



## wwPDB EM Validation Summary Report ⓘ

Dec 18, 2022 – 10:18 am GMT

PDB ID : 6YNY  
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](mailto: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>.

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

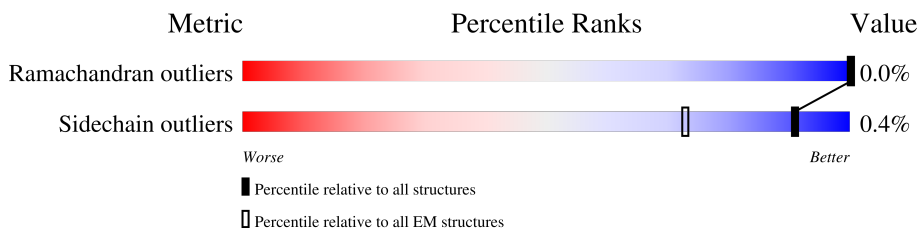
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.70 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.



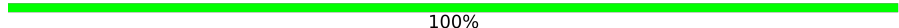
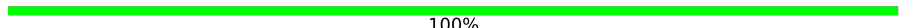
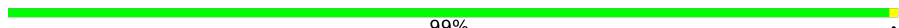
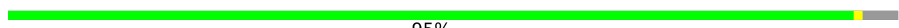
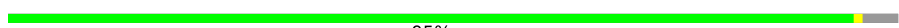








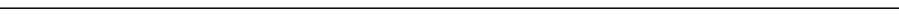

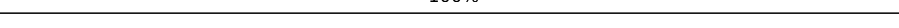




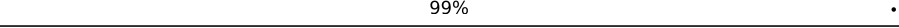
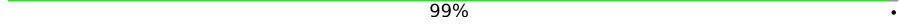


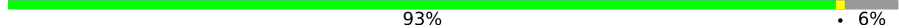
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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% .

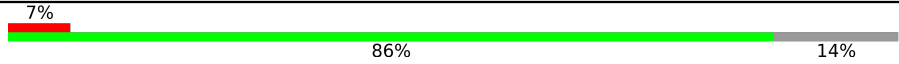
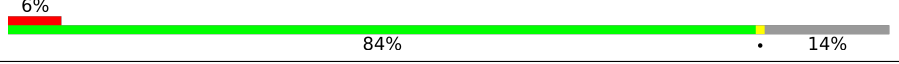
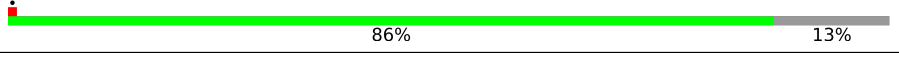


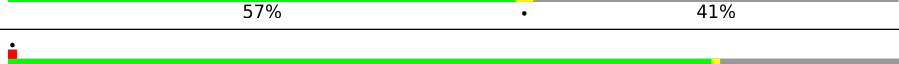


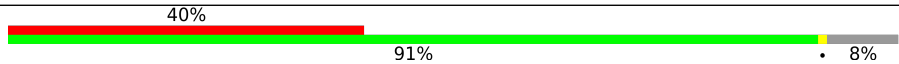
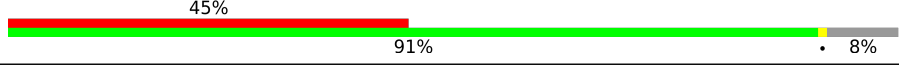
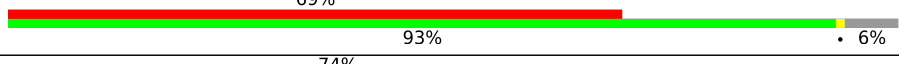
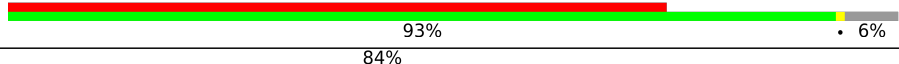

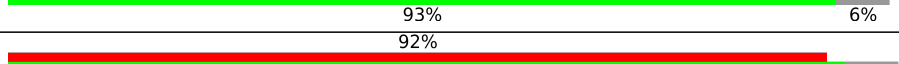
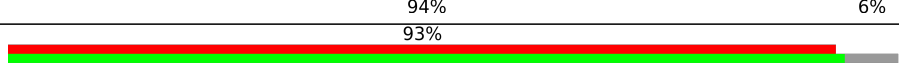
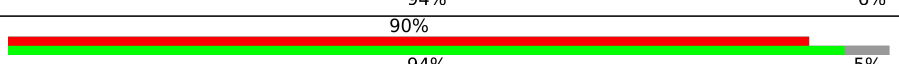
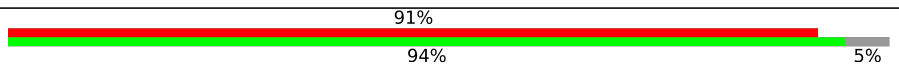
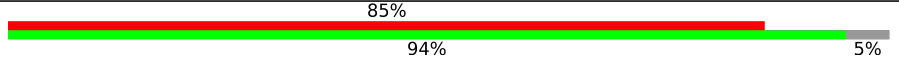
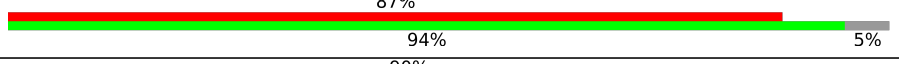
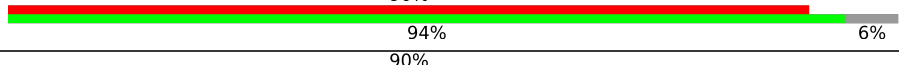
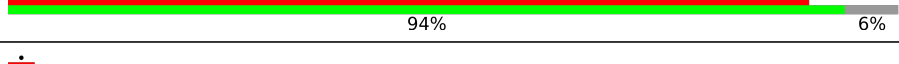
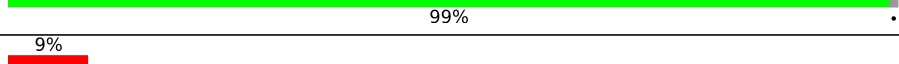
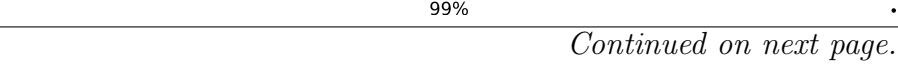


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Mol	Chain	Length	Quality of chain
5	i	209	 100%
6	K	179	 100%
6	k	179	 99%
7	C	100	 95%
7	c	100	 95%
8	G	286	 89%
8	g	286	 89%
9	H	268	 86%
9	h	268	 86%
10	J	273	 98%
10	j	273	 99%
11	L	247	 99%
11	l	247	 99%
12	M	221	 100%
12	m	221	 100%
13	N	179	 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	9% 96%
26	I2	76	12% 99%
26	J1	76	8% 99%
26	J2	76	12% 99%
26	K1	76	12% 99%
26	K2	76	17% 97%
26	L1	76	16% 99%
26	L2	76	22% 99%
26	M1	76	13% 99%
26	M2	76	14% 99%
26	N1	76	8% 99%
26	N2	76	12% 99%
26	O1	76	16% 99%
26	O2	76	11% 99%
26	P1	76	8% 99%
26	P2	76	5% 99%
26	Q1	76	7% 99%
26	Q2	76	• 99%
27	d1	158	31% 84% 15%
27	d2	158	32% 84% 15%
28	e1	71	30% 96%
28	e2	71	39% 94%

## 2 Entry composition [i](#)

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
			Total	C	H	N	O	S		
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
			Total	C	H	N	O	S		
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
			Total	C	H	N	O	S		
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
			Total	C	H	N	O	S		
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	
			Total	C	H	N	O			S
5	i	209	Total 3462	C 1121	H 1742	N 304	O 285	S 10	0	0
5	I	209	Total 3460	C 1121	H 1740	N 304	O 285	S 10	0	0

- Molecule 6 is a protein called subunit k.

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

- Molecule 7 is a protein called subunit 8.

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

- Molecule 8 is a protein called ATPTT3.

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

- Molecule 9 is a protein called ATPTT4.

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

- Molecule 10 is a protein called ATPTT5.

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

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

- Molecule 11 is a protein called ATPTT6.

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

- Molecule 12 is a protein called ATPTT7.

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

- Molecule 13 is a protein called ATPTT8.

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

- Molecule 14 is a protein called ATPTT9.

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

- Molecule 15 is a protein called ATPTT10.

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



- Molecule 16 is a protein called ATPTT11.

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

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

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

- Molecule 23 is a protein called subunit gamma.

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

- Molecule 24 is a protein called subunit alpha.

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

- Molecule 25 is a protein called subunit beta.

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

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

- Molecule 26 is a protein called subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
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		

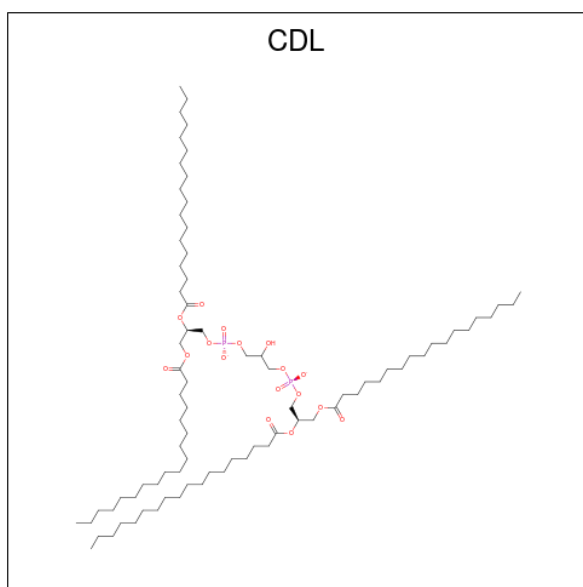
- Molecule 27 is a protein called subunit delta.

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 (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
29	a	1	Total 512	C 162	H 312	O 34	P 4	0
29	a	1	Total 512	C 162	H 312	O 34	P 4	0
29	b	1	Total 256	C 81	H 156	O 17	P 2	0
29	f	1	Total 768	C 243	H 468	O 51	P 6	0
29	f	1	Total 768	C 243	H 468	O 51	P 6	0
29	f	1	Total 768	C 243	H 468	O 51	P 6	0
29	i	1	Total 256	C 81	H 156	O 17	P 2	0
29	k	1	Total 512	C 162	H 312	O 34	P 4	0
29	k	1	Total 512	C 162	H 312	O 34	P 4	0
29	j	1	Total 512	C 162	H 312	O 34	P 4	0
29	j	1	Total 512	C 162	H 312	O 34	P 4	0
29	l	1	Total 512	C 162	H 312	O 34	P 4	0
29	l	1	Total 512	C 162	H 312	O 34	P 4	0
29	p	1	Total 256	C 81	H 156	O 17	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
29	r	1	256	81	156	17	2	0
29	A	1	256	81	156	17	2	0
29	B	1	1024	324	624	68	8	0
29	B	1	1024	324	624	68	8	0
29	B	1	1024	324	624	68	8	0
29	B	1	1024	324	624	68	8	0
29	F	1	256	81	156	17	2	0
29	I	1	512	162	312	34	4	0
29	I	1	512	162	312	34	4	0
29	K	1	512	162	312	34	4	0
29	K	1	512	162	312	34	4	0
29	J	1	512	162	312	34	4	0
29	J	1	512	162	312	34	4	0
29	L	1	512	162	312	34	4	0
29	L	1	512	162	312	34	4	0
29	P	1	256	81	156	17	2	0

- Molecule 30 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: C<sub>44</sub>H<sub>88</sub>NO<sub>8</sub>P).



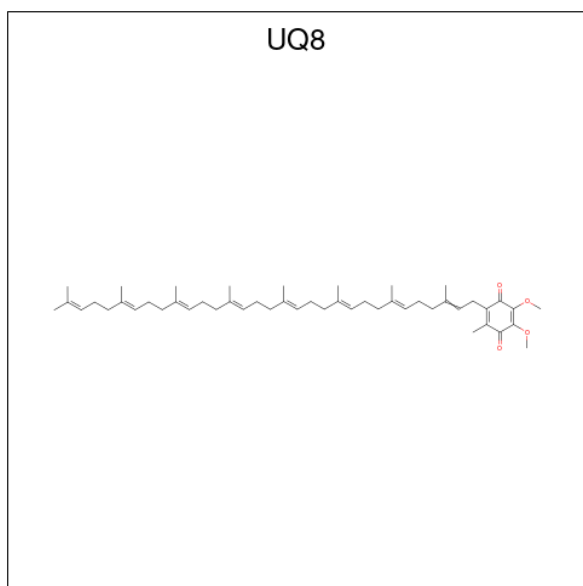
Mol	Chain	Residues	Atoms					AltConf		
			Total	C	H	N	O		P	
30	d	1	Total	142	44	88	1	8	1	0
30	g	1	Total	284	88	176	2	16	2	0
30	g	1	Total	284	88	176	2	16	2	0
30	D	1	Total	142	44	88	1	8	1	0
30	G	1	Total	284	88	176	2	16	2	0
30	G	1	Total	284	88	176	2	16	2	0

- Molecule 31 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

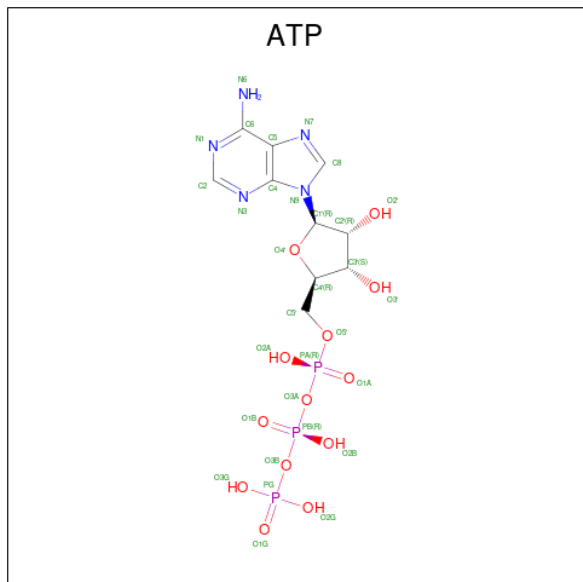
- Molecule 32 is Ubiquinone-8 (three-letter code: UQ8) (formula:  $C_{49}H_{74}O_4$ ).



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



- Molecule 33 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
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 (three-letter code: MG) (formula: Mg).

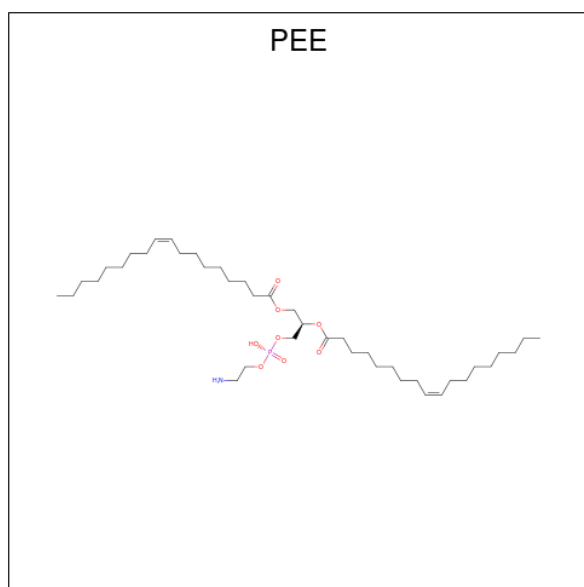
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
34	g	1	Total	Mg	0
			1	1	
34	G	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
34	C1	1	1	1	0
34	D1	1	1	1	0
34	B1	1	1	1	0
34	A1	1	1	1	0
34	E1	1	1	1	0
34	C2	1	1	1	0
34	D2	1	1	1	0
34	B2	1	1	1	0
34	A2	1	1	1	0
34	E2	1	1	1	0

- Molecule 35 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula:  $C_{41}H_{78}NO_8P$ ).



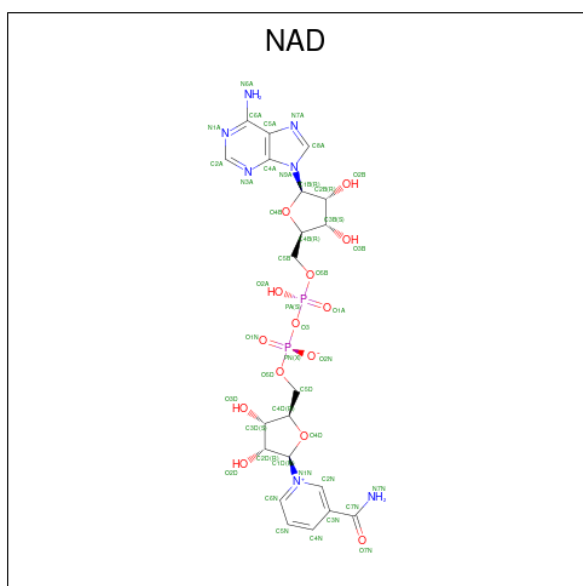
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
35	m	1	133	41	82	1	8	1	0

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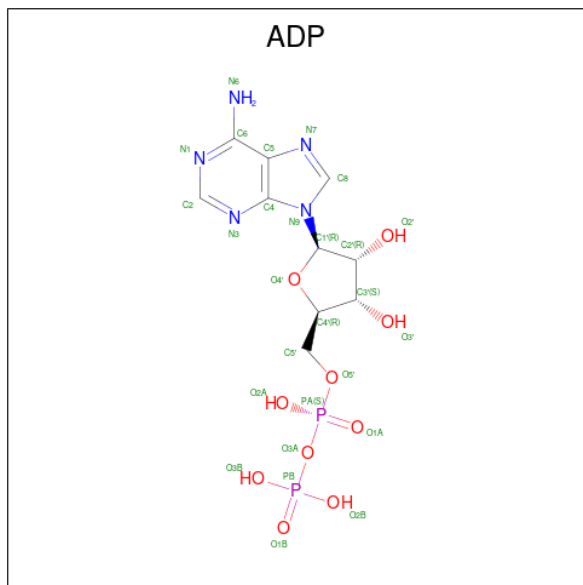
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
35	A	1	Total	C	H	N	O	P	0
			123	38	75	1	8	1	
35	J	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
35	L	1	Total	C	H	N	O	P	0
			123	38	75	1	8	1	

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



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
36	e	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	
36	E	1	Total	C	H	N	O	P	0
			70	21	26	7	14	2	

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



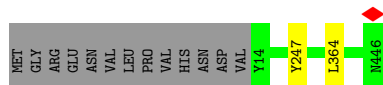
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
37	D1	1	38	10	11	5	10	2	0
37	B1	1	38	10	11	5	10	2	0
37	D2	1	38	10	11	5	10	2	0
37	B2	1	38	10	11	5	10	2	0

