (100%)	0	0	100	100
19	E	415/480 (86%)	406 (98%)	9 (2%)	0	100	100
19	e	415/480 (86%)	405 (98%)	10 (2%)	0	100	100
20	i1	64/108 (59%)	64 (100%)	0	0	100	100
20	i2	60/108 (56%)	60 (100%)	0	0	100	100
21	t	363/460 (79%)	360 (99%)	3 (1%)	0	100	100
22	G1	186/219 (85%)	176 (95%)	10 (5%)	0	100	100
22	G2	186/219 (85%)	176 (95%)	10 (5%)	0	100	100
23	g1	273/299 (91%)	265 (97%)	8 (3%)	0	100	100
23	g2	273/299 (91%)	265 (97%)	8 (3%)	0	100	100
24	A1	510/546 (93%)	503 (99%)	7 (1%)	0	100	100
24	A2	510/546 (93%)	503 (99%)	7 (1%)	0	100	100
24	B1	509/546 (93%)	498 (98%)	10 (2%)	1 (0%)	44	68
24	B2	509/546 (93%)	500 (98%)	8 (2%)	1 (0%)	44	68
24	C1	511/546 (94%)	509 (100%)	2 (0%)	0	100	100
24	C2	511/546 (94%)	507 (99%)	4 (1%)	0	100	100
25	D1	468/497 (94%)	461 (98%)	7 (2%)	0	100	100
25	D2	468/497 (94%)	463 (99%)	5 (1%)	0	100	100
25	E1	468/497 (94%)	459 (98%)	9 (2%)	0	100	100
25	E2	468/497 (94%)	459 (98%)	9 (2%)	0	100	100
25	F1	467/497 (94%)	454 (97%)	13 (3%)	0	100	100
25	F2	467/497 (94%)	455 (97%)	12 (3%)	0	100	100
26	H1	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	H2	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	I1	73/76 (96%)	73 (100%)	0	0	100	100
26	I2	73/76 (96%)	71 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	J1	73/76 (96%)	73 (100%)	0	0	100	100
26	J2	73/76 (96%)	73 (100%)	0	0	100	100
26	K1	73/76 (96%)	73 (100%)	0	0	100	100
26	K2	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	L1	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	L2	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
26	M1	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	M2	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	N1	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	N2	73/76 (96%)	73 (100%)	0	0	100	100
26	O1	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
26	O2	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	P1	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
26	P2	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
26	Q1	73/76 (96%)	71 (97%)	2 (3%)	0	100	100
26	Q2	73/76 (96%)	70 (96%)	3 (4%)	0	100	100
27	d1	132/158 (84%)	126 (96%)	6 (4%)	0	100	100
27	d2	132/158 (84%)	127 (96%)	5 (4%)	0	100	100
28	e1	66/71 (93%)	60 (91%)	6 (9%)	0	100	100
28	e2	66/71 (93%)	60 (91%)	6 (9%)	0	100	100
All	All	17171/18866 (91%)	16800 (98%)	369 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
24	B1	55	ASP
24	B2	55	ASP

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	397/409 (97%)	395 (100%)	2 (0%)	86	95
1	a	397/409 (97%)	395 (100%)	2 (0%)	86	95
2	B	306/331 (92%)	306 (100%)	0	100	100
2	b	306/331 (92%)	306 (100%)	0	100	100
3	D	183/206 (89%)	183 (100%)	0	100	100
3	d	183/206 (89%)	183 (100%)	0	100	100
4	F	175/178 (98%)	174 (99%)	1 (1%)	84	94
4	f	175/178 (98%)	174 (99%)	1 (1%)	84	94
5	I	182/182 (100%)	180 (99%)	2 (1%)	70	87
5	i	182/182 (100%)	181 (100%)	1 (0%)	86	95
6	K	152/152 (100%)	152 (100%)	0	100	100
6	k	152/152 (100%)	151 (99%)	1 (1%)	81	93
7	C	93/97 (96%)	92 (99%)	1 (1%)	70	87
7	c	93/97 (96%)	92 (99%)	1 (1%)	70	87
8	G	235/262 (90%)	234 (100%)	1 (0%)	89	96
8	g	235/262 (90%)	234 (100%)	1 (0%)	89	96
9	H	208/245 (85%)	207 (100%)	1 (0%)	86	95
9	h	208/245 (85%)	207 (100%)	1 (0%)	86	95
10	J	235/239 (98%)	234 (100%)	1 (0%)	89	96
10	j	235/239 (98%)	235 (100%)	0	100	100
11	L	219/220 (100%)	217 (99%)	2 (1%)	75	90
11	l	219/220 (100%)	218 (100%)	1 (0%)	86	95
12	M	202/202 (100%)	202 (100%)	0	100	100
12	m	202/202 (100%)	201 (100%)	1 (0%)	86	95
13	N	104/162 (64%)	104 (100%)	0	100	100
13	n	104/162 (64%)	103 (99%)	1 (1%)	73	89
14	O	89/142 (63%)	89 (100%)	0	100	100
14	o	89/142 (63%)	89 (100%)	0	100	100
15	P	131/133 (98%)	131 (100%)	0	100	100
15	p	131/133 (98%)	131 (100%)	0	100	100
16	Q	97/135 (72%)	97 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	q	97/135 (72%)	97 (100%)	0	100	100
17	R	120/129 (93%)	119 (99%)	1 (1%)	79	91
17	r	125/129 (97%)	124 (99%)	1 (1%)	79	91
18	S	112/131 (86%)	112 (100%)	0	100	100
18	s	111/131 (85%)	109 (98%)	2 (2%)	54	80
19	E	359/414 (87%)	357 (99%)	2 (1%)	84	94
19	e	359/414 (87%)	358 (100%)	1 (0%)	91	97
20	i1	64/101 (63%)	64 (100%)	0	100	100
20	i2	61/101 (60%)	59 (97%)	2 (3%)	33	62
21	t	325/414 (78%)	322 (99%)	3 (1%)	75	90
22	G1	166/195 (85%)	166 (100%)	0	100	100
22	G2	166/195 (85%)	166 (100%)	0	100	100
23	g1	234/254 (92%)	230 (98%)	4 (2%)	56	81
23	g2	234/254 (92%)	231 (99%)	3 (1%)	65	85
24	A1	422/453 (93%)	419 (99%)	3 (1%)	81	93
24	A2	422/453 (93%)	419 (99%)	3 (1%)	81	93
24	B1	422/453 (93%)	419 (99%)	3 (1%)	81	93
24	B2	422/453 (93%)	421 (100%)	1 (0%)	92	98
24	C1	424/453 (94%)	423 (100%)	1 (0%)	92	98
24	C2	424/453 (94%)	423 (100%)	1 (0%)	92	98
25	D1	381/402 (95%)	380 (100%)	1 (0%)	91	97
25	D2	381/402 (95%)	380 (100%)	1 (0%)	91	97
25	E1	381/402 (95%)	380 (100%)	1 (0%)	91	97
25	E2	381/402 (95%)	380 (100%)	1 (0%)	91	97
25	F1	380/402 (94%)	380 (100%)	0	100	100
25	F2	380/402 (94%)	380 (100%)	0	100	100
26	H1	59/59 (100%)	59 (100%)	0	100	100
26	H2	59/59 (100%)	59 (100%)	0	100	100
26	I1	59/59 (100%)	57 (97%)	2 (3%)	32	61
26	I2	59/59 (100%)	59 (100%)	0	100	100
26	J1	59/59 (100%)	59 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	J2	59/59 (100%)	59 (100%)	0	100	100
26	K1	59/59 (100%)	59 (100%)	0	100	100
26	K2	59/59 (100%)	58 (98%)	1 (2%)	56	81
26	L1	59/59 (100%)	59 (100%)	0	100	100
26	L2	59/59 (100%)	59 (100%)	0	100	100
26	M1	59/59 (100%)	59 (100%)	0	100	100
26	M2	59/59 (100%)	59 (100%)	0	100	100
26	N1	59/59 (100%)	59 (100%)	0	100	100
26	N2	59/59 (100%)	59 (100%)	0	100	100
26	O1	59/59 (100%)	59 (100%)	0	100	100
26	O2	59/59 (100%)	59 (100%)	0	100	100
26	P1	59/59 (100%)	59 (100%)	0	100	100
26	P2	59/59 (100%)	59 (100%)	0	100	100
26	Q1	59/59 (100%)	59 (100%)	0	100	100
26	Q2	59/59 (100%)	59 (100%)	0	100	100
27	d1	117/139 (84%)	116 (99%)	1 (1%)	75	90
27	d2	117/139 (84%)	116 (99%)	1 (1%)	75	90
28	e1	57/60 (95%)	57 (100%)	0	100	100
28	e2	57/60 (95%)	57 (100%)	0	100	100
All	All	14800/16160 (92%)	14738 (100%)	62 (0%)	88	96

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	E	391	LEU
24	B2	300	ASP
23	g1	194	TYR
25	D2	437	PHE
25	E2	386	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
27	d1	63	ASN

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Mol	Chain	Res	Type
22	G2	161	GLN
25	E2	92	GLN
9	H	101	GLN
5	I	209	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 70 ligands modelled in this entry, 12 are monoatomic - leaving 58 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
29	CDL	i	301	-	99,99,99	0.88	8 (8%)	105,111,111	1.07	4 (3%)
30	PC1	d	301	3	53,53,53	0.93	4 (7%)	59,61,61	1.07	2 (3%)
37	ADP	D1	501	34	24,29,29	3.65	9 (37%)	29,45,45	3.77	7 (24%)
37	ADP	B2	603	34,24	24,29,29	3.71	9 (37%)	29,45,45	3.57	7 (24%)
33	ATP	C2	601	34	26,33,33	4.79	8 (30%)	31,52,52	2.43	7 (22%)
33	ATP	B1	601	25,34,24	26,33,33	4.80	9 (34%)	31,52,52	2.45	8 (25%)
29	CDL	b	401	2,4	99,99,99	0.87	8 (8%)	105,111,111	1.11	4 (3%)
35	PEE	A	501	-	47,47,50	1.18	6 (12%)	50,52,55	1.16	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	ATP	B2	601	25,34,24	26,33,33	4.80	8 (30%)	31,52,52	2.45	8 (25%)
29	CDL	k	201	6	99,99,99	0.89	8 (8%)	105,111,111	1.02	4 (3%)
29	CDL	K	201	-	99,99,99	0.88	8 (8%)	105,111,111	1.03	4 (3%)
29	CDL	B	401	-	99,99,99	0.87	8 (8%)	105,111,111	0.99	4 (3%)
29	CDL	J	302	-	99,99,99	0.87	8 (8%)	105,111,111	1.00	4 (3%)
29	CDL	B	402	2	99,99,99	0.87	7 (7%)	105,111,111	1.13	5 (4%)
33	ATP	G	301	34	26,33,33	4.77	7 (26%)	31,52,52	2.44	7 (22%)
29	CDL	a	502	-	99,99,99	0.88	8 (8%)	105,111,111	1.09	6 (5%)
33	ATP	g	301	34	26,33,33	4.78	7 (26%)	31,52,52	2.42	7 (22%)
35	PEE	L	303	-	47,47,50	1.17	6 (12%)	50,52,55	1.16	3 (6%)
29	CDL	P	201	-	99,99,99	0.88	7 (7%)	105,111,111	1.03	5 (4%)
30	PC1	G	303	-	53,53,53	0.96	4 (7%)	59,61,61	0.98	2 (3%)
31	PO4	F	301	-	4,4,4	1.04	0	6,6,6	0.44	0
33	ATP	C1	601	34	26,33,33	4.79	8 (30%)	31,52,52	2.40	7 (22%)
29	CDL	f	303	-	99,99,99	0.88	8 (8%)	105,111,111	1.09	5 (4%)
29	CDL	l	302	-	99,99,99	0.89	8 (8%)	105,111,111	1.05	4 (3%)
29	CDL	B	403	-	99,99,99	0.88	7 (7%)	105,111,111	1.05	4 (3%)
35	PEE	m	301	-	50,50,50	1.15	6 (12%)	53,55,55	1.08	4 (7%)
29	CDL	j	302	-	99,99,99	0.88	7 (7%)	105,111,111	1.01	4 (3%)
32	UQ8	I	303	-	53,53,53	1.79	7 (13%)	64,67,67	1.68	17 (26%)
29	CDL	a	501	-	99,99,99	0.89	7 (7%)	105,111,111	1.05	5 (4%)
36	NAD	E	900	-	42,48,48	3.82	19 (45%)	50,73,73	2.13	7 (14%)
30	PC1	G	304	8	53,53,53	0.95	4 (7%)	59,61,61	1.00	2 (3%)
30	PC1	g	304	8	53,53,53	0.96	4 (7%)	59,61,61	0.93	2 (3%)
29	CDL	r	201	-	99,99,99	0.87	8 (8%)	105,111,111	1.03	4 (3%)
29	CDL	f	302	-	99,99,99	0.87	7 (7%)	105,111,111	1.04	4 (3%)
29	CDL	k	202	-	99,99,99	0.88	7 (7%)	105,111,111	1.12	5 (4%)
29	CDL	B	404	2	99,99,99	0.88	8 (8%)	105,111,111	1.09	5 (4%)
29	CDL	l	301	-	99,99,99	0.88	6 (6%)	105,111,111	1.05	5 (4%)
29	CDL	K	202	-	99,99,99	0.88	7 (7%)	105,111,111	1.10	5 (4%)
31	PO4	f	301	-	4,4,4	1.04	0	6,6,6	0.44	0
29	CDL	L	302	-	99,99,99	0.88	7 (7%)	105,111,111	1.03	3 (2%)
29	CDL	J	301	-	99,99,99	0.89	6 (6%)	105,111,111	1.08	4 (3%)
29	CDL	j	301	-	99,99,99	0.88	7 (7%)	105,111,111	1.09	4 (3%)
32	UQ8	i	302	-	53,53,53	1.79	7 (13%)	64,67,67	1.65	16 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CDL	I	301	5	99,99,99	0.87	7 (7%)	105,111,111	0.99	4 (3%)
29	CDL	p	201	-	99,99,99	0.88	8 (8%)	105,111,111	1.04	4 (3%)
33	ATP	A1	601	34	26,33,33	4.82	8 (30%)	31,52,52	2.41	7 (22%)
29	CDL	L	301	-	99,99,99	0.89	7 (7%)	105,111,111	1.01	4 (3%)
30	PC1	D	301	3	53,53,53	0.94	4 (7%)	59,61,61	1.10	2 (3%)
29	CDL	I	302	-	99,99,99	0.88	8 (8%)	105,111,111	1.04	4 (3%)
37	ADP	D2	501	34	24,29,29	3.68	9 (37%)	29,45,45	3.54	7 (24%)
30	PC1	g	303	-	53,53,53	0.96	4 (7%)	59,61,61	0.97	2 (3%)
35	PEE	J	303	-	50,50,50	1.15	6 (12%)	53,55,55	1.16	3 (5%)
37	ADP	B1	603	34,24	24,29,29	3.70	9 (37%)	29,45,45	3.58	7 (24%)
29	CDL	A	502	-	99,99,99	0.88	7 (7%)	105,111,111	1.08	4 (3%)
36	NAD	e	900	-	42,48,48	3.83	19 (45%)	50,73,73	2.14	7 (14%)
33	ATP	A2	601	34	26,33,33	4.83	8 (30%)	31,52,52	2.40	7 (22%)
29	CDL	f	304	-	99,99,99	0.89	7 (7%)	105,111,111	1.05	4 (3%)
29	CDL	F	302	-	99,99,99	0.88	8 (8%)	105,111,111	1.07	4 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CDL	i	301	-	-	38/110/110/110	-
30	PC1	d	301	3	-	23/57/57/57	-
37	ADP	D1	501	34	-	2/12/32/32	0/3/3/3
37	ADP	B2	603	34,24	-	2/12/32/32	0/3/3/3
33	ATP	C2	601	34	-	4/18/38/38	0/3/3/3
33	ATP	B1	601	25,34,24	-	2/18/38/38	0/3/3/3
29	CDL	b	401	2,4	-	44/110/110/110	-
35	PEE	A	501	-	-	21/51/51/54	-
33	ATP	B2	601	25,34,24	-	2/18/38/38	0/3/3/3
29	CDL	k	201	6	-	37/110/110/110	-
29	CDL	K	201	-	-	27/110/110/110	-
29	CDL	B	401	-	-	43/110/110/110	-
29	CDL	J	302	-	-	41/110/110/110	-
29	CDL	B	402	2	-	40/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	ATP	G	301	34	-	0/18/38/38	0/3/3/3
29	CDL	a	502	-	-	39/110/110/110	-
33	ATP	g	301	34	-	0/18/38/38	0/3/3/3
35	PEE	L	303	-	-	22/51/51/54	-
29	CDL	P	201	-	-	36/110/110/110	-
30	PC1	G	303	-	-	29/57/57/57	-
33	ATP	C1	601	34	-	5/18/38/38	0/3/3/3
35	PEE	m	301	-	-	24/54/54/54	-
29	CDL	f	303	-	-	41/110/110/110	-
29	CDL	l	302	-	-	40/110/110/110	-
29	CDL	B	403	-	-	33/110/110/110	-
29	CDL	j	302	-	-	41/110/110/110	-
32	UQ8	I	303	-	-	9/51/75/75	0/1/1/1
29	CDL	a	501	-	-	33/110/110/110	-
36	NAD	E	900	-	-	7/26/62/62	0/5/5/5
30	PC1	G	304	8	-	19/57/57/57	-
30	PC1	g	304	8	-	19/57/57/57	-
29	CDL	r	201	-	-	36/110/110/110	-
29	CDL	f	302	-	-	54/110/110/110	-
29	CDL	k	202	-	-	35/110/110/110	-
29	CDL	B	404	2	-	46/110/110/110	-
29	CDL	l	301	-	-	39/110/110/110	-
29	CDL	K	202	-	-	36/110/110/110	-
29	CDL	L	302	-	-	45/110/110/110	-
29	CDL	J	301	-	-	42/110/110/110	-
29	CDL	j	301	-	-	40/110/110/110	-
32	UQ8	i	302	-	-	8/51/75/75	0/1/1/1
29	CDL	I	301	5	-	42/110/110/110	-
29	CDL	p	201	-	-	44/110/110/110	-
33	ATP	A1	601	34	-	5/18/38/38	0/3/3/3
29	CDL	L	301	-	-	38/110/110/110	-
30	PC1	D	301	3	-	21/57/57/57	-
29	CDL	I	302	-	-	38/110/110/110	-
37	ADP	D2	501	34	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	PC1	g	303	-	-	22/57/57/57	-
35	PEE	J	303	-	-	29/54/54/54	-
37	ADP	B1	603	34,24	-	1/12/32/32	0/3/3/3
29	CDL	A	502	-	-	46/110/110/110	-
36	NAD	e	900	-	-	6/26/62/62	0/5/5/5
33	ATP	A2	601	34	-	5/18/38/38	0/3/3/3
29	CDL	f	304	-	-	49/110/110/110	-
29	CDL	F	302	-	-	47/110/110/110	-

The worst 5 of 421 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	A2	601	ATP	C2'-C1'	-17.27	1.27	1.53
33	B2	601	ATP	C2'-C1'	-17.23	1.27	1.53
33	A1	601	ATP	C2'-C1'	-17.22	1.27	1.53
33	B1	601	ATP	C2'-C1'	-17.21	1.27	1.53
33	g	301	ATP	C2'-C1'	-17.19	1.27	1.53

The worst 5 of 286 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	D1	501	ADP	C1'-N9-C4	15.98	154.72	126.64
37	B1	603	ADP	C1'-N9-C4	14.91	152.83	126.64
37	B2	603	ADP	C1'-N9-C4	14.89	152.81	126.64
37	D2	501	ADP	C1'-N9-C4	14.61	152.31	126.64
36	e	900	NAD	C1B-N9A-C4A	-8.49	111.73	126.64

There are no chirality outliers.

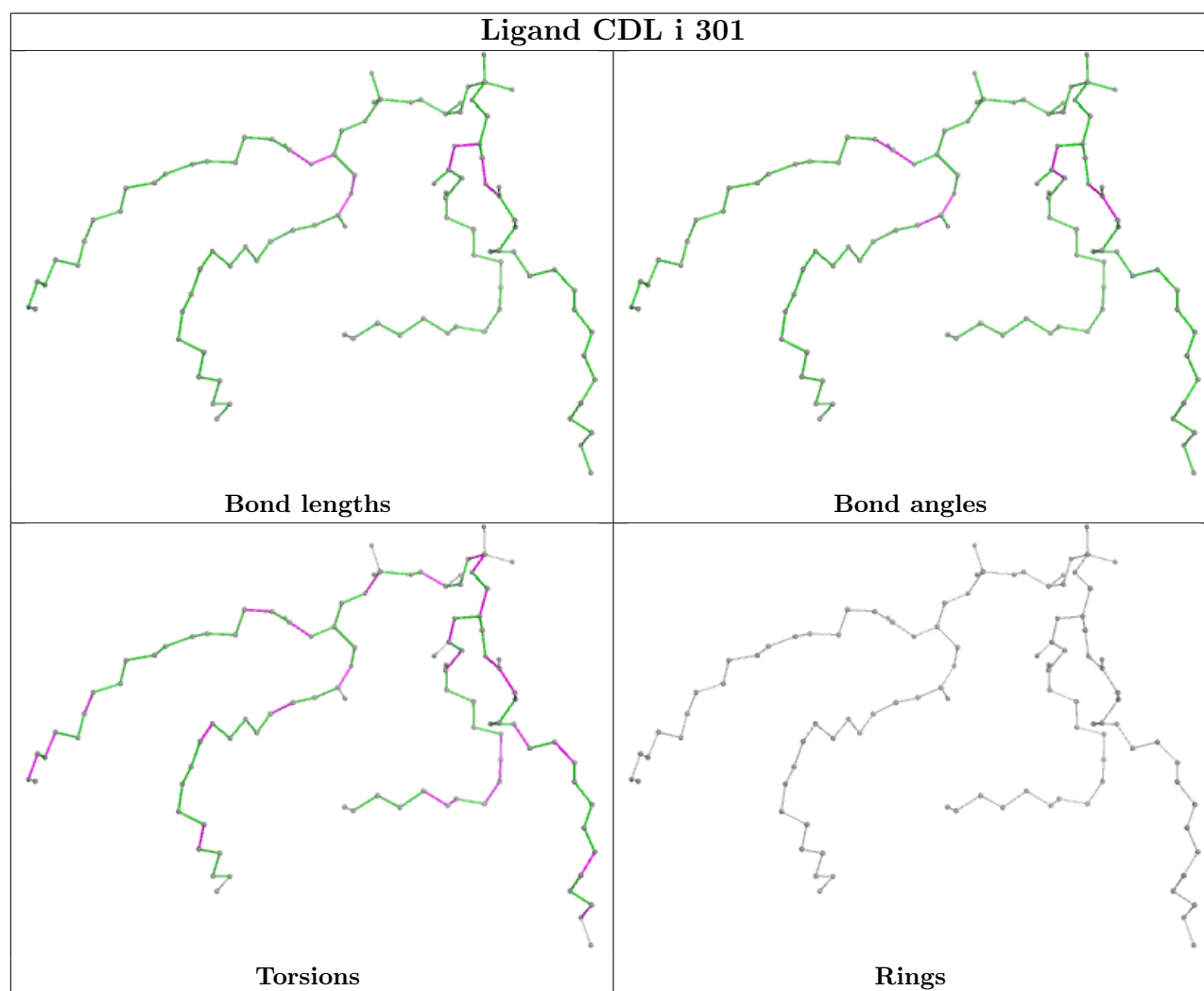
5 of 1499 torsion outliers are listed below:

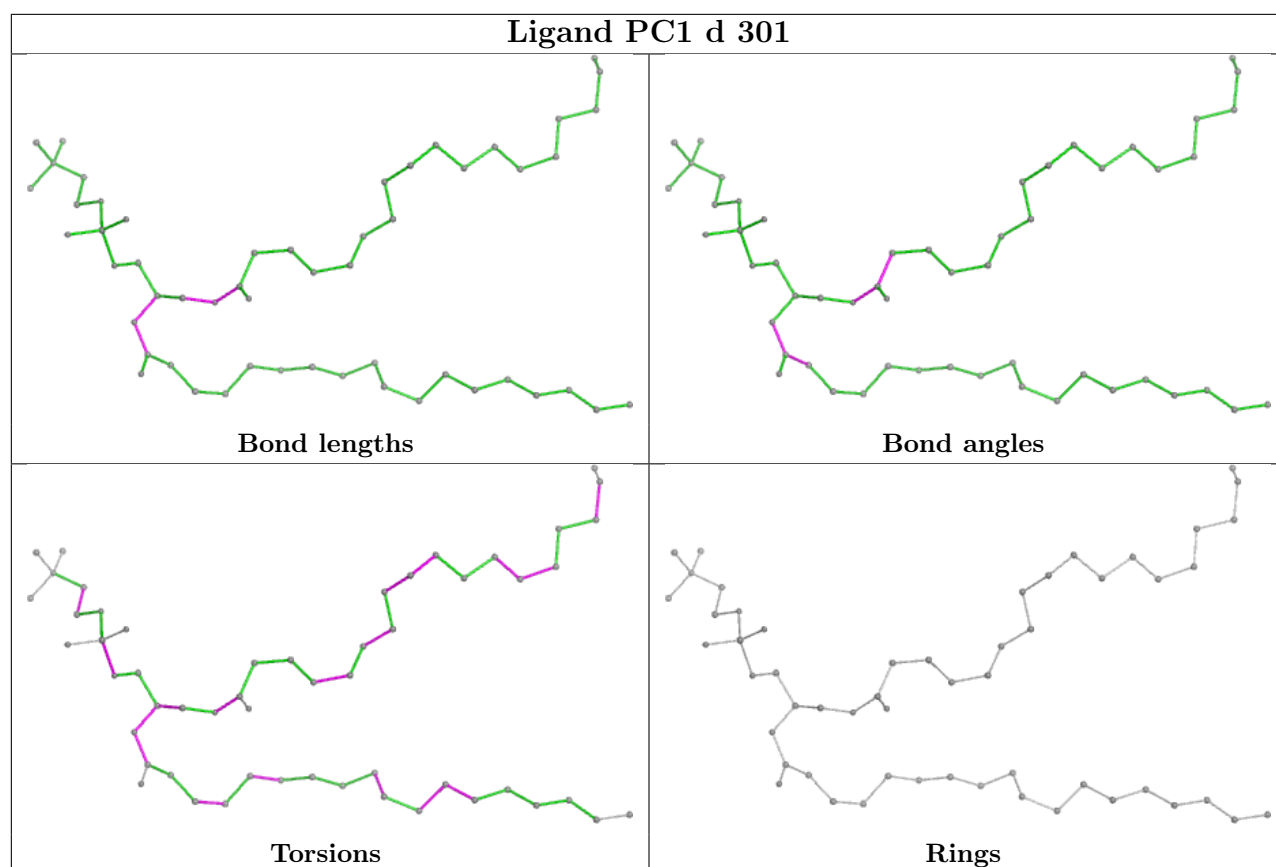
Mol	Chain	Res	Type	Atoms
29	a	501	CDL	OA5-CA3-CA4-OA6
29	a	501	CDL	CB3-OB5-PB2-OB4
29	a	501	CDL	OB7-CB5-OB6-CB4
29	a	501	CDL	C51-CB5-OB6-CB4
29	a	502	CDL	CA3-OA5-PA1-OA3

There are no ring outliers.

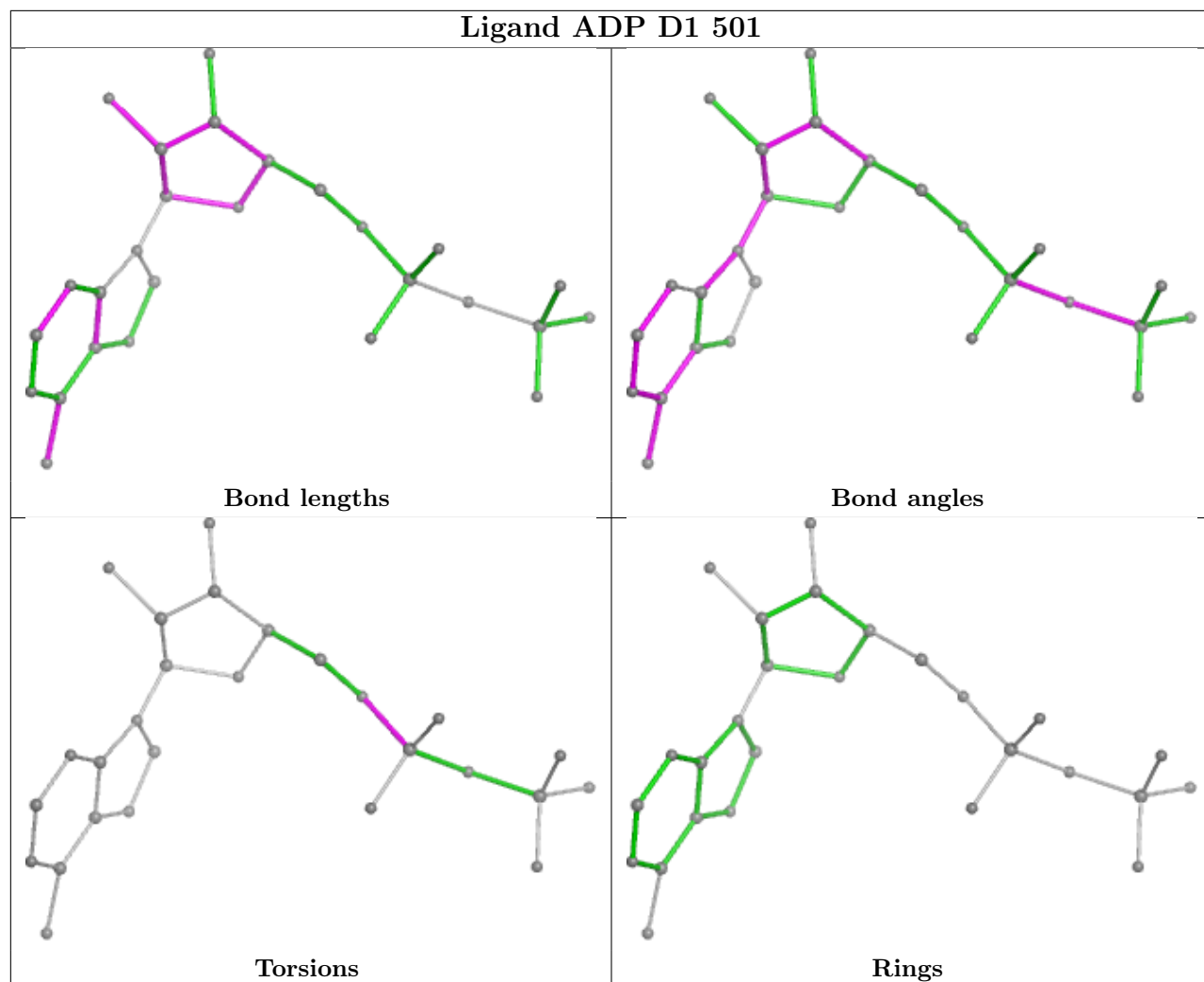
No monomer is involved in short contacts.

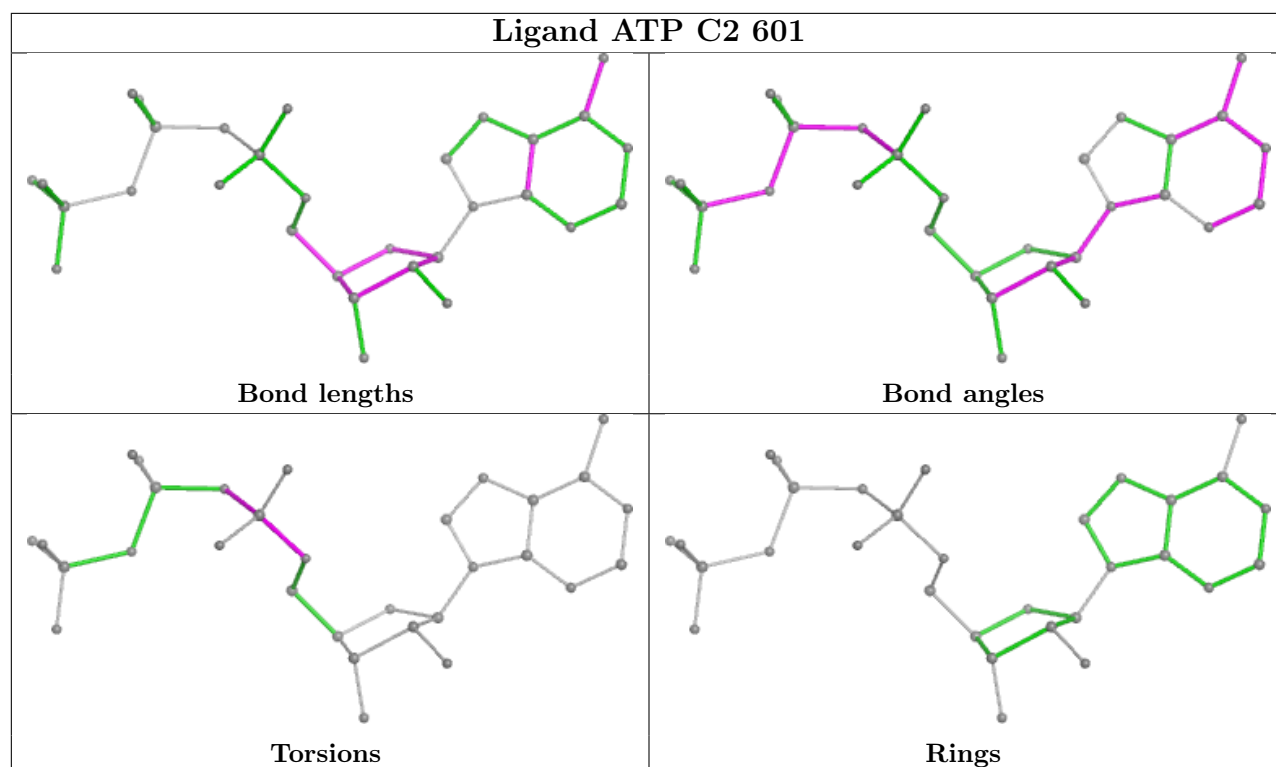
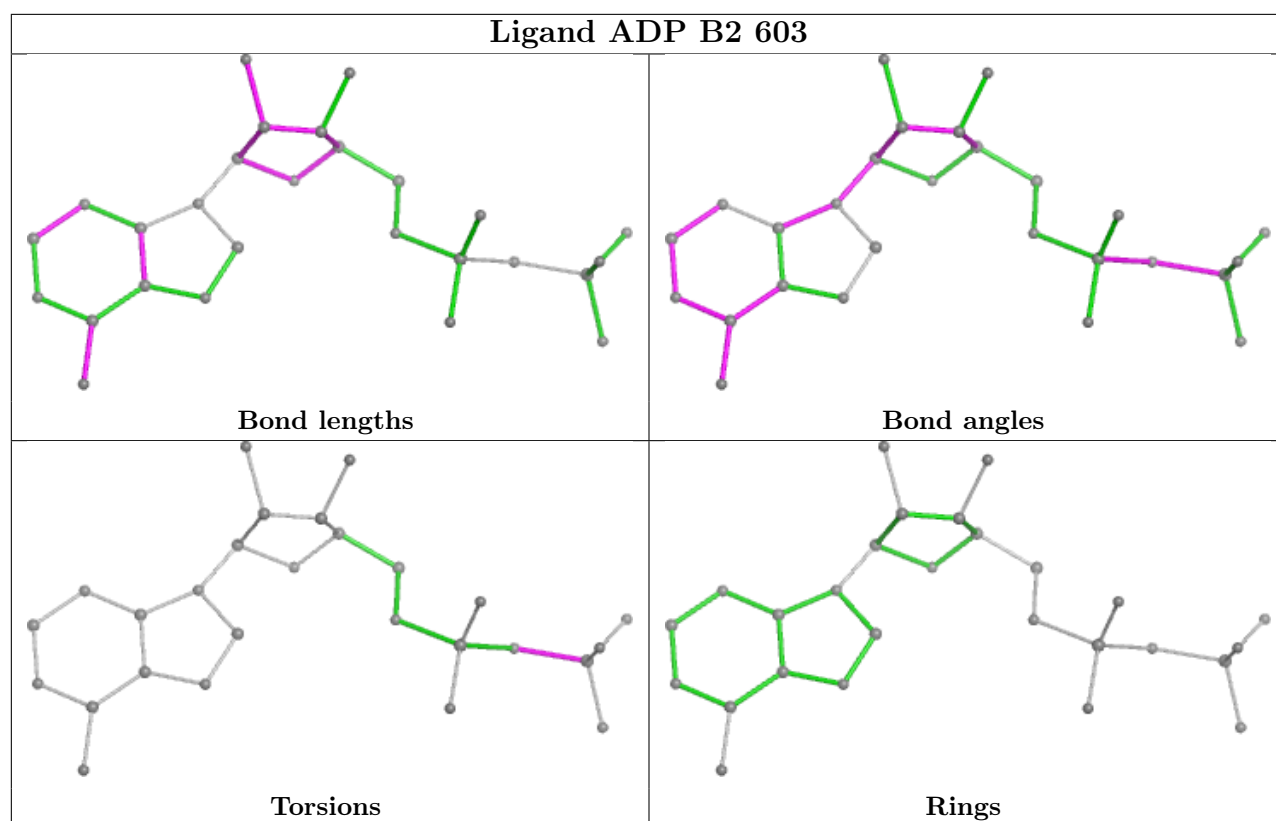
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

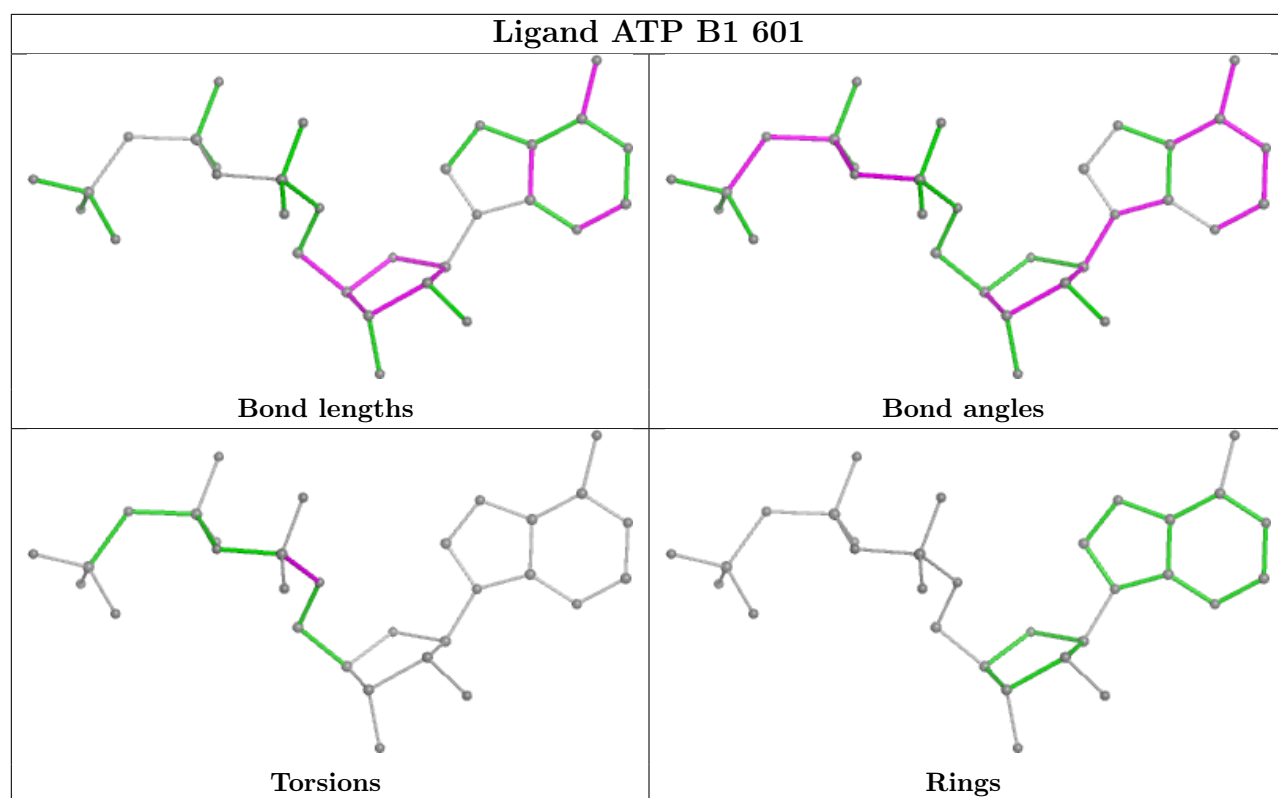


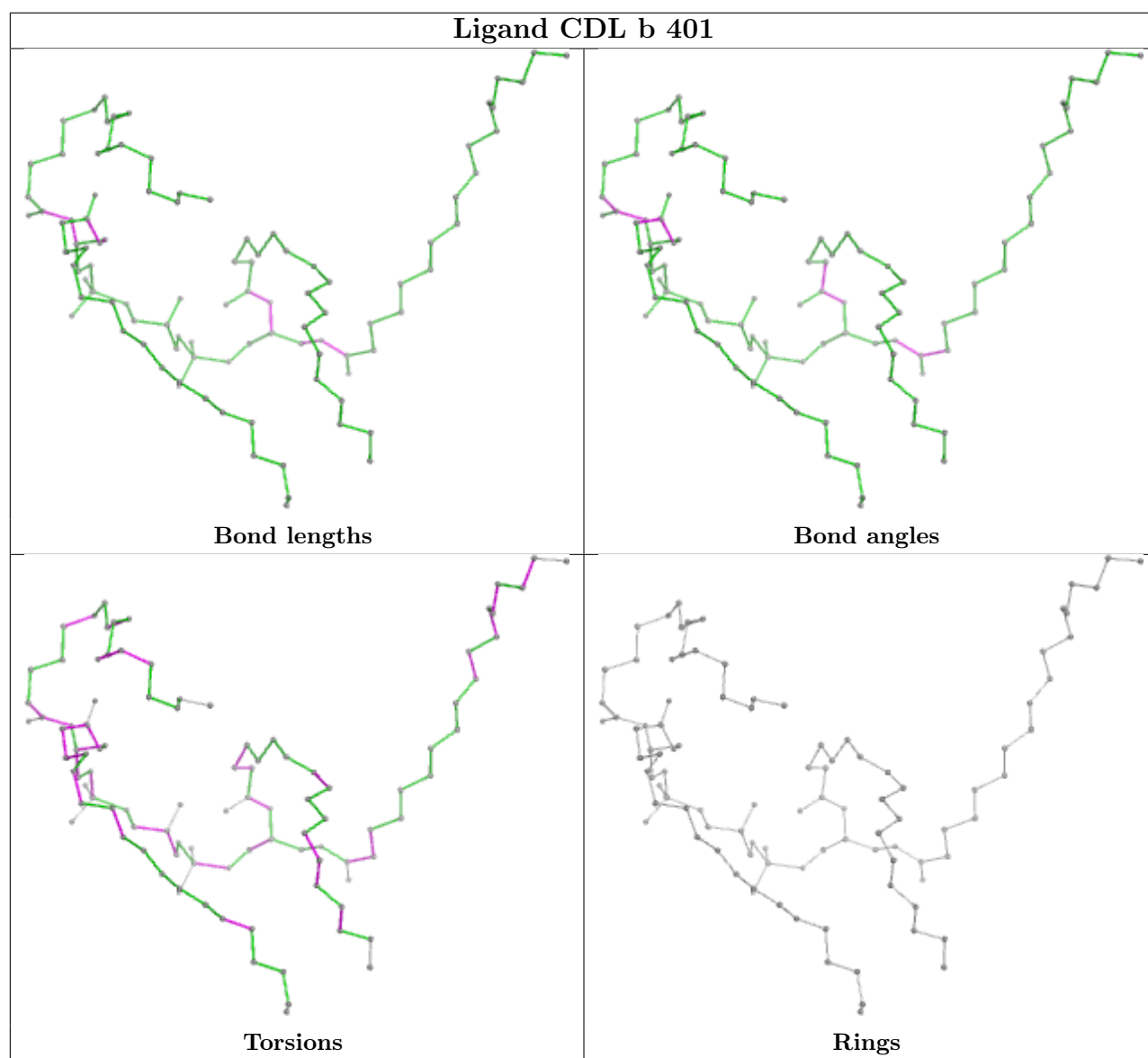


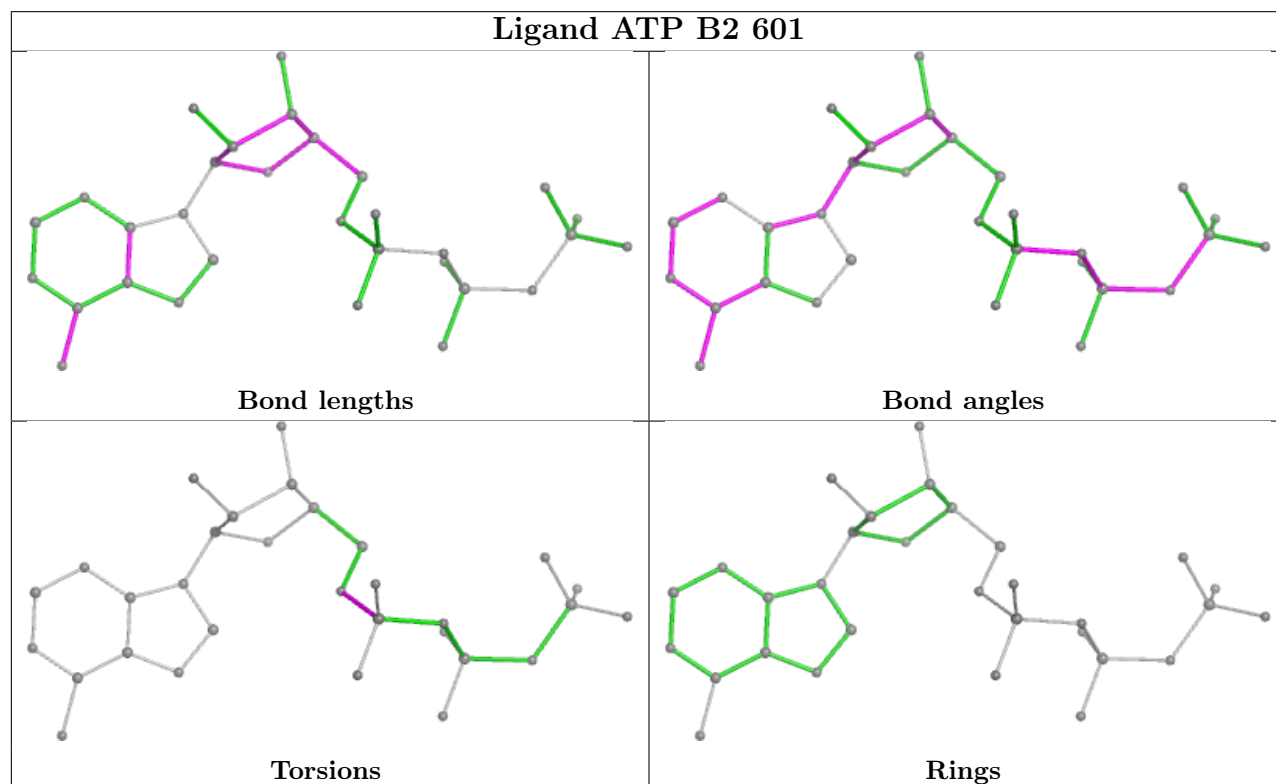
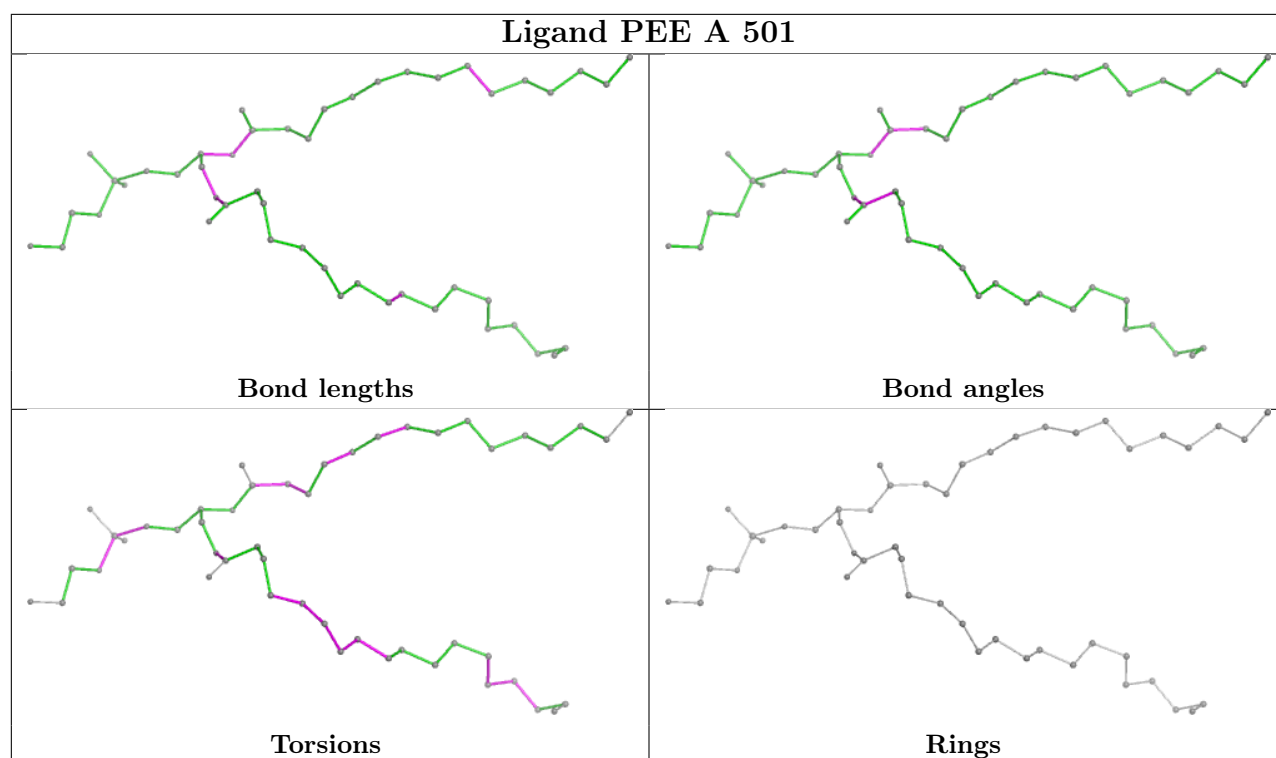
Ligand ADP D1 501