### 3 Residue-property plots [i](#)

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

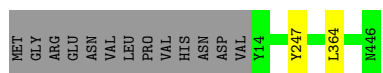
- Molecule 1: subunit a

Chain a:  97%

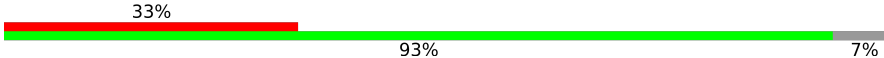


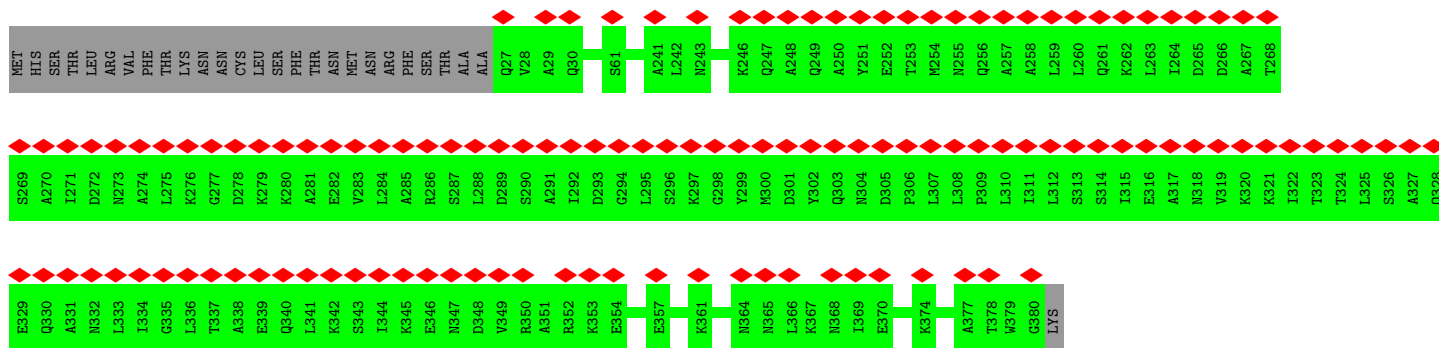
- Molecule 1: subunit a

Chain A:  97%



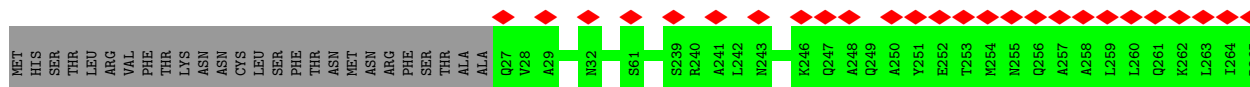
- Molecule 2: subunit b

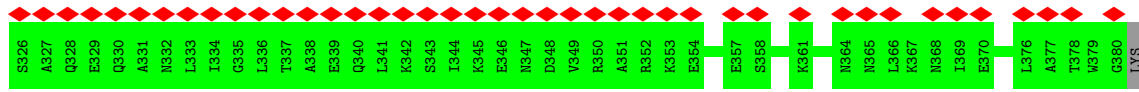
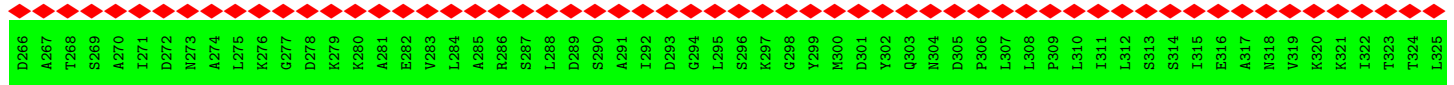
Chain b:  33% 93% 7%



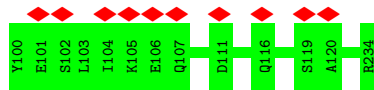
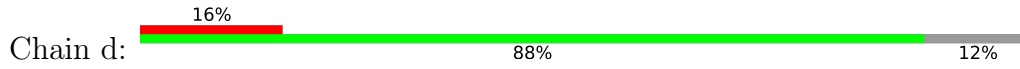
- Molecule 2: subunit b

Chain B:  34% 93% 7%

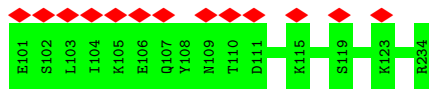
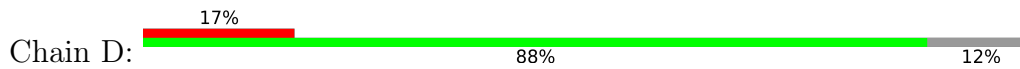




• Molecule 3: subunit d



• Molecule 3: subunit d



• Molecule 4: subunit f



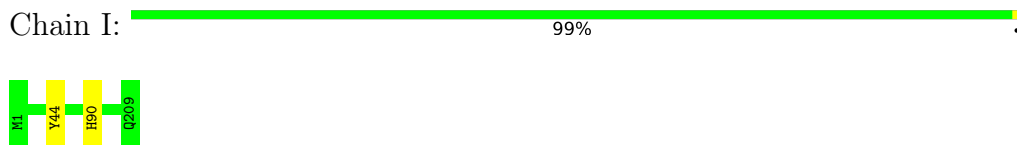
• Molecule 4: subunit f



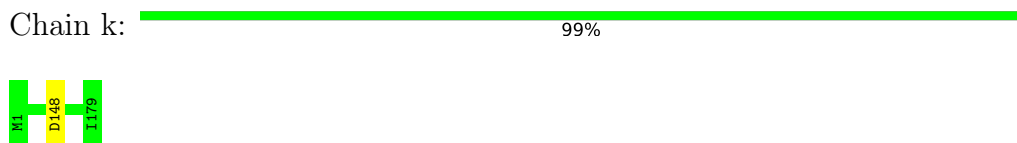
• Molecule 5: subunit i/j



• Molecule 5: subunit i/j



• Molecule 6: subunit k

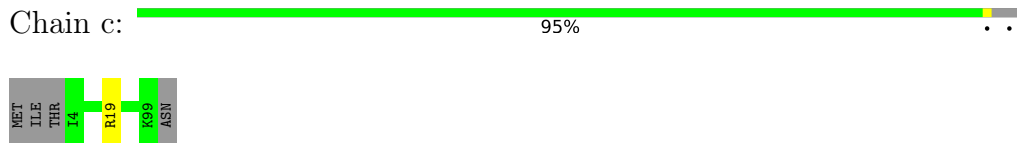


• Molecule 6: subunit k

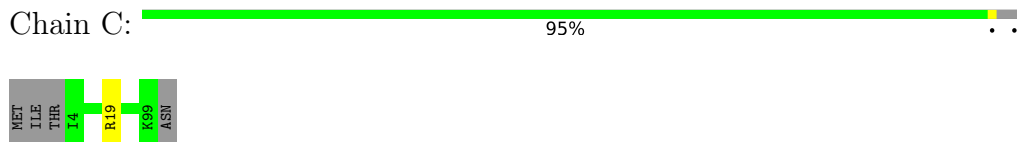


There are no outlier residues recorded for this chain.

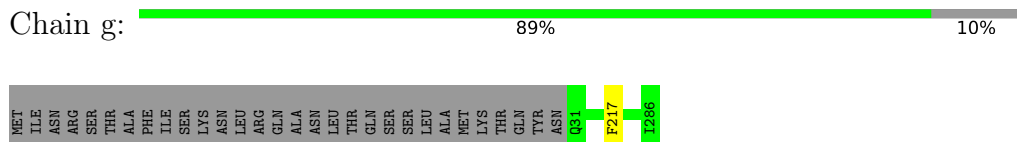
• Molecule 7: subunit 8



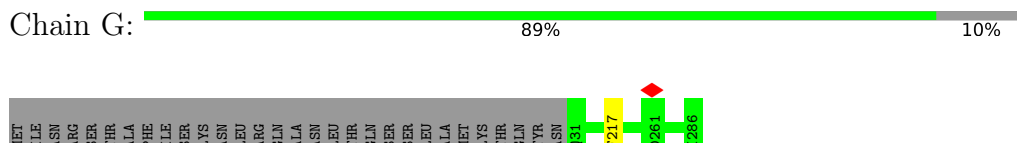
• Molecule 7: subunit 8



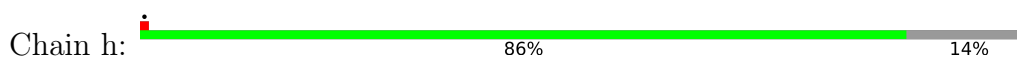
• Molecule 8: ATPPT3

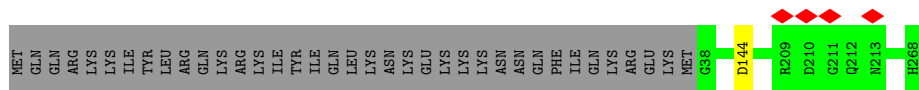


• Molecule 8: ATPPT3

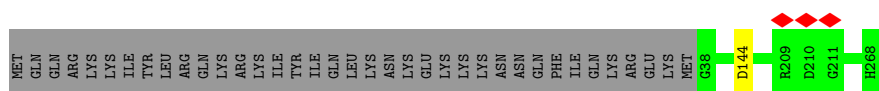
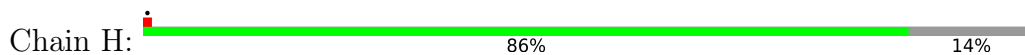


• Molecule 9: ATPPT4

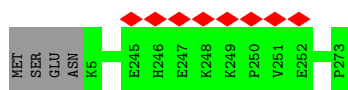




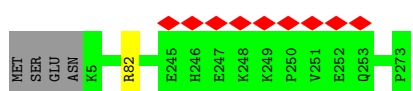
• Molecule 9: ATPTT4



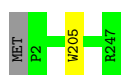
• Molecule 10: ATPTT5



• Molecule 10: ATPTT5



• Molecule 11: ATPTT6



• Molecule 11: ATPTT6



• Molecule 12: ATPTT7



• Molecule 12: ATPTT7





There are no outlier residues recorded for this chain.

• Molecule 13: ATPTT8



MET	GLU	GLY	PHE	ILE	GLN	ASN	ARG	LYS	LYS	LYS	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	SER	LYS	GLU	LYS	ARG	LYS	GLN	ILE	ASN	GLN	LEU	ASN	LYS	GLN	LYS	LYS	GLN	GLN	GLU	GLU	GLU	GLU	LYS	LYS	TYR	TYR	GLN	GLN	LYS	LYS	ASP	GLN	LYS	ARG	LYS	TYR	LEU	TYR	GLN	ARG	LYS	GLU	MET
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• Molecule 13: ATPTT8



MET	GLU	GLY	PHE	ILE	GLN	ASN	LYS	ARG	LYS	LYS	LYS	GLU	GLU	GLU	GLU	GLU	GLU	GLU	SER	LYS	GLU	LYS	ARG	LYS	GLN	ILE	ASN	GLN	LEU	ASN	LYS	GLN	LYS	LYS	GLN	GLN	GLU	GLU	GLU	GLU	LYS	LYS	TYR	TYR	GLN	LYS	ASP	GLN	LYS	ARG	LYS	TYR	LEU	TYR	GLN	ARG	LYS	GLU	MET
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• Molecule 14: ATPTT9



MET	LYS	GLN	LYS	ILE	ASN	LYS	LEU	LEU	ASN	LYS	GLY	VAL	GLN	ASP	LYS	TYR	LYS	TYR	LEU	SER	LYS	LEU	ILE	LEU	ASP	GLN	GLU	ILE	LYS	GLY	LYS	LYS	ILE	ARG	LYS	ASN	LYS	LYS	LYS	GLU	GLU	LYS	GLN	LYS	ARG	LYS	ASN	LYS	LEU	LEU	ILE	GLU	GLU	M65	K153	ASN
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• Molecule 14: ATPTT9



MET	LYS	GLN	LYS	ILE	ASN	LYS	LEU	LEU	ASN	LYS	GLY	VAL	GLN	ASP	LYS	TYR	LYS	TYR	LEU	SER	LYS	LEU	ILE	LEU	ASP	GLN	GLU	ILE	LYS	GLY	LYS	LYS	ILE	ARG	LYS	ASN	LYS	LYS	LYS	GLU	GLU	LYS	GLN	LYS	ARG	LYS	ASN	LYS	LEU	LEU	ILE	GLU	GLU	M65	K153	ASN
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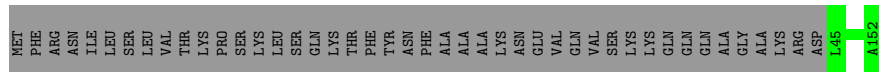
• Molecule 15: ATPTT10



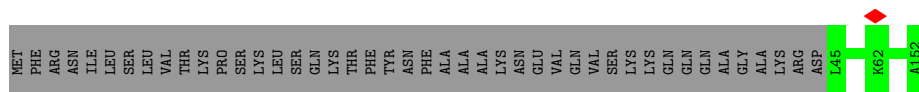
• Molecule 15: ATPTT10



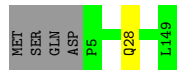
• Molecule 16: ATPTT11



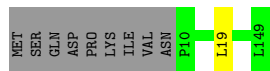
• Molecule 16: ATPTT11



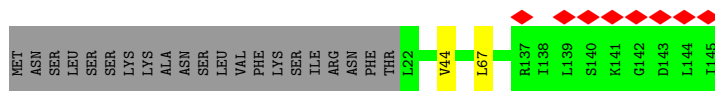
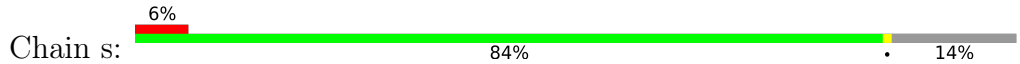
• Molecule 17: ATPTT12



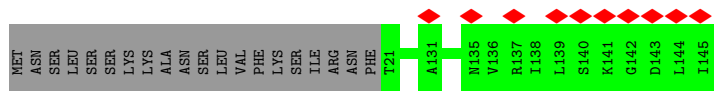
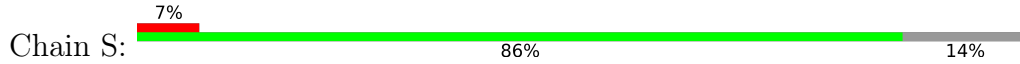
• Molecule 17: ATPTT12



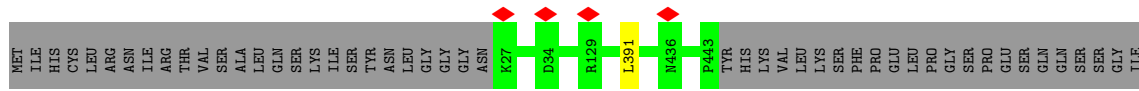
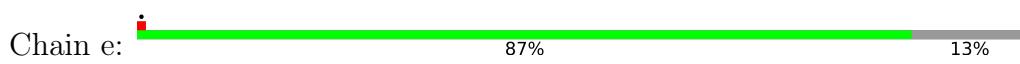
• Molecule 18: ATPTT13



• Molecule 18: ATPTT13

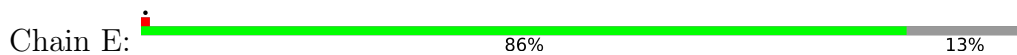


• Molecule 19: ATPTT1



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

• Molecule 19: ATPTT1



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

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

• Molecule 20: Inhibitor of F1 (IF1)



MET ASN ARG SER VAL ILE ALA LYS ASN LEU ILE GLN THR TYR ARG ALA MET SER VAL GLN SER ARG 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 M62 T63

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

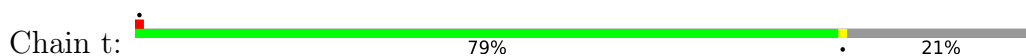
• Molecule 20: Inhibitor of F1 (IF1)



MET ASN ARG SER VAL ILE ALA LYS ASN LEU ILE GLN THR TYR ARG ALA MET SER VAL GLN SER ARG 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 M62 T63 THR SER LYS

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

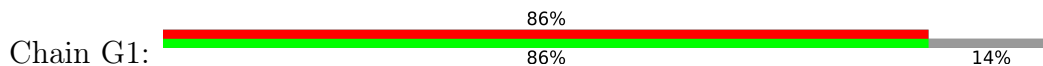
• Molecule 21: ATPTT2

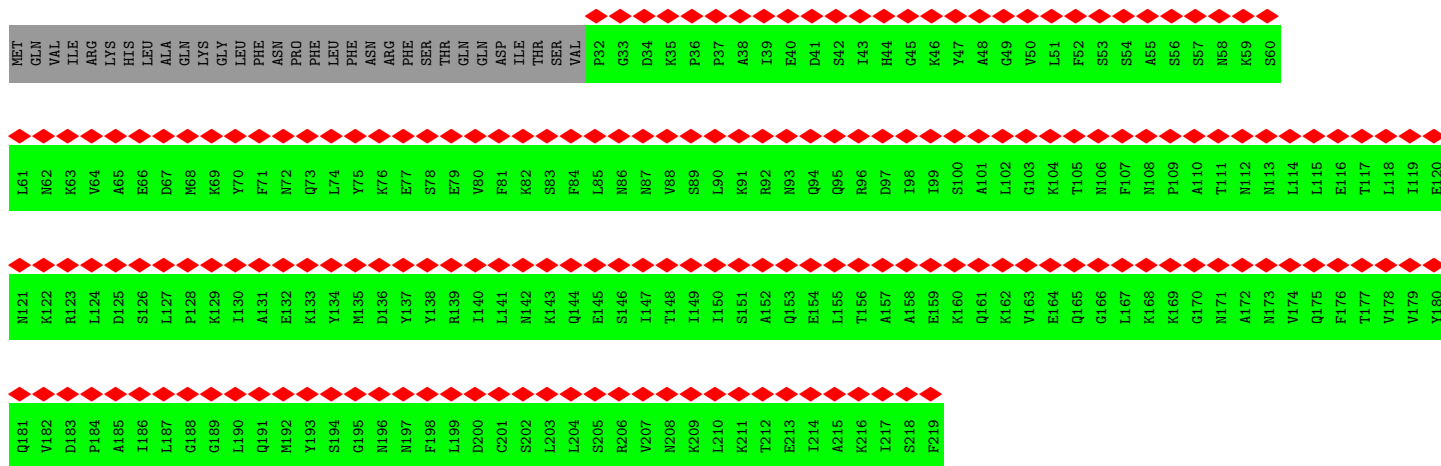


MET LYS MET TYR LEU GLN SER GLU TYR GLY LYS ASP ALA ILE ASN ARG LYS ILE HIS LYS GLU TYR LYS TRP GLY ALA PRO TYR ASN PHE S94 E135 T140 R158 A288 K289 T290 Q291 M458 GLN

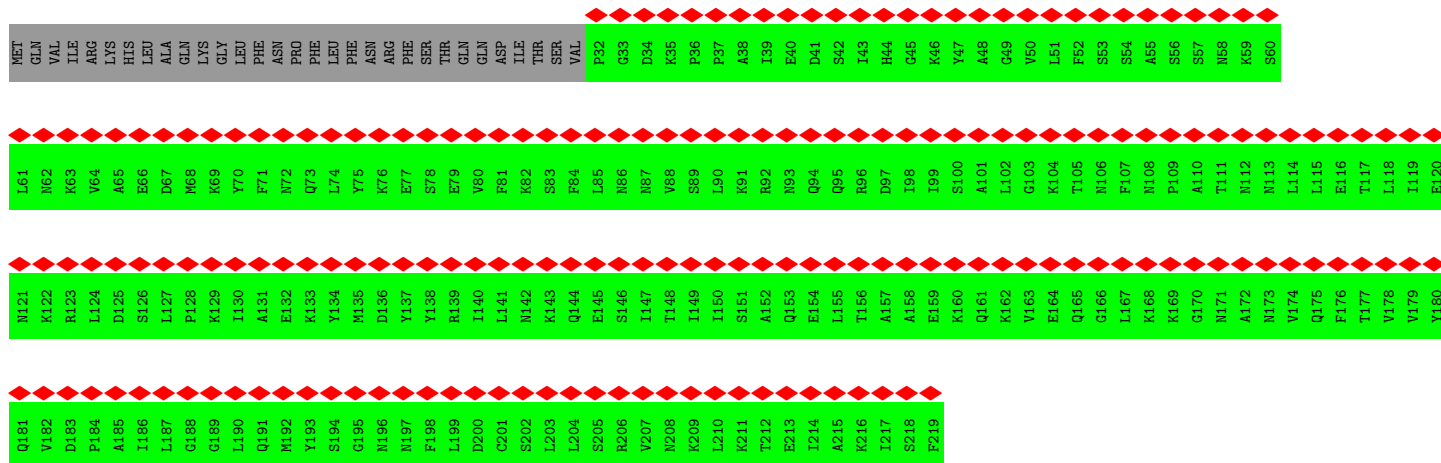
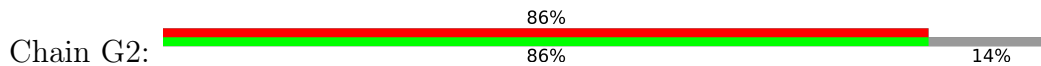
ILE GLN SER ASN GLN ARG LYS LYS MET ILE ASN THR LYS VAL PHE CYS LEU TRP GLY ALA PRO TYR ASN PHE S94 E135 T140 R158 A288 K289 T290 Q291 M458 GLN