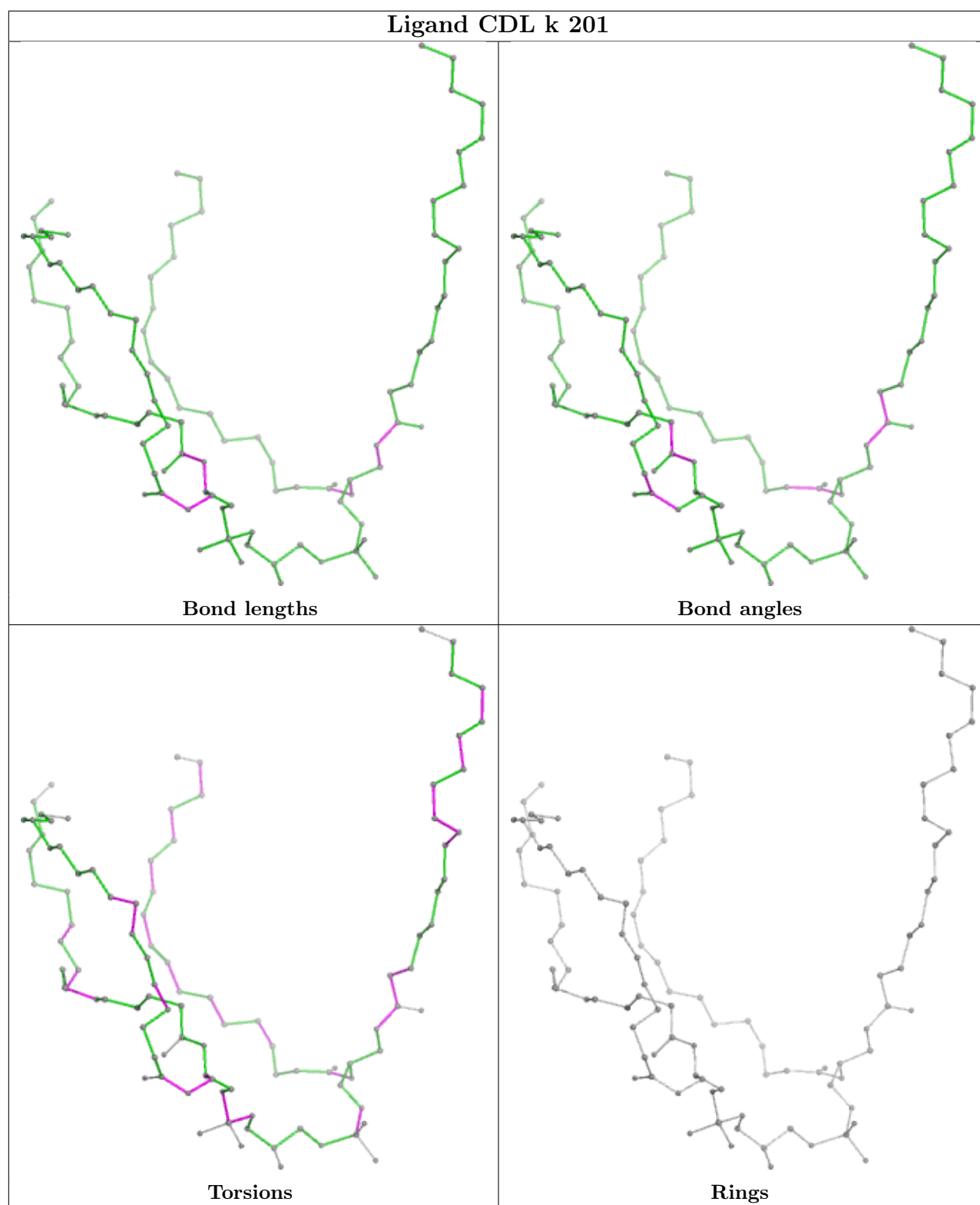


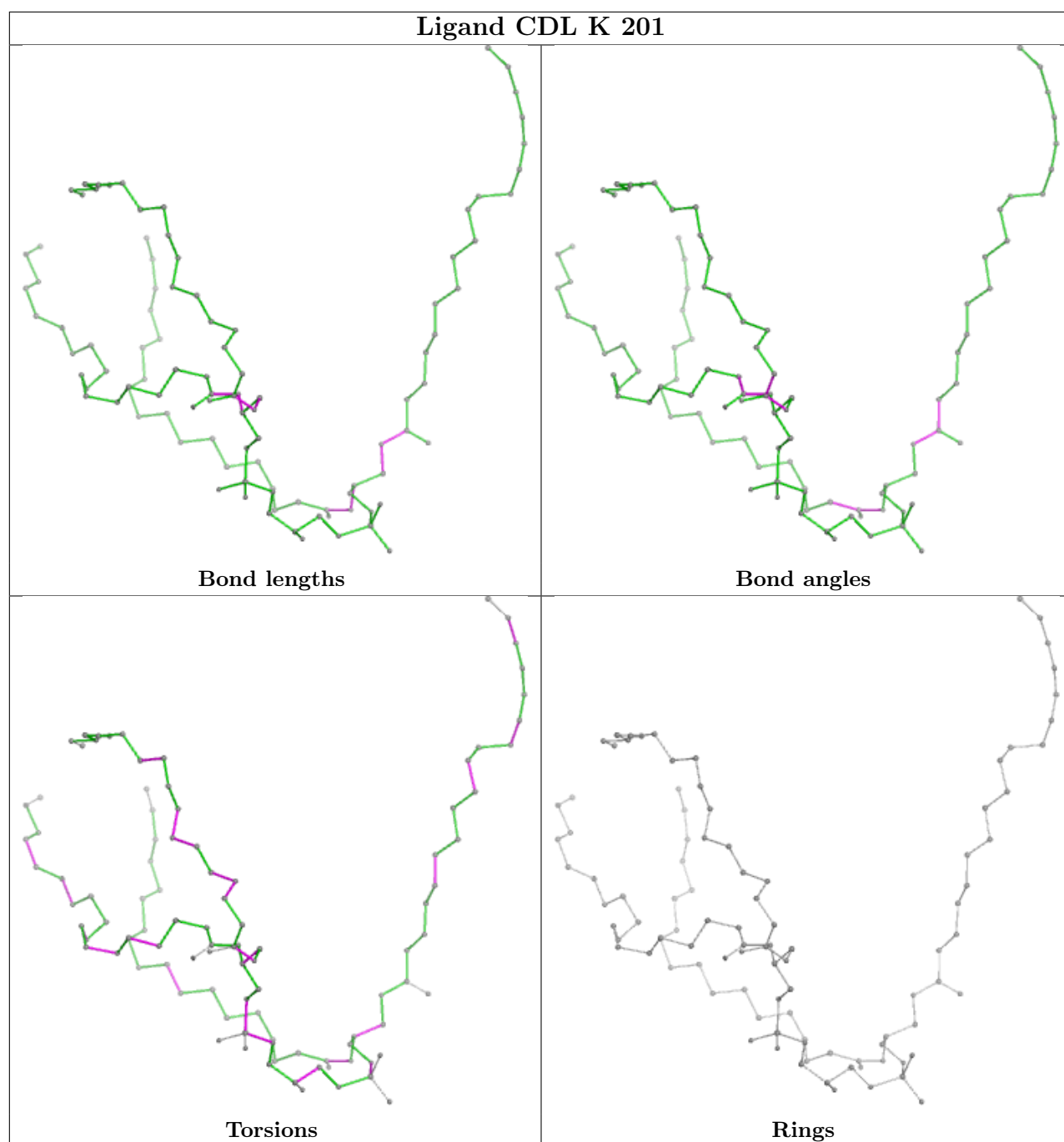


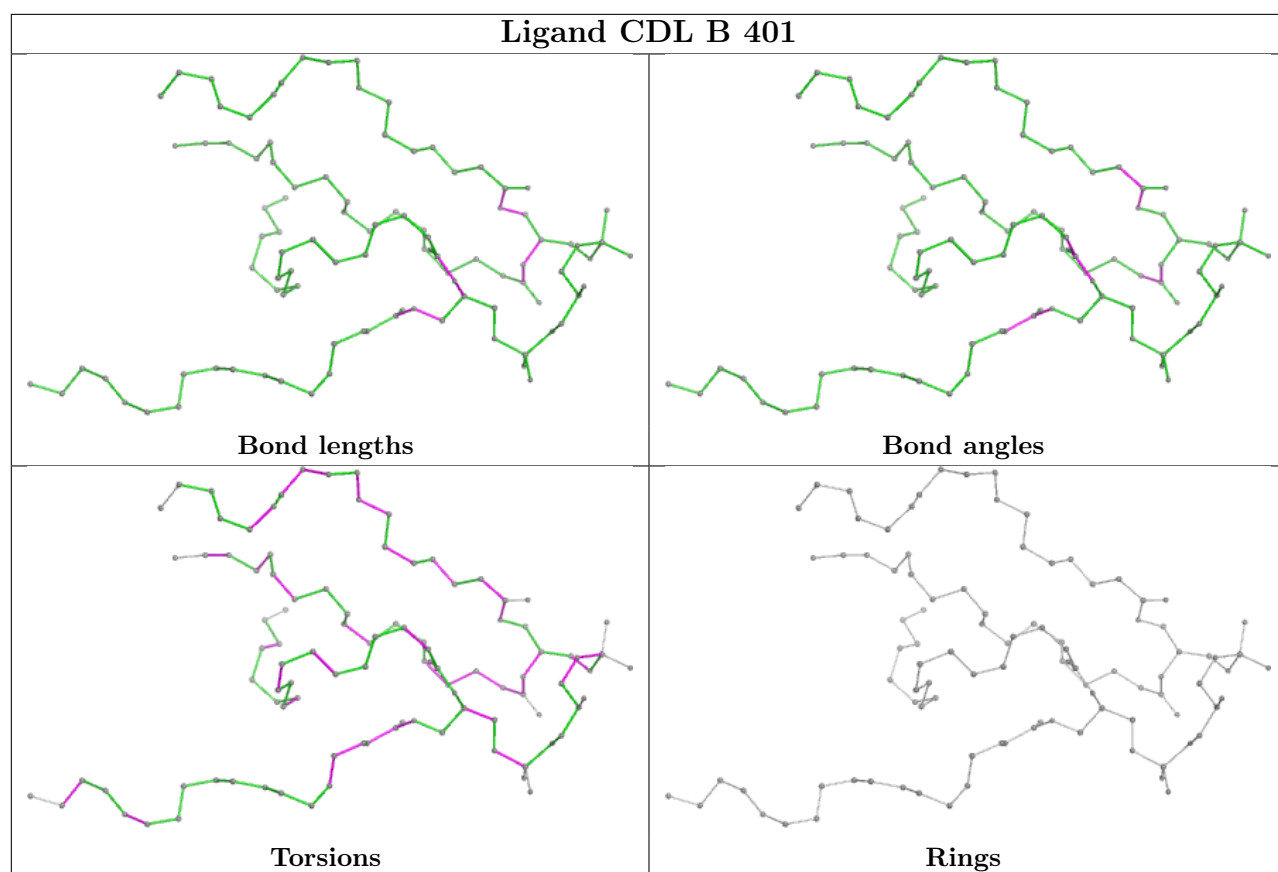


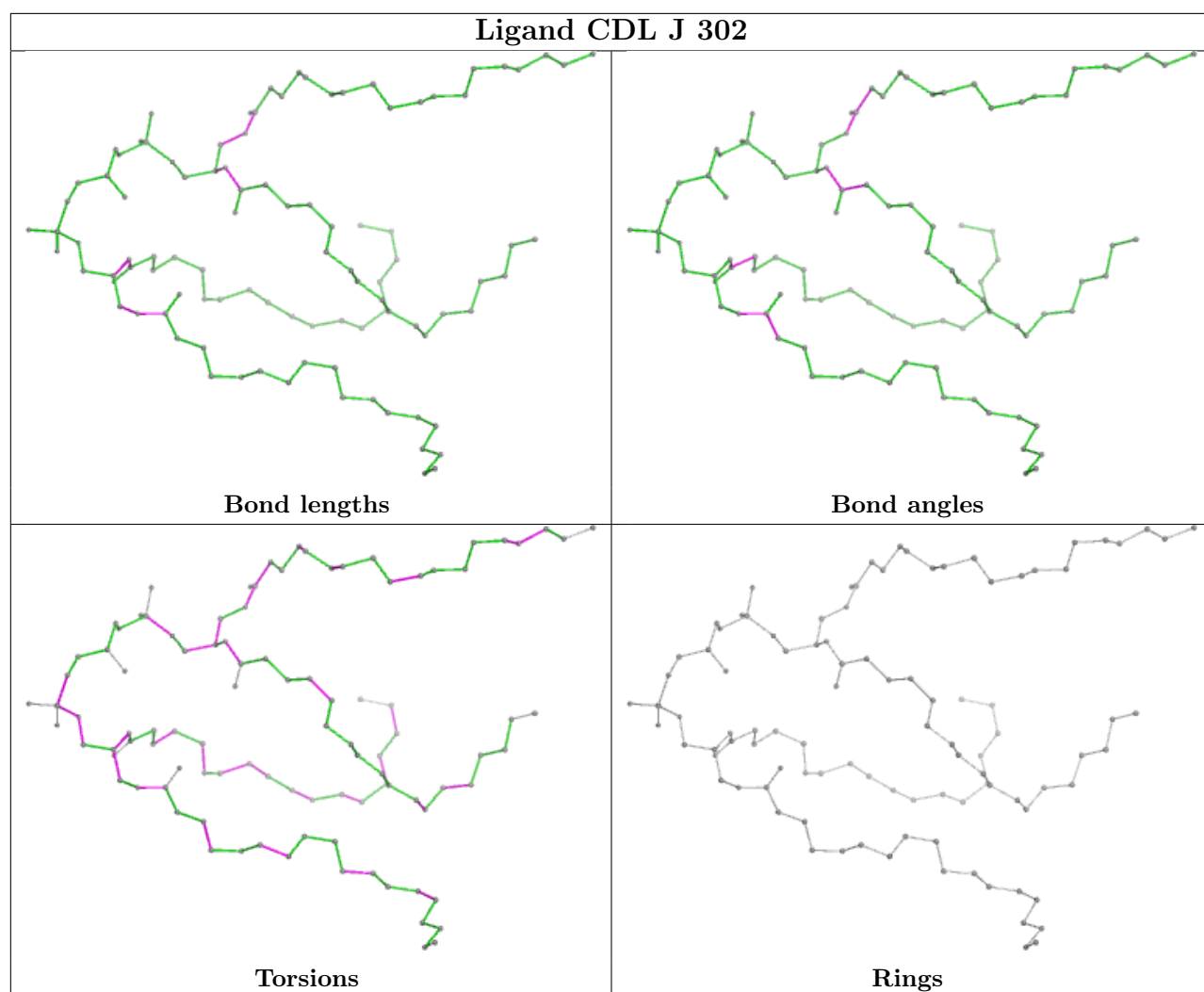


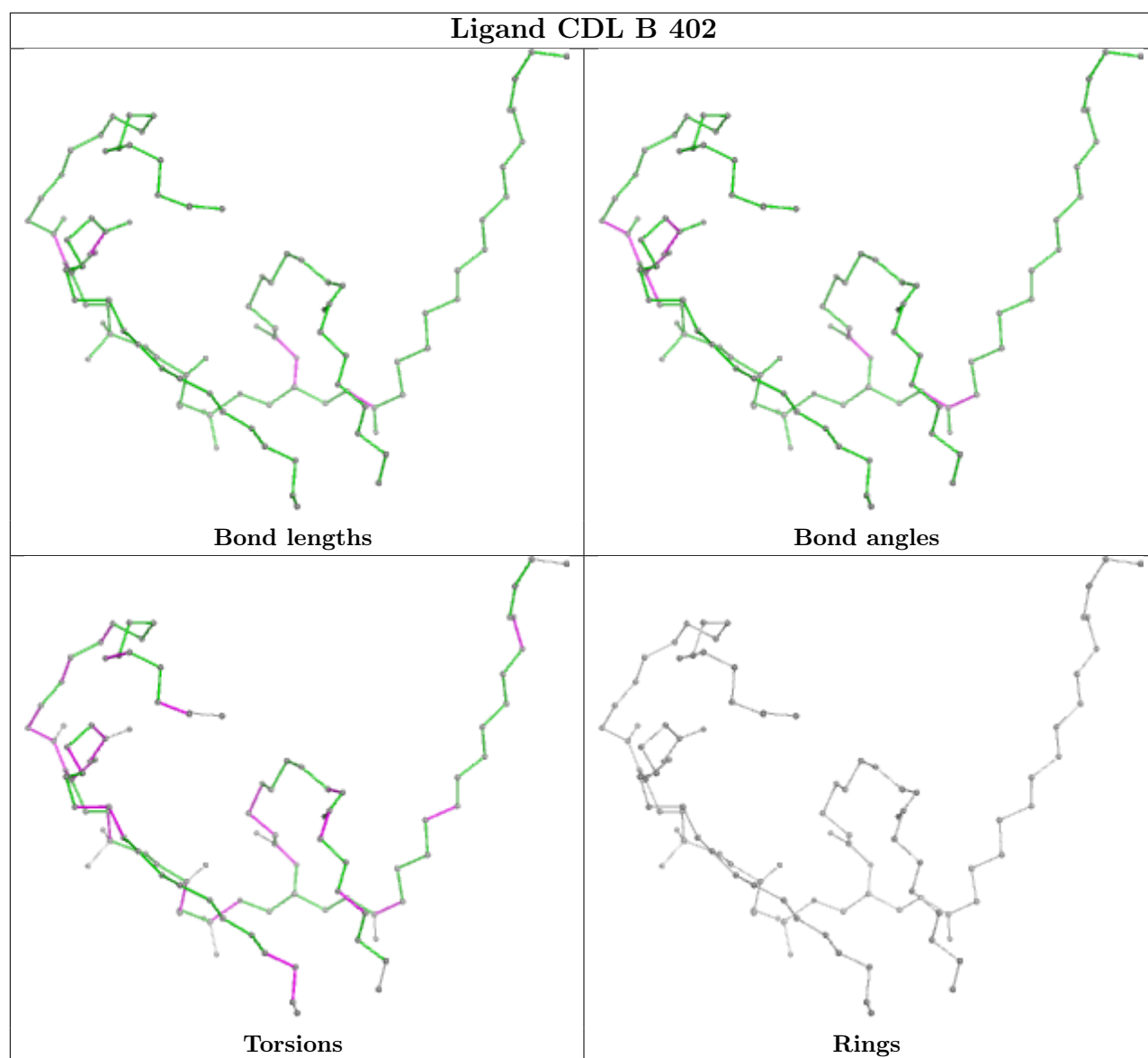


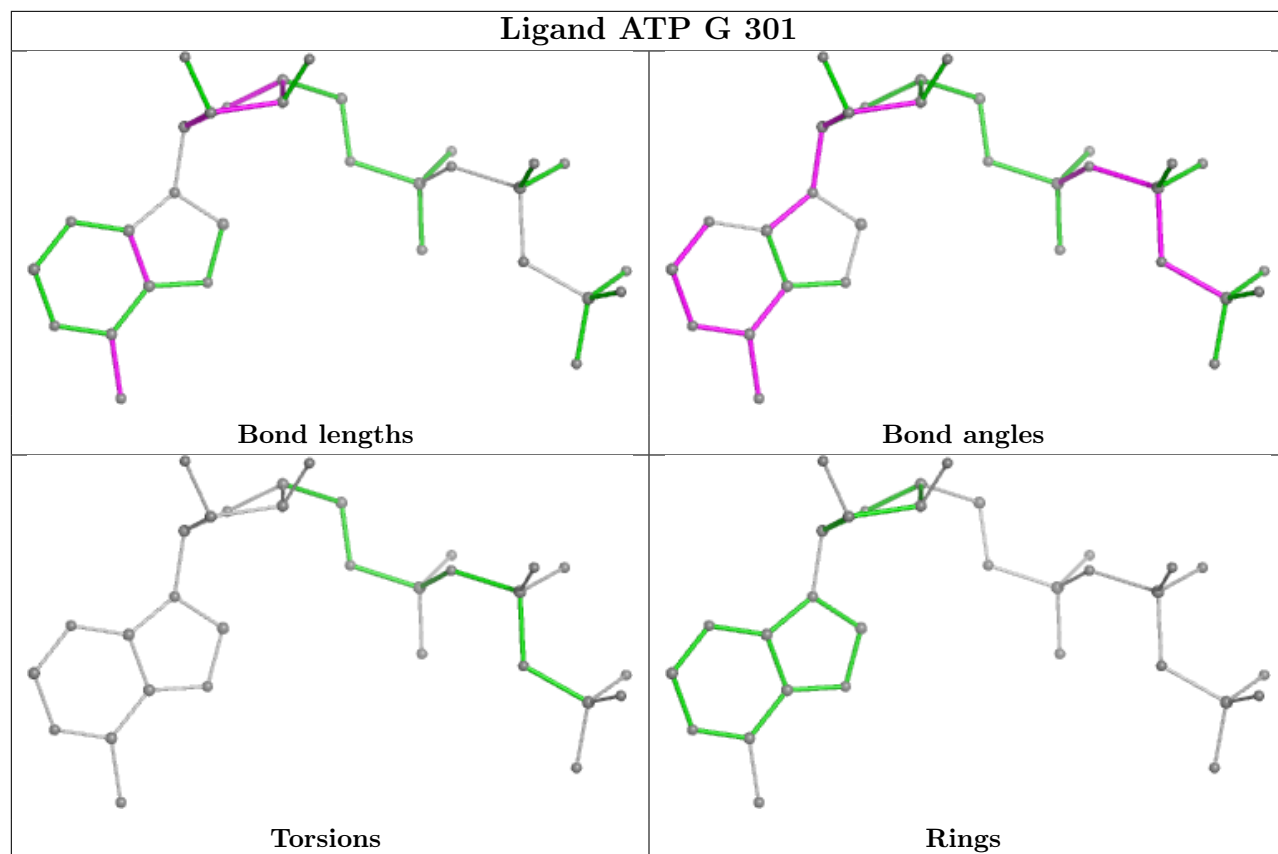


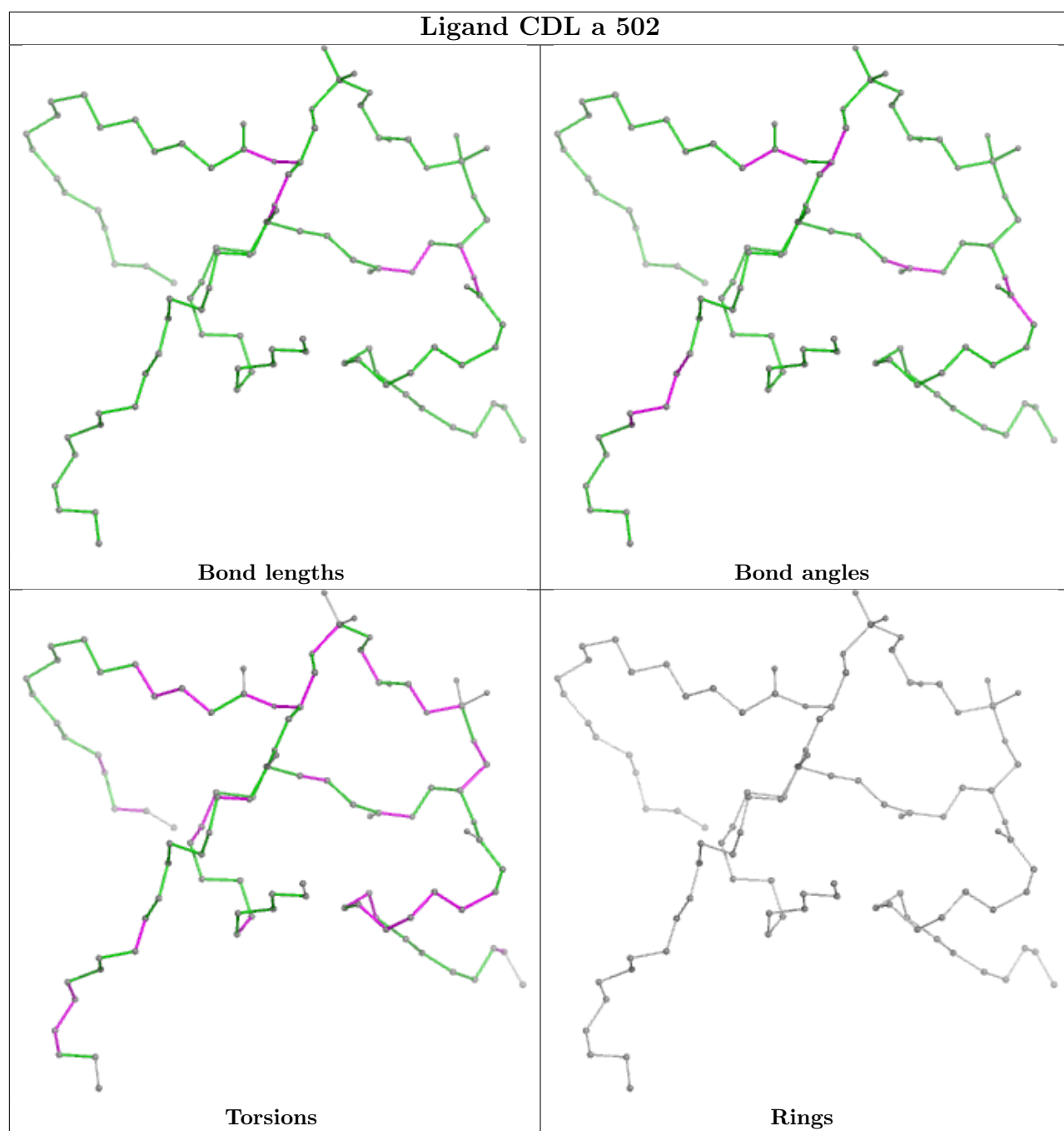


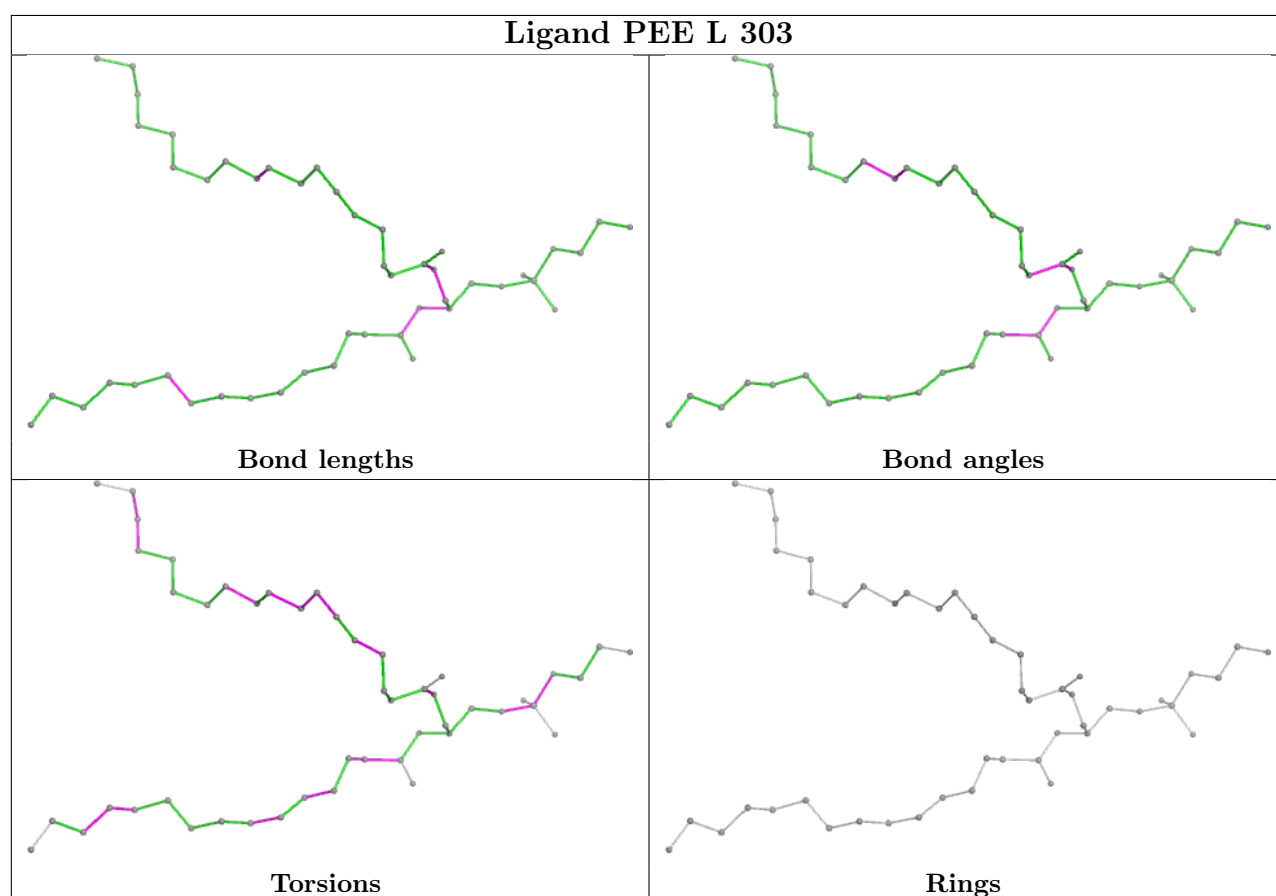
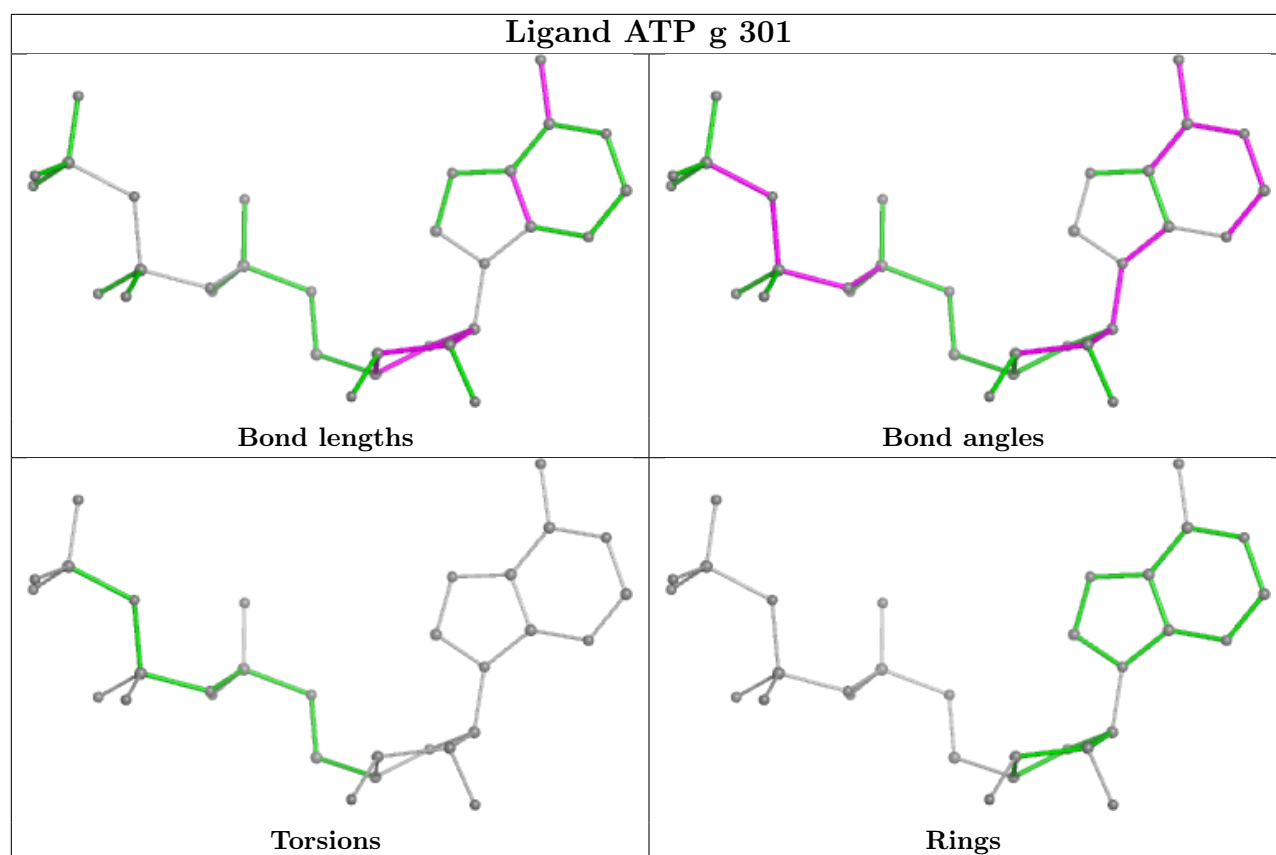


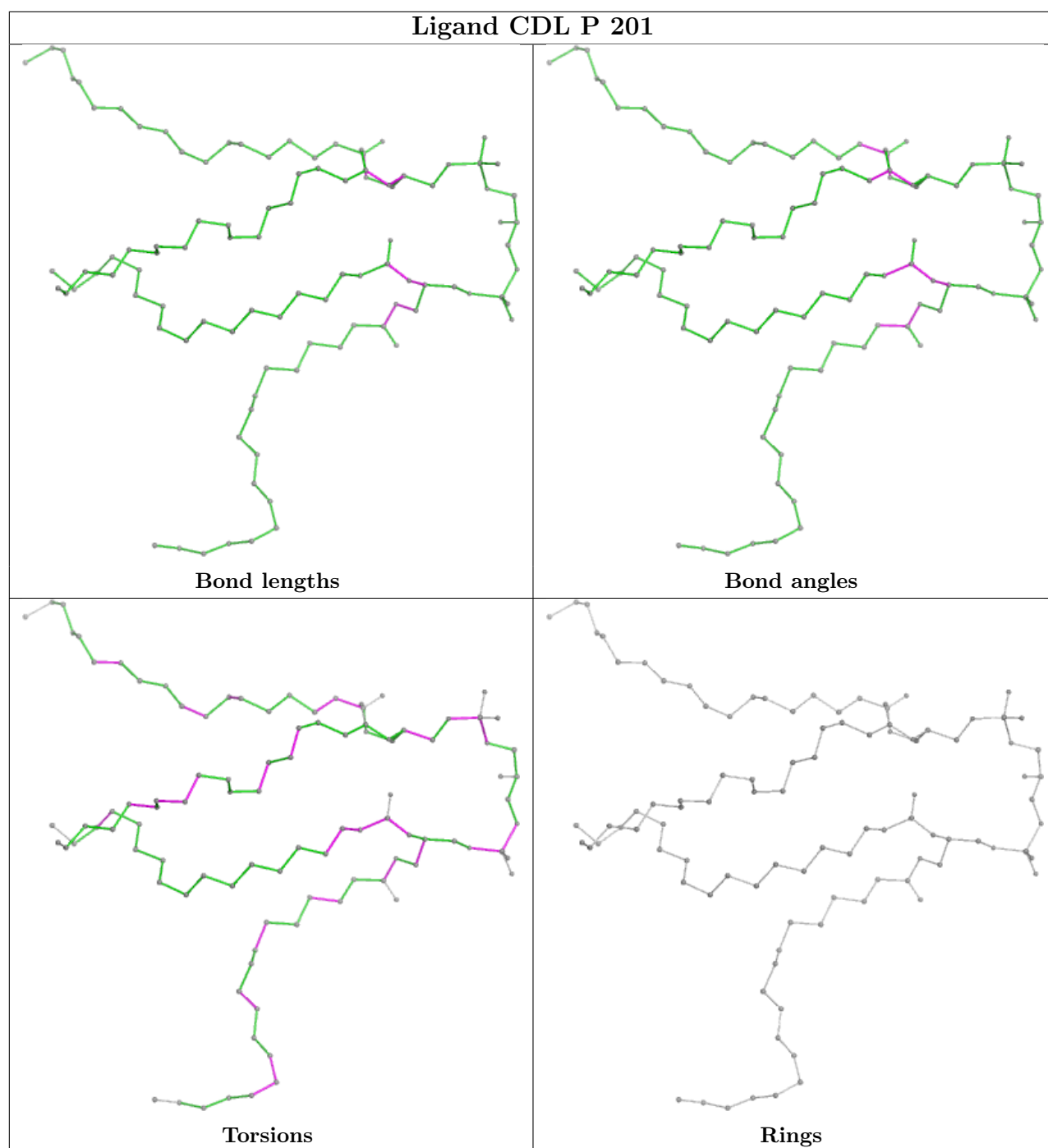


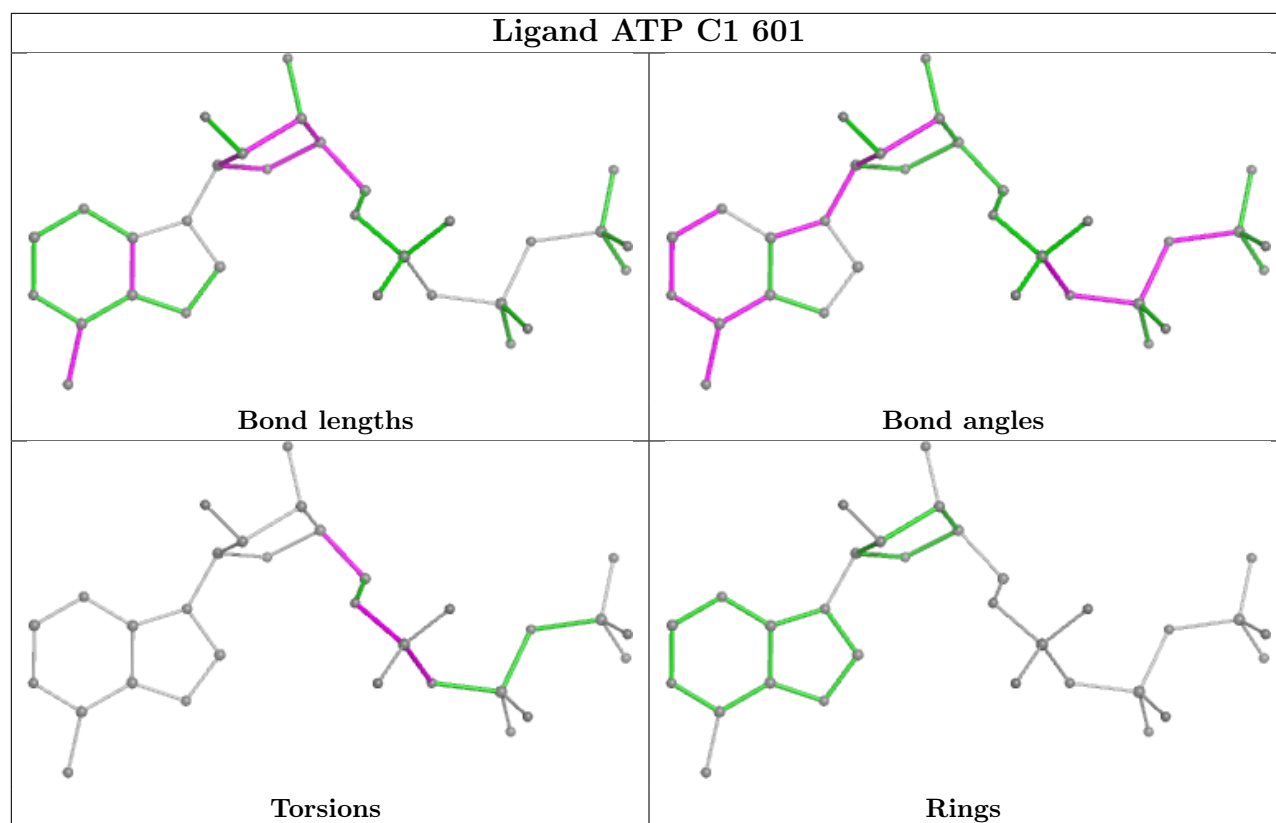
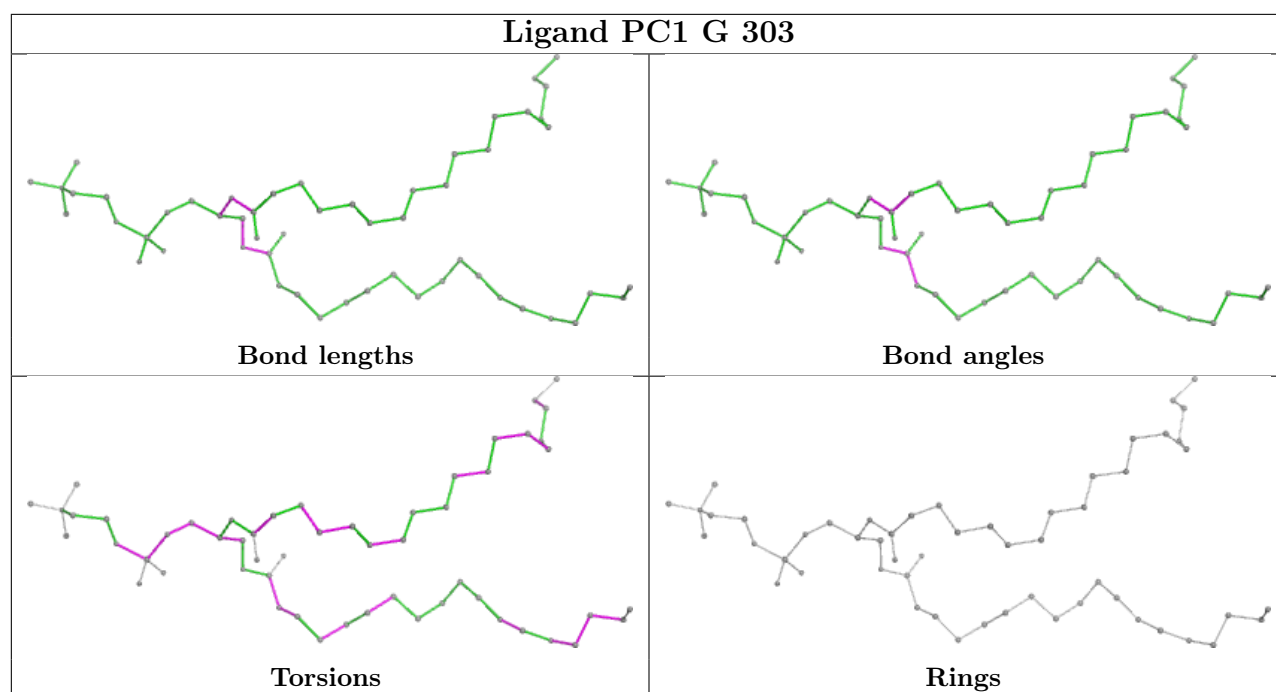


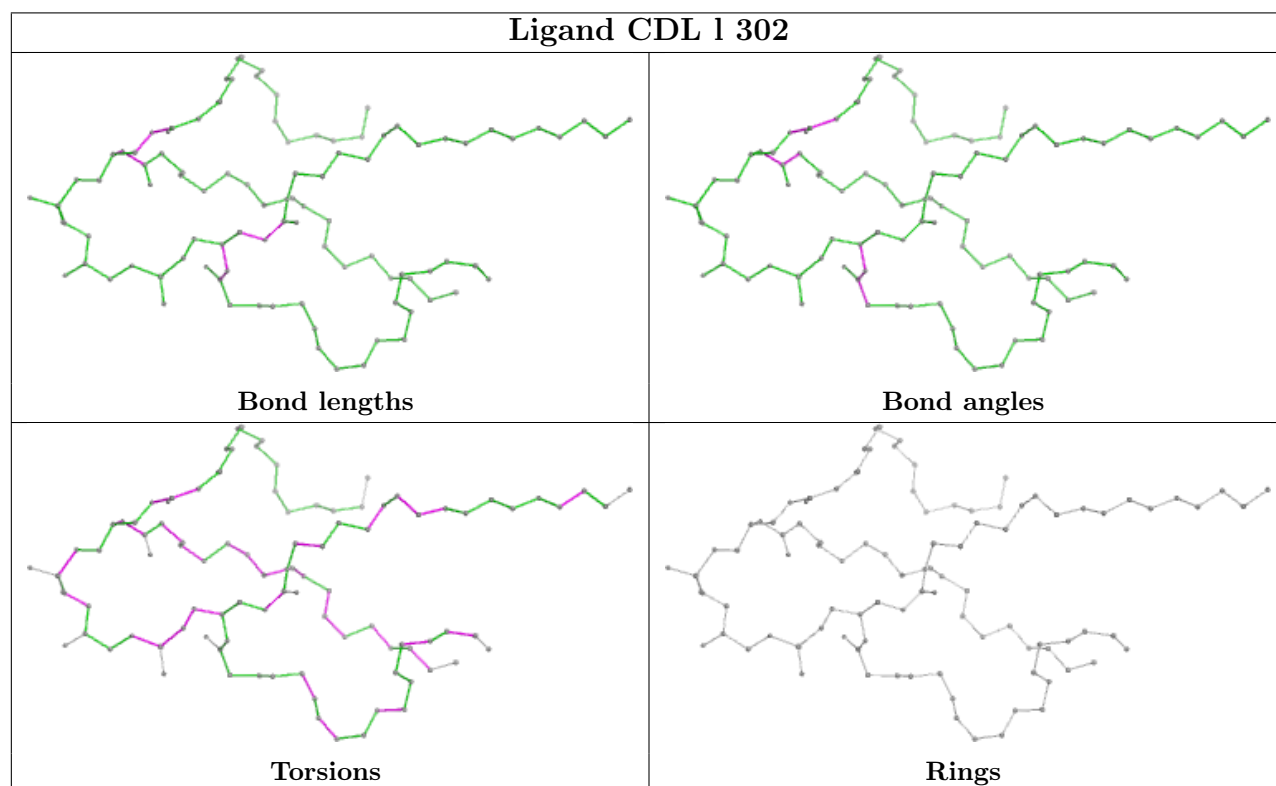
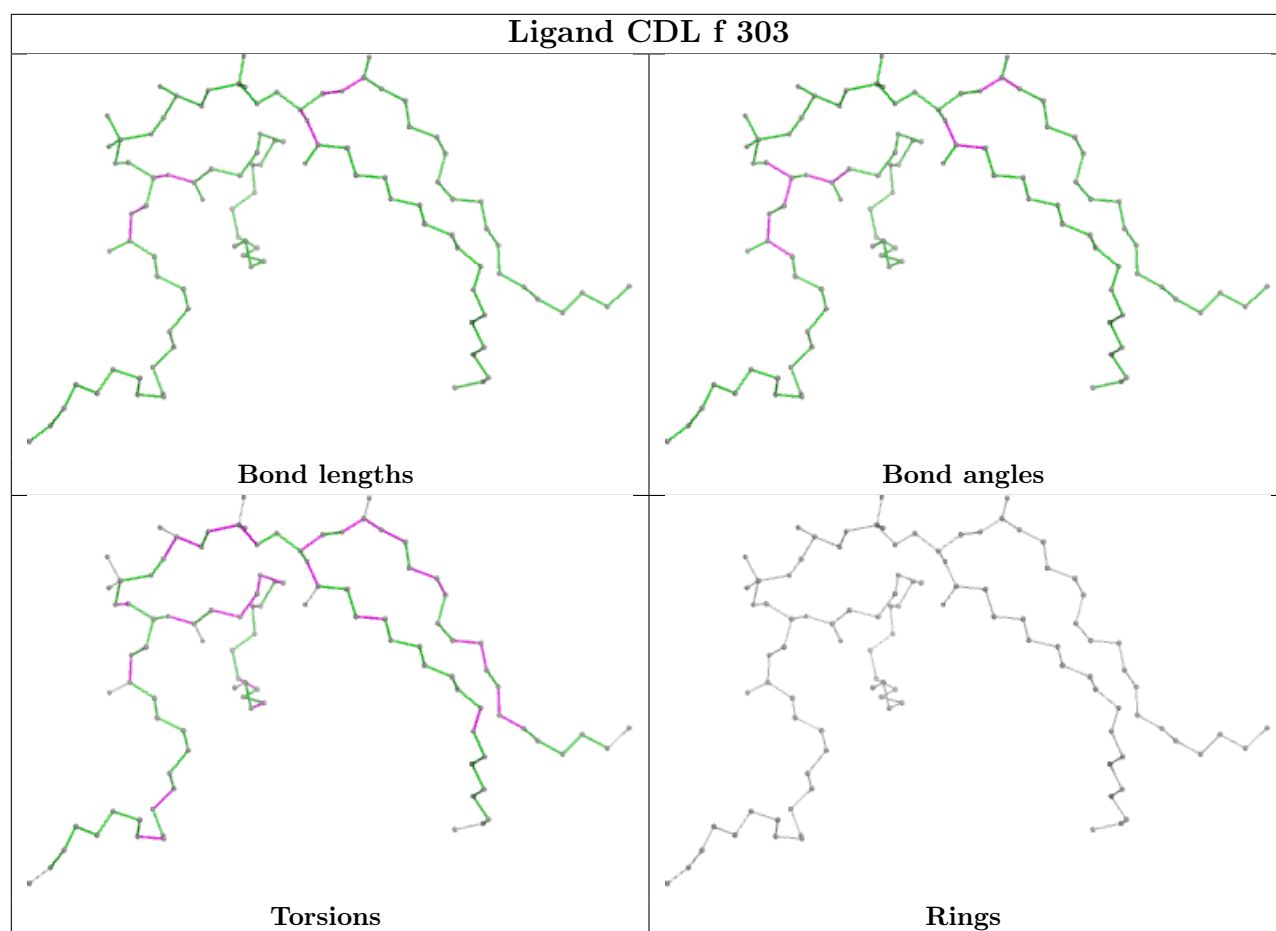


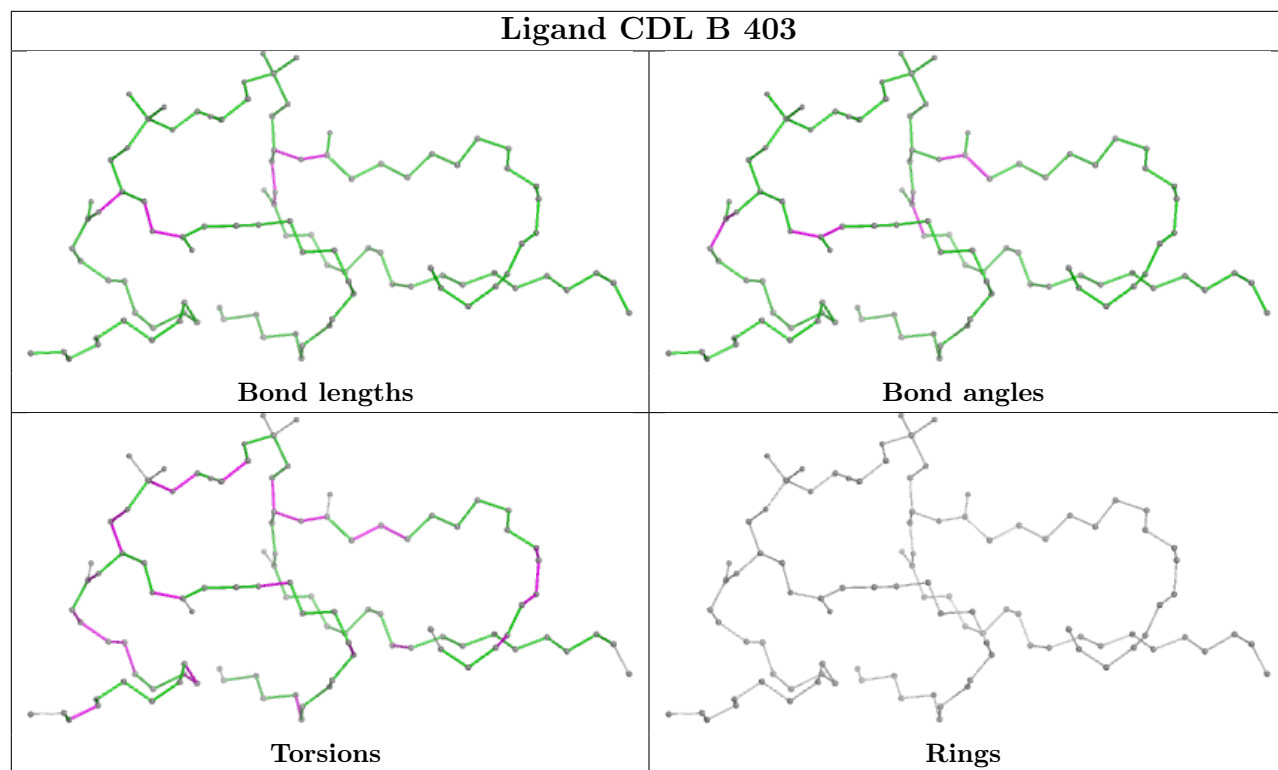


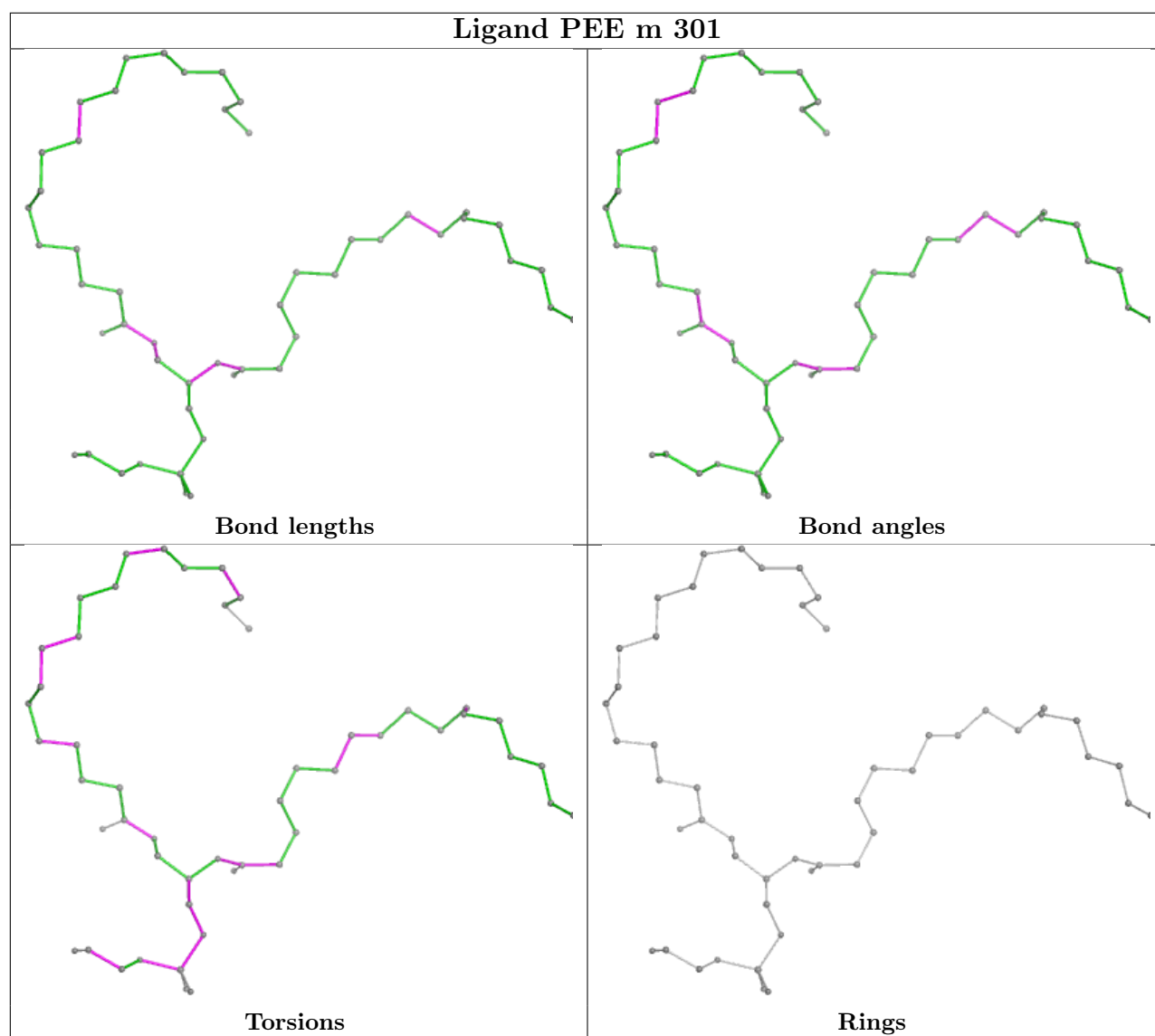




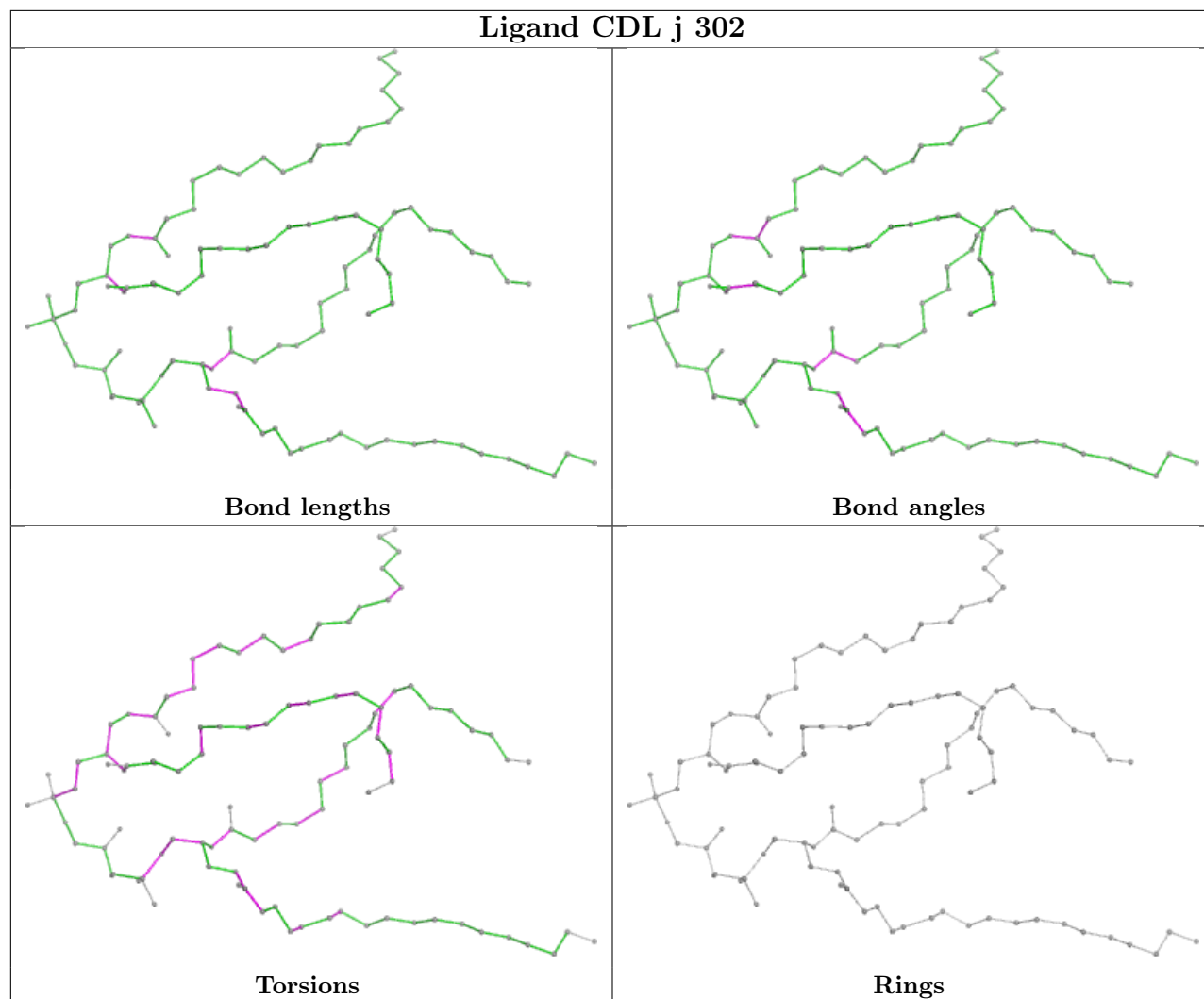


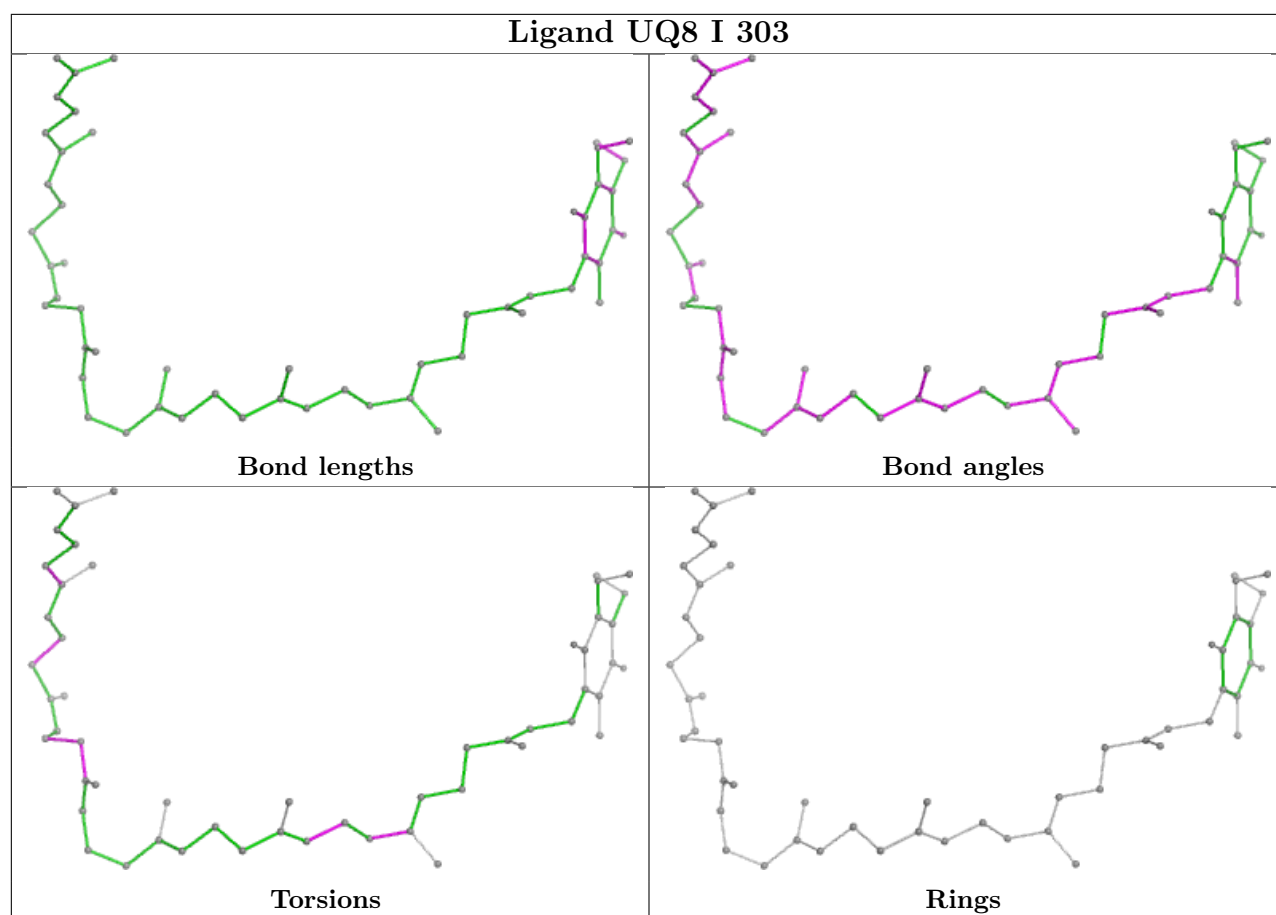


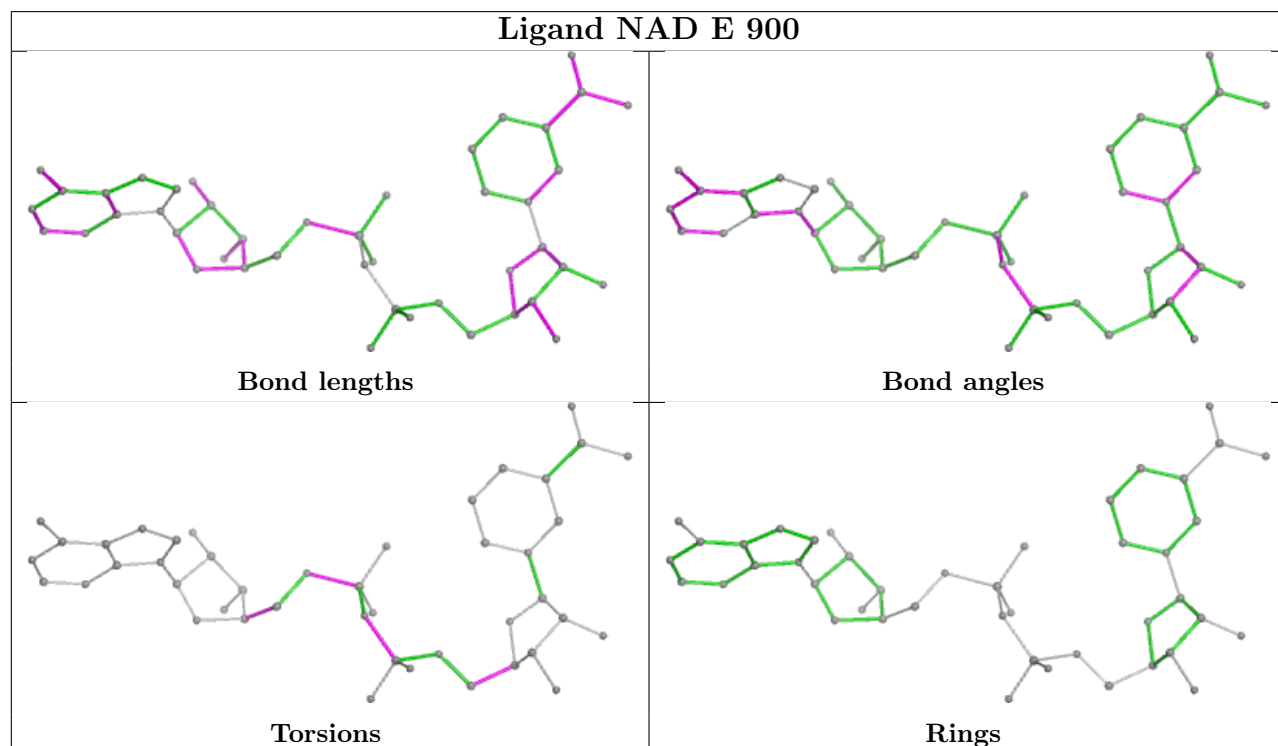
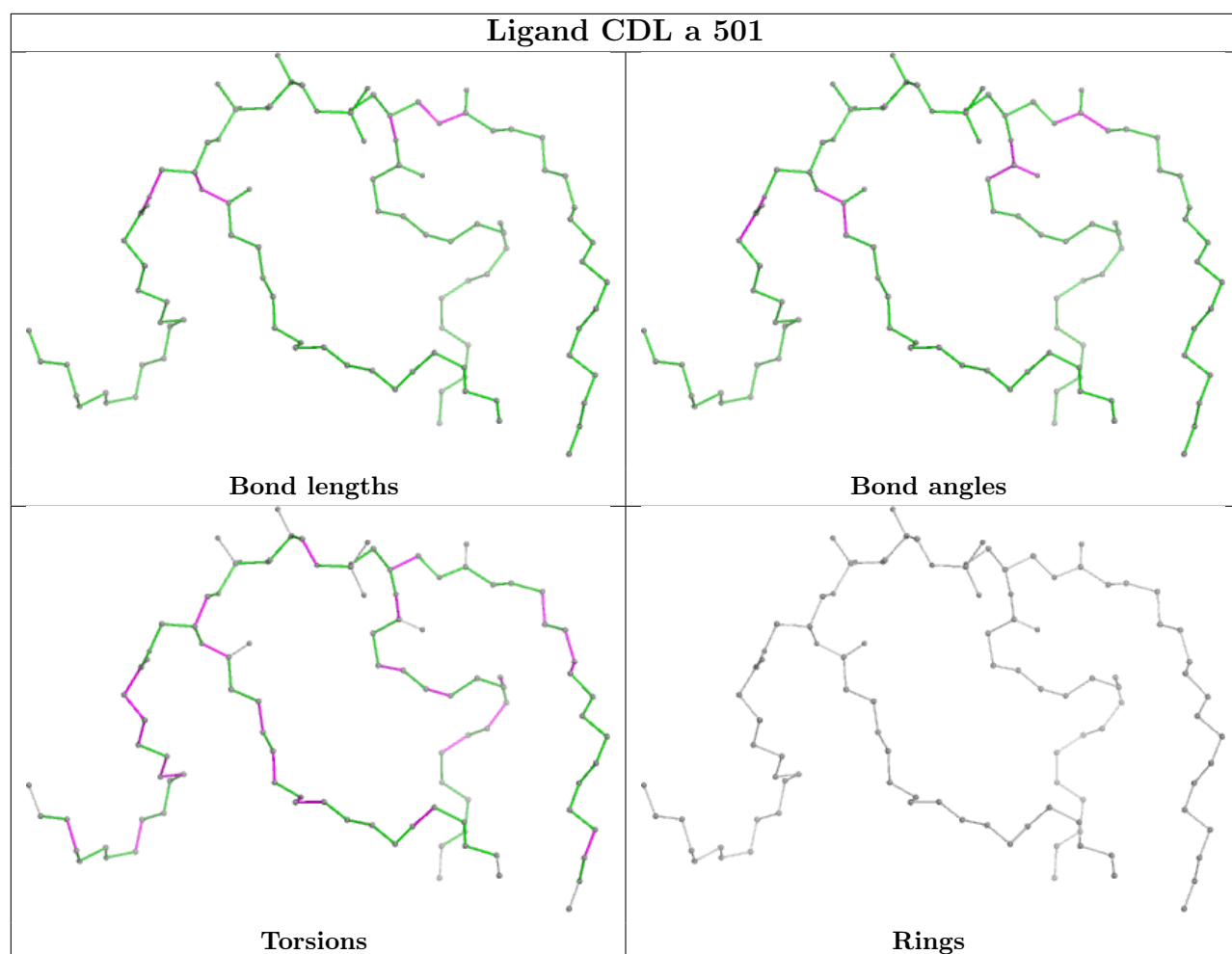