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

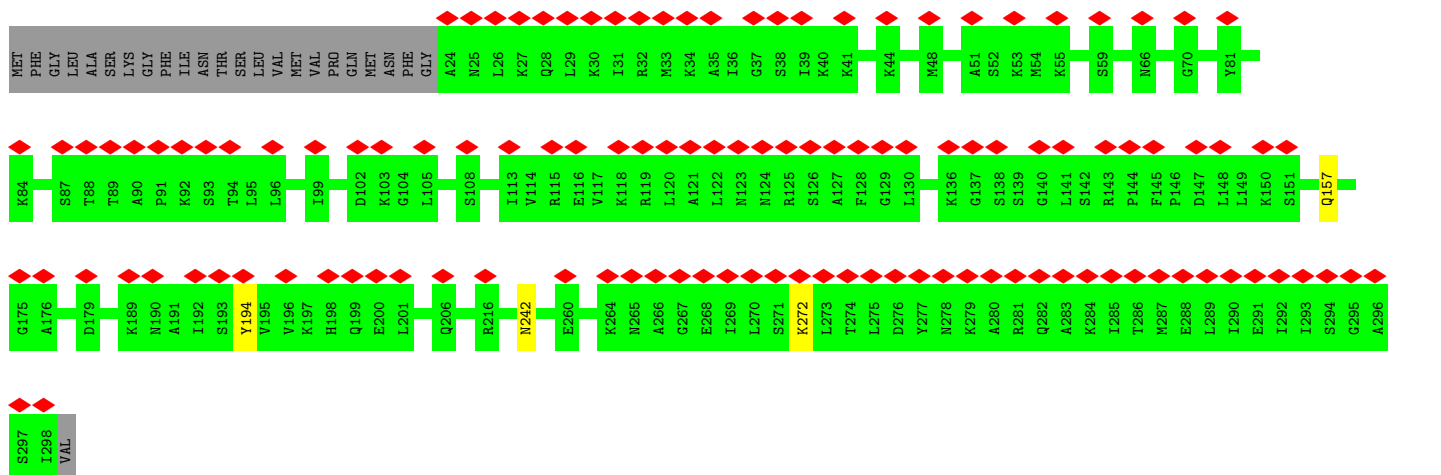
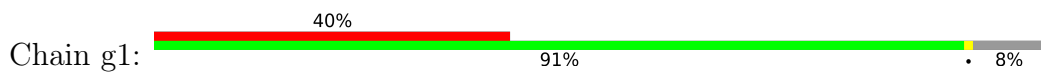




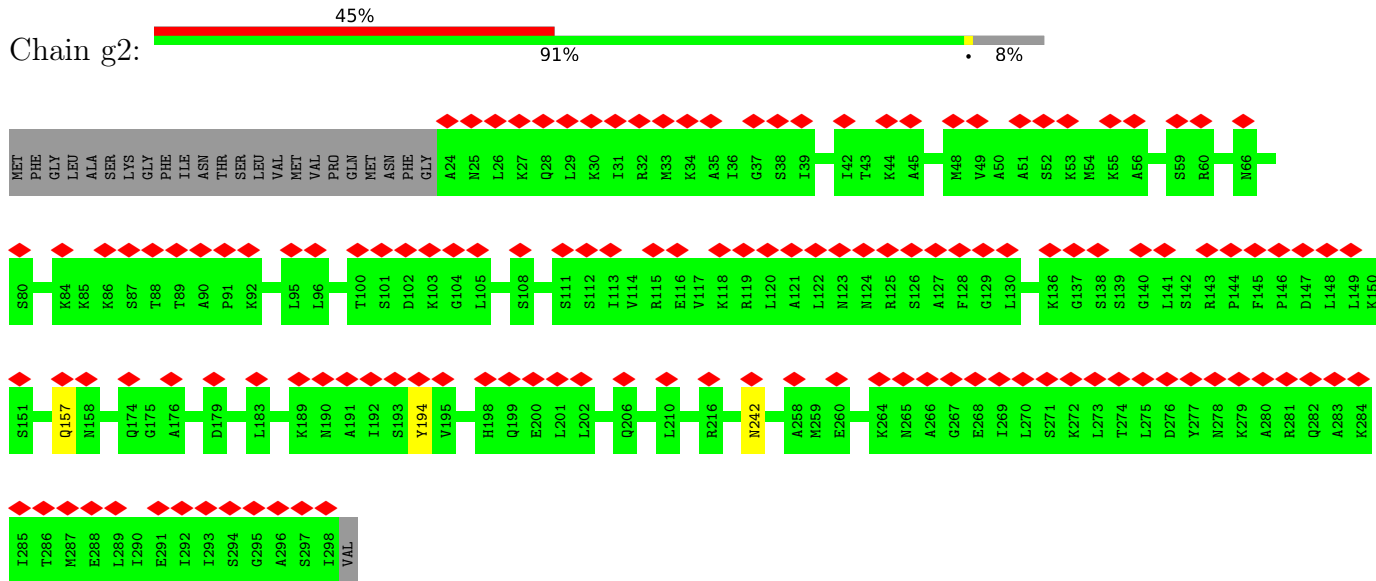
• Molecule 22: Oligomycin sensitivity-conferring protein (OSCP)



• Molecule 23: subunit gamma

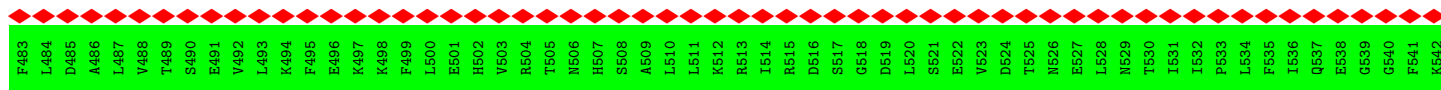


• Molecule 23: subunit gamma

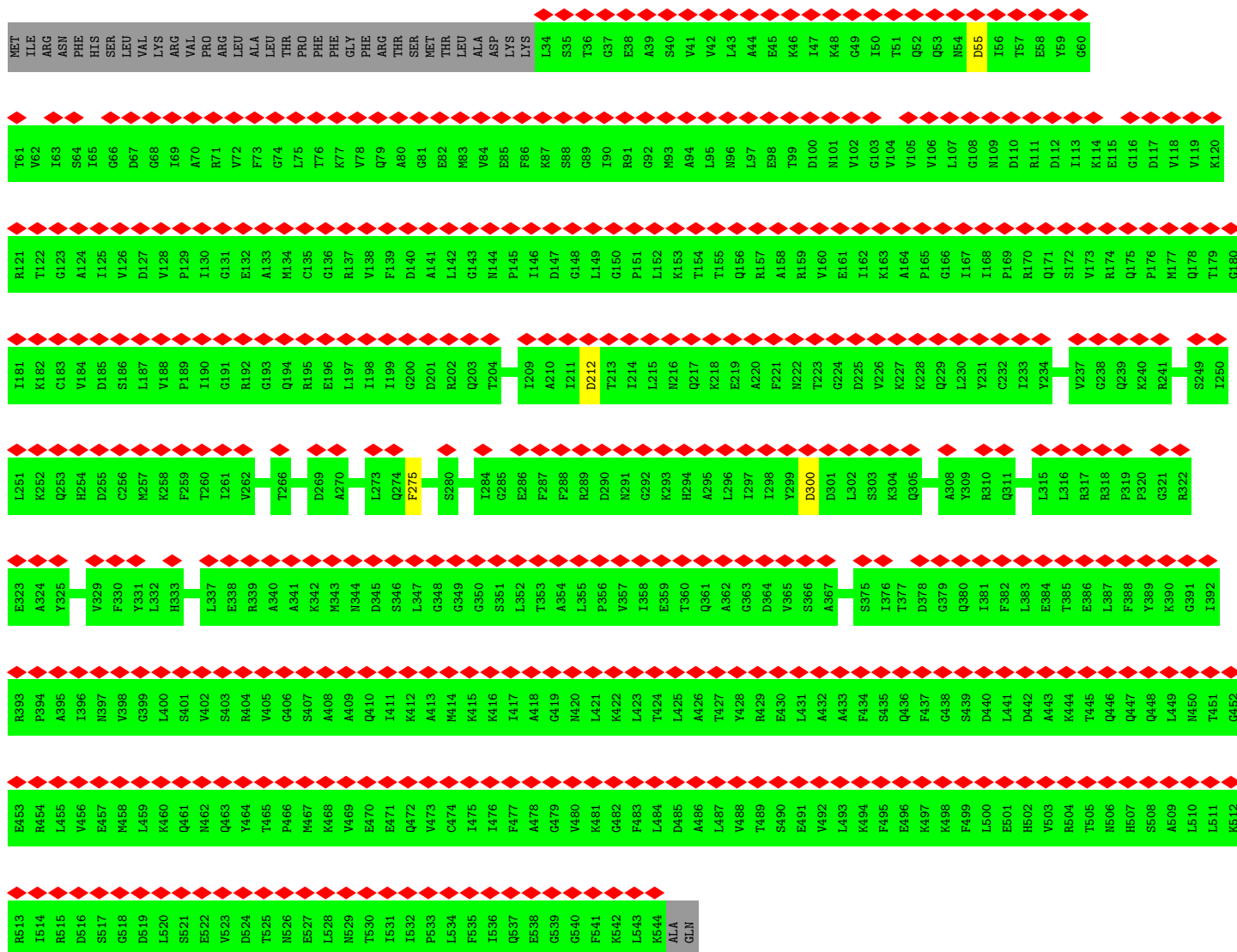
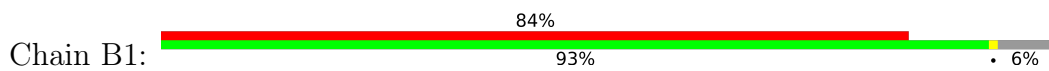


• Molecule 24: subunit alpha

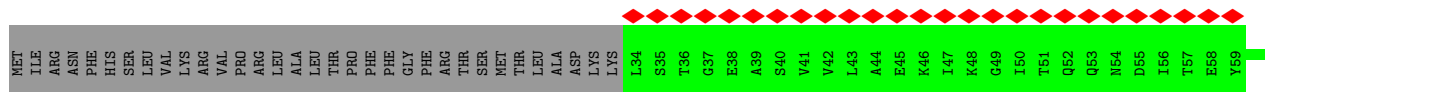


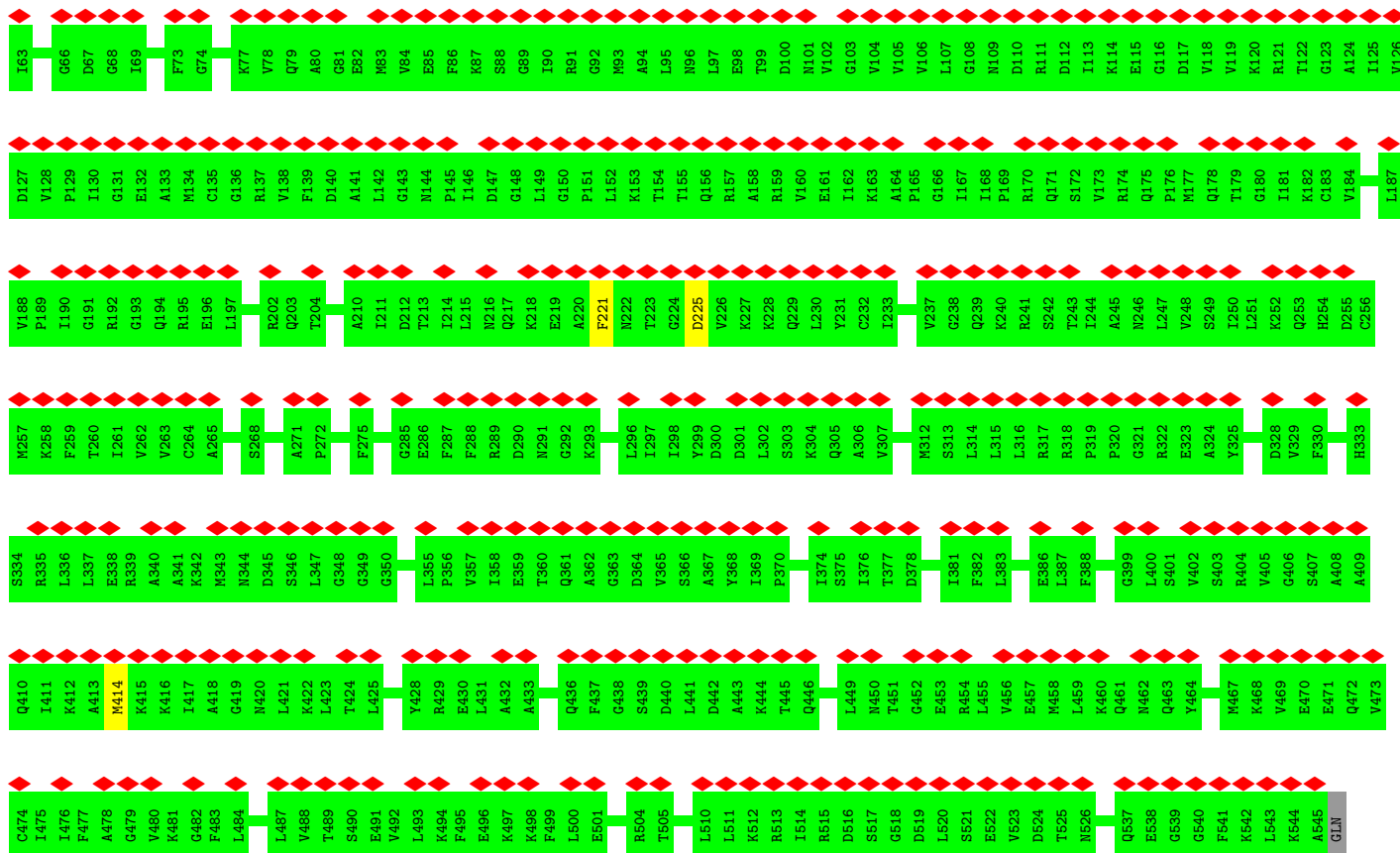


• Molecule 24: subunit alpha

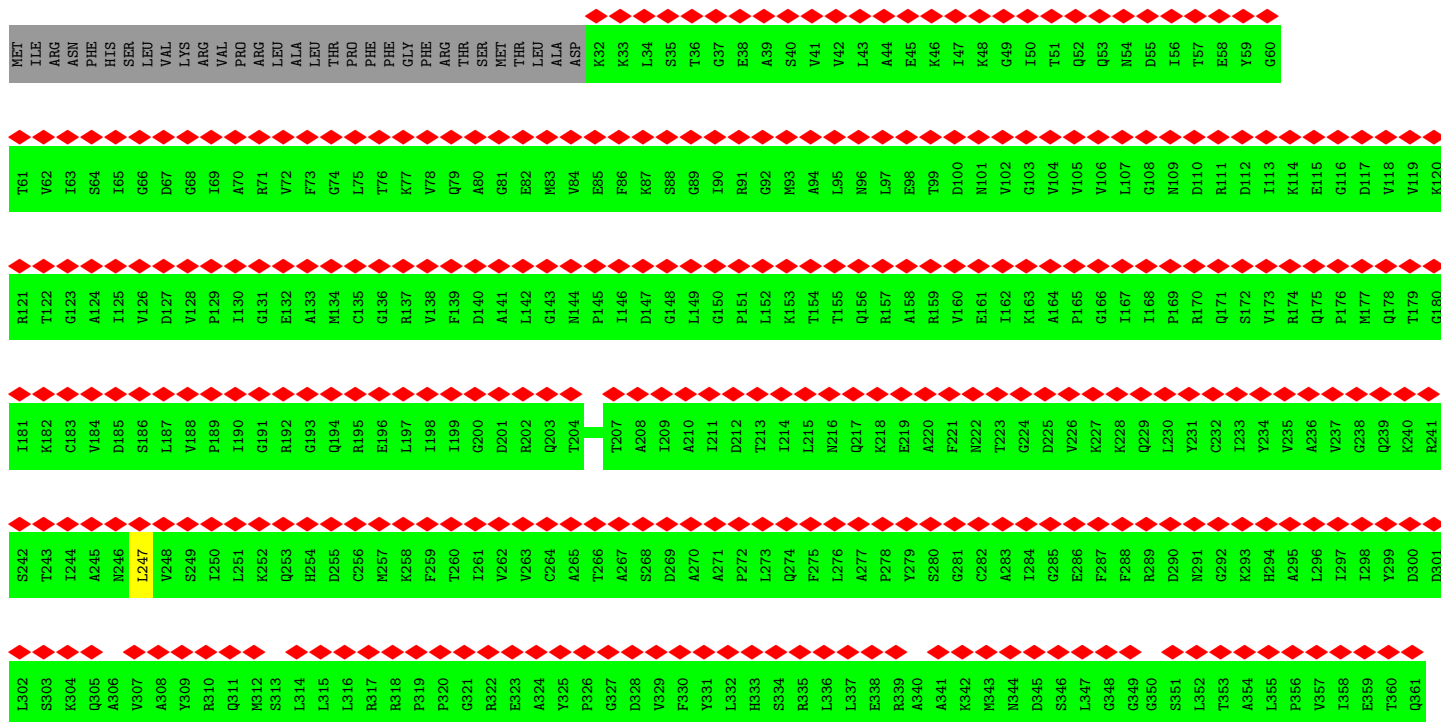


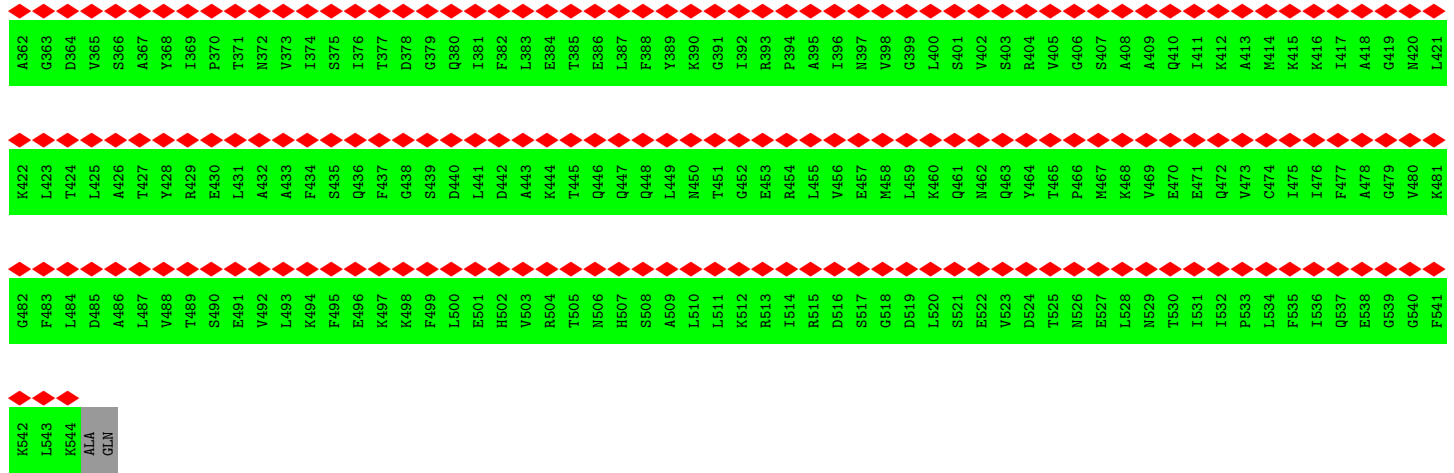
• Molecule 24: subunit alpha



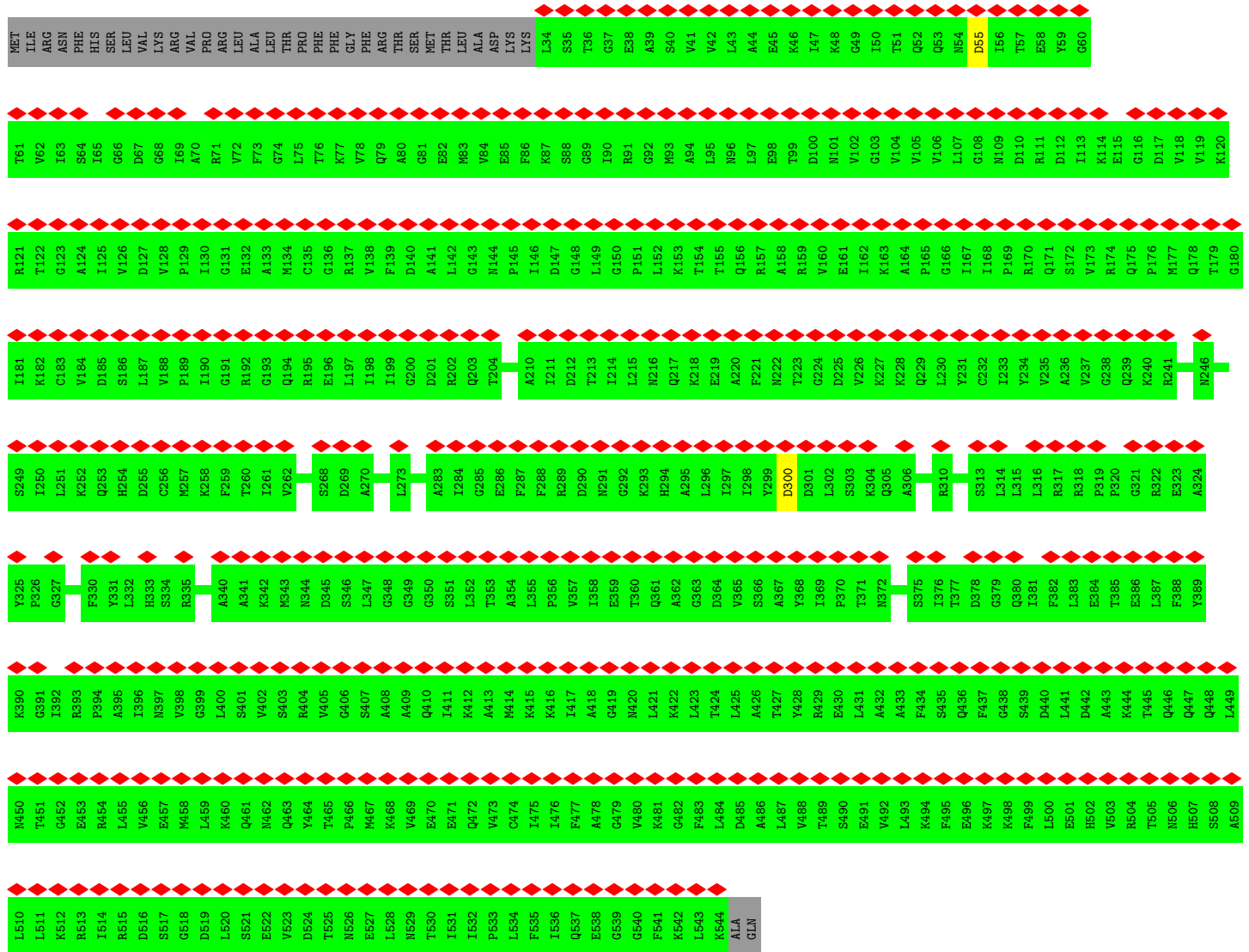
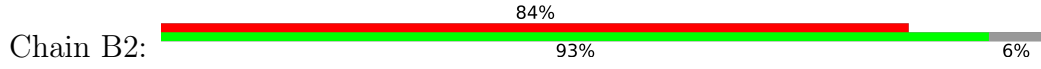


• Molecule 24: subunit alpha





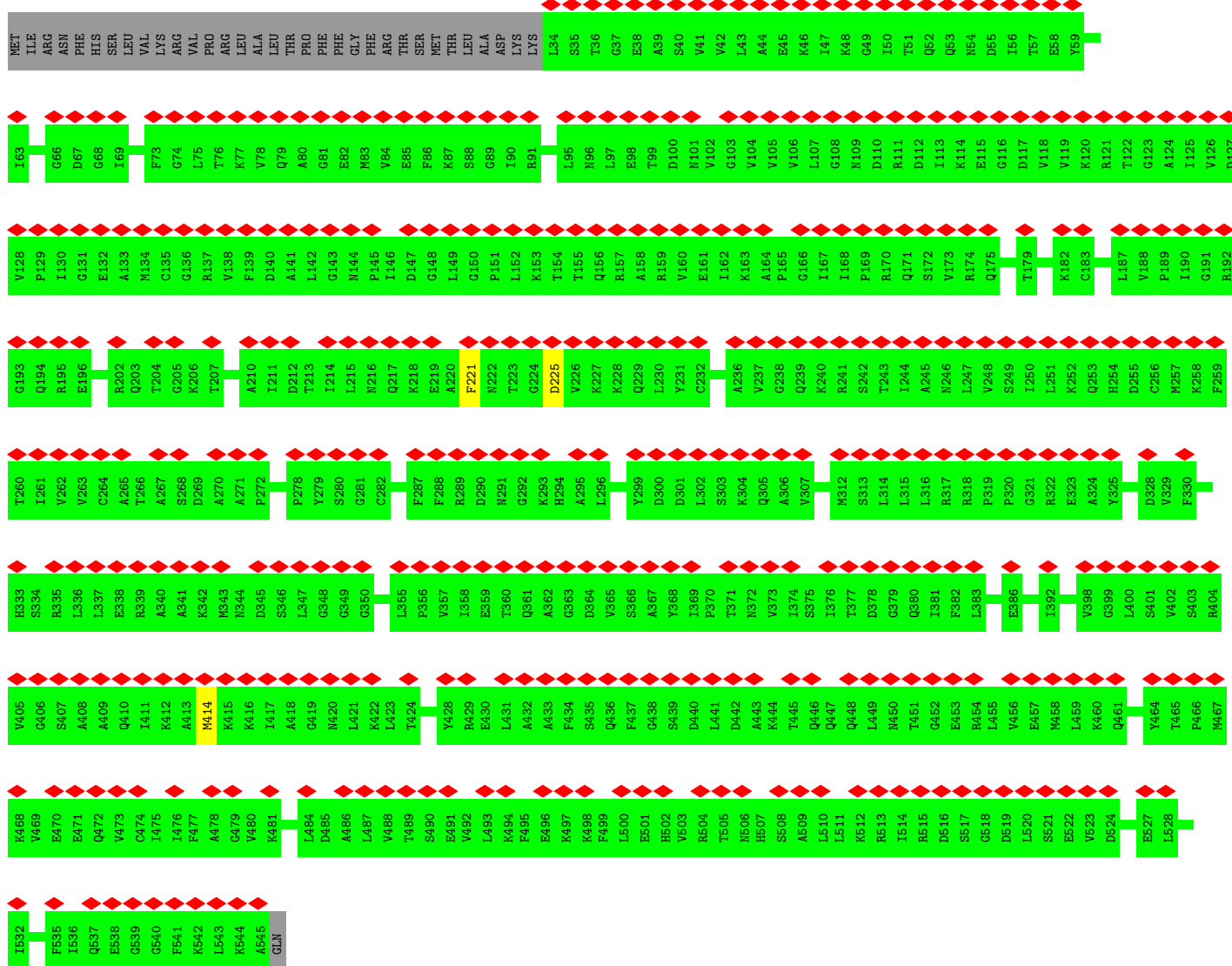
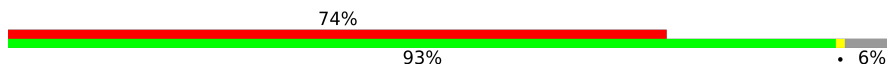
• Molecule 24: subunit alpha





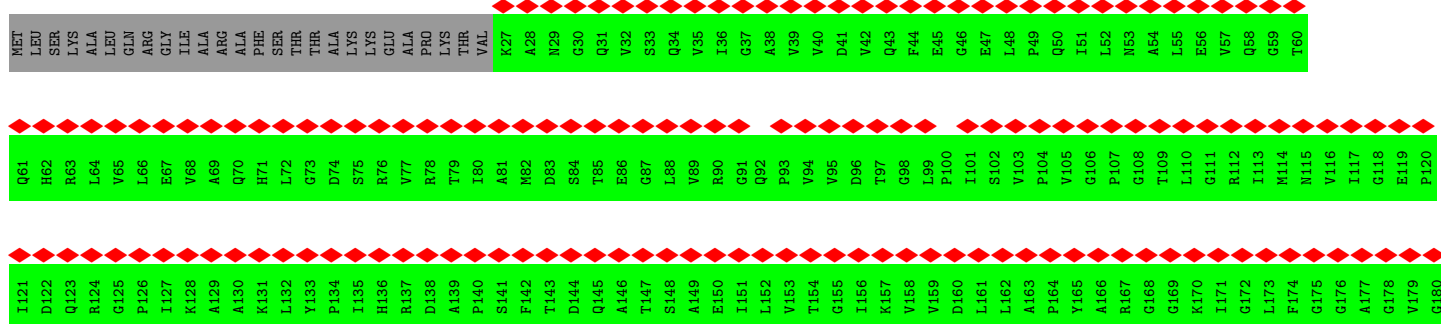
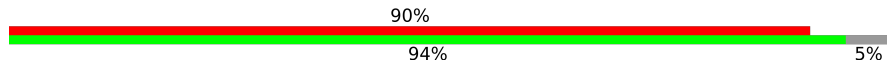
• Molecule 24: subunit alpha

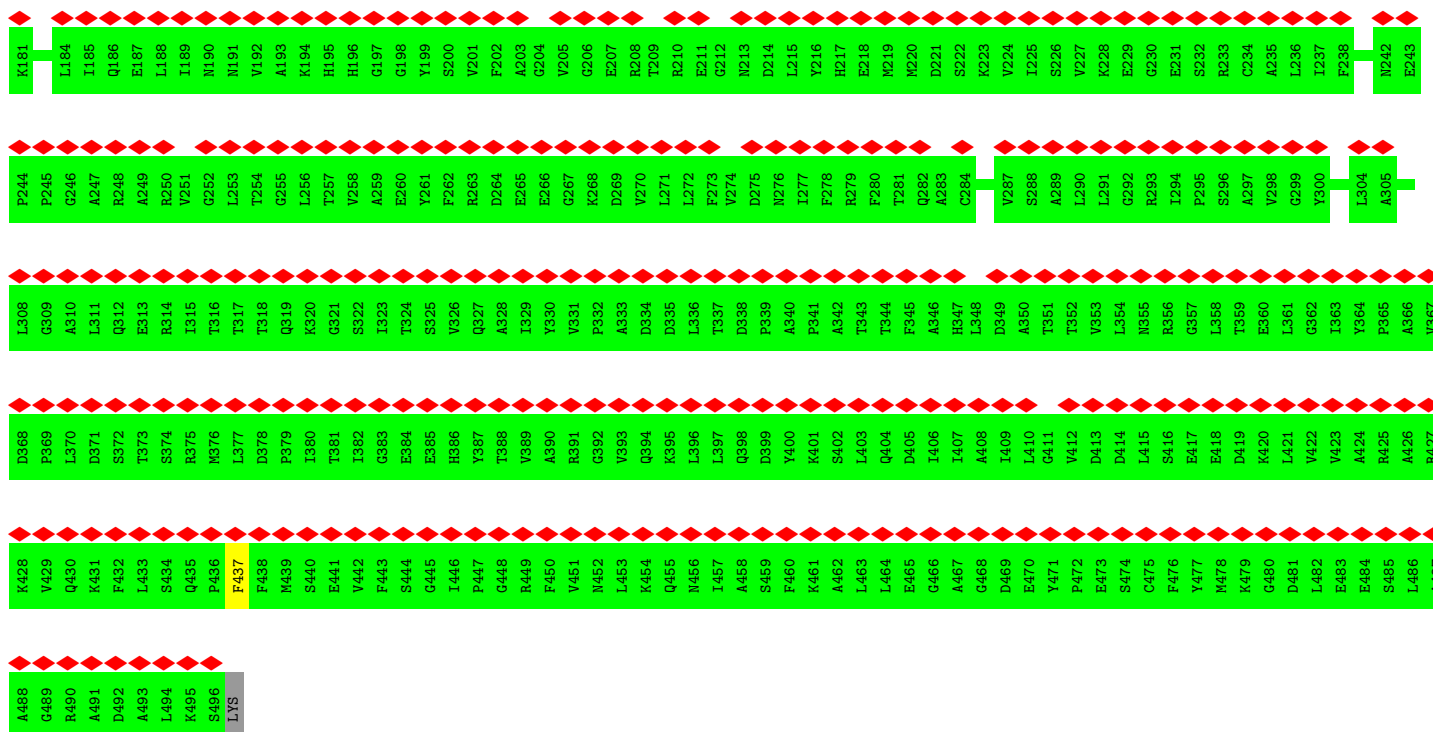
Chain A2:



• Molecule 25: subunit beta

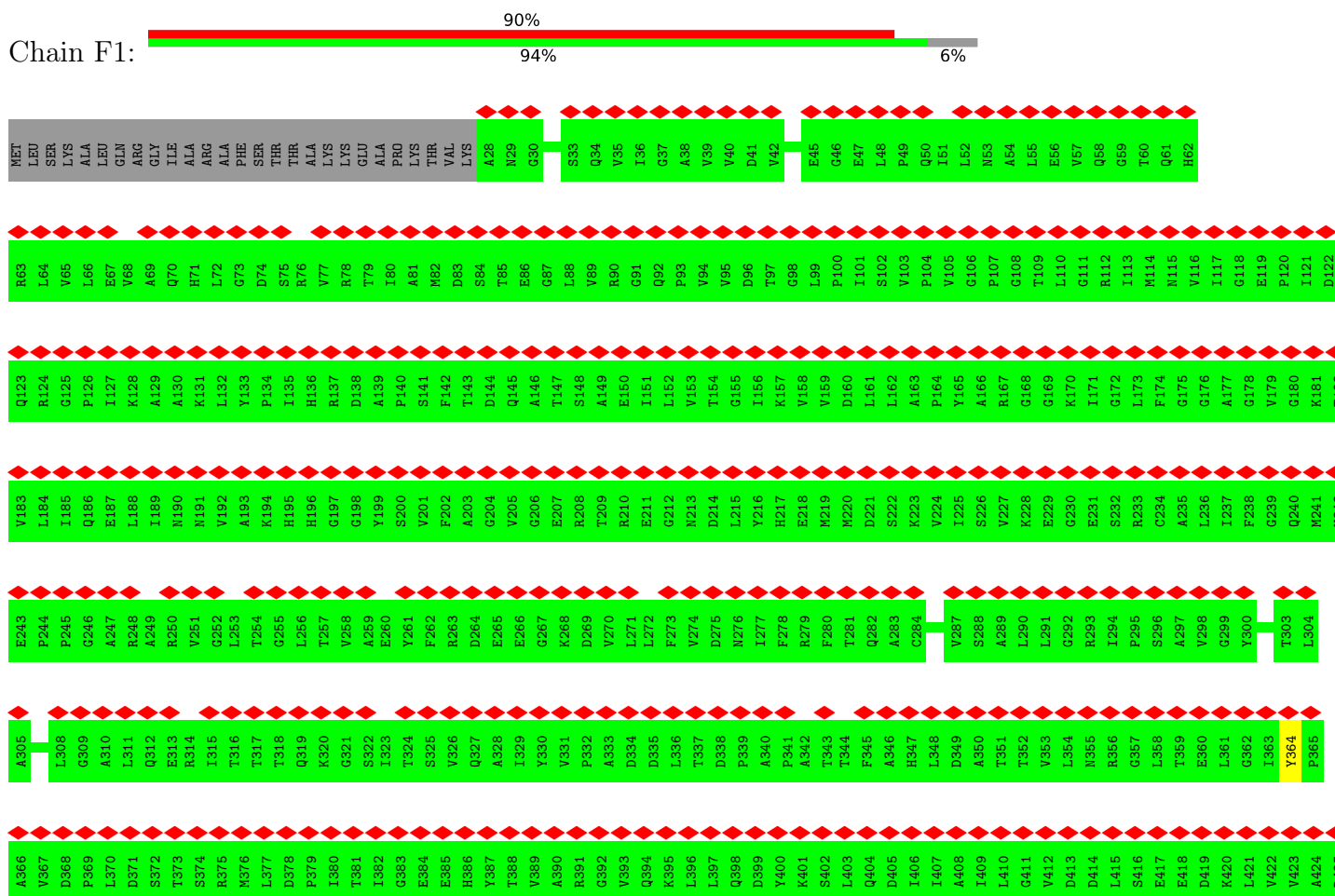
Chain D1:

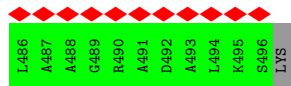
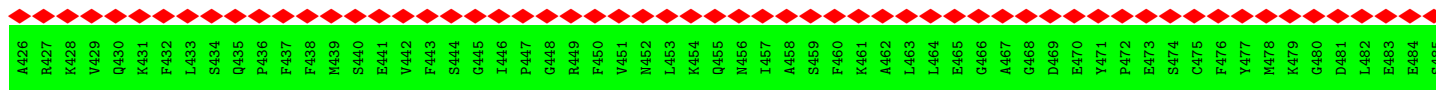




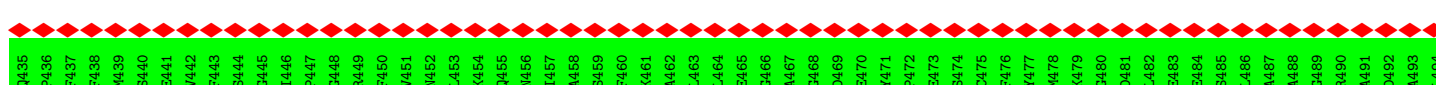
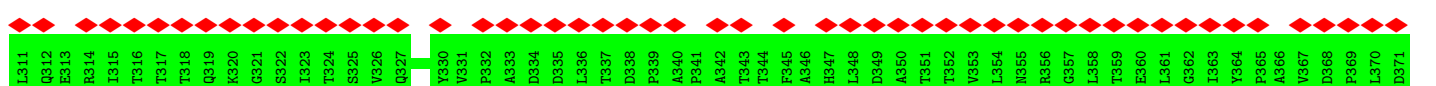
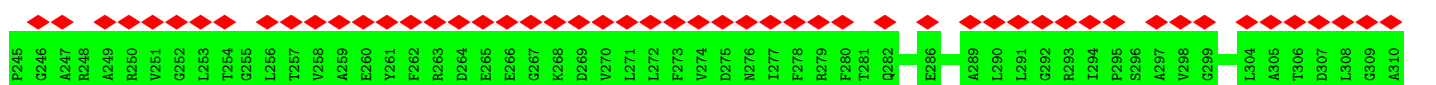
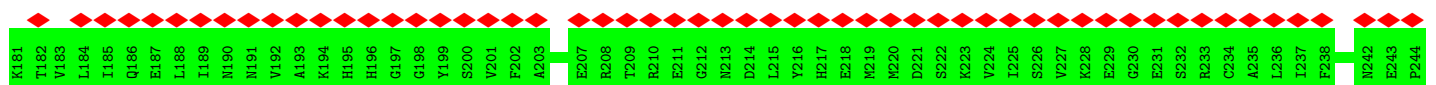
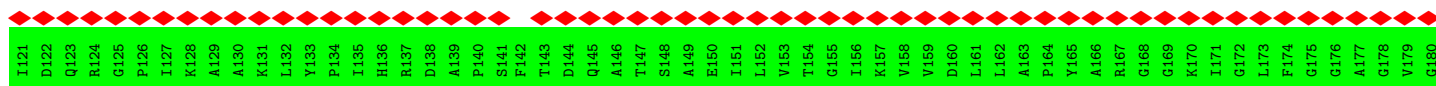
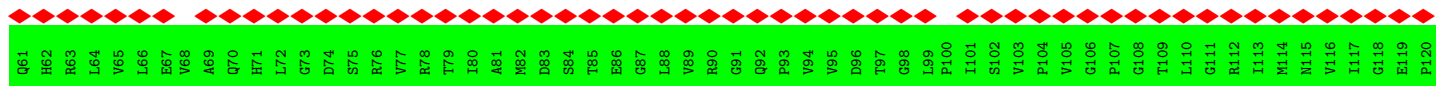
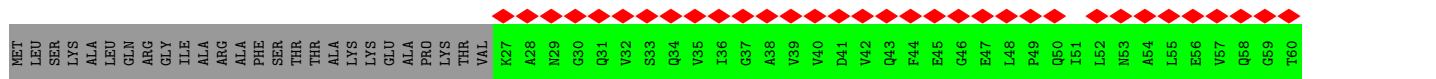
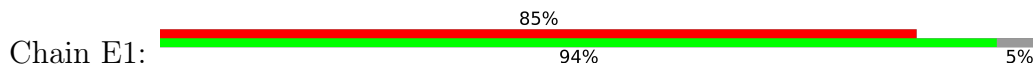
• Molecule 25: subunit beta