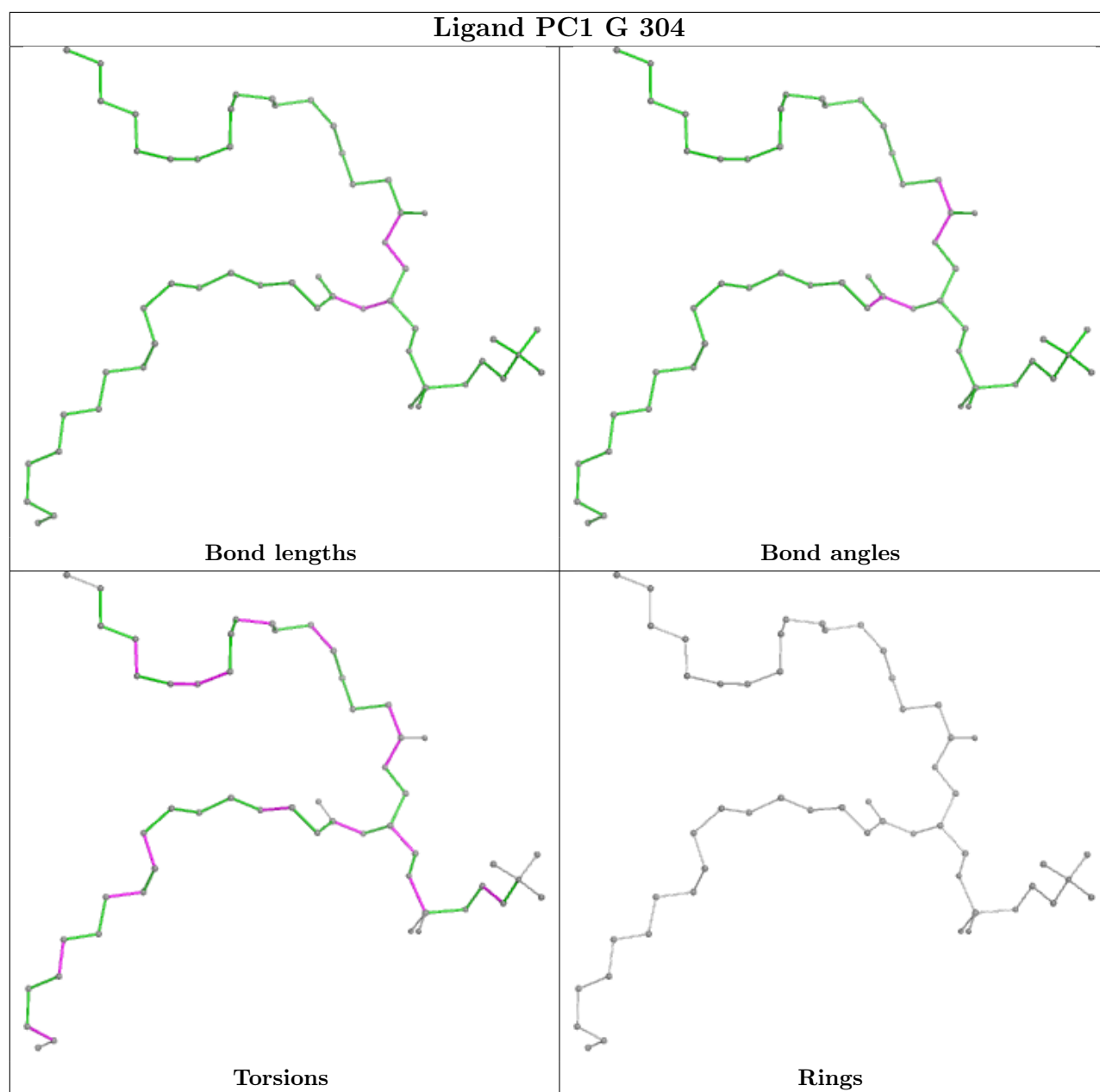


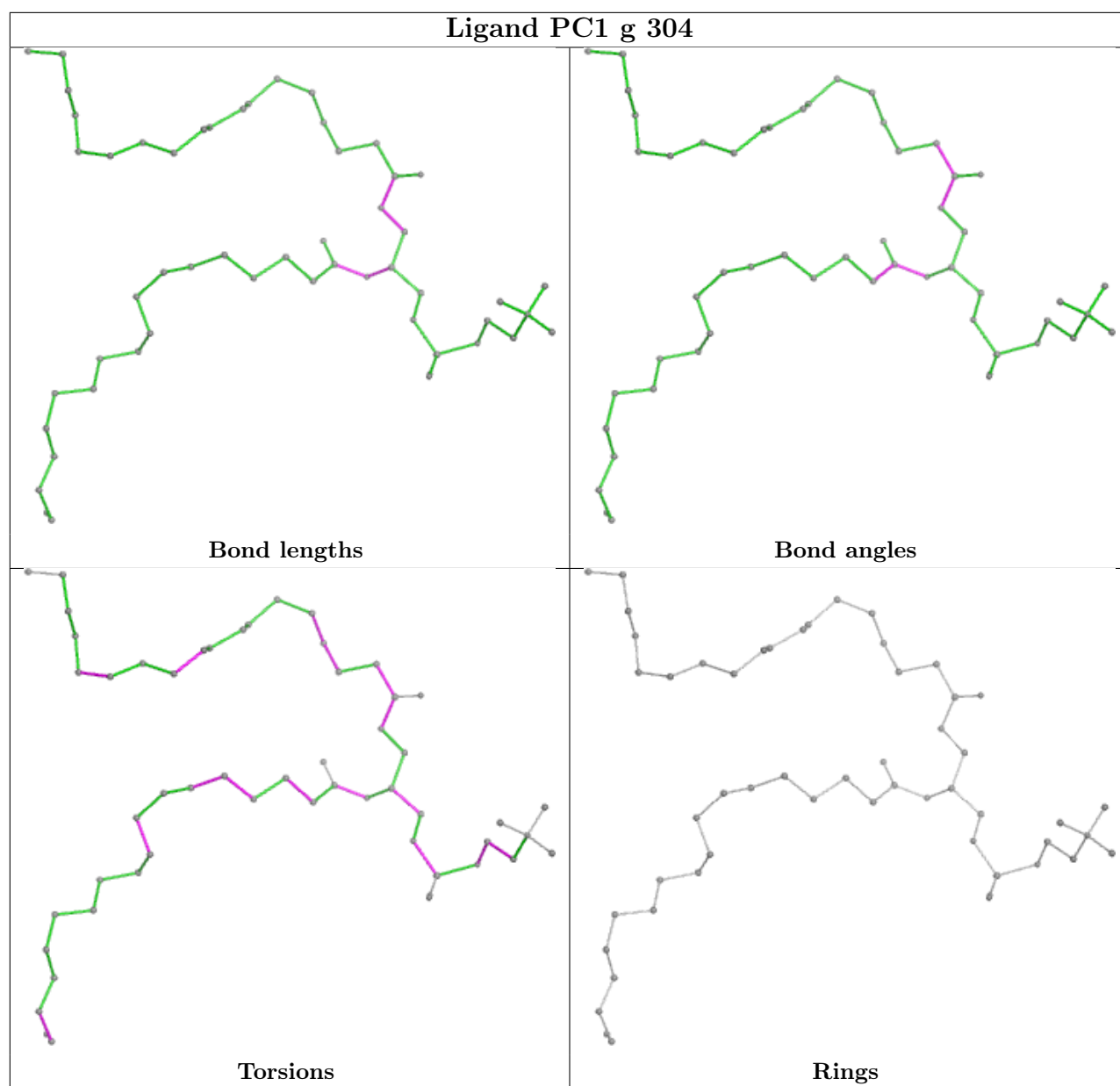
Ligand CDL j 302

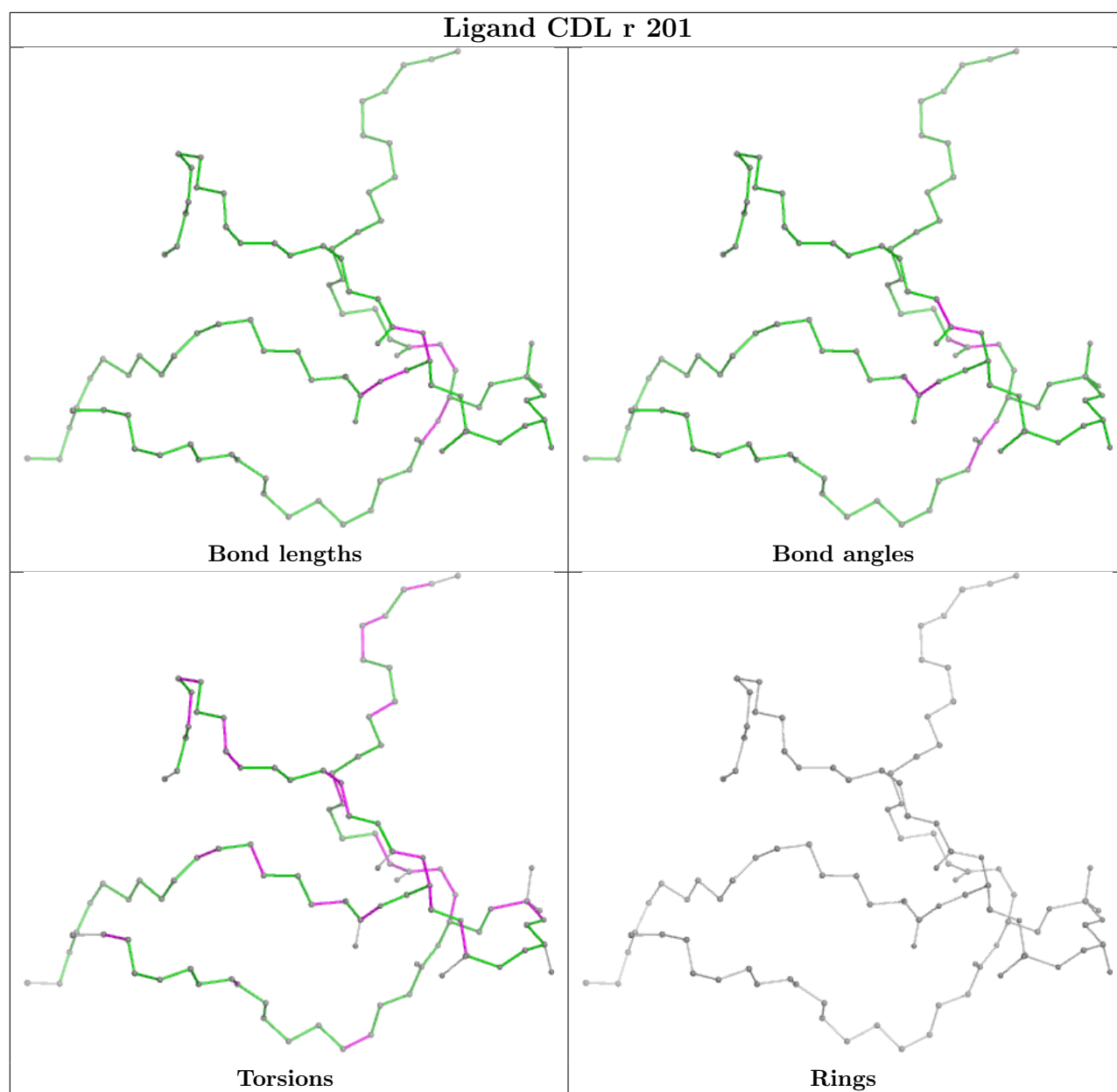


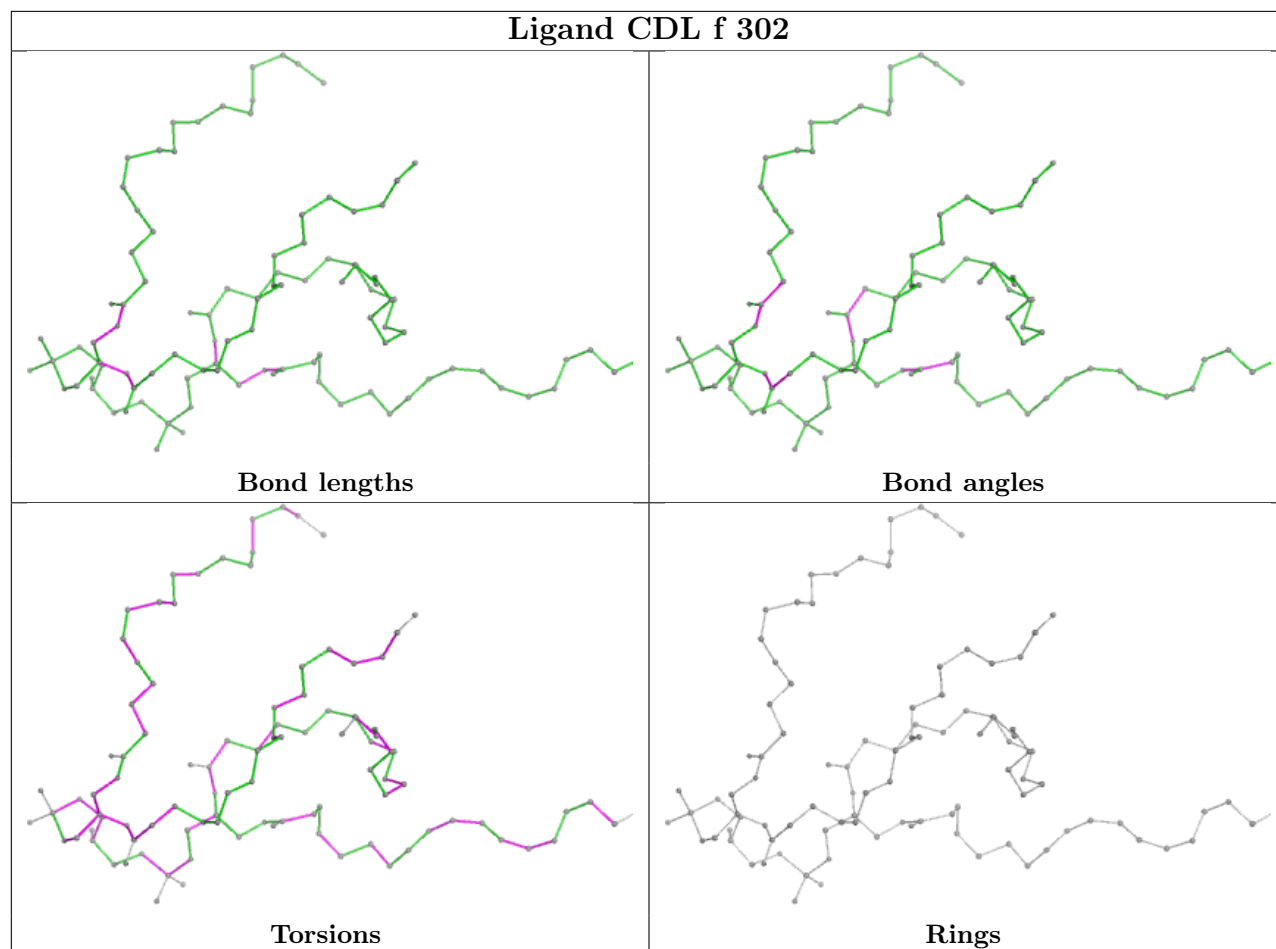
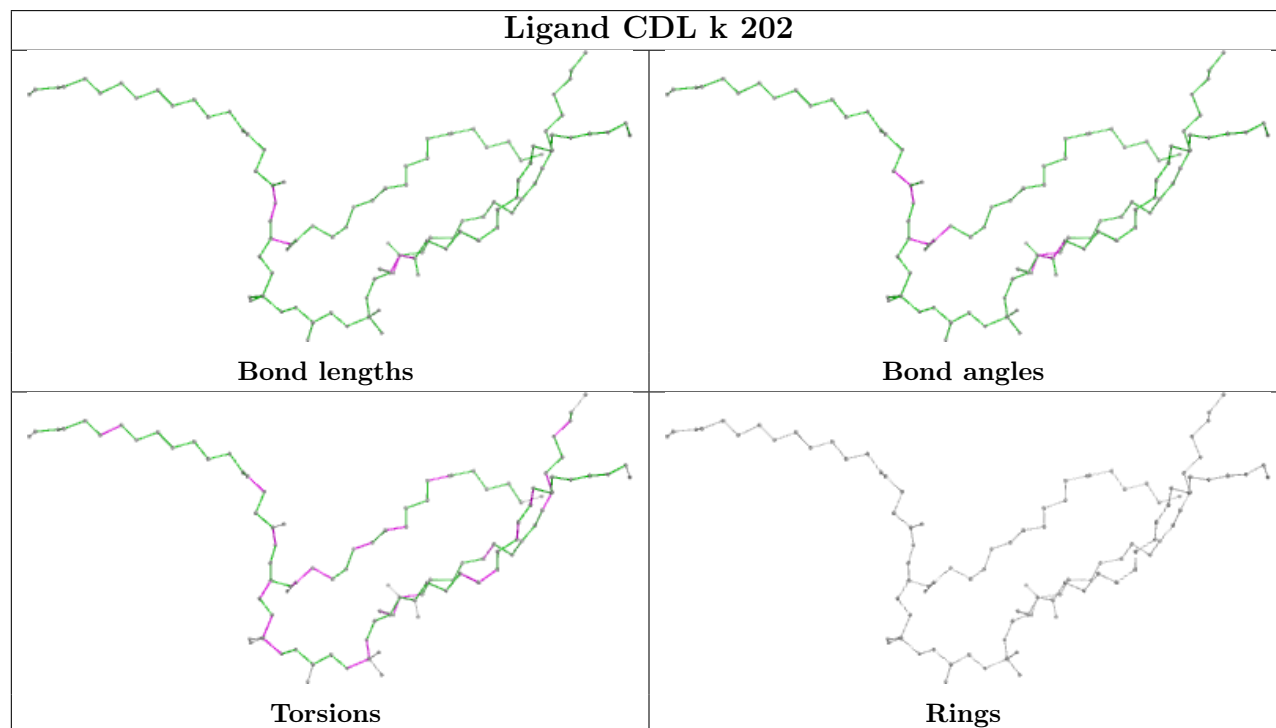


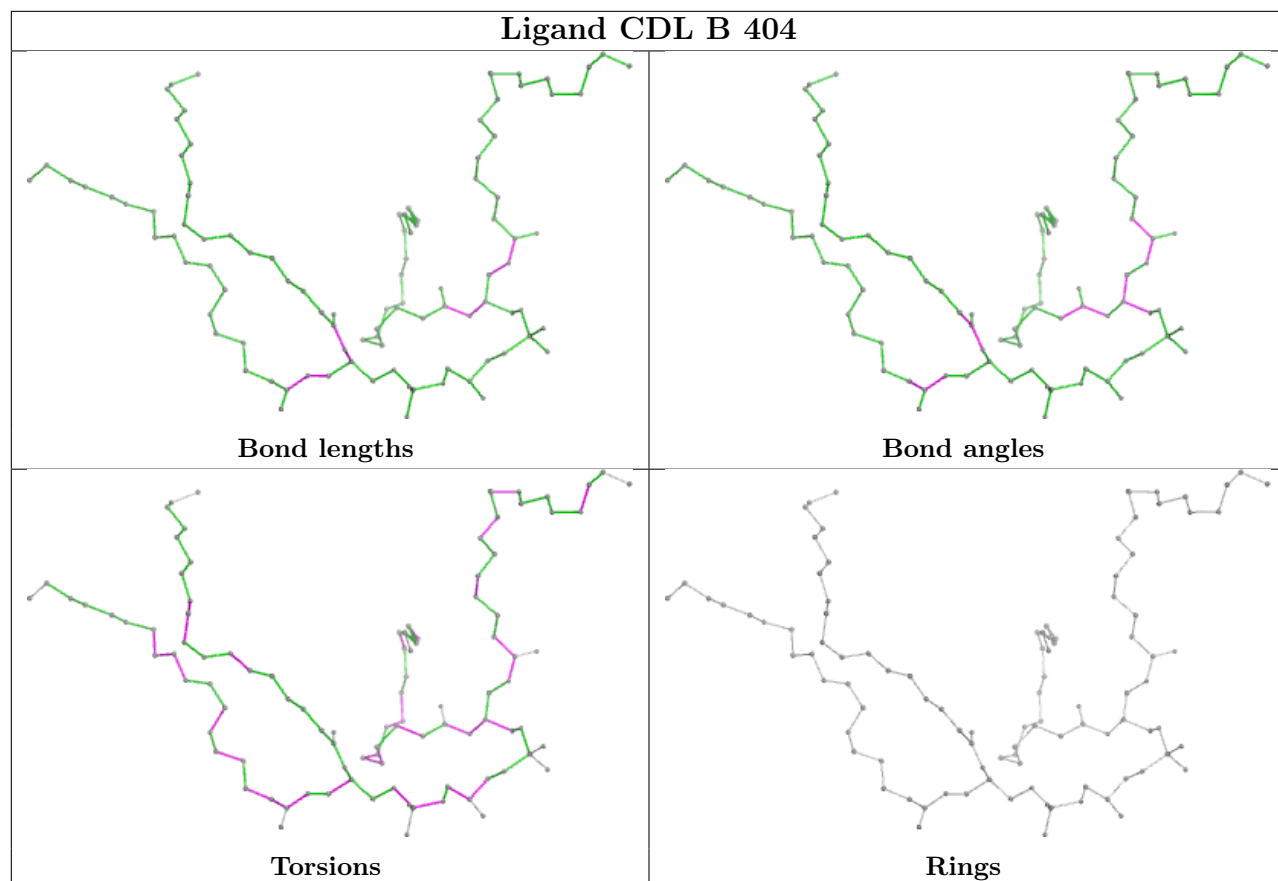


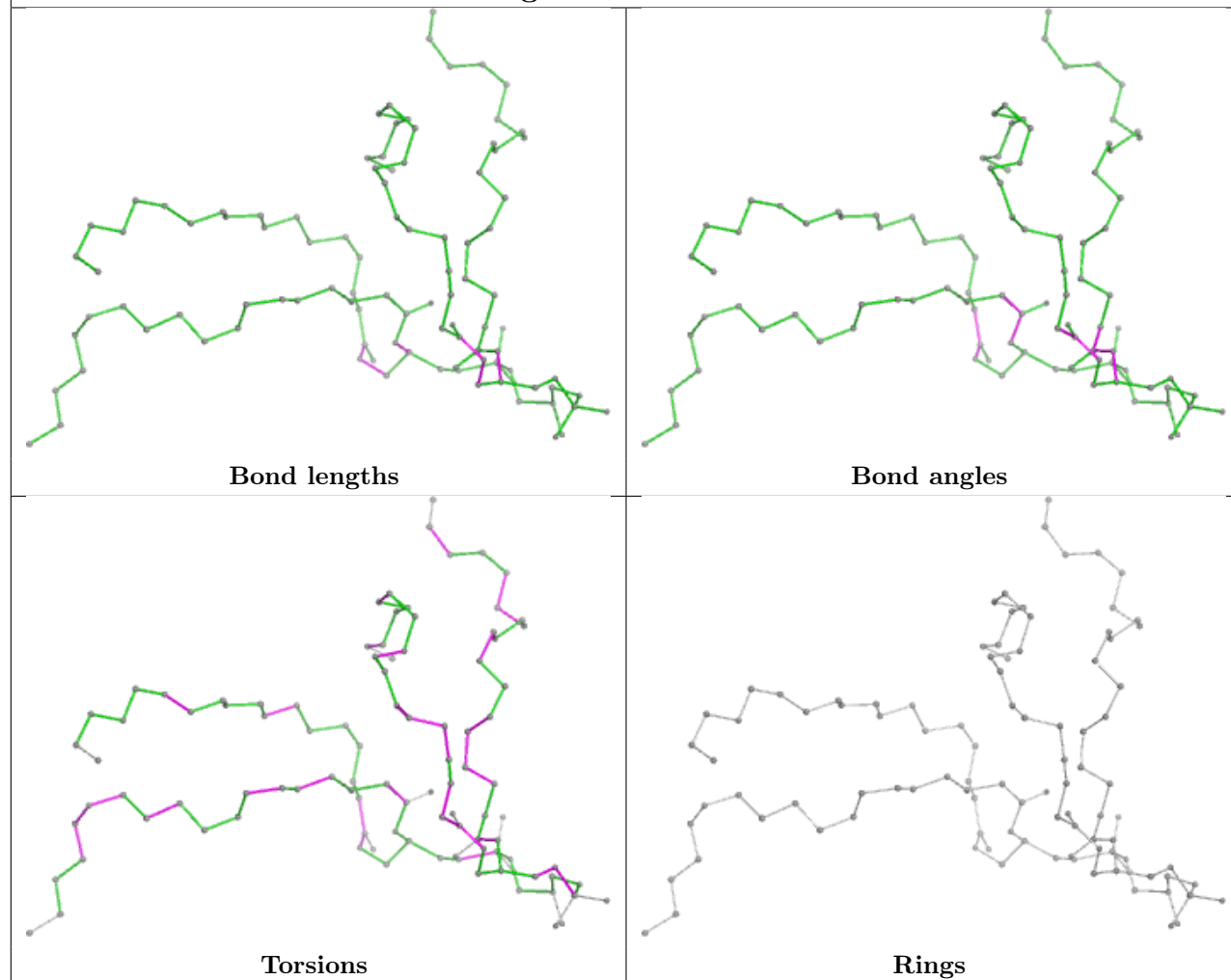
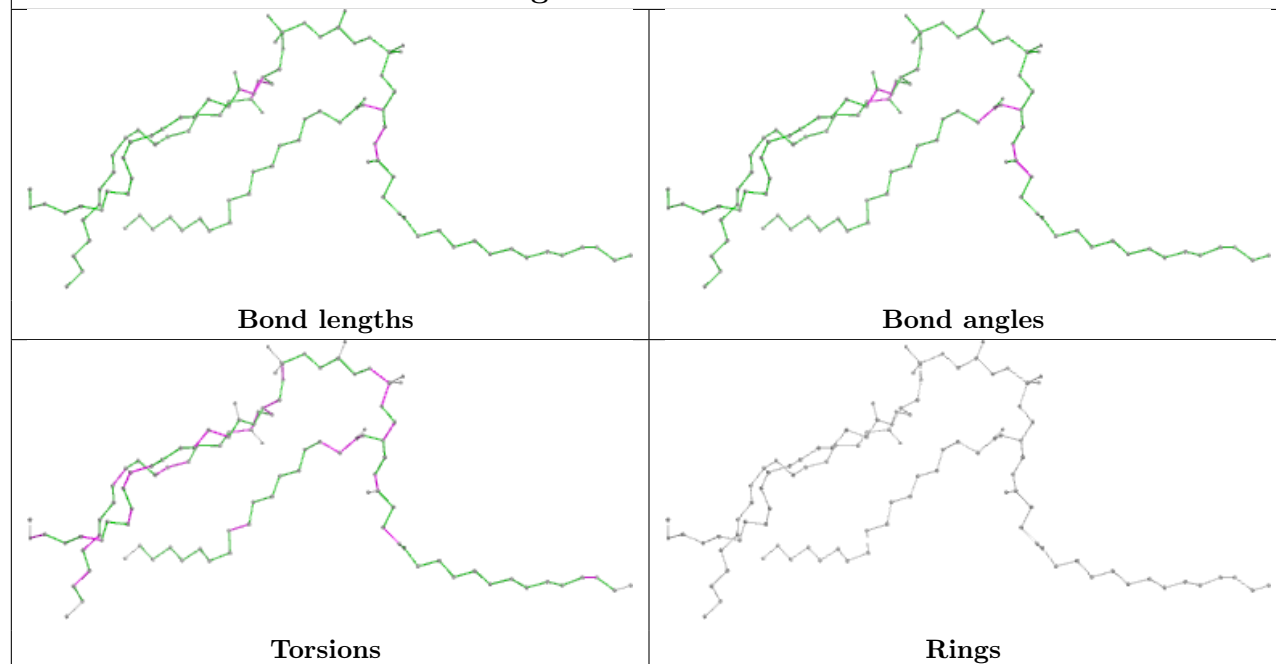


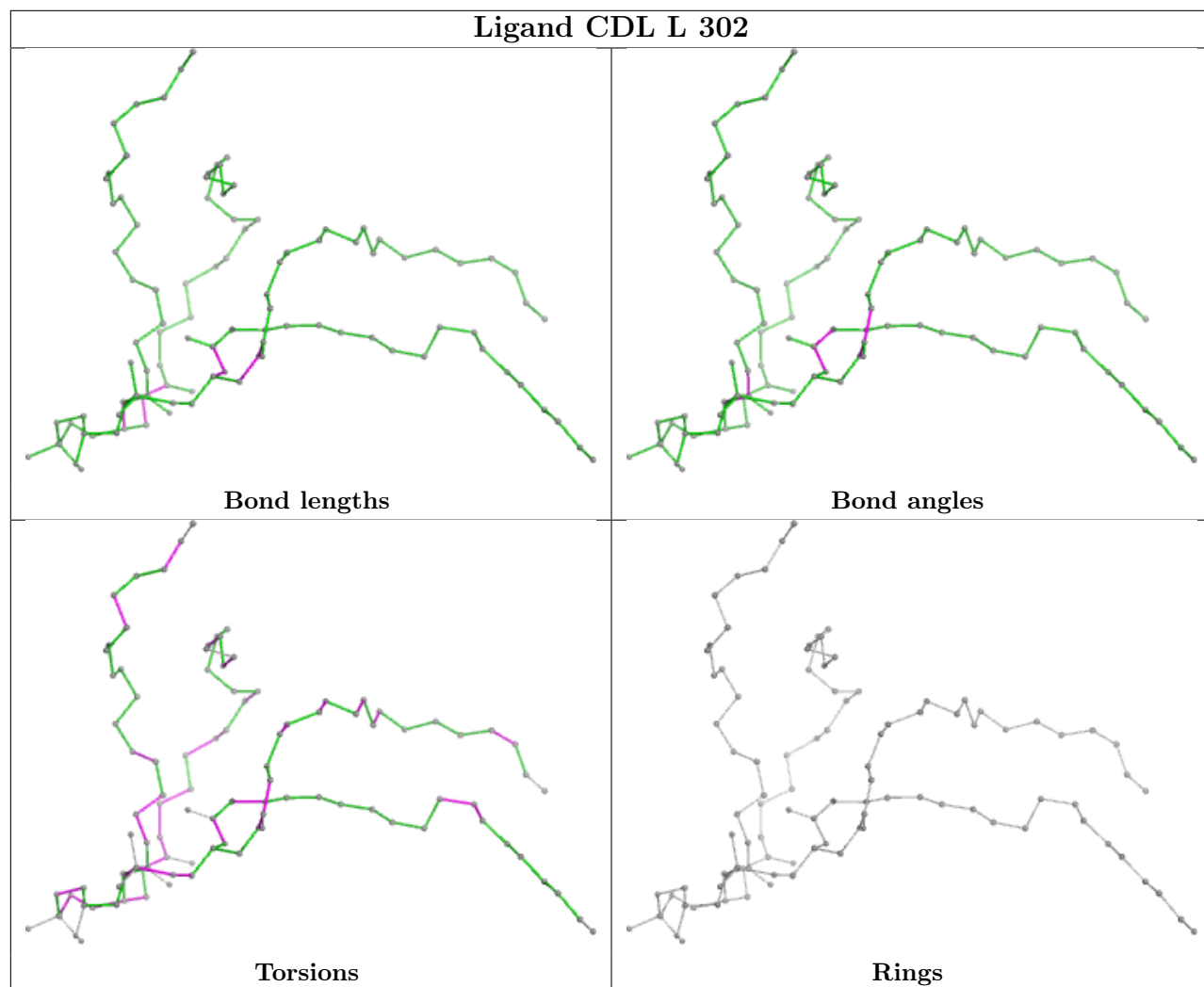


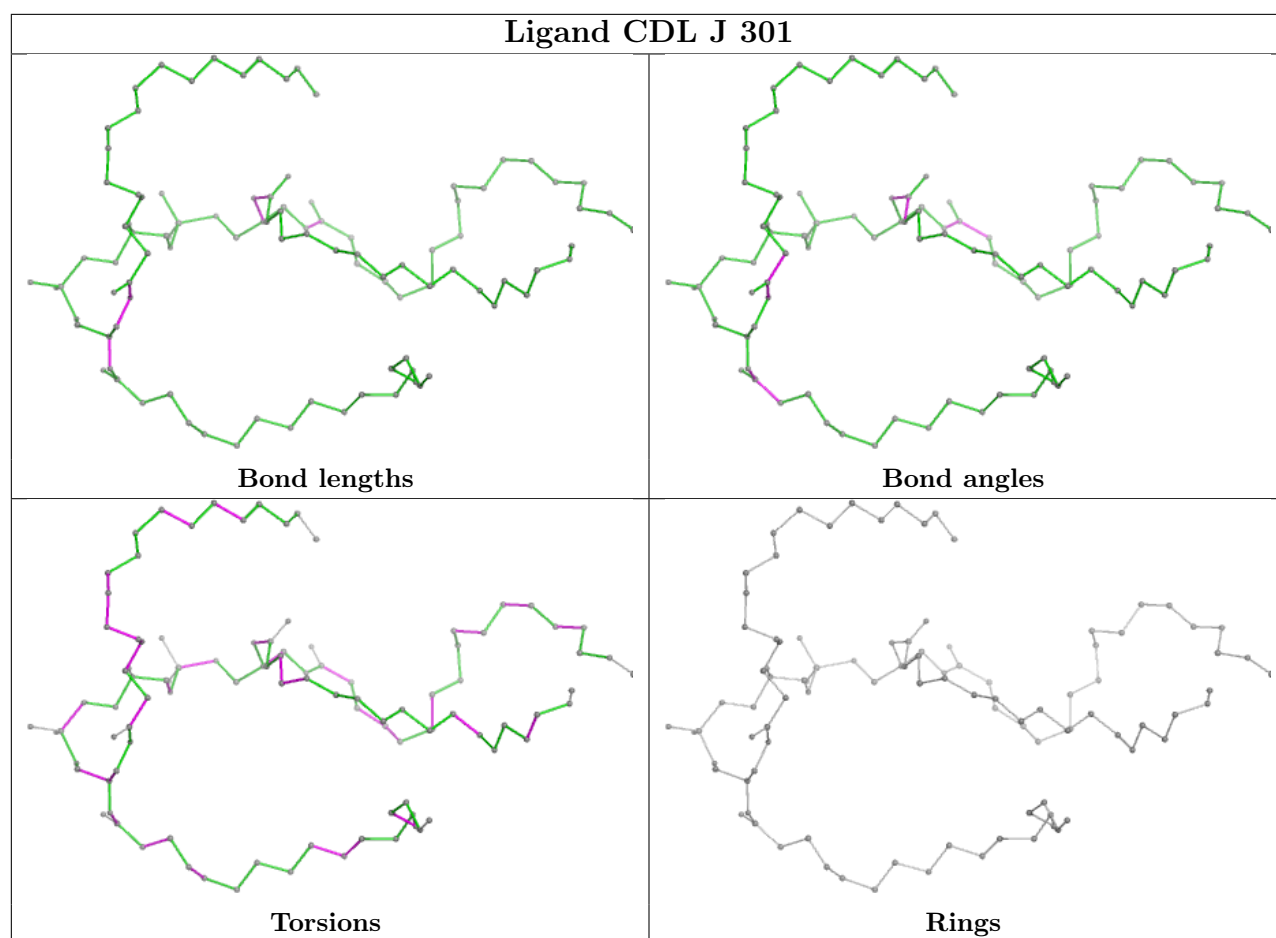


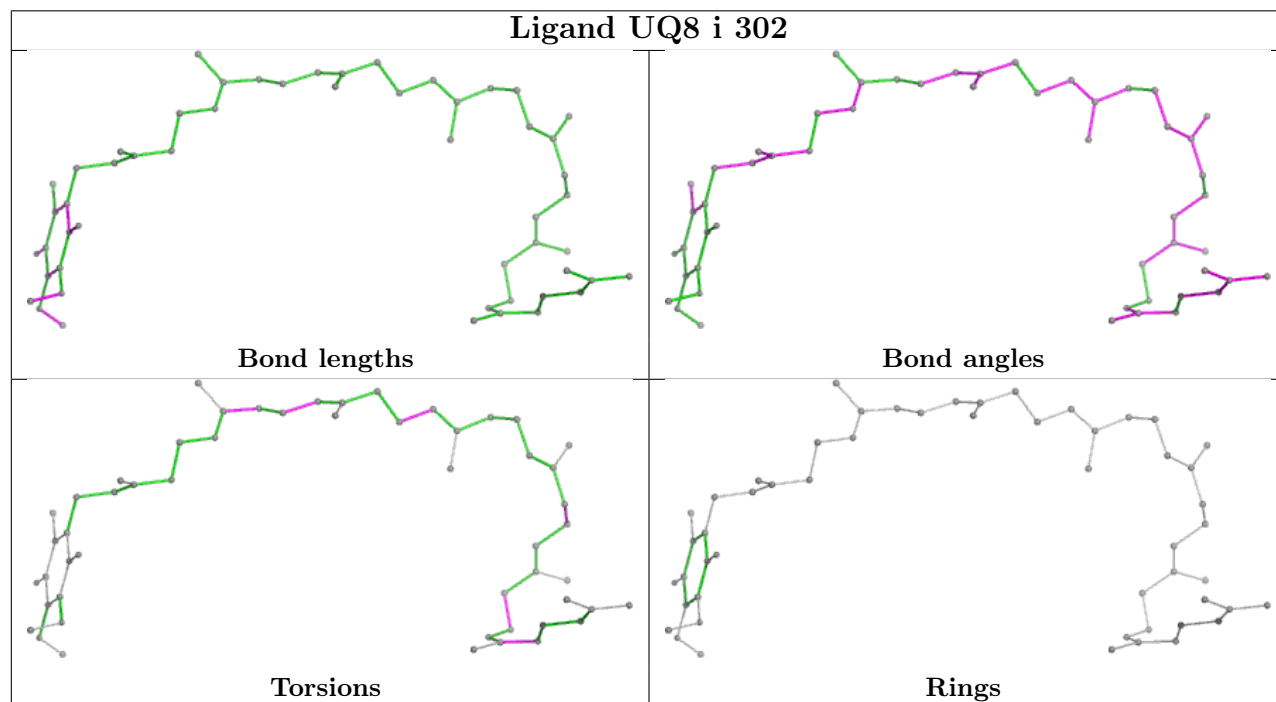
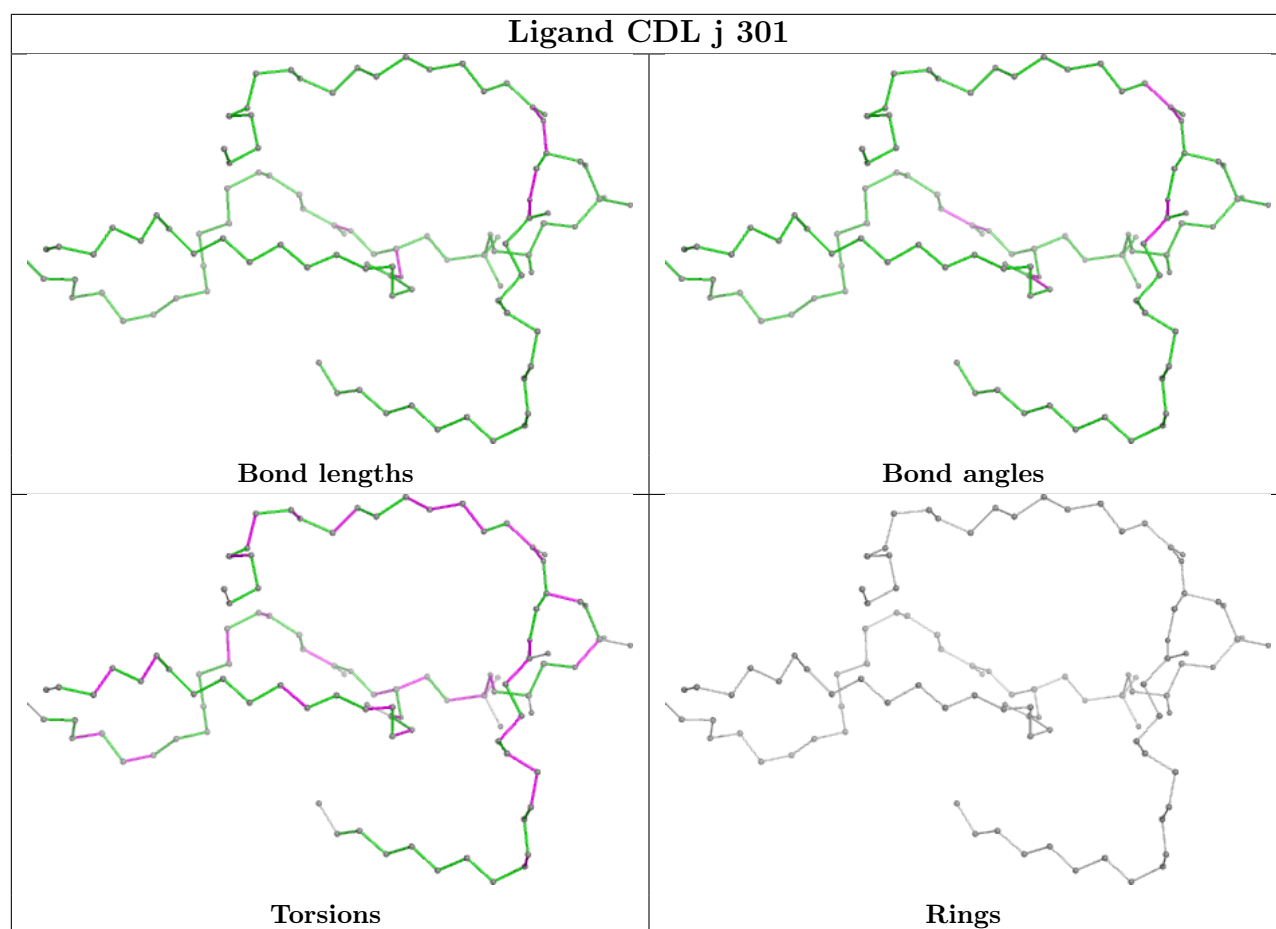
Ligand CDL f 302**Ligand CDL k 202**