Chain F1:

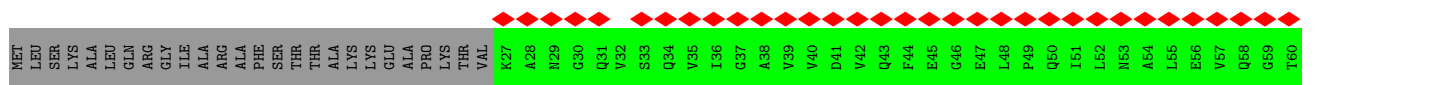


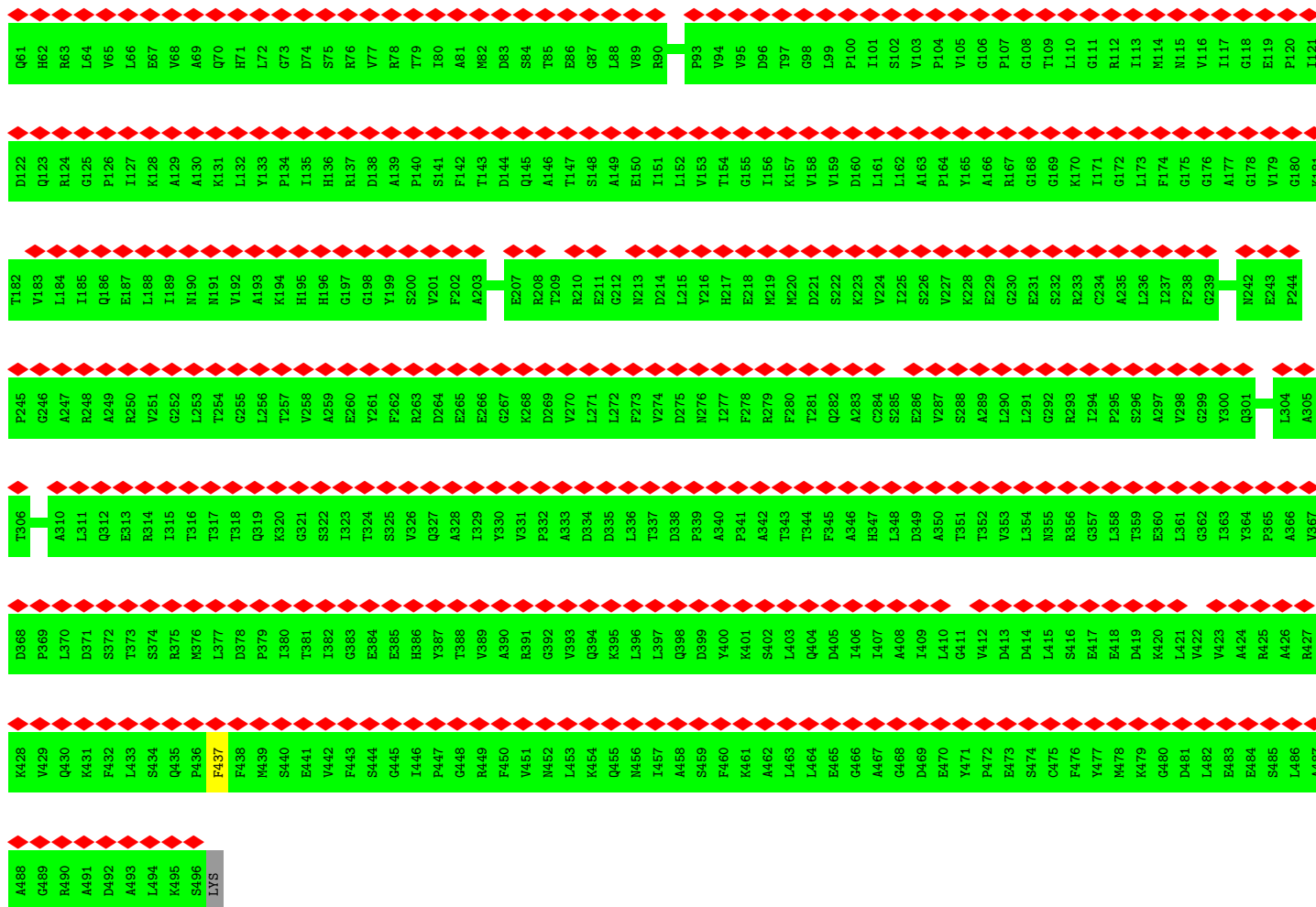


• Molecule 25: subunit beta

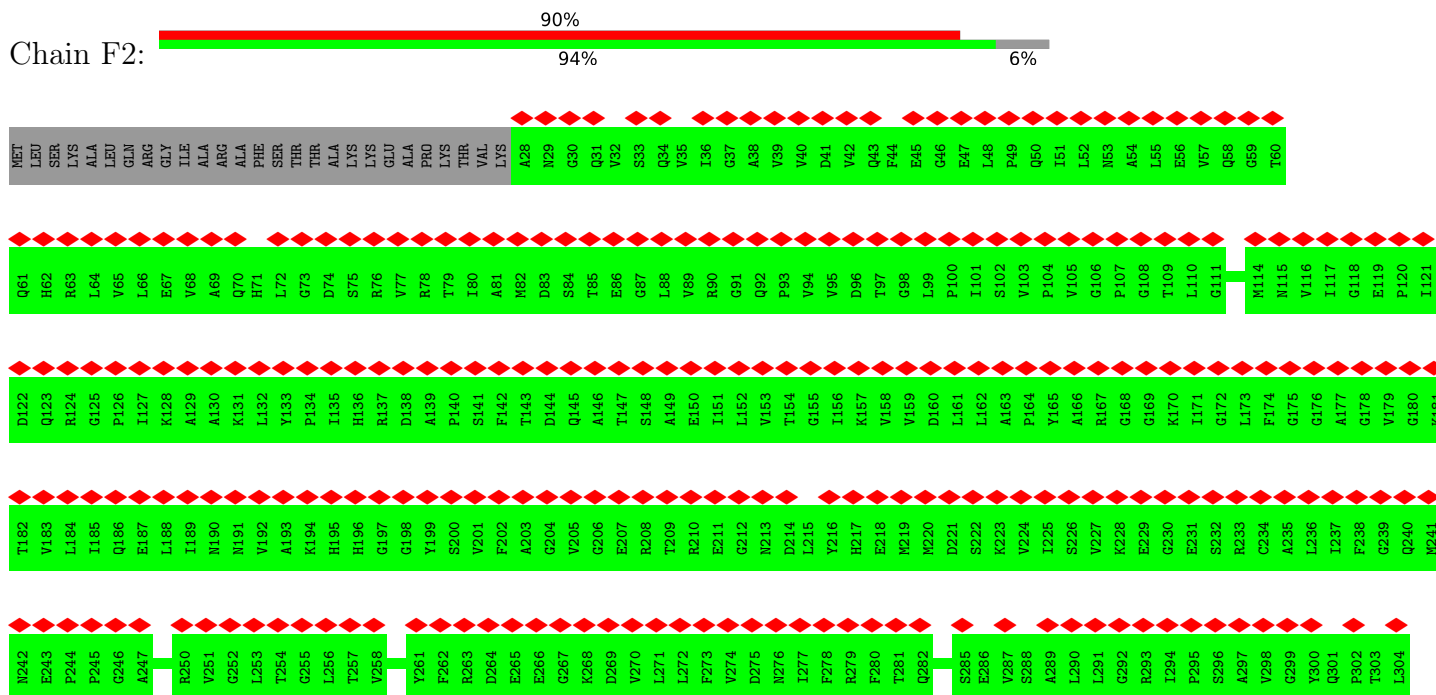


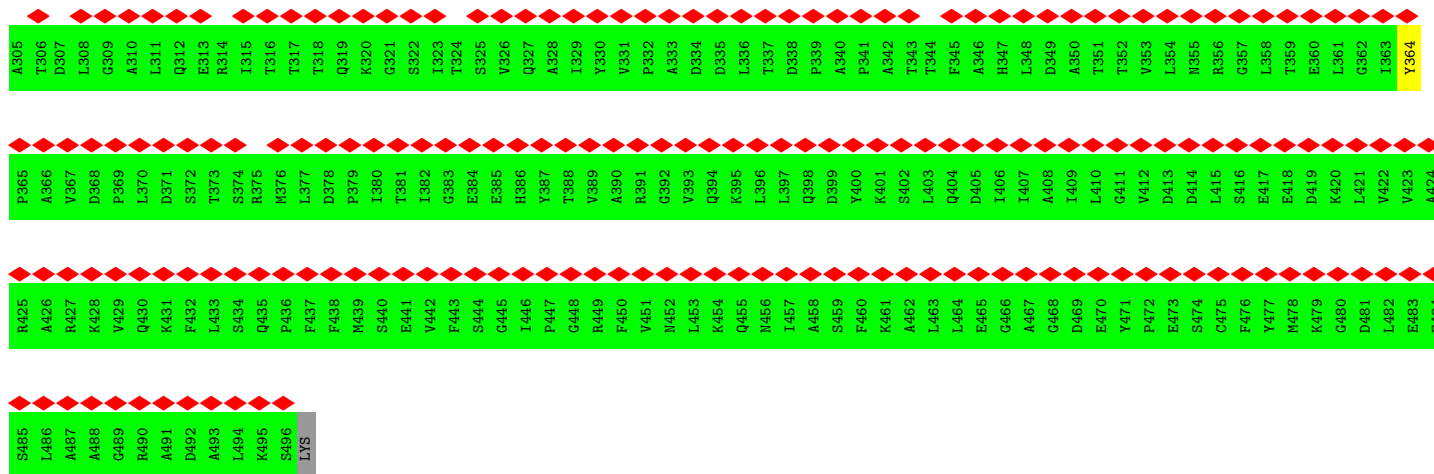
• Molecule 25: subunit beta



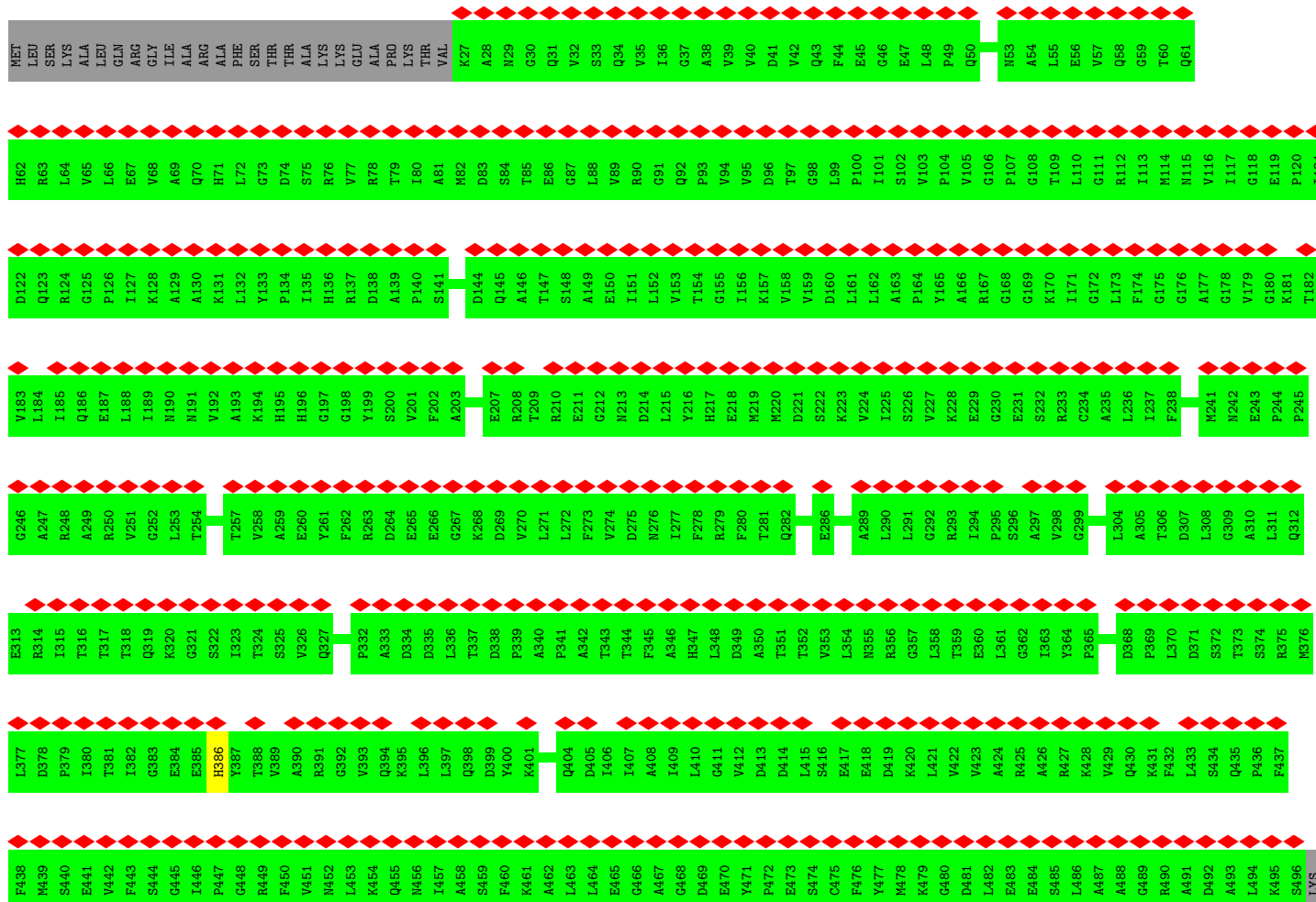
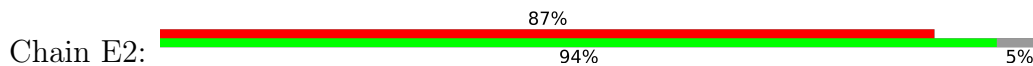


- Molecule 25: subunit beta





• Molecule 25: subunit beta



• Molecule 26: subunit c

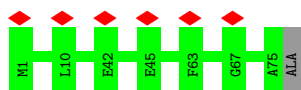




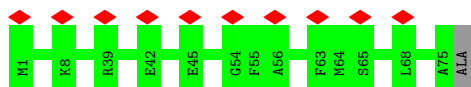
- Molecule 26: subunit c



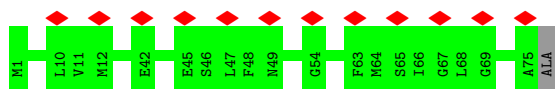
- Molecule 26: subunit c



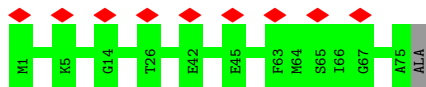
- Molecule 26: subunit c



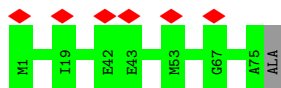
- Molecule 26: subunit c



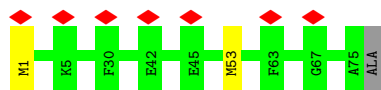
- Molecule 26: subunit c



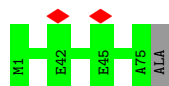
- Molecule 26: subunit c



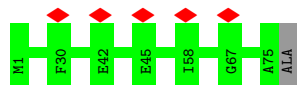
- Molecule 26: subunit c



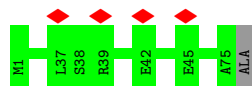
- Molecule 26: subunit c



- Molecule 26: subunit c



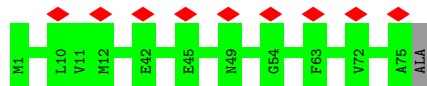
- Molecule 26: subunit c



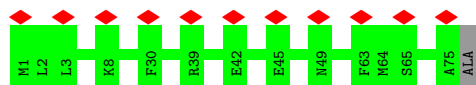
- Molecule 26: subunit c



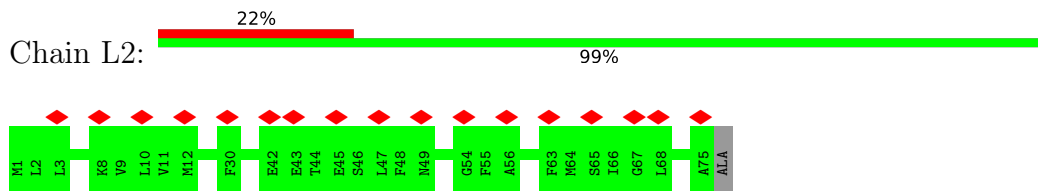
- Molecule 26: subunit c



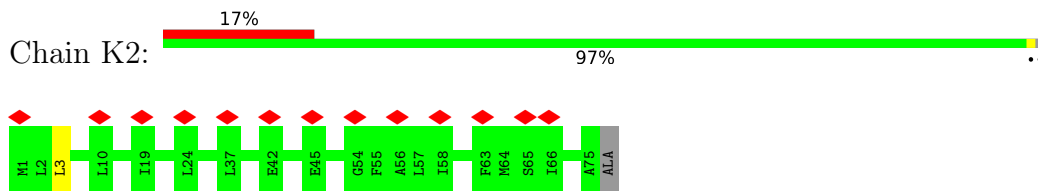
- Molecule 26: subunit c



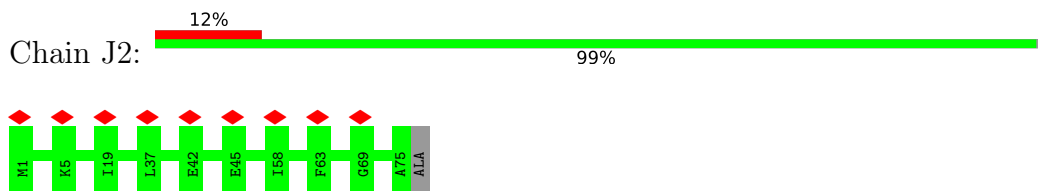
• Molecule 26: subunit c



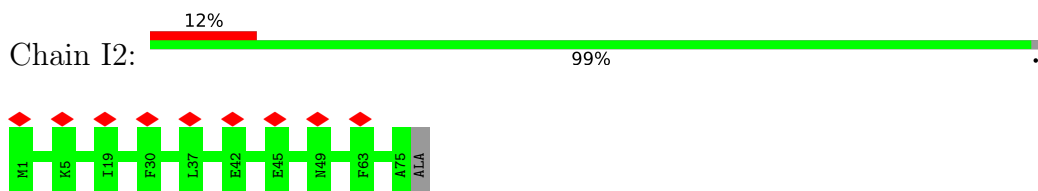
• Molecule 26: subunit c



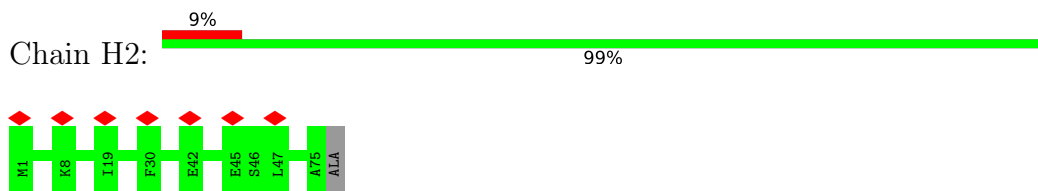
• Molecule 26: subunit c



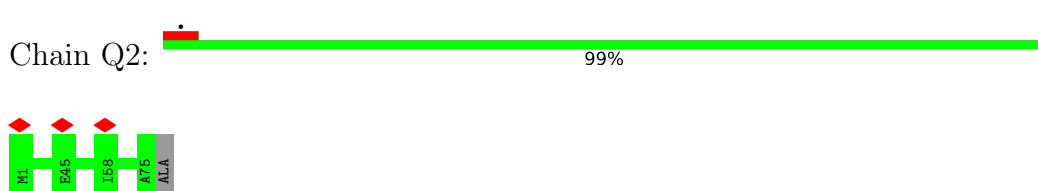
• Molecule 26: subunit c



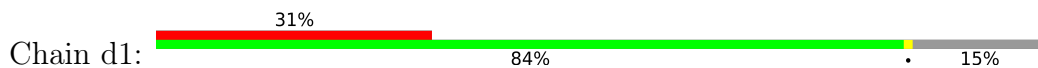
• Molecule 26: subunit c



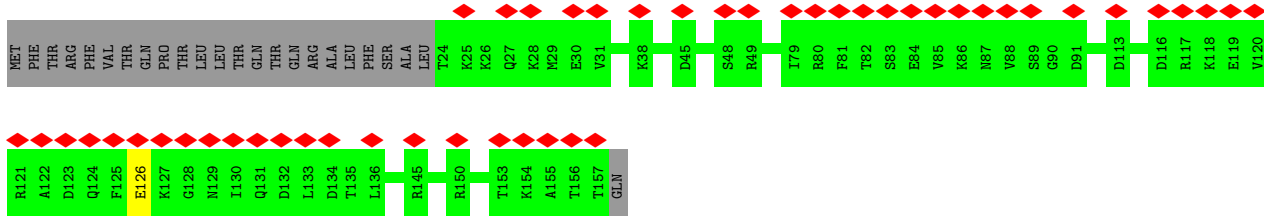
• Molecule 26: subunit c



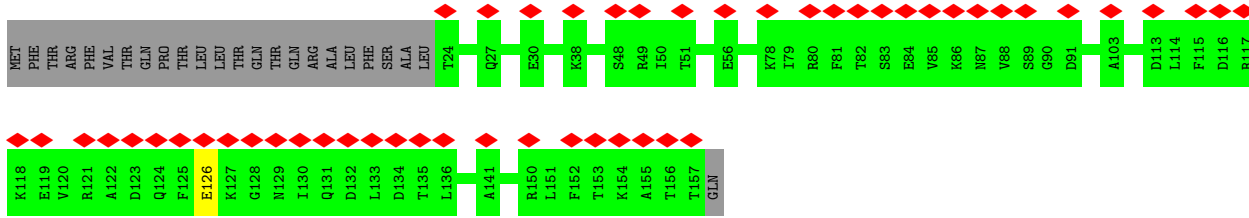
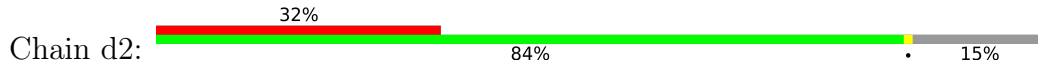
• Molecule 27: subunit delta



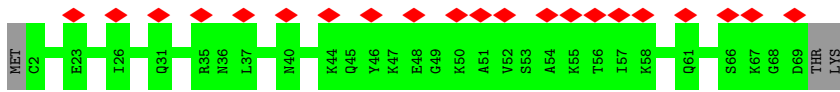




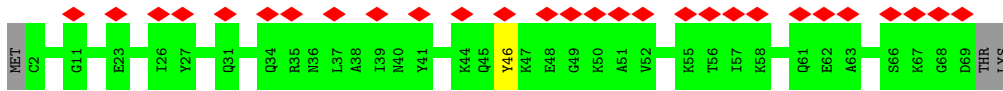
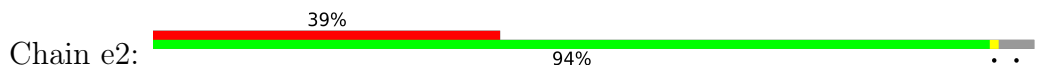
• Molecule 27: subunit delta



• 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: ATP, NAD, CDL, MG, UQ8, PO4, ADP, PC1, PEE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	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

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

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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%)	47	73
24	B2	509/546 (93%)	500 (98%)	8 (2%)	1 (0%)	47	73
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 [i](#)

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

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



analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	397/409 (97%)	395 (100%)	2 (0%)	88	96
1	a	397/409 (97%)	395 (100%)	2 (0%)	88	96
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%)	86	95
4	f	175/178 (98%)	174 (99%)	1 (1%)	86	95
5	I	182/182 (100%)	180 (99%)	2 (1%)	73	90
5	i	182/182 (100%)	181 (100%)	1 (0%)	88	96
6	K	152/152 (100%)	152 (100%)	0	100	100
6	k	152/152 (100%)	151 (99%)	1 (1%)	84	94
7	C	93/97 (96%)	92 (99%)	1 (1%)	73	90
7	c	93/97 (96%)	92 (99%)	1 (1%)	73	90
8	G	235/262 (90%)	234 (100%)	1 (0%)	91	97
8	g	235/262 (90%)	234 (100%)	1 (0%)	91	97
9	H	208/245 (85%)	207 (100%)	1 (0%)	88	96
9	h	208/245 (85%)	207 (100%)	1 (0%)	88	96
10	J	235/239 (98%)	234 (100%)	1 (0%)	91	97
10	j	235/239 (98%)	235 (100%)	0	100	100
11	L	219/220 (100%)	217 (99%)	2 (1%)	78	92
11	l	219/220 (100%)	218 (100%)	1 (0%)	88	96
12	M	202/202 (100%)	202 (100%)	0	100	100
12	m	202/202 (100%)	201 (100%)	1 (0%)	88	96
13	N	104/162 (64%)	104 (100%)	0	100	100
13	n	104/162 (64%)	103 (99%)	1 (1%)	76	91
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%)	81	93
17	r	125/129 (97%)	124 (99%)	1 (1%)	81	93
18	S	112/131 (86%)	112 (100%)	0	100	100
18	s	111/131 (85%)	109 (98%)	2 (2%)	59	83
19	E	359/414 (87%)	357 (99%)	2 (1%)	86	95
19	e	359/414 (87%)	358 (100%)	1 (0%)	92	98
20	i1	64/101 (63%)	64 (100%)	0	100	100
20	i2	61/101 (60%)	59 (97%)	2 (3%)	38	67
21	t	325/414 (78%)	322 (99%)	3 (1%)	78	92
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%)	60	84
23	g2	234/254 (92%)	231 (99%)	3 (1%)	69	87
24	A1	422/453 (93%)	419 (99%)	3 (1%)	84	94
24	A2	422/453 (93%)	419 (99%)	3 (1%)	84	94
24	B1	422/453 (93%)	419 (99%)	3 (1%)	84	94
24	B2	422/453 (93%)	421 (100%)	1 (0%)	93	98
24	C1	424/453 (94%)	423 (100%)	1 (0%)	93	98
24	C2	424/453 (94%)	423 (100%)	1 (0%)	93	98
25	D1	381/402 (95%)	380 (100%)	1 (0%)	92	98
25	D2	381/402 (95%)	380 (100%)	1 (0%)	92	98
25	E1	381/402 (95%)	380 (100%)	1 (0%)	92	98
25	E2	381/402 (95%)	380 (100%)	1 (0%)	92	98
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%)	37	66
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%)	60	84
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%)	78	92
27	d2	117/139 (84%)	116 (99%)	1 (1%)	78	92
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%)	91	97

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 [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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	K	202	-	99,99,99	0.88	7 (7%)	105,111,111	1.10	5 (4%)
29	CDL	k	201	6	99,99,99	0.89	8 (8%)	105,111,111	1.02	4 (3%)
30	PC1	g	303	-	53,53,53	0.96	4 (7%)	59,61,61	0.97	2 (3%)
33	ATP	g	301	34	26,33,33	4.78	7 (26%)	31,52,52	2.42	7 (22%)
33	ATP	B2	601	25,24,34	26,33,33	4.80	8 (30%)	31,52,52	2.45	8 (25%)
37	ADP	D2	501	34	24,29,29	3.68	9 (37%)	29,45,45	3.54	7 (24%)
29	CDL	L	301	-	99,99,99	0.89	7 (7%)	105,111,111	1.01	4 (3%)
29	CDL	K	201	-	99,99,99	0.88	8 (8%)	105,111,111	1.03	4 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	PC1	G	303	-	53,53,53	0.96	4 (7%)	59,61,61	0.98	2 (3%)
29	CDL	B	403	-	99,99,99	0.88	7 (7%)	105,111,111	1.05	4 (3%)
31	PO4	f	301	-	4,4,4	1.04	0	6,6,6	0.44	0
37	ADP	B2	603	24,34	24,29,29	3.71	9 (37%)	29,45,45	3.57	7 (24%)
29	CDL	p	201	-	99,99,99	0.88	8 (8%)	105,111,111	1.04	4 (3%)
30	PC1	d	301	3	53,53,53	0.93	4 (7%)	59,61,61	1.07	2 (3%)
36	NAD	E	900	-	42,48,48	3.82	19 (45%)	50,73,73	2.13	7 (14%)
29	CDL	J	301	-	99,99,99	0.89	6 (6%)	105,111,111	1.08	4 (3%)
29	CDL	A	502	-	99,99,99	0.88	7 (7%)	105,111,111	1.08	4 (3%)
32	UQ8	I	303	-	53,53,53	1.79	7 (13%)	64,67,67	1.68	17 (26%)
30	PC1	D	301	3	53,53,53	0.94	4 (7%)	59,61,61	1.10	2 (3%)
33	ATP	G	301	34	26,33,33	4.77	7 (26%)	31,52,52	2.44	7 (22%)
37	ADP	B1	603	24,34	24,29,29	3.70	9 (37%)	29,45,45	3.58	7 (24%)
29	CDL	L	302	-	99,99,99	0.88	7 (7%)	105,111,111	1.03	3 (2%)
37	ADP	D1	501	34	24,29,29	3.65	9 (37%)	29,45,45	3.77	7 (24%)
29	CDL	B	401	-	99,99,99	0.87	8 (8%)	105,111,111	0.99	4 (3%)
33	ATP	C2	601	34	26,33,33	4.79	8 (30%)	31,52,52	2.43	7 (22%)
29	CDL	j	301	-	99,99,99	0.88	7 (7%)	105,111,111	1.09	4 (3%)
29	CDL	j	302	-	99,99,99	0.88	7 (7%)	105,111,111	1.01	4 (3%)
33	ATP	B1	601	25,24,34	26,33,33	4.80	9 (34%)	31,52,52	2.45	8 (25%)
29	CDL	P	201	-	99,99,99	0.88	7 (7%)	105,111,111	1.03	5 (4%)
35	PEE	m	301	-	50,50,50	1.15	6 (12%)	53,55,55	1.08	4 (7%)
29	CDL	f	302	-	99,99,99	0.87	7 (7%)	105,111,111	1.04	4 (3%)
29	CDL	f	304	-	99,99,99	0.89	7 (7%)	105,111,111	1.05	4 (3%)
36	NAD	e	900	-	42,48,48	3.83	19 (45%)	50,73,73	2.14	7 (14%)
30	PC1	G	304	8	53,53,53	0.95	4 (7%)	59,61,61	1.00	2 (3%)
29	CDL	I	302	-	99,99,99	0.88	8 (8%)	105,111,111	1.04	4 (3%)
35	PEE	J	303	-	50,50,50	1.15	6 (12%)	53,55,55	1.16	3 (5%)
29	CDL	r	201	-	99,99,99	0.87	8 (8%)	105,111,111	1.03	4 (3%)
29	CDL	b	401	4,2	99,99,99	0.87	8 (8%)	105,111,111	1.11	4 (3%)
33	ATP	C1	601	34	26,33,33	4.79	8 (30%)	31,52,52	2.40	7 (22%)
35	PEE	A	501	-	47,47,50	1.18	6 (12%)	50,52,55	1.16	2 (4%)
33	ATP	A1	601	34	26,33,33	4.82	8 (30%)	31,52,52	2.41	7 (22%)
29	CDL	B	402	2	99,99,99	0.87	7 (7%)	105,111,111	1.13	5 (4%)
33	ATP	A2	601	34	26,33,33	4.83	8 (30%)	31,52,52	2.40	7 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CDL	B	404	2	99,99,99	0.88	8 (8%)	105,111,111	1.09	5 (4%)
35	PEE	L	303	-	47,47,50	1.17	6 (12%)	50,52,55	1.16	3 (6%)
29	CDL	k	202	-	99,99,99	0.88	7 (7%)	105,111,111	1.12	5 (4%)
29	CDL	F	302	-	99,99,99	0.88	8 (8%)	105,111,111	1.07	4 (3%)
29	CDL	l	301	-	99,99,99	0.88	6 (6%)	105,111,111	1.05	5 (4%)
29	CDL	i	301	-	99,99,99	0.88	8 (8%)	105,111,111	1.07	4 (3%)
31	PO4	F	301	-	4,4,4	1.04	0	6,6,6	0.44	0
29	CDL	l	302	-	99,99,99	0.89	8 (8%)	105,111,111	1.05	4 (3%)
29	CDL	J	302	-	99,99,99	0.87	8 (8%)	105,111,111	1.00	4 (3%)
29	CDL	f	303	-	99,99,99	0.88	8 (8%)	105,111,111	1.09	5 (4%)
32	UQ8	i	302	-	53,53,53	1.79	7 (13%)	64,67,67	1.65	16 (25%)
29	CDL	a	501	-	99,99,99	0.89	7 (7%)	105,111,111	1.05	5 (4%)
29	CDL	I	301	5	99,99,99	0.87	7 (7%)	105,111,111	0.99	4 (3%)
29	CDL	a	502	-	99,99,99	0.88	8 (8%)	105,111,111	1.09	6 (5%)
30	PC1	g	304	8	53,53,53	0.96	4 (7%)	59,61,61	0.93	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CDL	K	202	-	-	36/110/110/110	-
29	CDL	k	201	6	-	37/110/110/110	-
30	PC1	g	303	-	-	22/57/57/57	-
33	ATP	g	301	34	-	0/18/38/38	0/3/3/3
33	ATP	B2	601	25,24,34	-	2/18/38/38	0/3/3/3
37	ADP	D2	501	34	-	2/12/32/32	0/3/3/3
29	CDL	L	301	-	-	38/110/110/110	-
29	CDL	K	201	-	-	27/110/110/110	-
30	PC1	G	303	-	-	29/57/57/57	-
29	CDL	B	403	-	-	33/110/110/110	-
37	ADP	B2	603	24,34	-	2/12/32/32	0/3/3/3
29	CDL	p	201	-	-	44/110/110/110	-
30	PC1	d	301	3	-	23/57/57/57	-
36	NAD	E	900	-	-	7/26/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CDL	J	301	-	-	42/110/110/110	-
29	CDL	A	502	-	-	46/110/110/110	-
32	UQ8	I	303	-	-	9/51/75/75	0/1/1/1
30	PC1	D	301	3	-	21/57/57/57	-
33	ATP	G	301	34	-	0/18/38/38	0/3/3/3
37	ADP	B1	603	24,34	-	1/12/32/32	0/3/3/3
29	CDL	L	302	-	-	45/110/110/110	-
37	ADP	D1	501	34	-	2/12/32/32	0/3/3/3
29	CDL	B	401	-	-	43/110/110/110	-
33	ATP	C2	601	34	-	4/18/38/38	0/3/3/3
29	CDL	j	301	-	-	40/110/110/110	-
29	CDL	j	302	-	-	41/110/110/110	-
33	ATP	B1	601	25,24,34	-	2/18/38/38	0/3/3/3
29	CDL	P	201	-	-	36/110/110/110	-
35	PEE	m	301	-	-	24/54/54/54	-
29	CDL	f	302	-	-	54/110/110/110	-
29	CDL	f	304	-	-	49/110/110/110	-
36	NAD	e	900	-	-	6/26/62/62	0/5/5/5
30	PC1	G	304	8	-	19/57/57/57	-
29	CDL	I	302	-	-	38/110/110/110	-
35	PEE	J	303	-	-	29/54/54/54	-
29	CDL	r	201	-	-	36/110/110/110	-
29	CDL	b	401	4,2	-	44/110/110/110	-
33	ATP	C1	601	34	-	5/18/38/38	0/3/3/3
35	PEE	A	501	-	-	21/51/51/54	-
33	ATP	A1	601	34	-	5/18/38/38	0/3/3/3
29	CDL	B	402	2	-	40/110/110/110	-
33	ATP	A2	601	34	-	5/18/38/38	0/3/3/3
29	CDL	B	404	2	-	46/110/110/110	-
35	PEE	L	303	-	-	22/51/51/54	-
29	CDL	k	202	-	-	35/110/110/110	-
29	CDL	F	302	-	-	47/110/110/110	-
29	CDL	l	301	-	-	39/110/110/110	-
29	CDL	i	301	-	-	38/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CDL	l	302	-	-	40/110/110/110	-
29	CDL	J	302	-	-	41/110/110/110	-
29	CDL	f	303	-	-	41/110/110/110	-
32	UQ8	i	302	-	-	8/51/75/75	0/1/1/1
29	CDL	a	501	-	-	33/110/110/110	-
29	CDL	I	301	5	-	42/110/110/110	-
29	CDL	a	502	-	-	39/110/110/110	-
30	PC1	g	304	8	-	19/57/57/57	-

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:

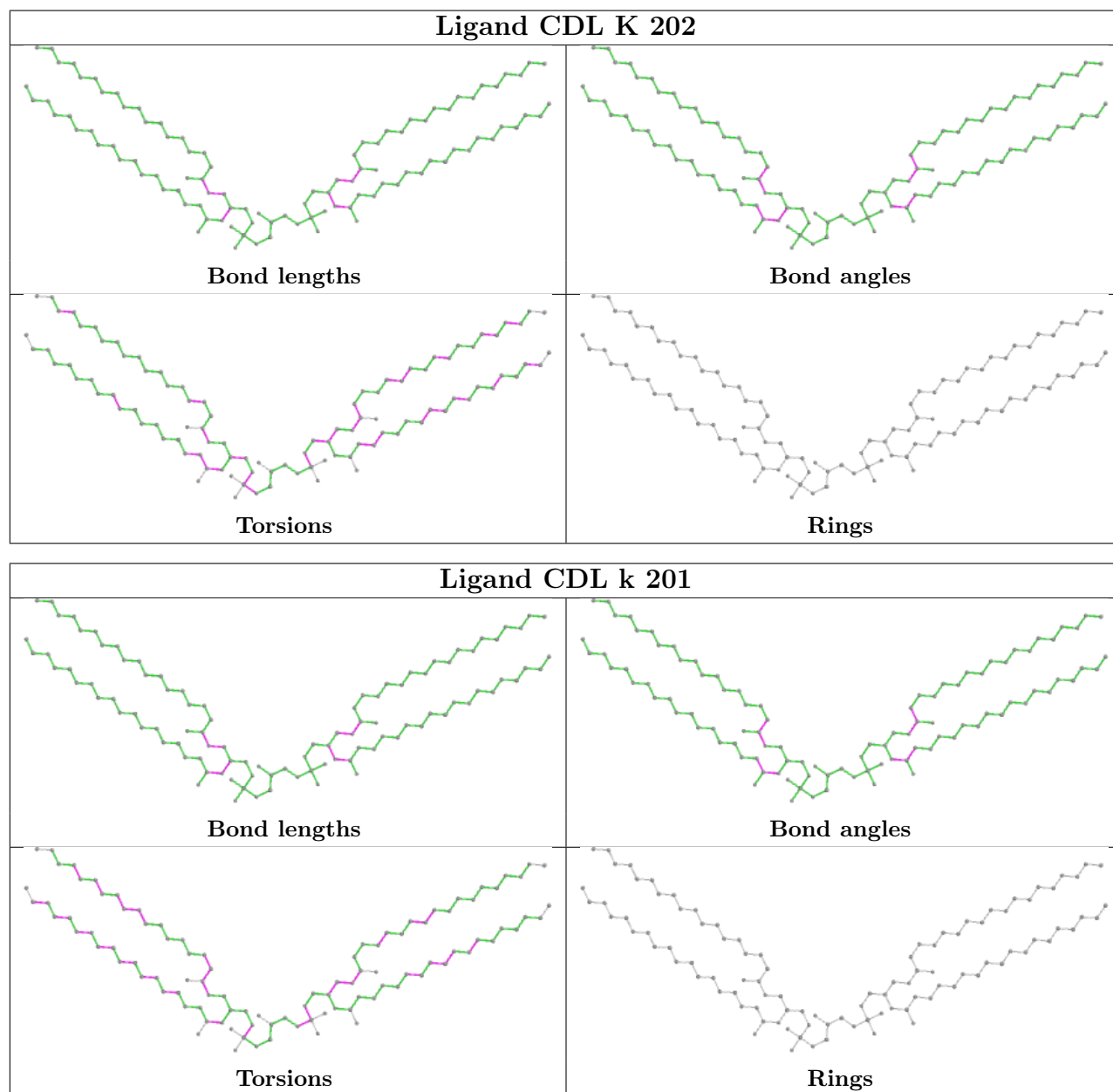
Mol	Chain	Res	Type	Atoms
29	a	501	CDL	OA5-CA3-CA4-OA6
29	a	501	CDL	CB3-OB5-PB2-OB4
29	a	501	CDL	OB7-CB5-OB6-CB4
29	a	501	CDL	C51-CB5-OB6-CB4
29	a	502	CDL	CA3-OA5-PA1-OA3

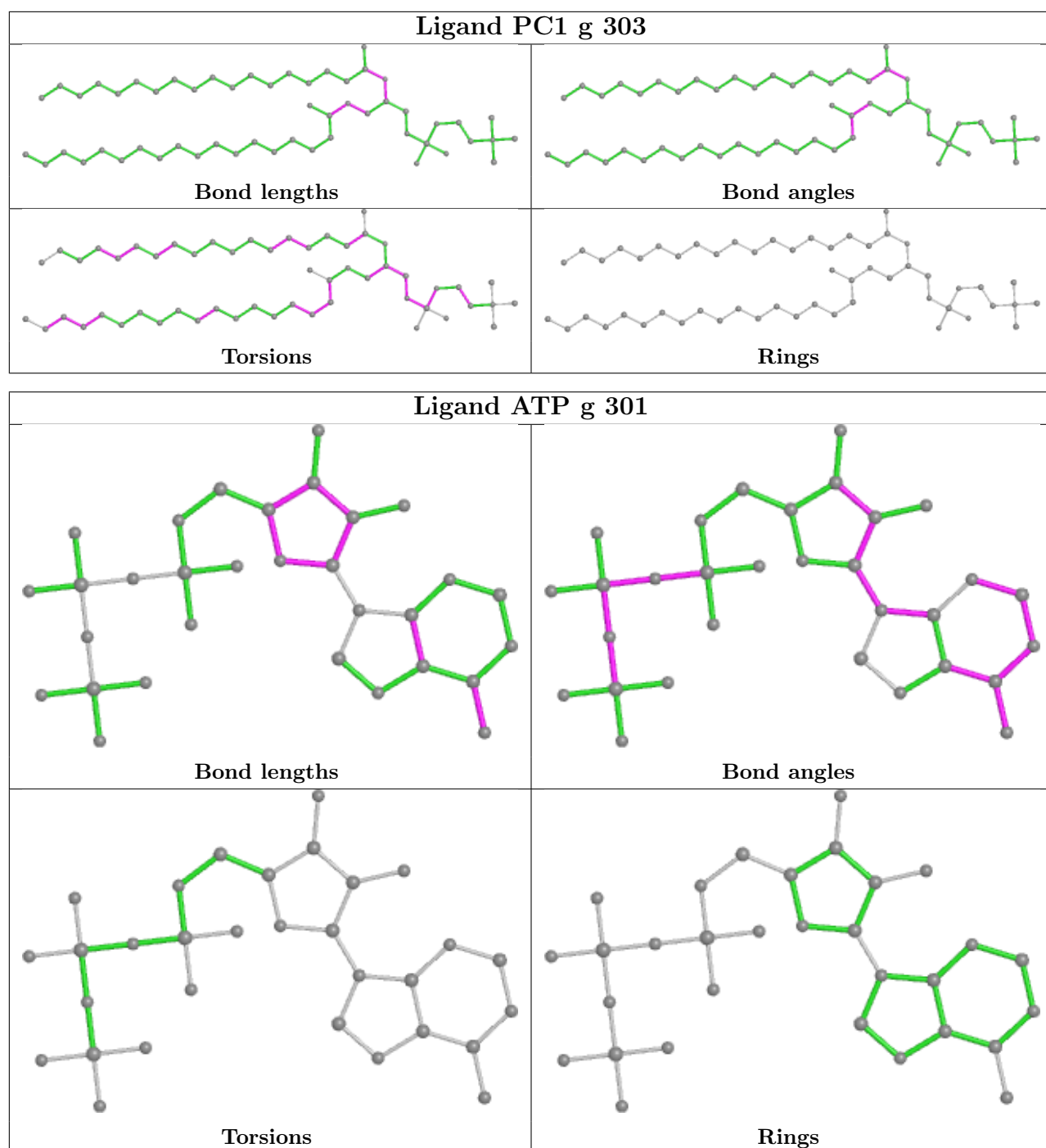
There are no ring outliers.

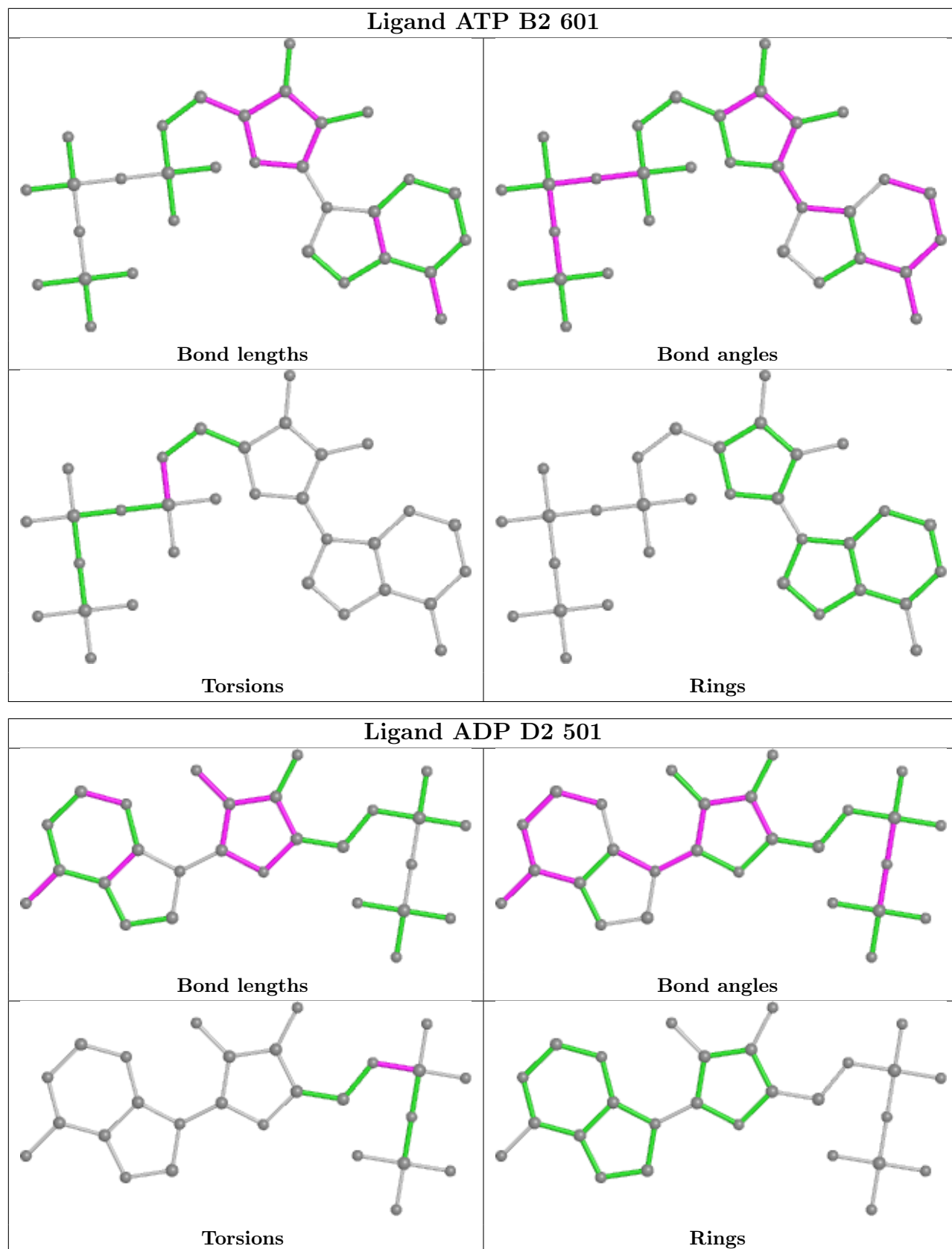
No monomer is involved in short contacts.

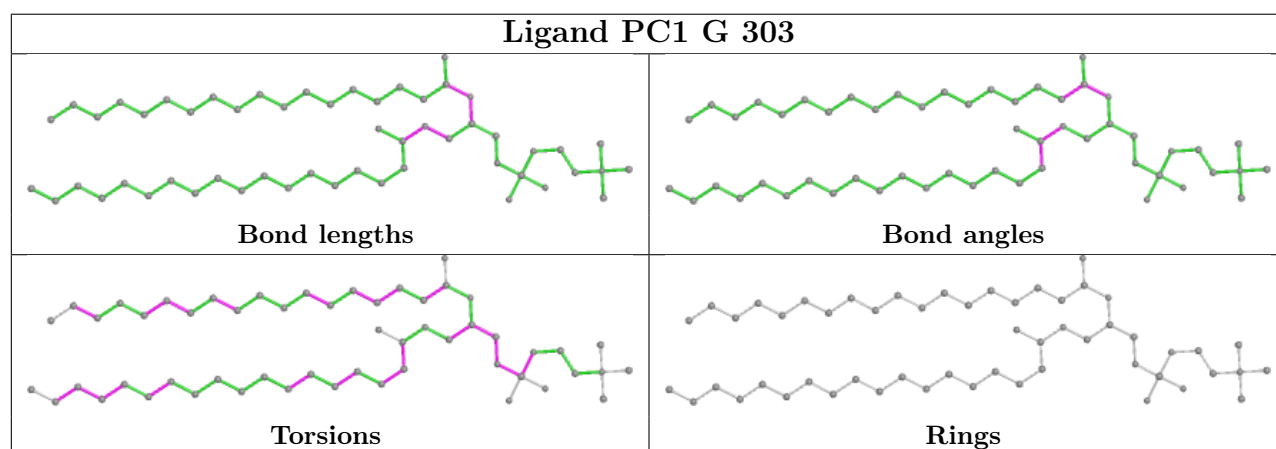
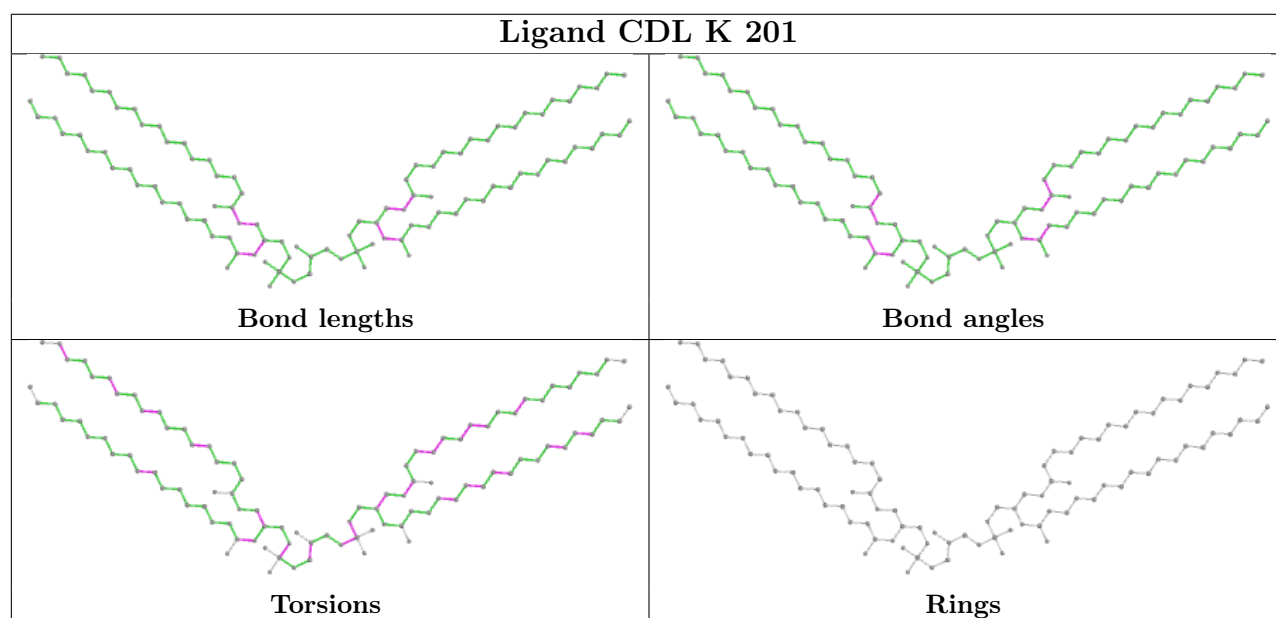
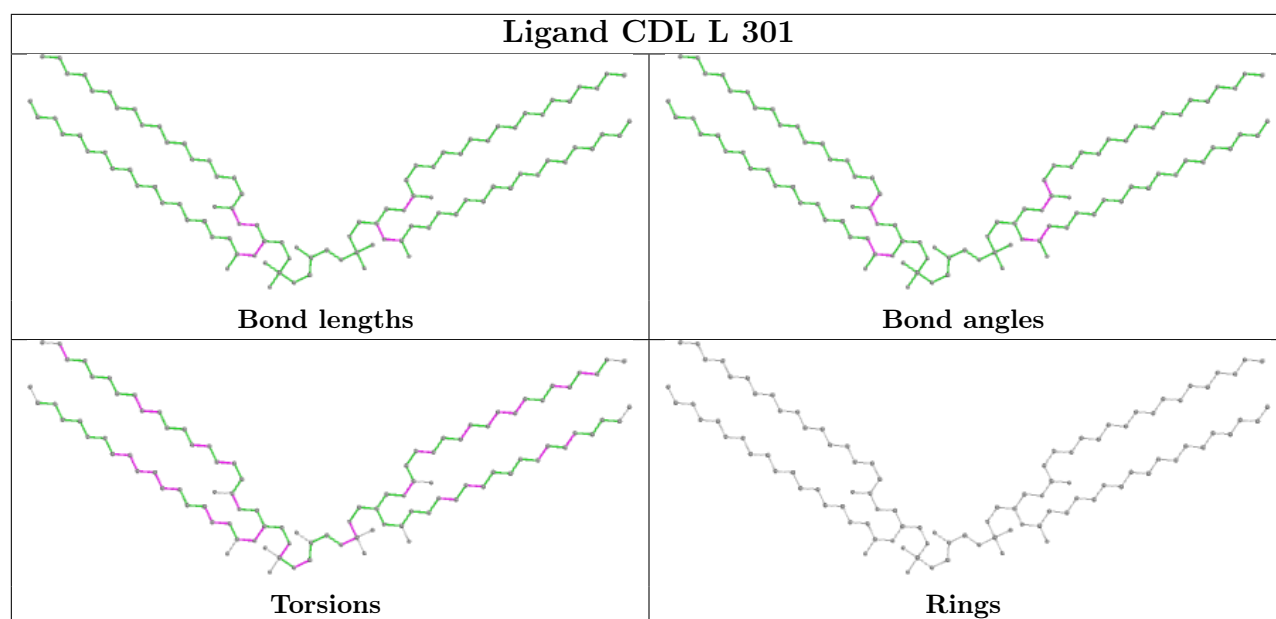