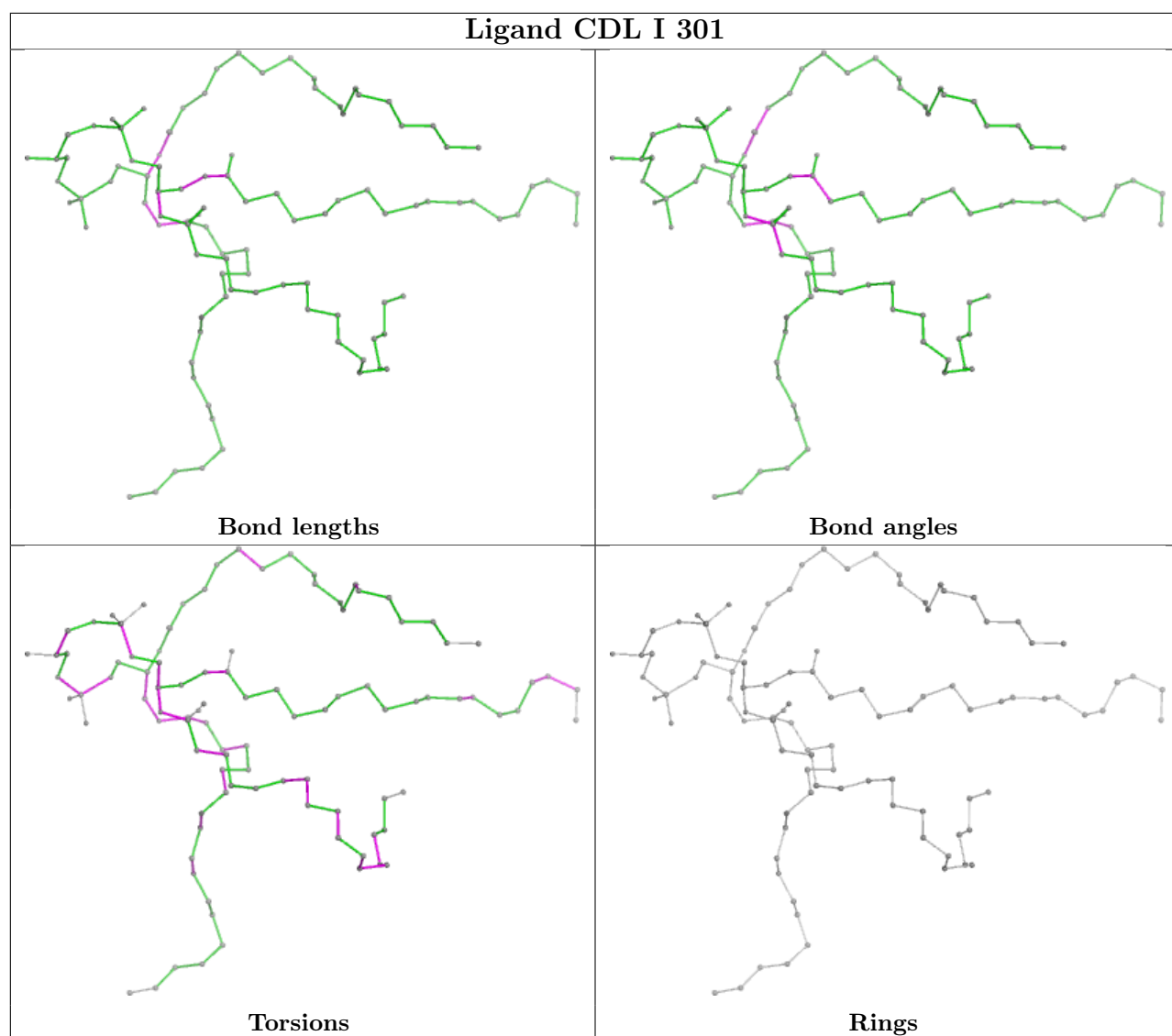


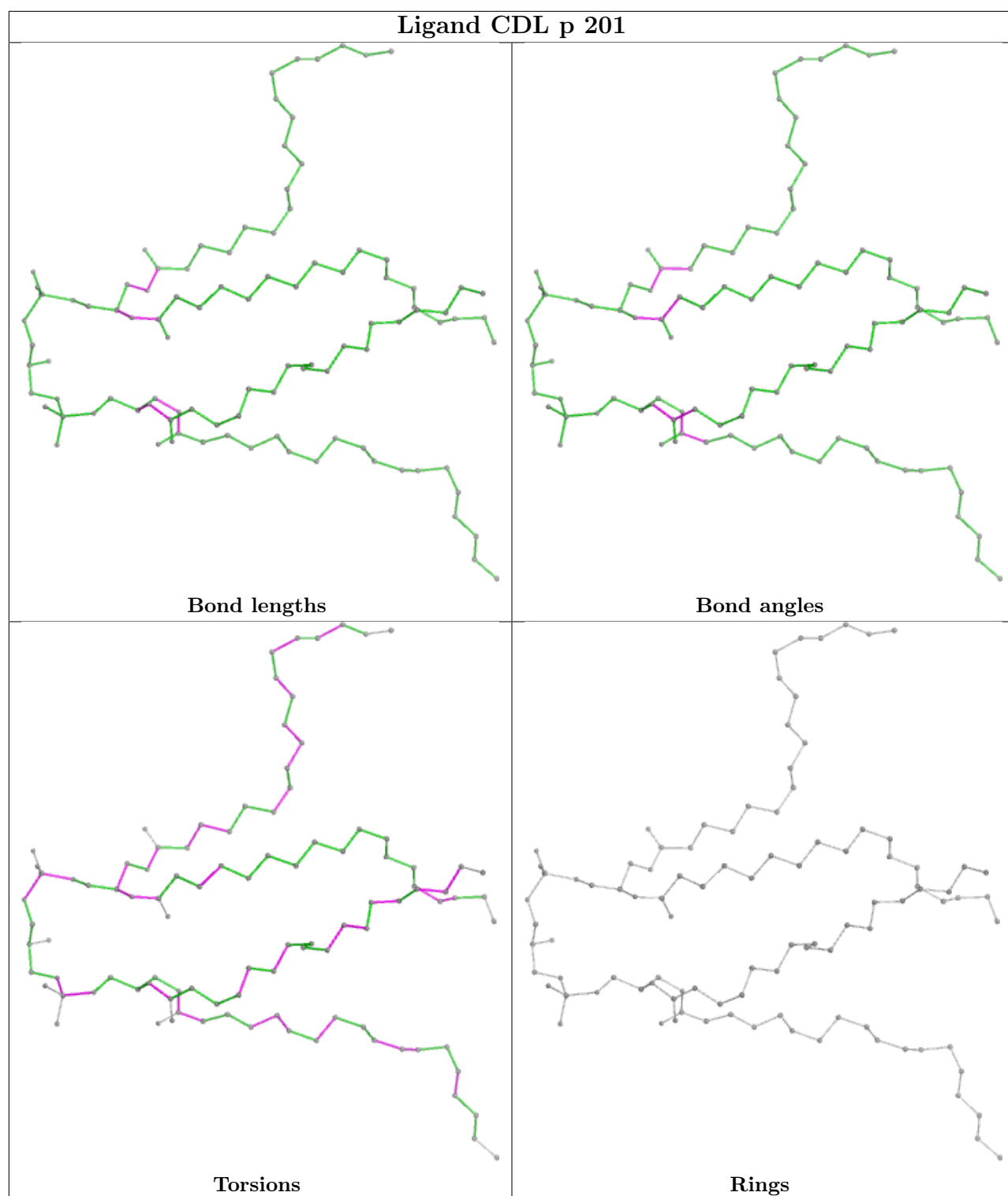
Ligand CDL I 301**Ligand CDL K 202**

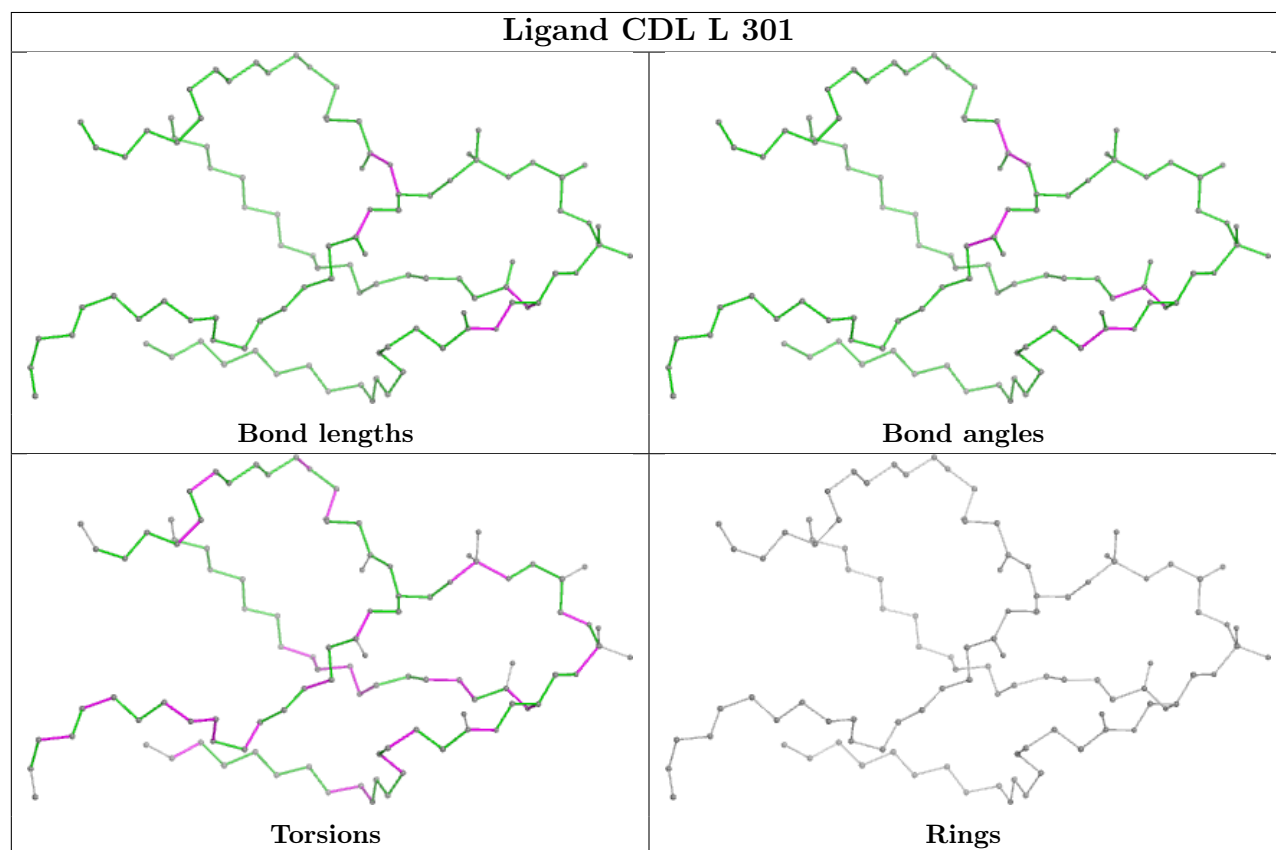
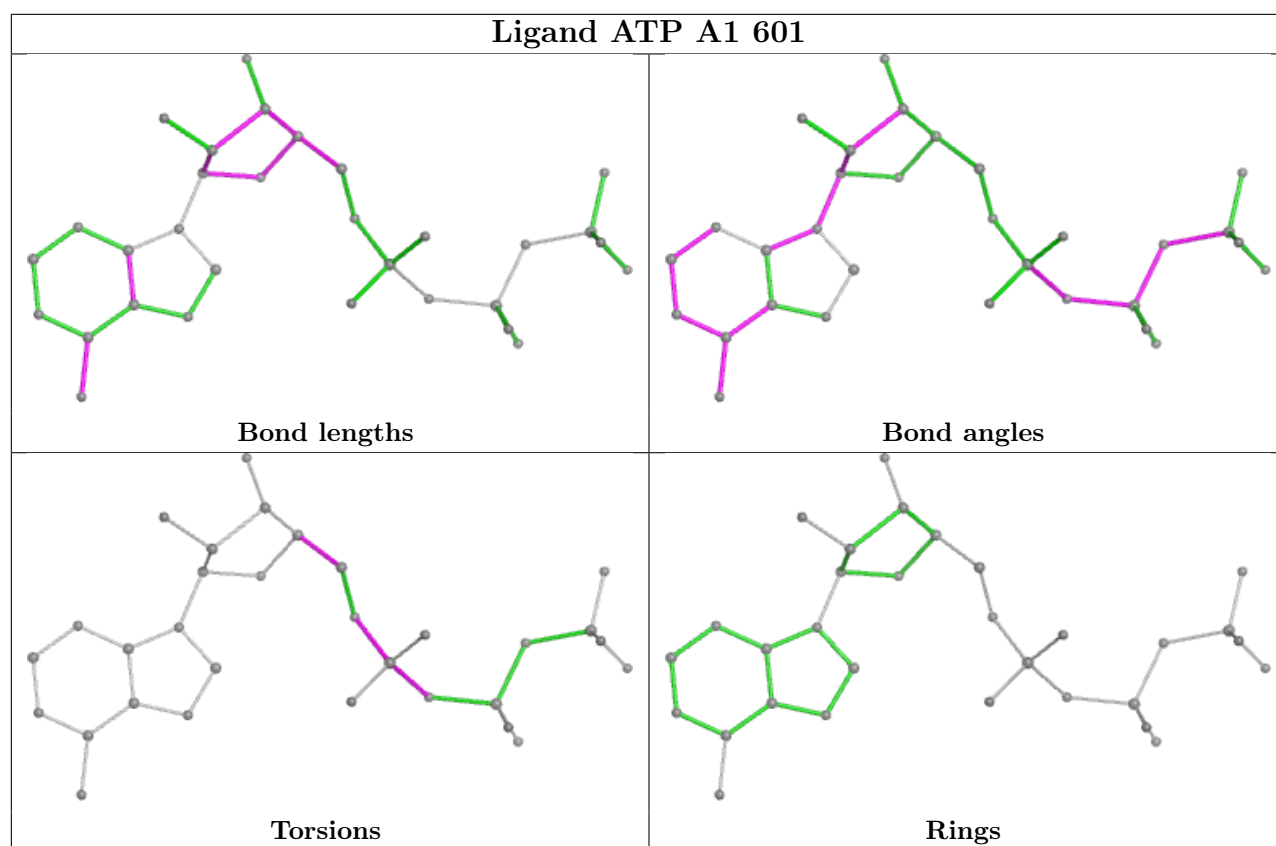
Ligand CDL L 302

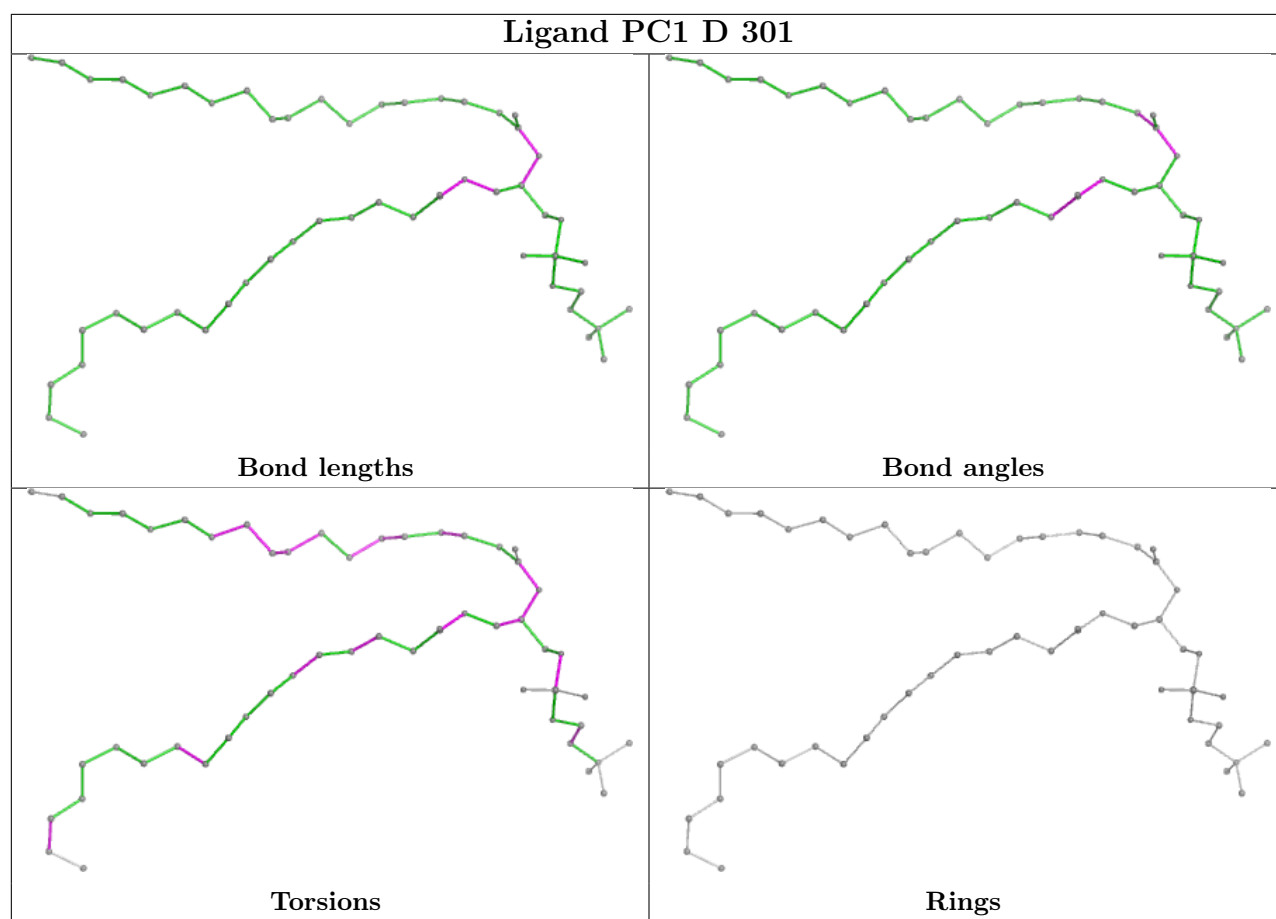


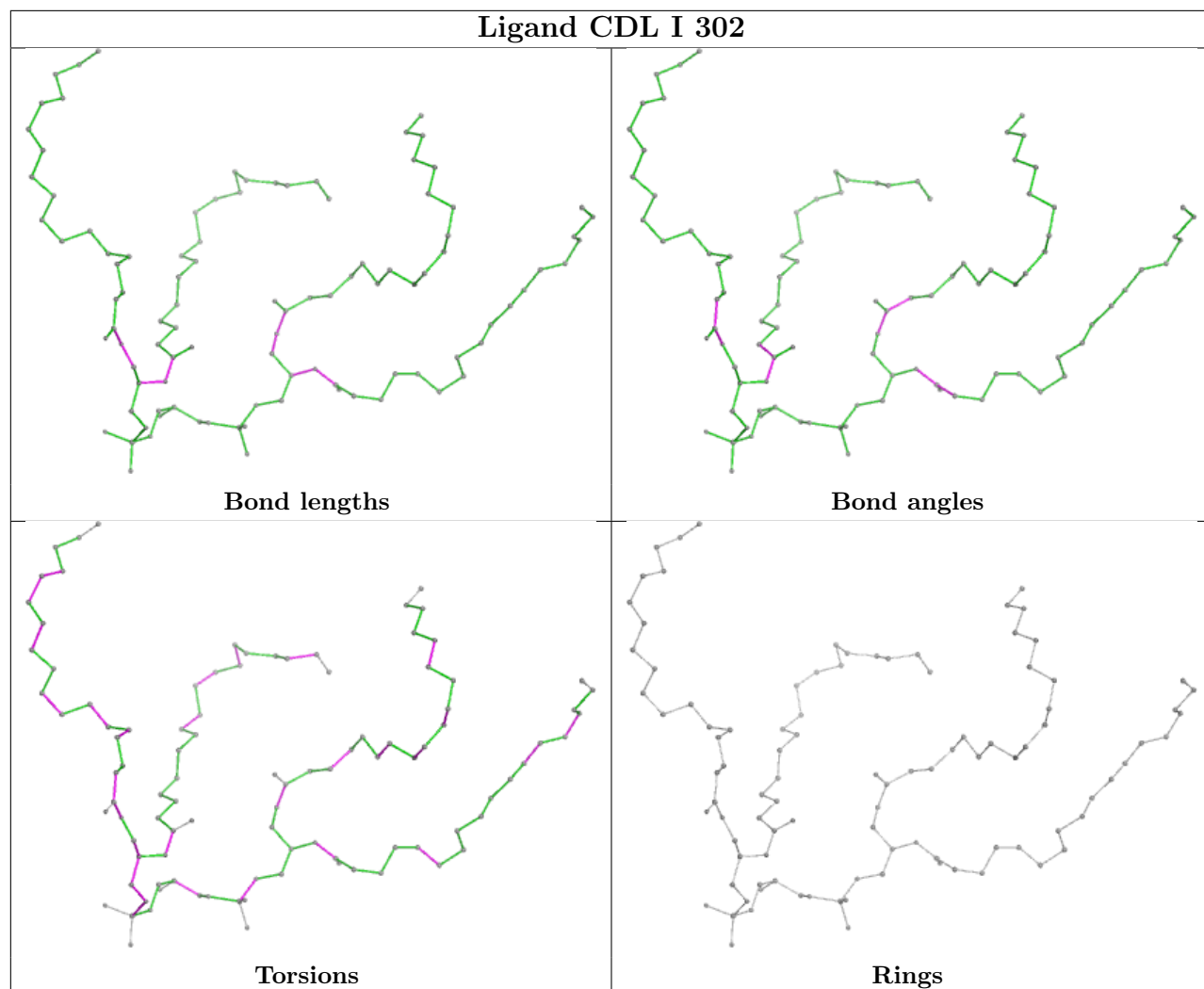


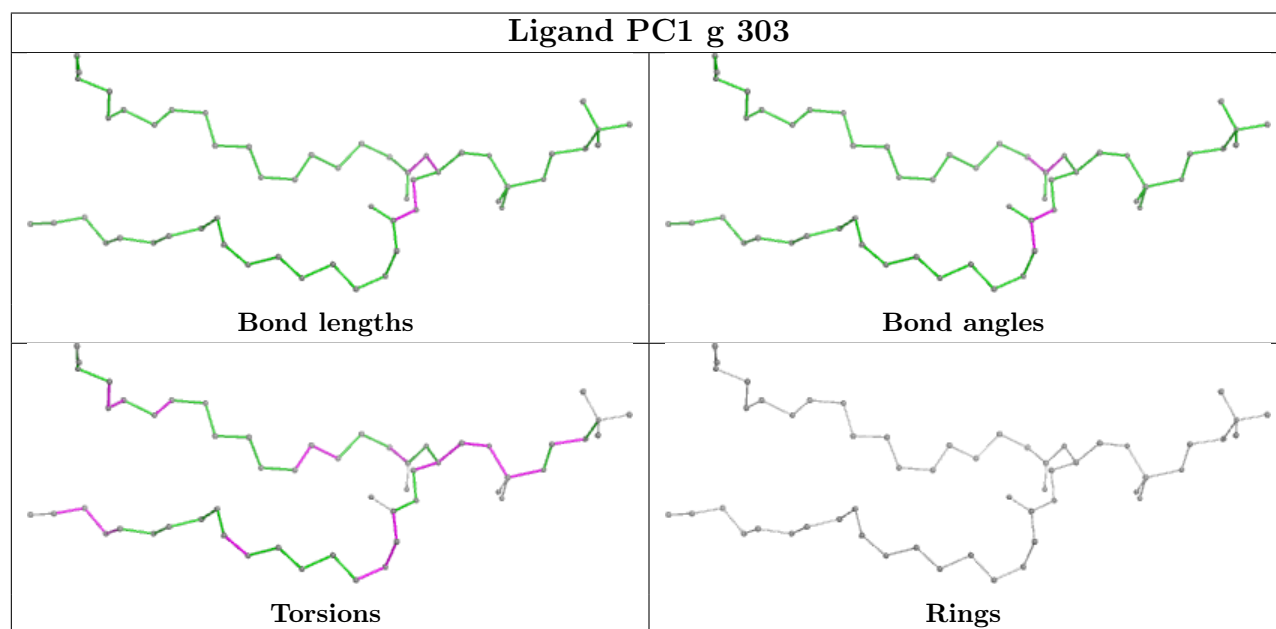
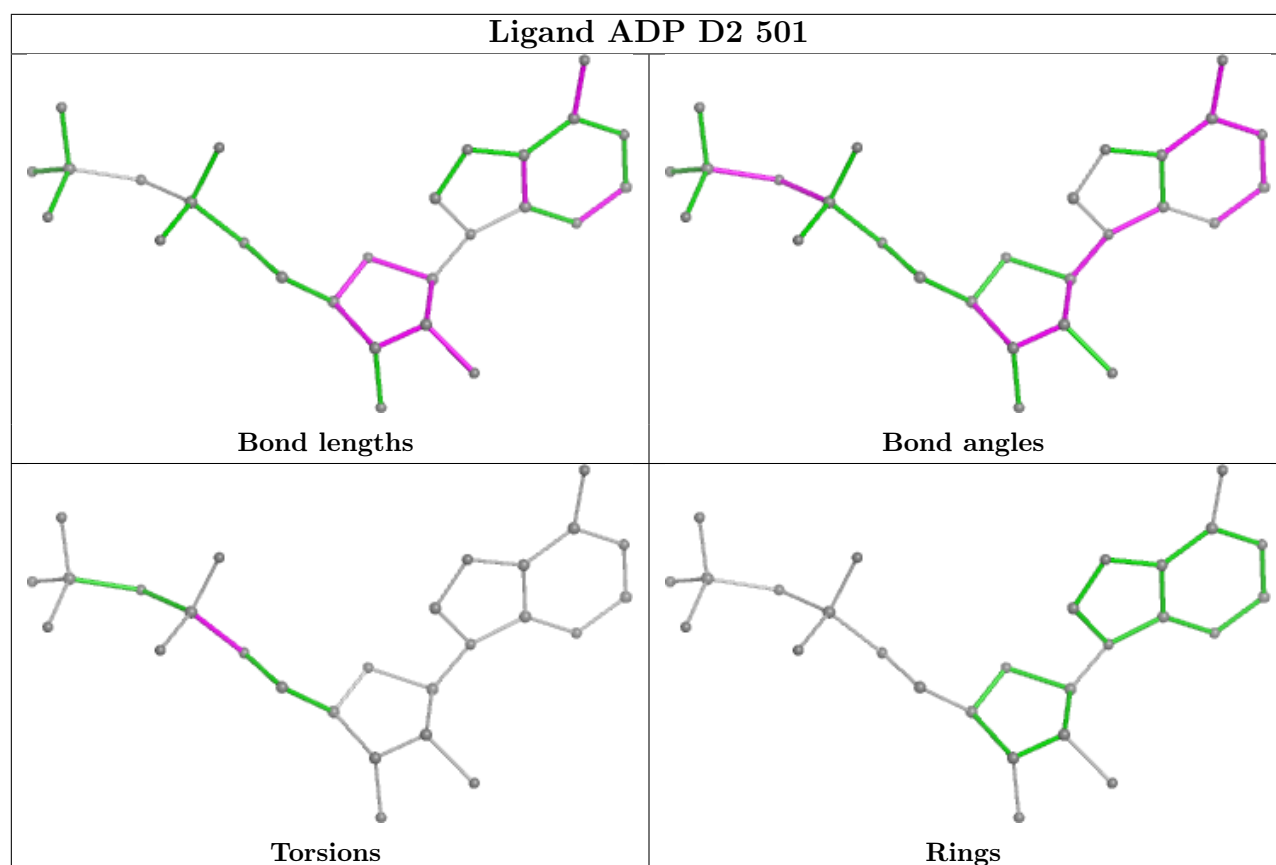


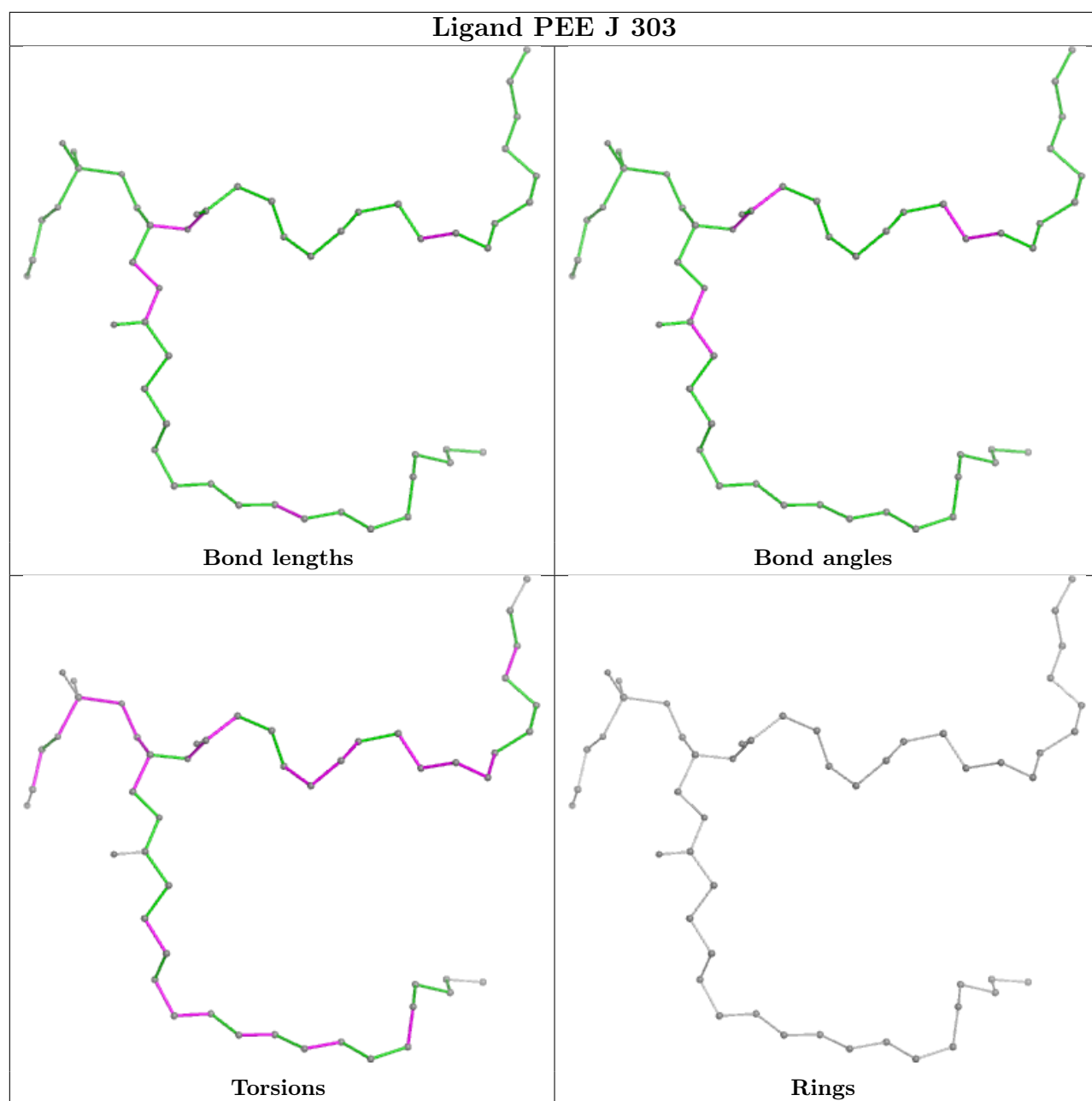


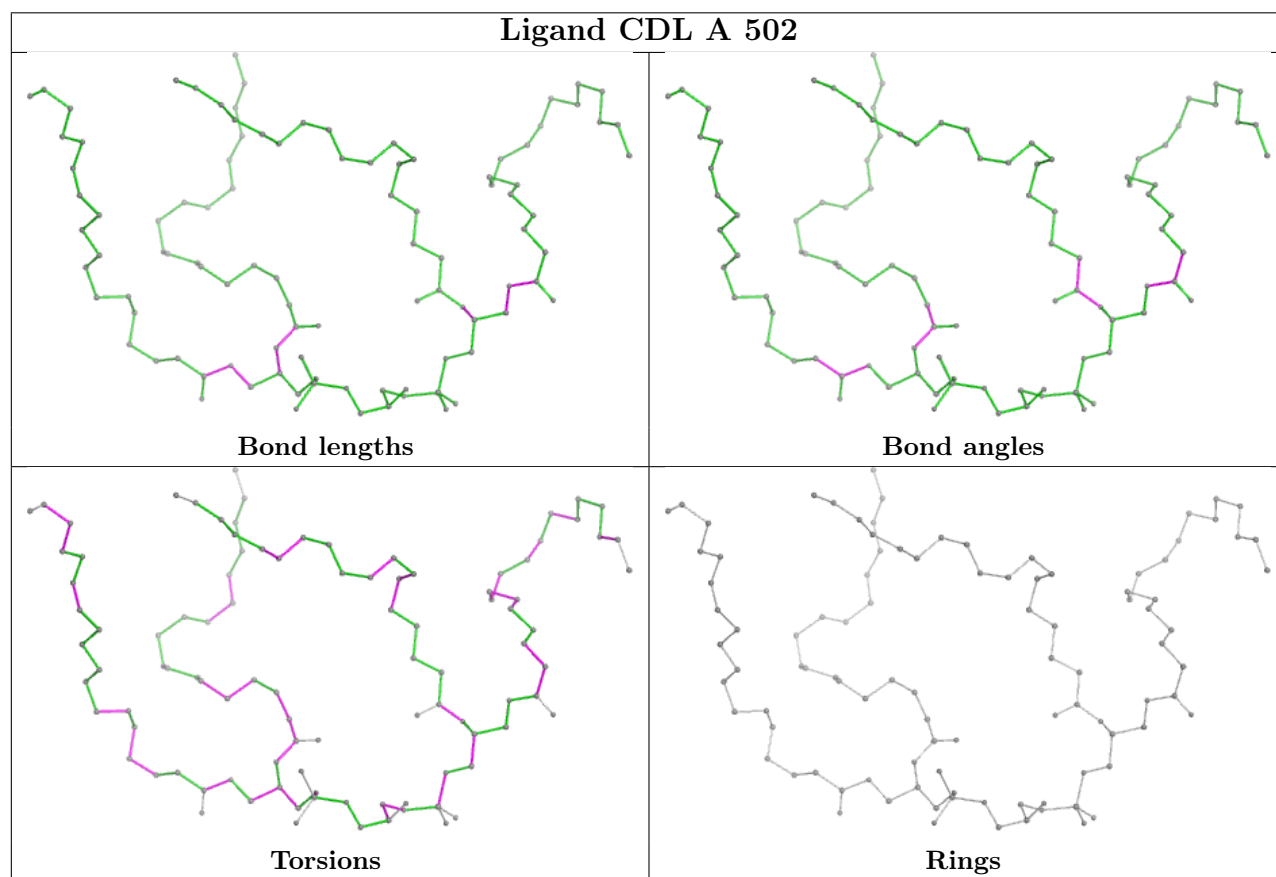
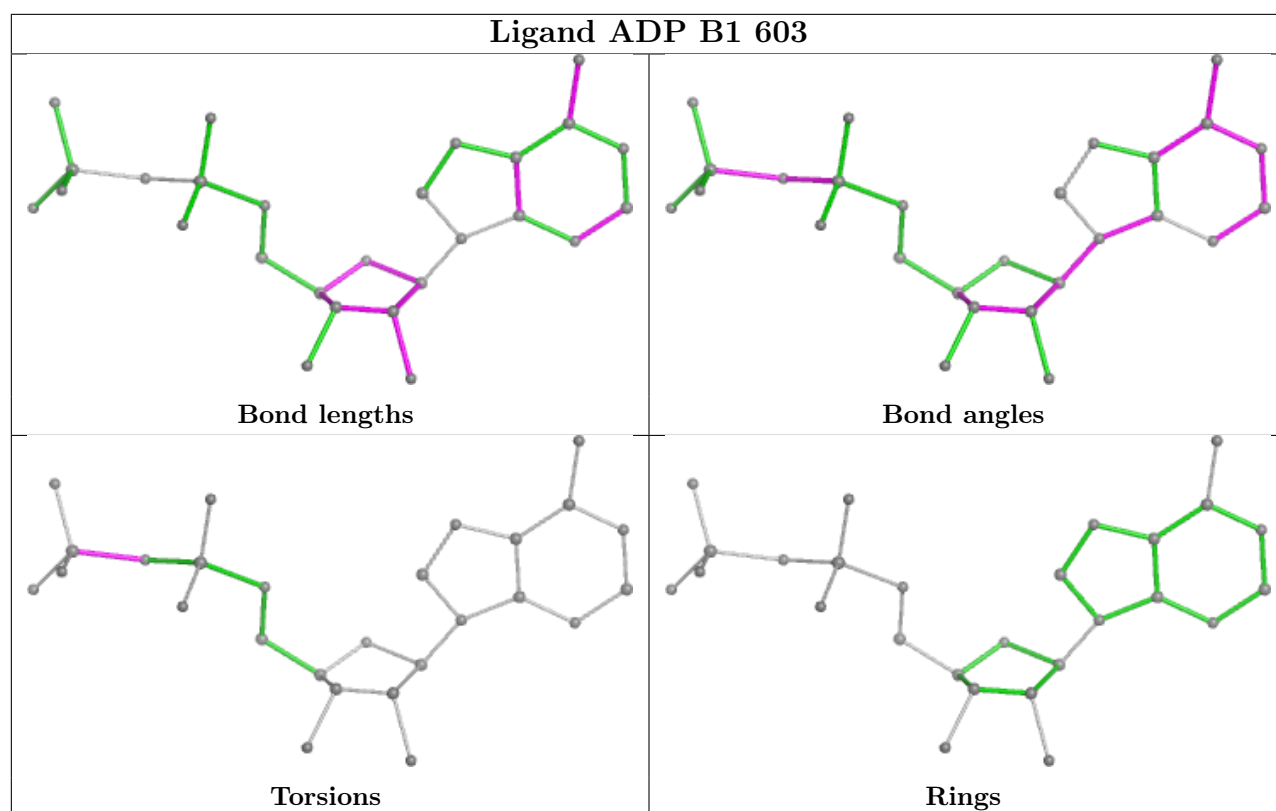


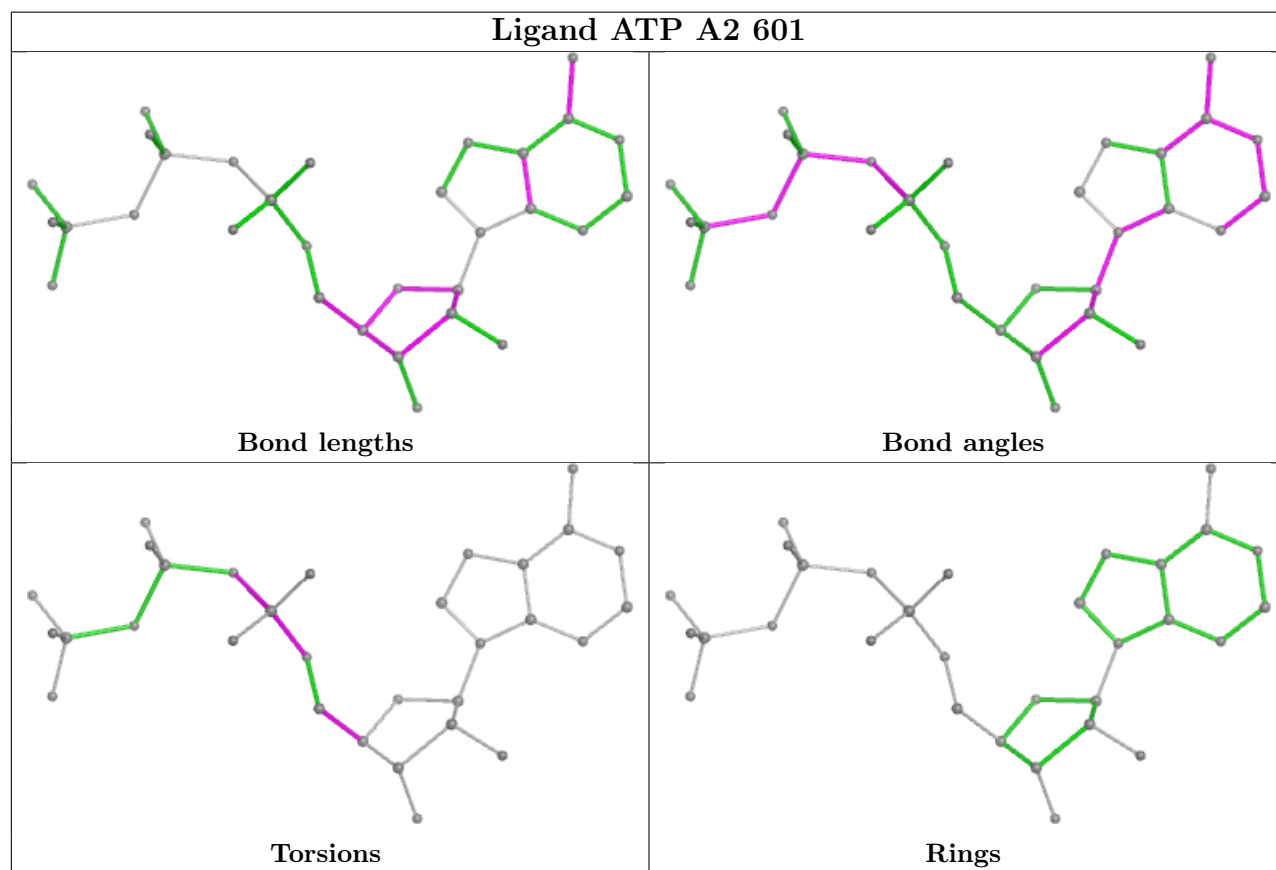
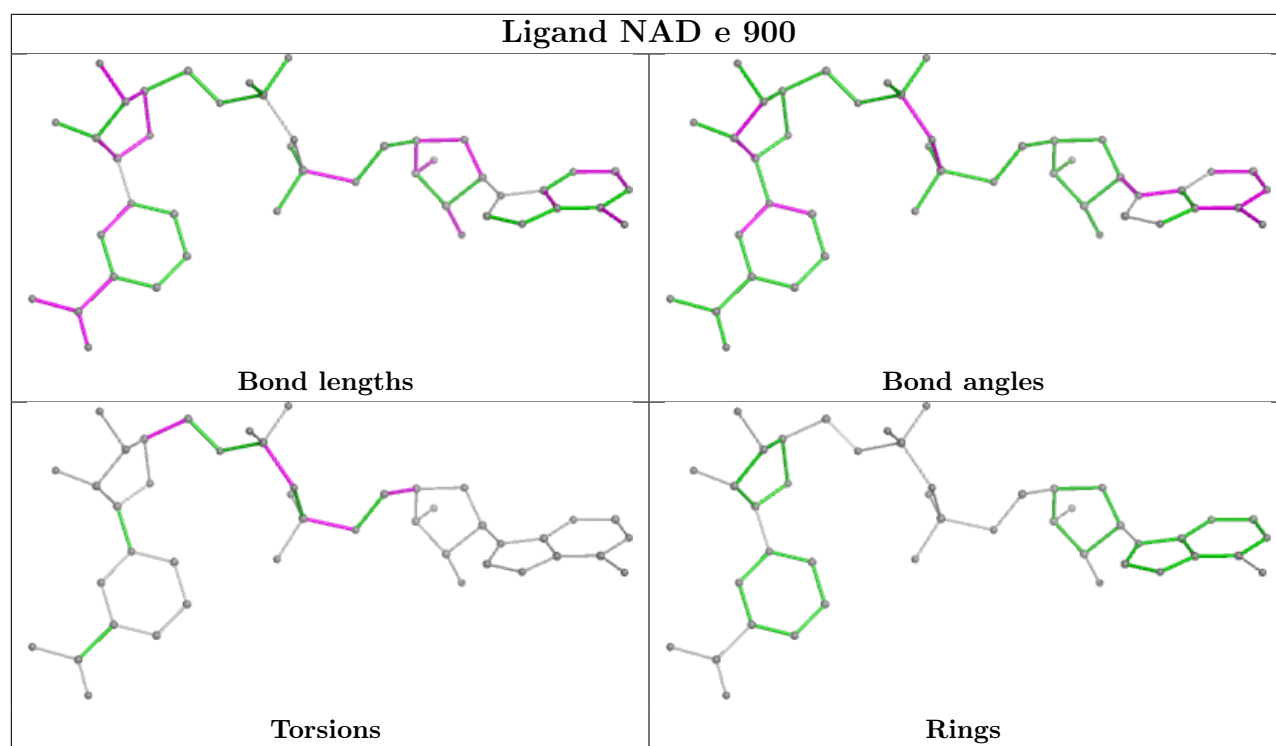


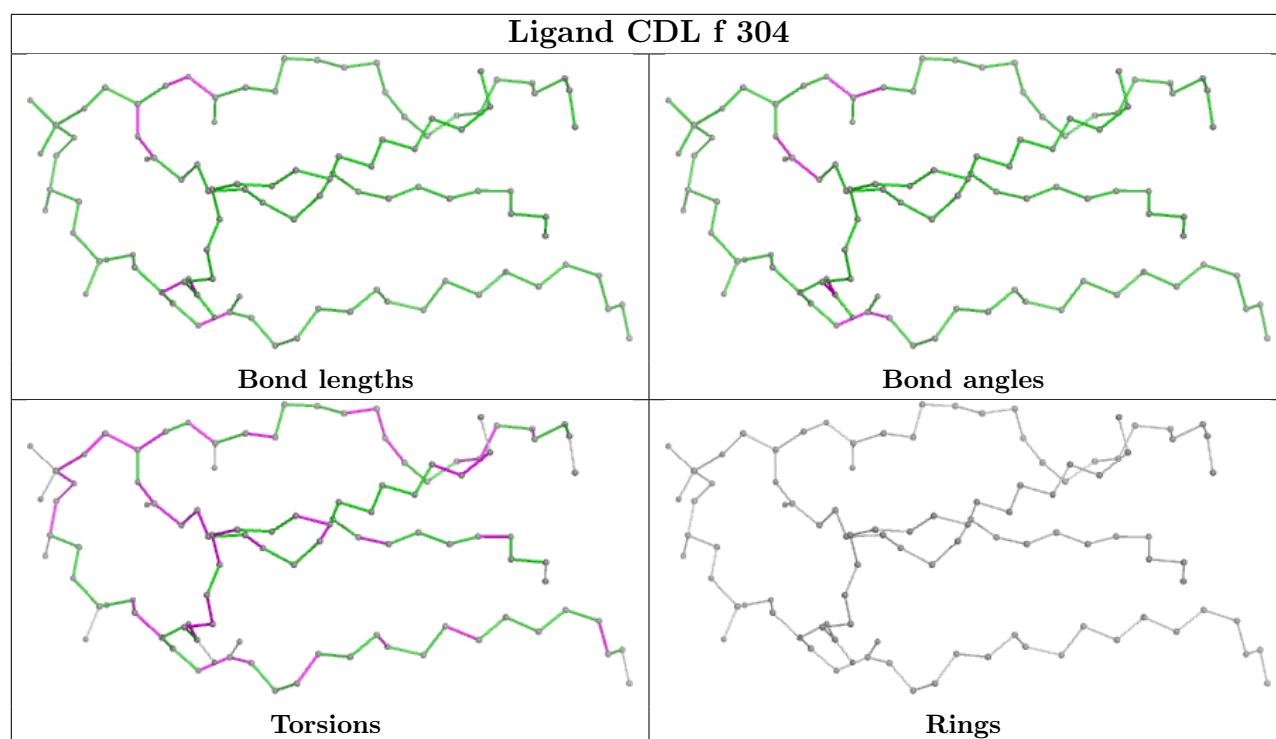


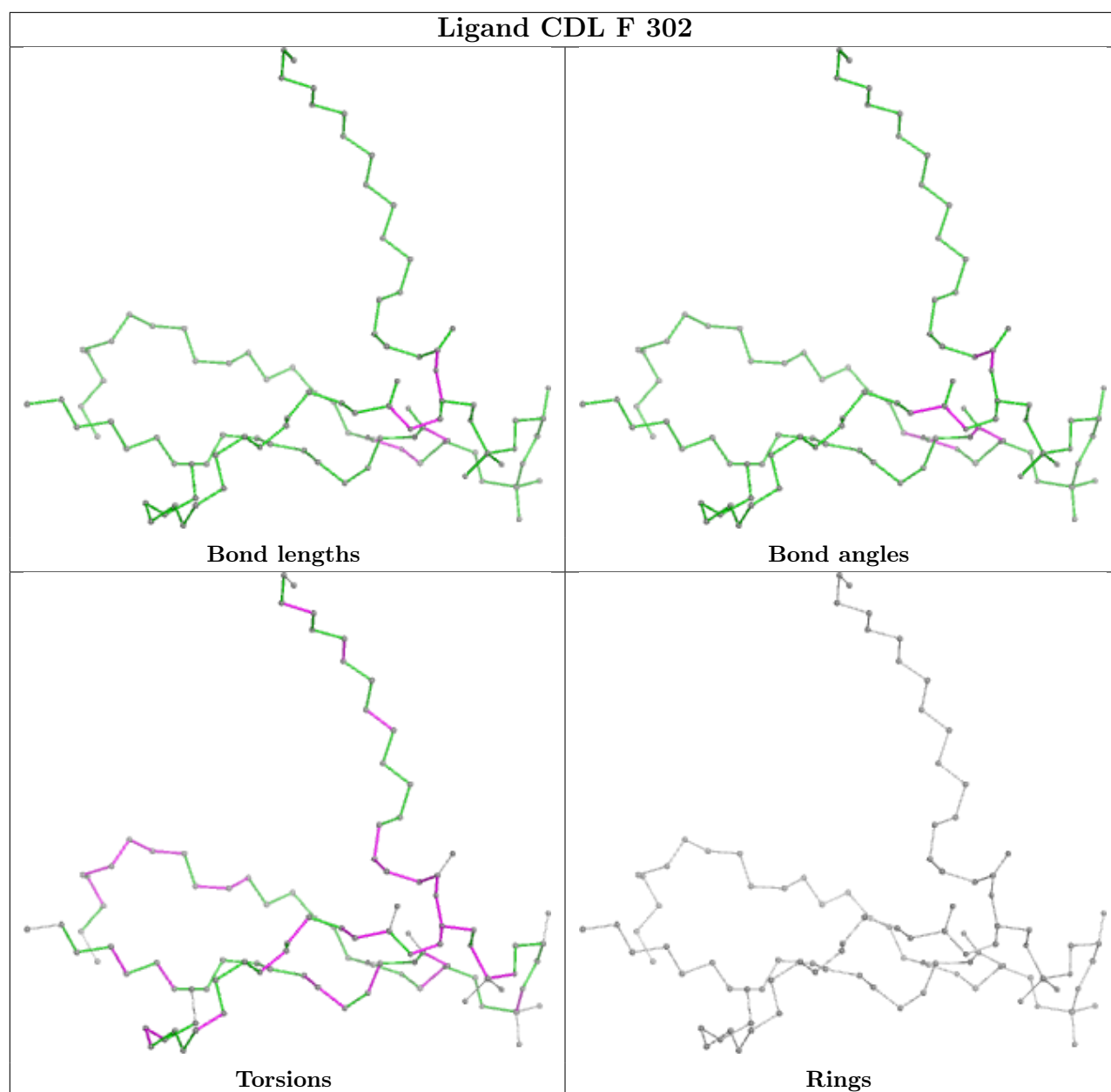












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

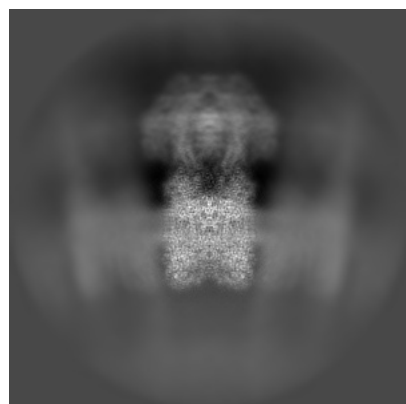
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10860. These allow visual inspection of the internal detail of the map and identification of artifacts.

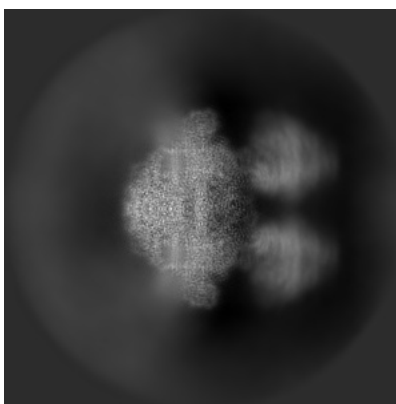
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

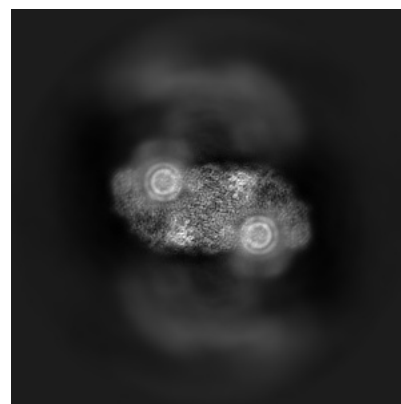
6.1.1 Primary map



X

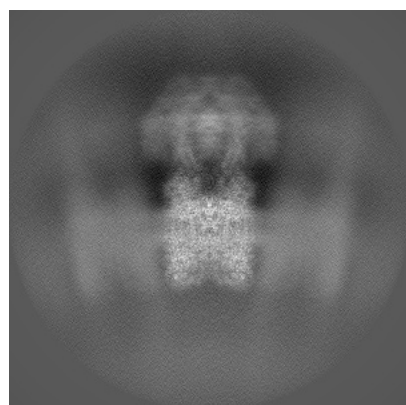


Y

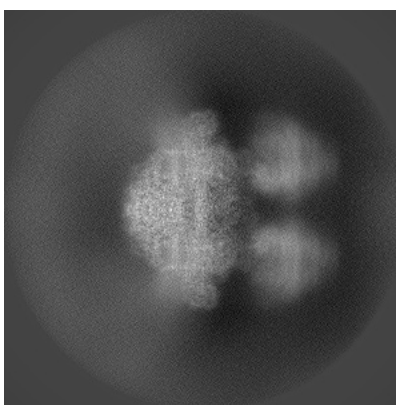


Z

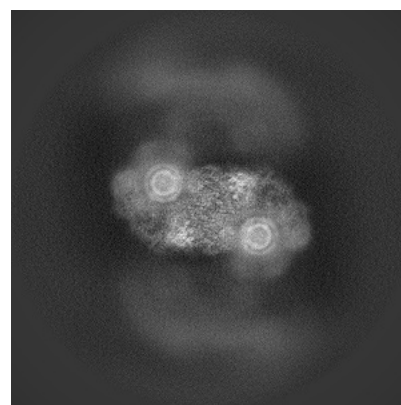
6.1.2 Raw map



X



Y

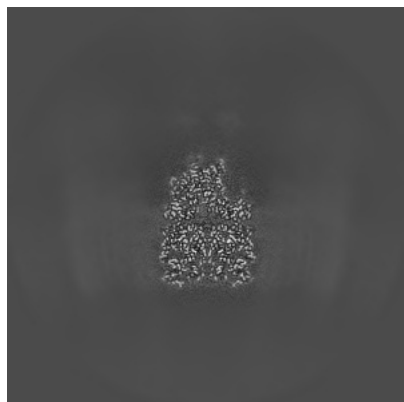


Z

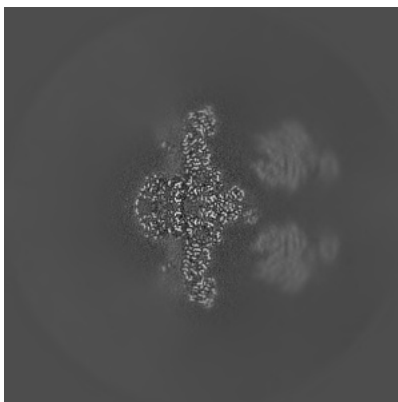
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 300

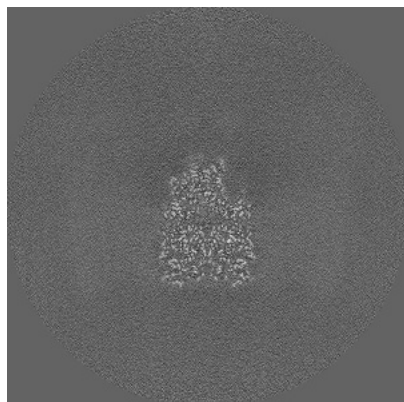


Y Index: 300

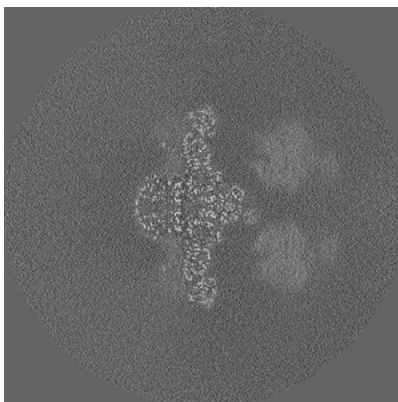


Z Index: 300

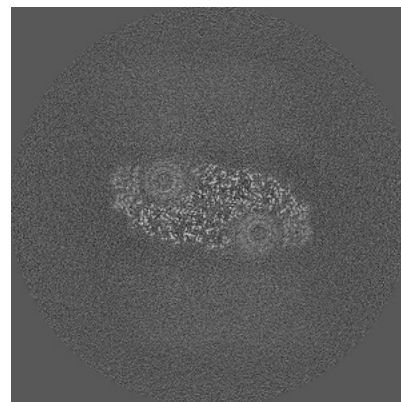
6.2.2 Raw map



X Index: 300



Y Index: 300

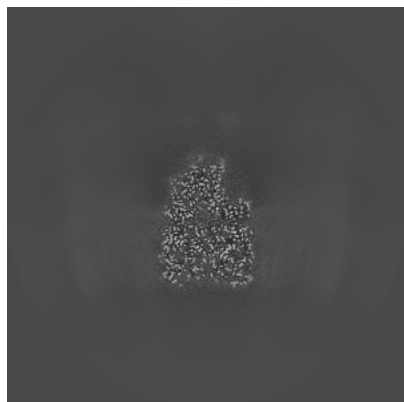


Z Index: 300

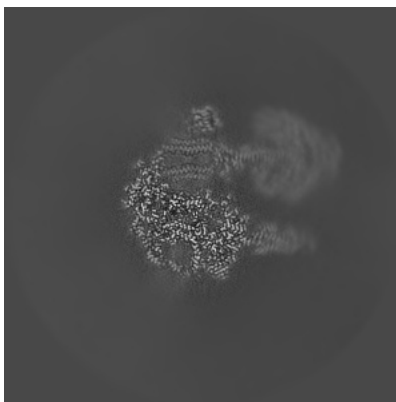
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

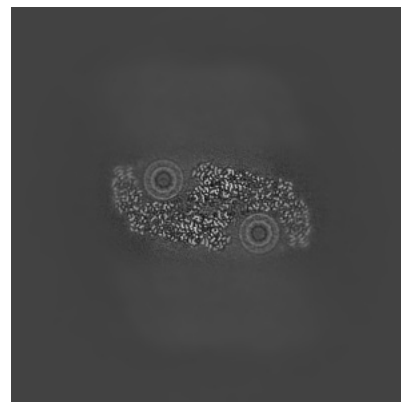
6.3.1 Primary map



X Index: 298

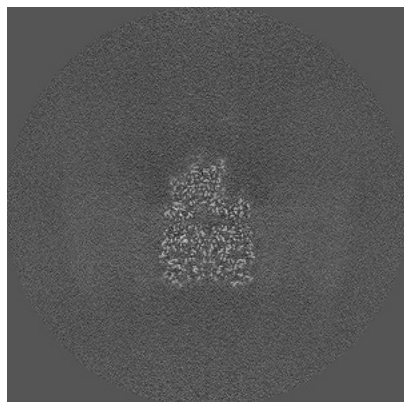


Y Index: 258

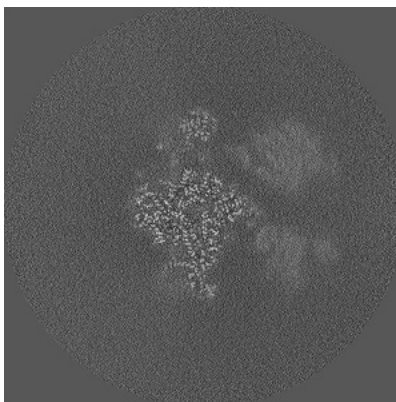


Z Index: 292

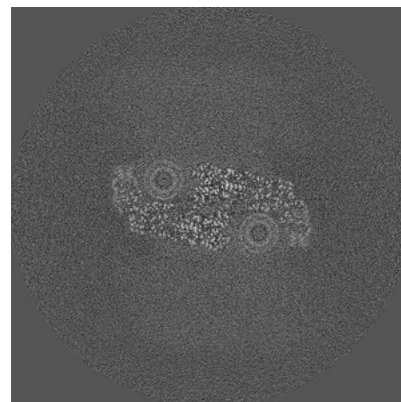
6.3.2 Raw map



X Index: 299



Y Index: 290

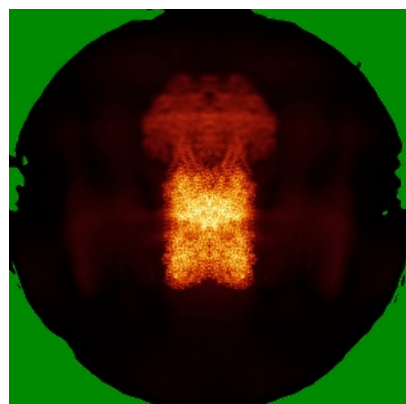


Z Index: 292

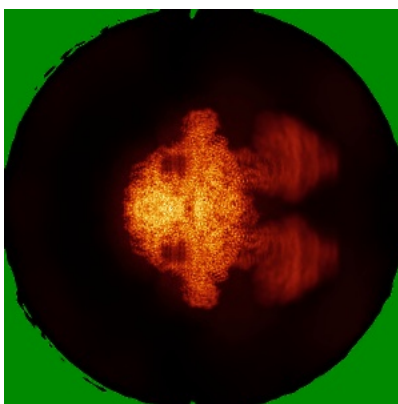
The images above show the largest variance slices of the map in three orthogonal directions.

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

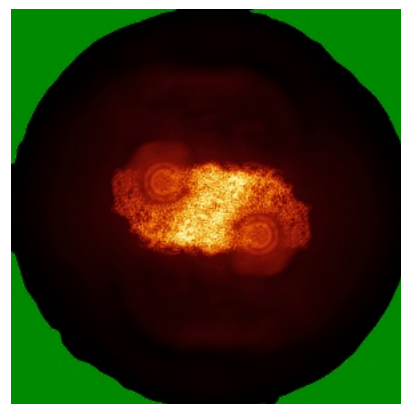
6.4.1 Primary map



X

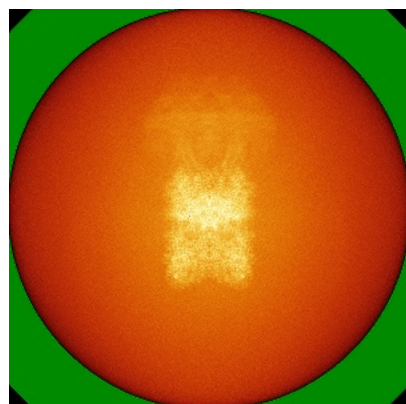


Y

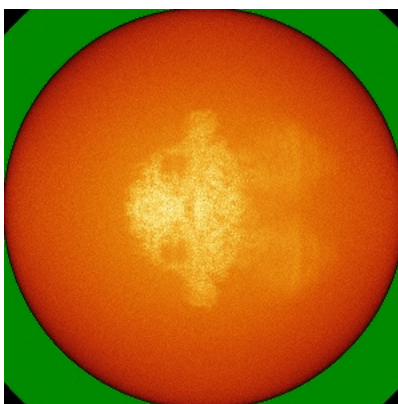


Z

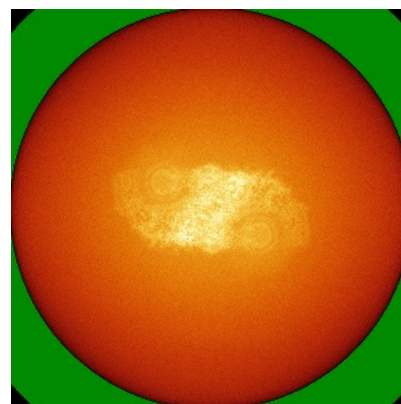
6.4.2 Raw map



X



Y

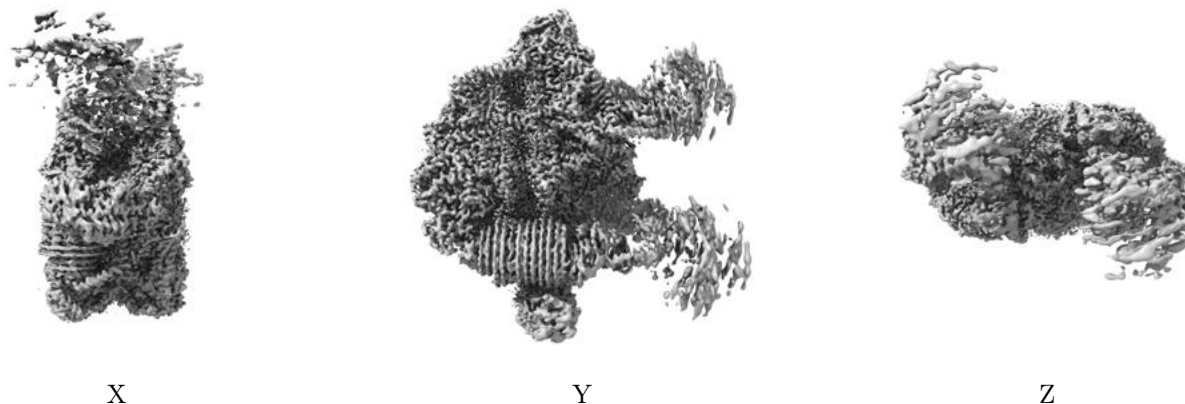


Z

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

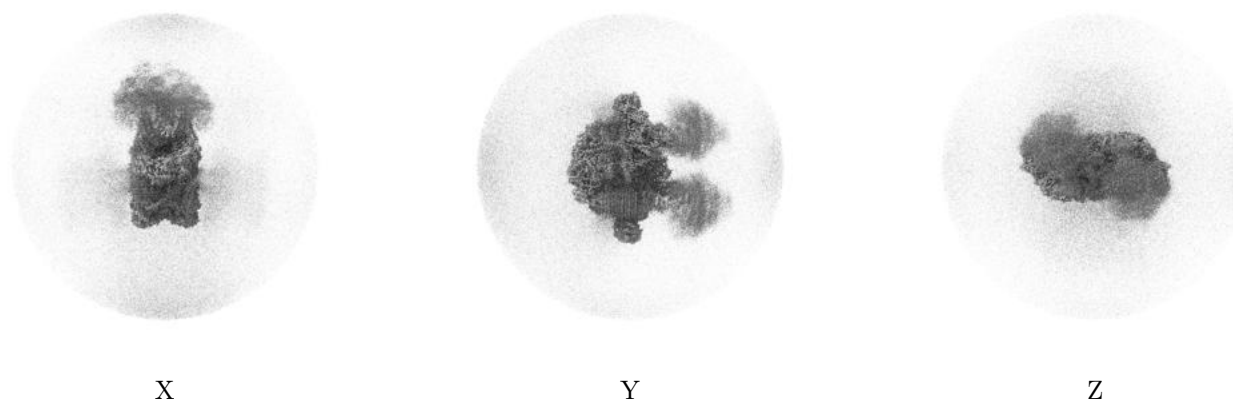
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

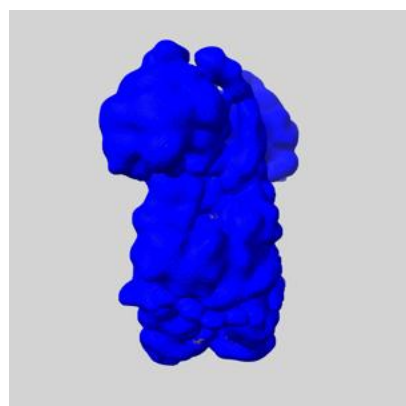
6.6 Mask visualisation [i](#)

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

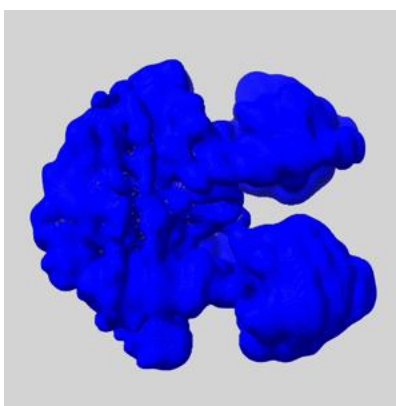
A mask typically either:

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

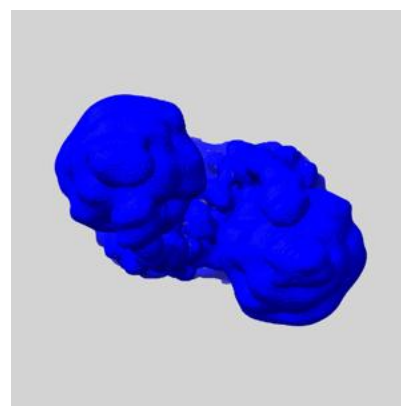
6.6.1 emd_10860_msk_1.map [i](#)



X



Y

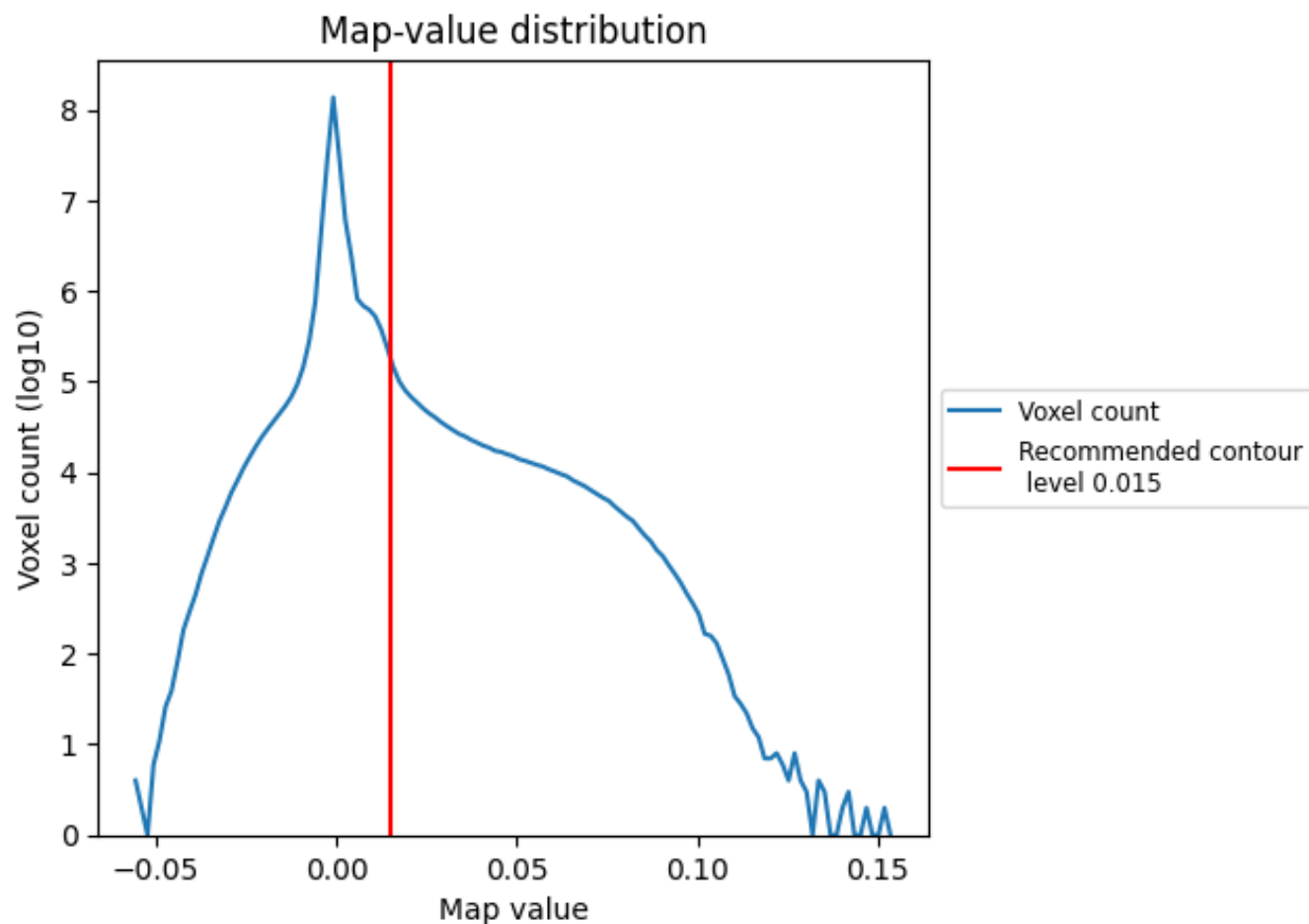


Z

7 Map analysis [i](#)

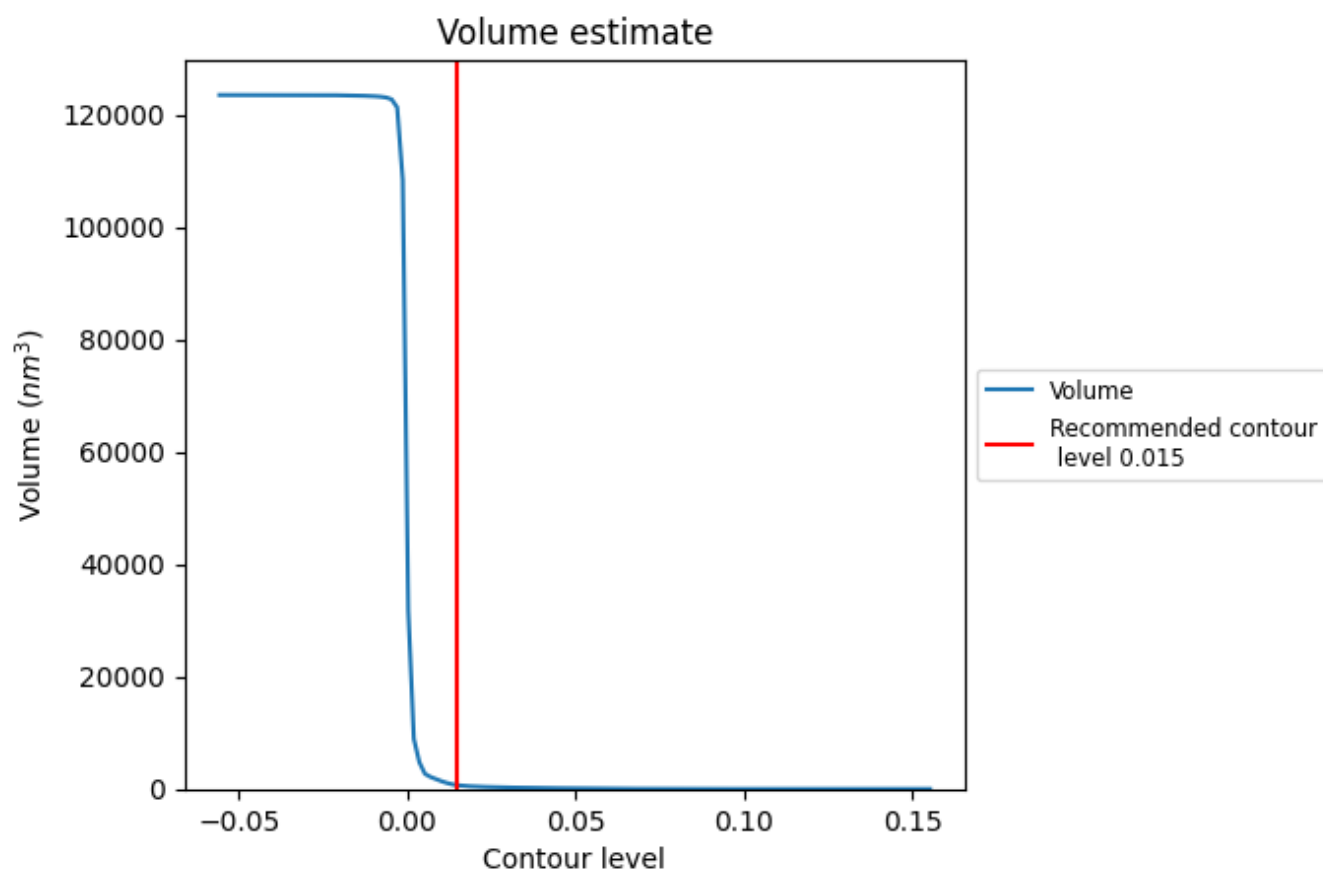
This section contains the results of statistical analysis of the map.

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.

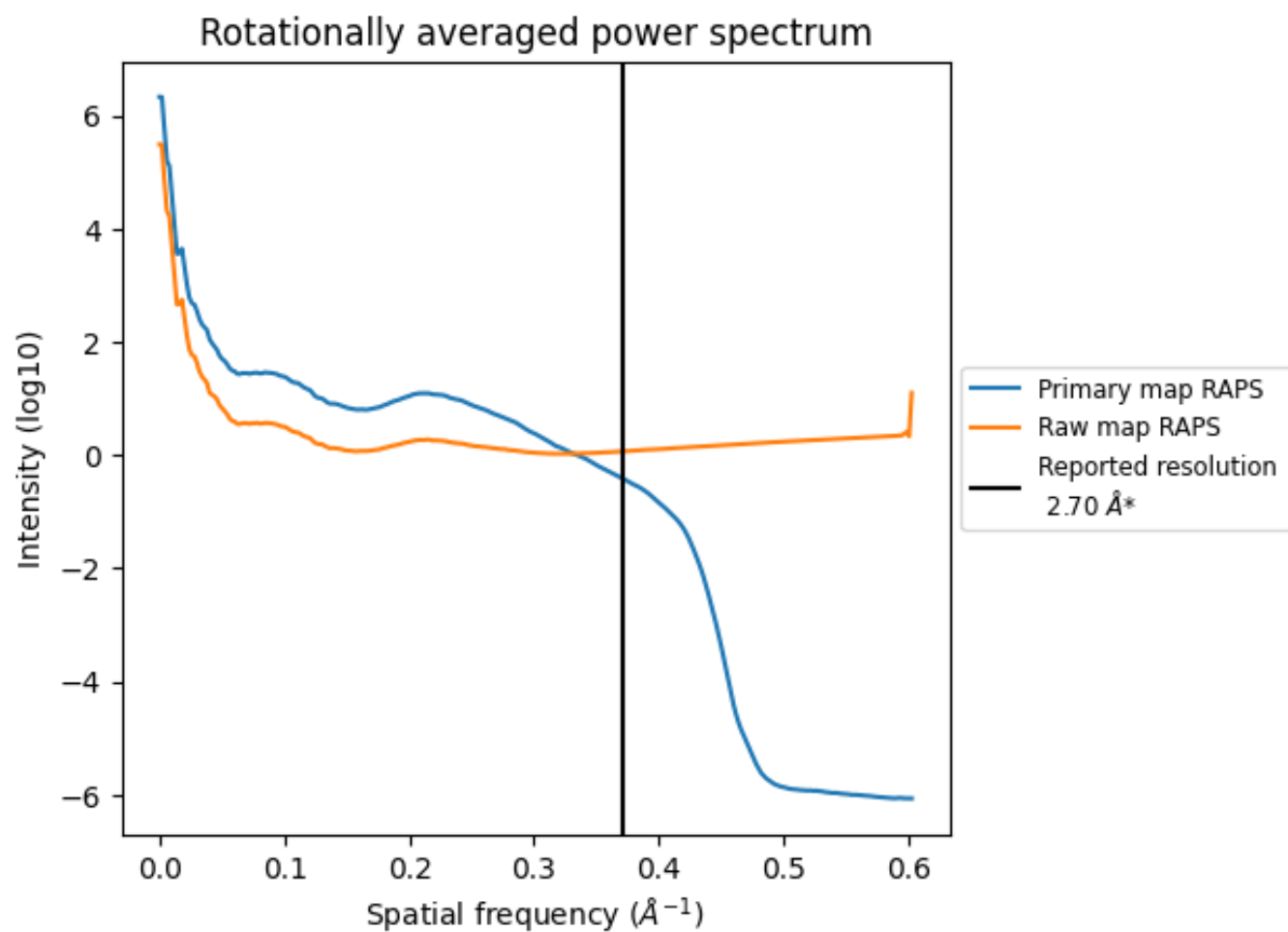
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 665 nm^3 ; this corresponds to an approximate mass of 600 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

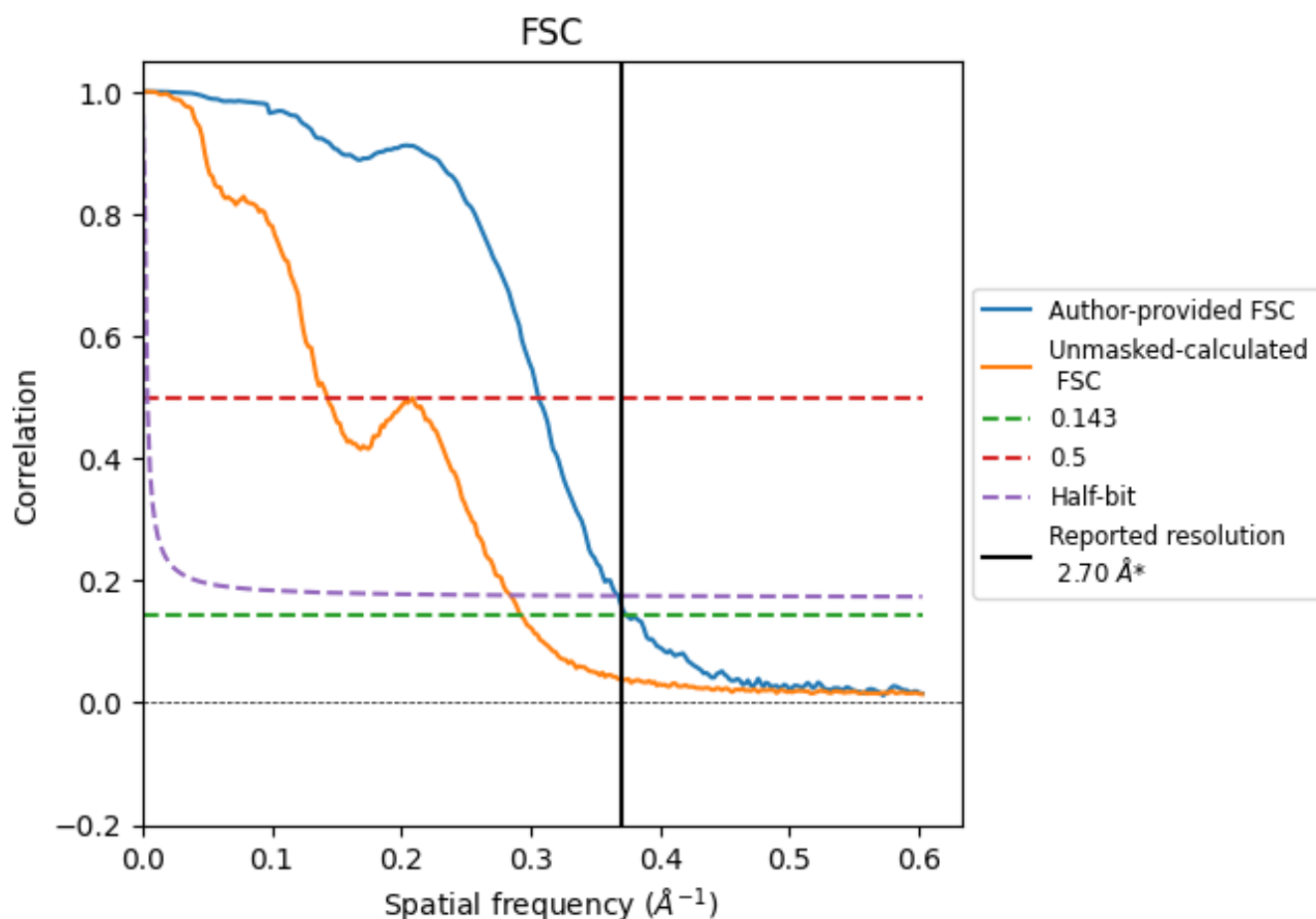


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 \AA^{-1}

8.2 Resolution estimates [i](#)

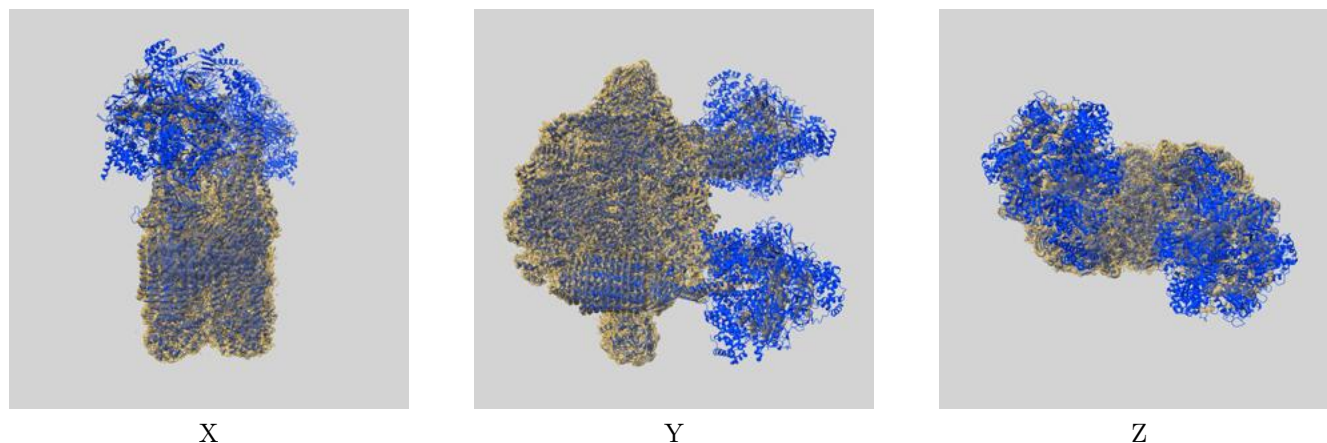
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.67	3.27	2.72
Unmasked-calculated*	3.42	7.00	3.52

*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 2.7 by more than 10 %

9 Map-model fit [i](#)

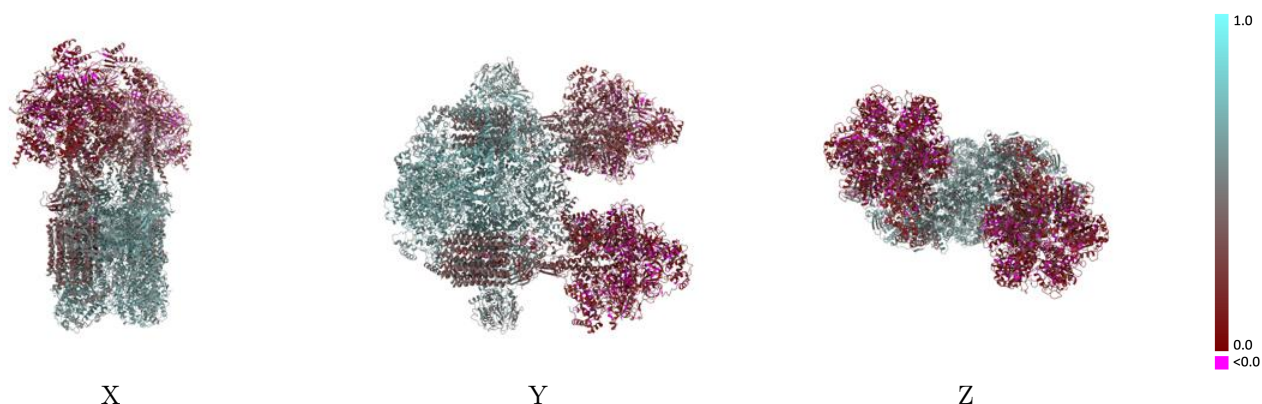
This section contains information regarding the fit between EMDB map EMD-10860 and PDB model 6YNY. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



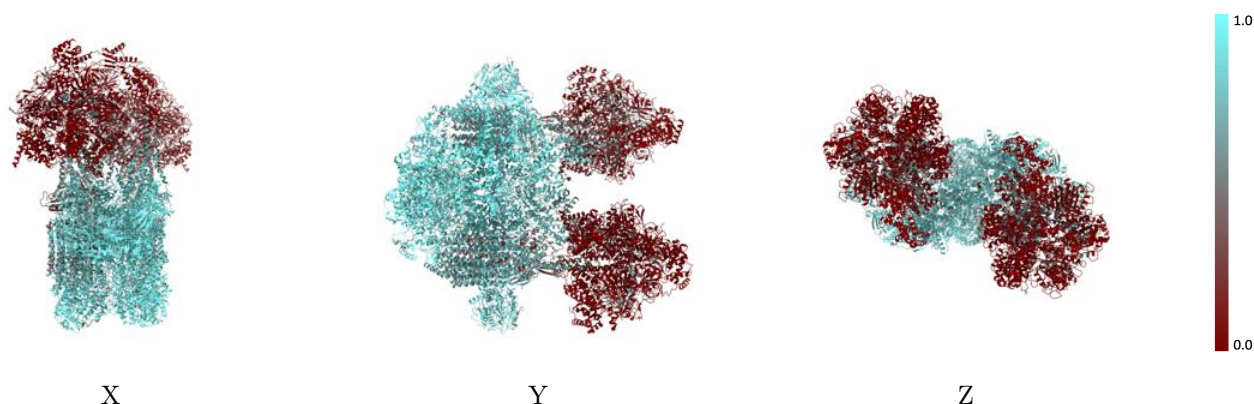
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



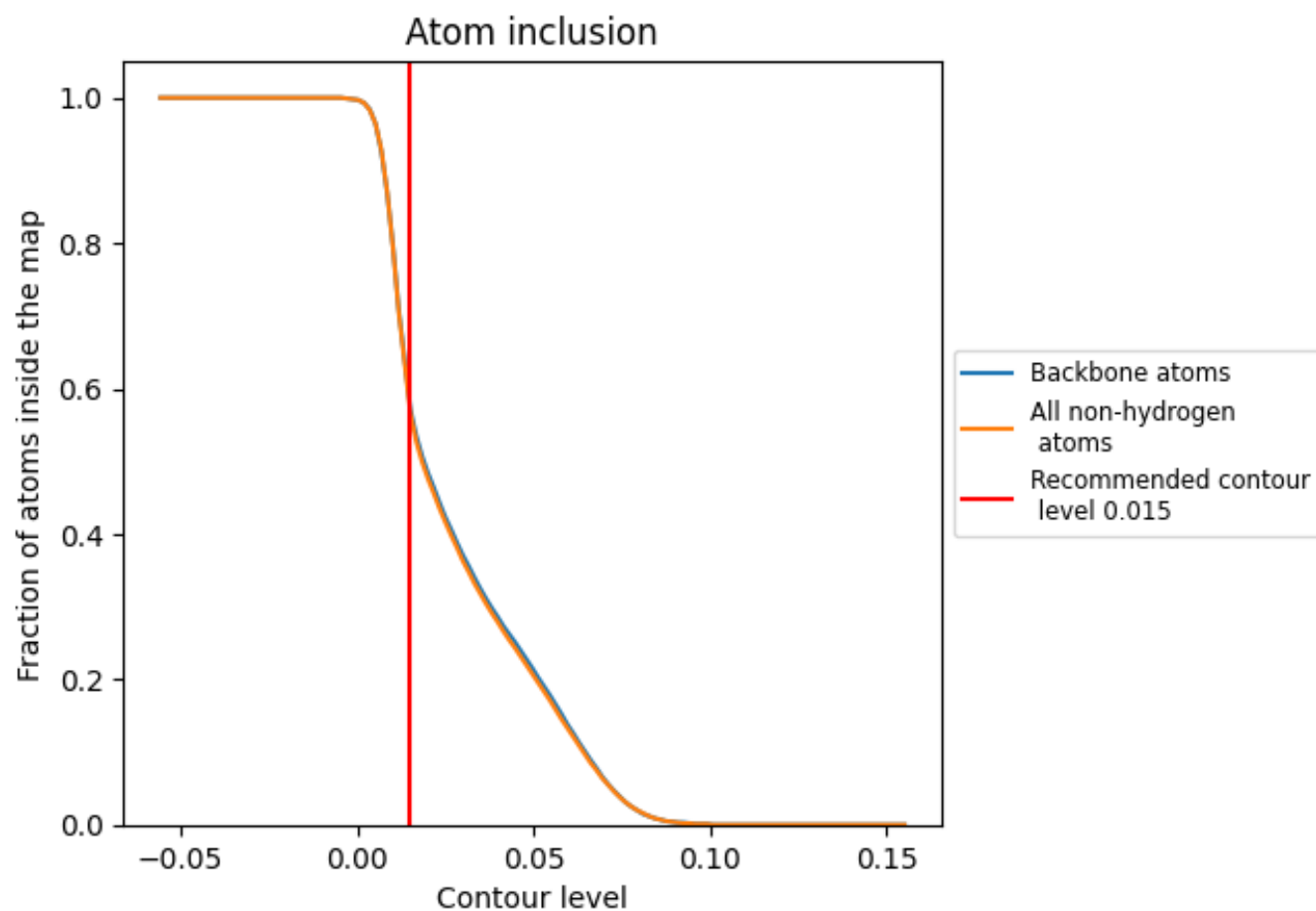
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 57% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5700	 0.4030
A	 0.9540	 0.6410
A1	 0.2440	 0.2160
A2	 0.2050	 0.2000
B	 0.6040	 0.4500
B1	 0.0900	 0.1260
B2	 0.0880	 0.1250
C	 0.9740	 0.6530
C1	 0.0270	 0.1220
C2	 0.0250	 0.1070
D	 0.7480	 0.5130
D1	 0.0540	 0.1330
D2	 0.0470	 0.1300
E	 0.8520	 0.5130
E1	 0.1000	 0.1640
E2	 0.0830	 0.1510
F	 0.9580	 0.6580
F1	 0.0490	 0.1230
F2	 0.0600	 0.1210
G	 0.9160	 0.6040
G1	 0.0000	 0.1260
G2	 0.0000	 0.1340
H	 0.9270	 0.6200
H1	 0.7570	 0.4040
H2	 0.7100	 0.3980
I	 0.9040	 0.6100
I1	 0.6830	 0.3880
I2	 0.6740	 0.3670
J	 0.8810	 0.5980
J1	 0.6960	 0.3790
J2	 0.6760	 0.3790
K	 0.8500	 0.5560
K1	 0.6670	 0.3780
K2	 0.6150	 0.3680
L	 0.9210	 0.6280













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Chain	Atom inclusion	Q-score
L1	 0.6490	 0.3630
L2	 0.6260	 0.3660
M	 0.9690	 0.6440
M1	 0.6940	 0.3700
M2	 0.6640	 0.3670
N	 0.9660	 0.6470
N1	 0.7030	 0.3780
N2	 0.6910	 0.3690
O	 0.9430	 0.6110
O1	 0.6920	 0.3810
O2	 0.6820	 0.3750
P	 0.8320	 0.5540
P1	 0.7010	 0.3740
P2	 0.6960	 0.3710
Q	 0.9260	 0.6100
Q1	 0.7320	 0.3910
Q2	 0.7170	 0.3900
R	 0.9470	 0.6320
S	 0.8480	 0.5740
a	 0.9430	 0.6340
b	 0.6110	 0.4510
c	 0.9790	 0.6570
d	 0.7490	 0.5210
d1	 0.4870	 0.3030
d2	 0.4570	 0.2940
e	 0.8560	 0.5170
e1	 0.5150	 0.3110
e2	 0.4530	 0.2710
f	 0.9220	 0.6320
g	 0.9180	 0.6060
g1	 0.4620	 0.3030
g2	 0.4180	 0.2790
h	 0.9400	 0.6270
i	 0.9140	 0.6180
i1	 0.4320	 0.3210
i2	 0.3790	 0.3130
j	 0.8840	 0.6010
k	 0.8440	 0.5500
l	 0.9270	 0.6260
m	 0.9650	 0.6410
n	 0.9610	 0.6460
o	 0.9370	 0.6100

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Chain	Atom inclusion	Q-score
p	 0.8330	 0.5540
q	 0.9290	 0.6130
r	 0.9380	 0.6240
s	 0.8440	 0.5570
t	 0.9280	 0.6170