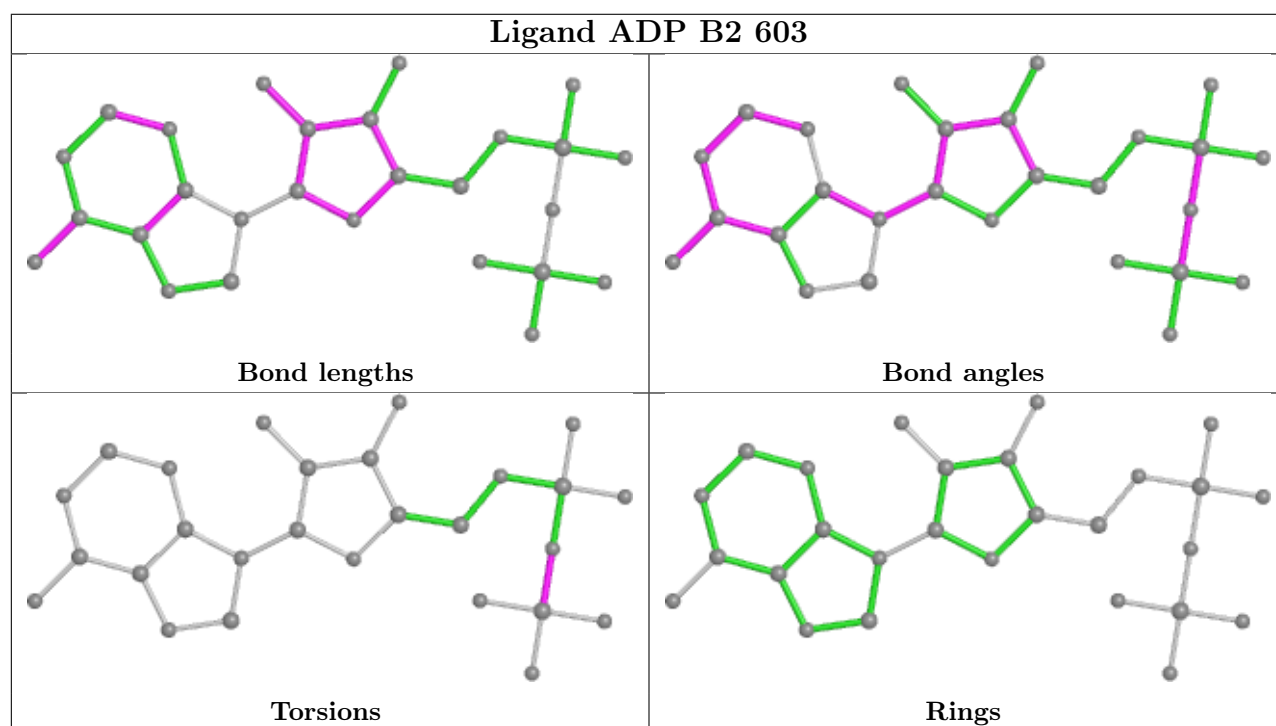
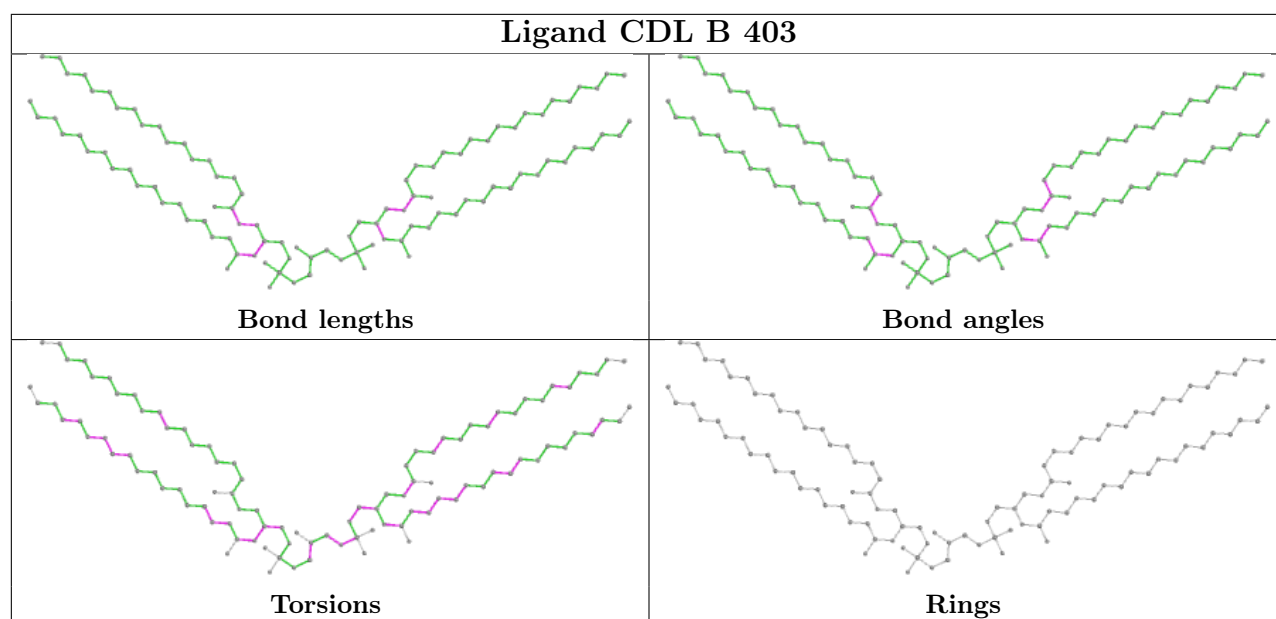
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

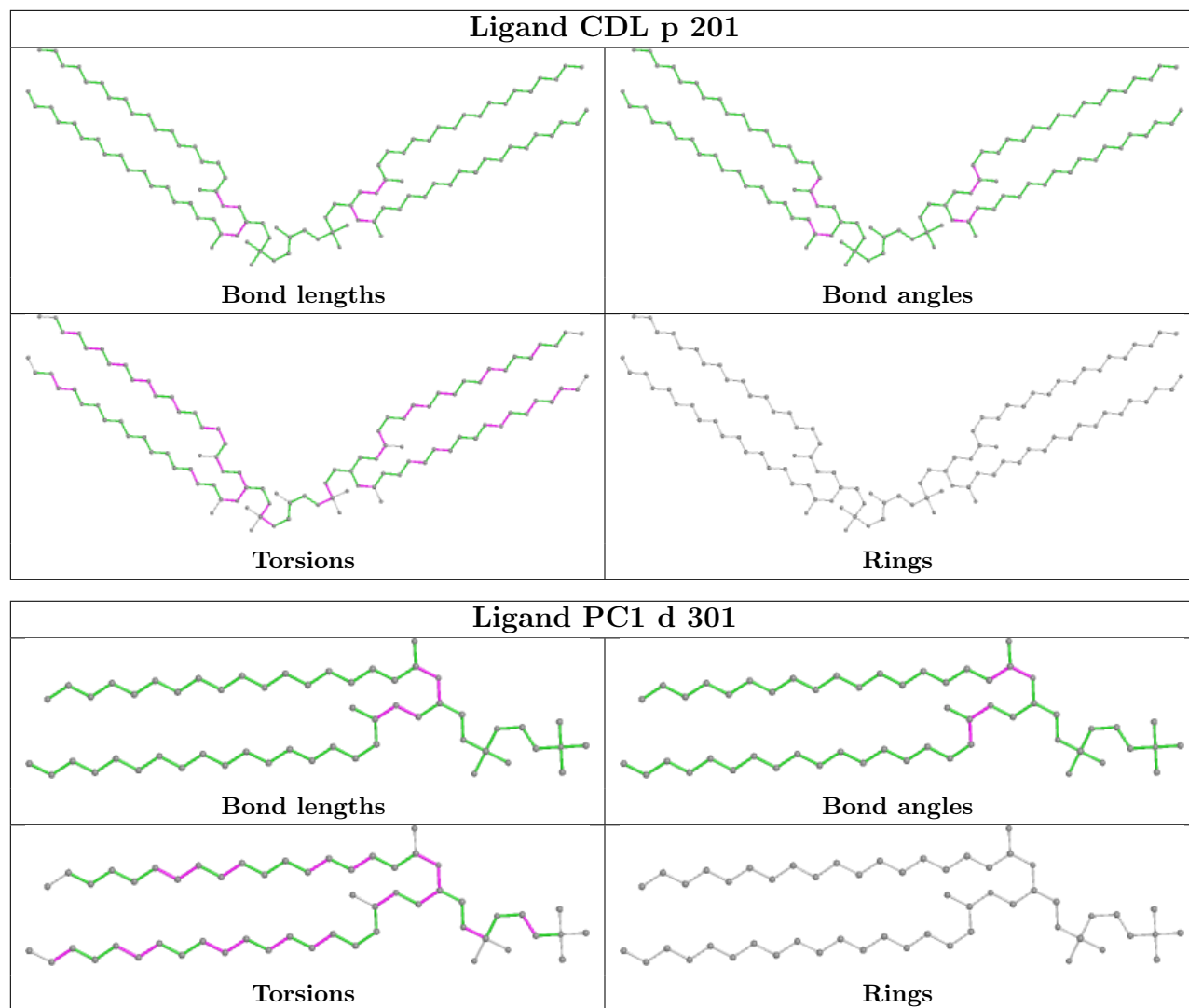


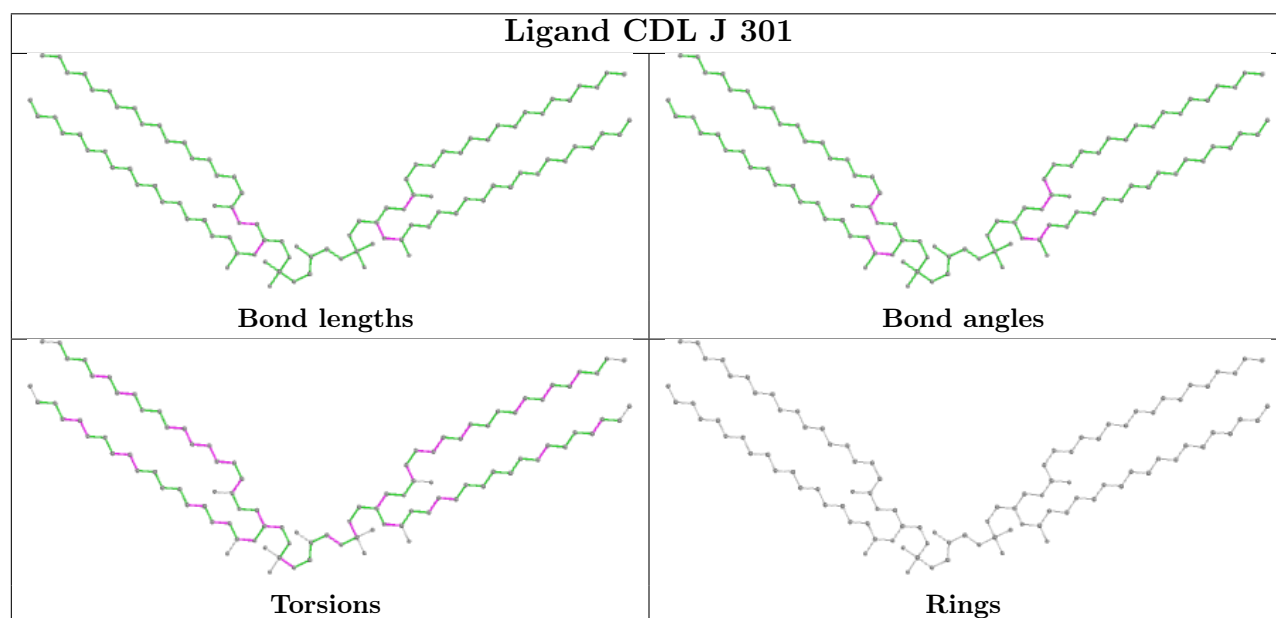
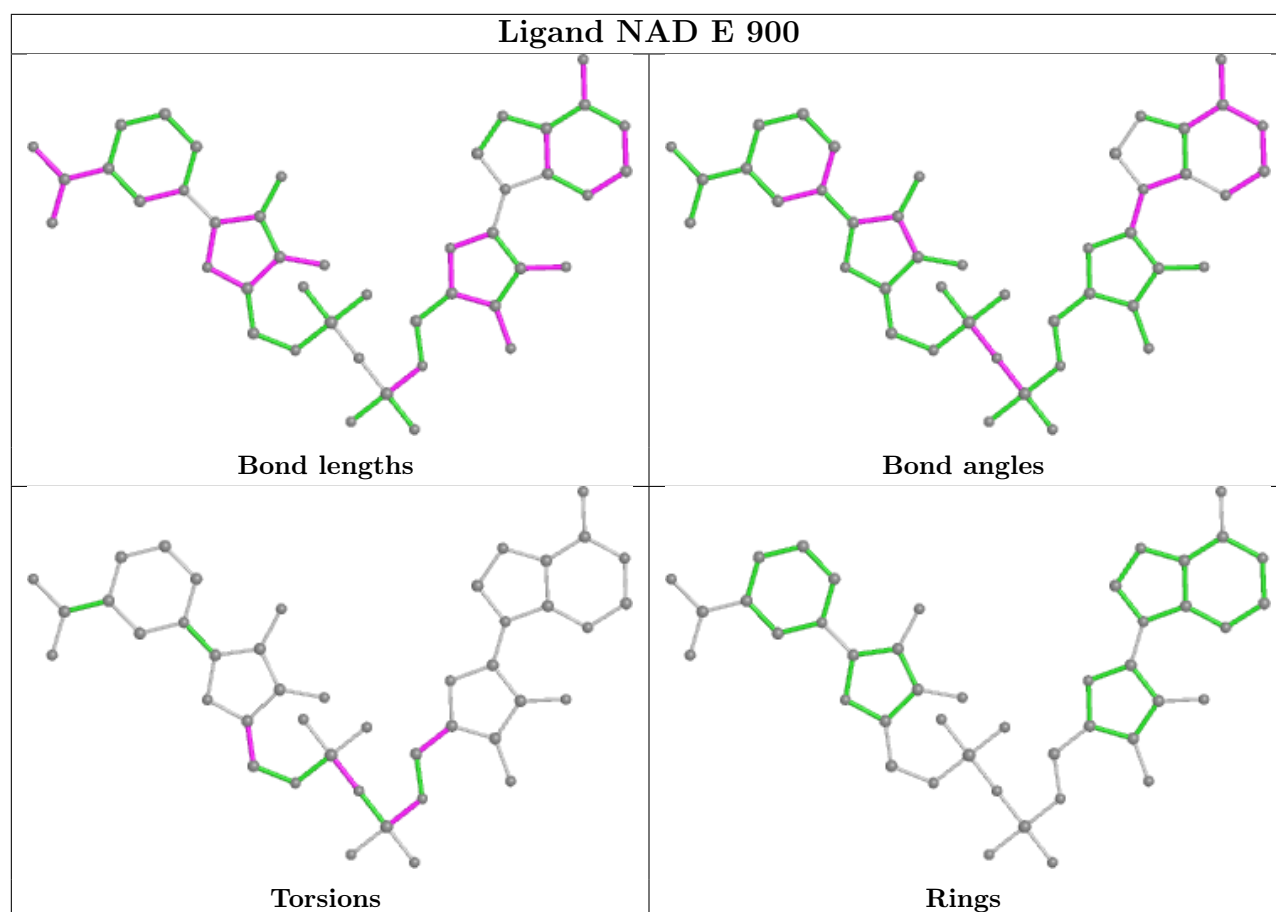


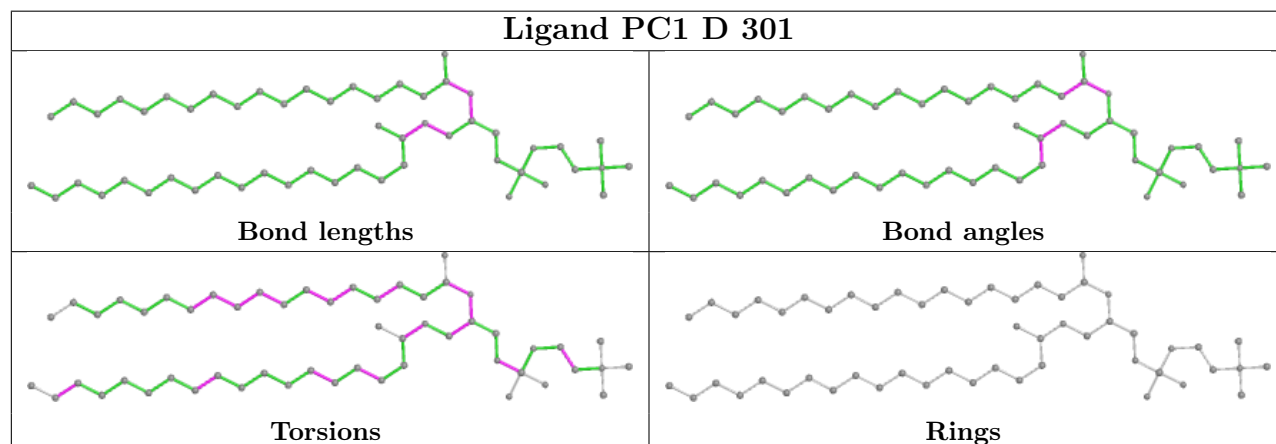
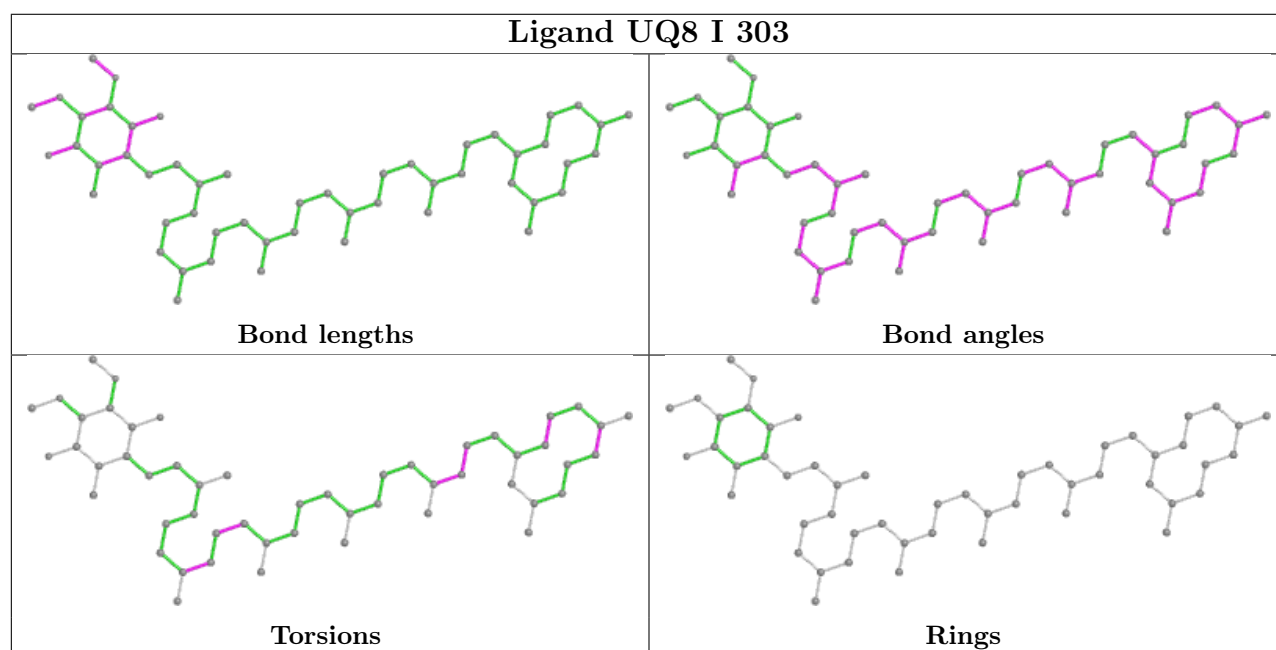
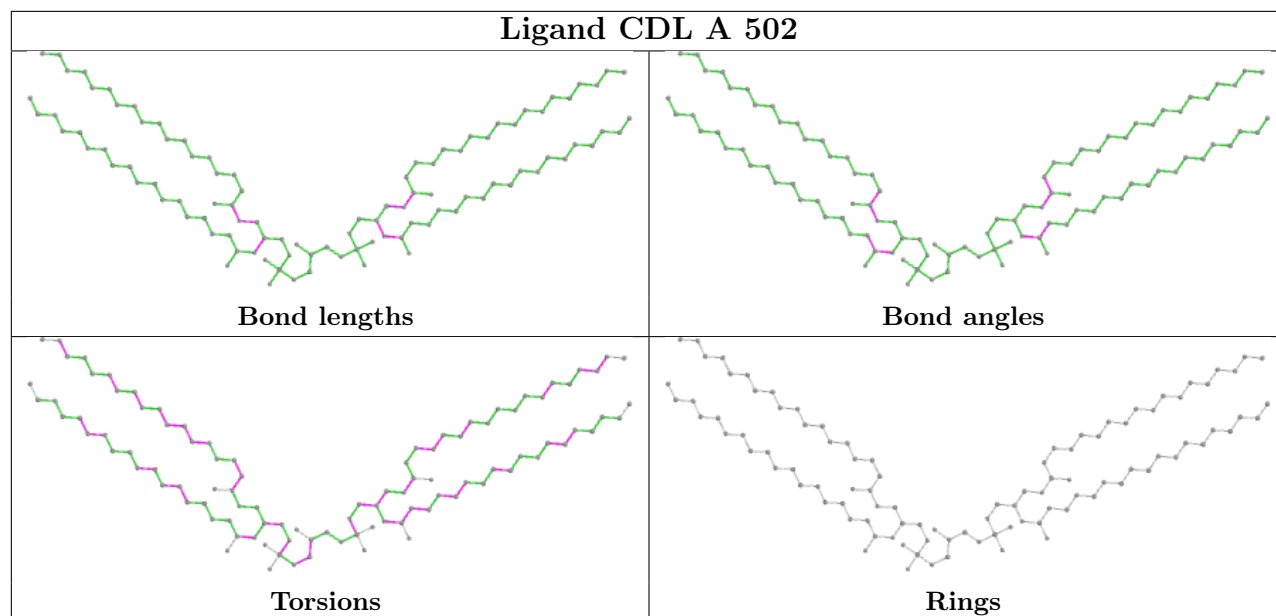




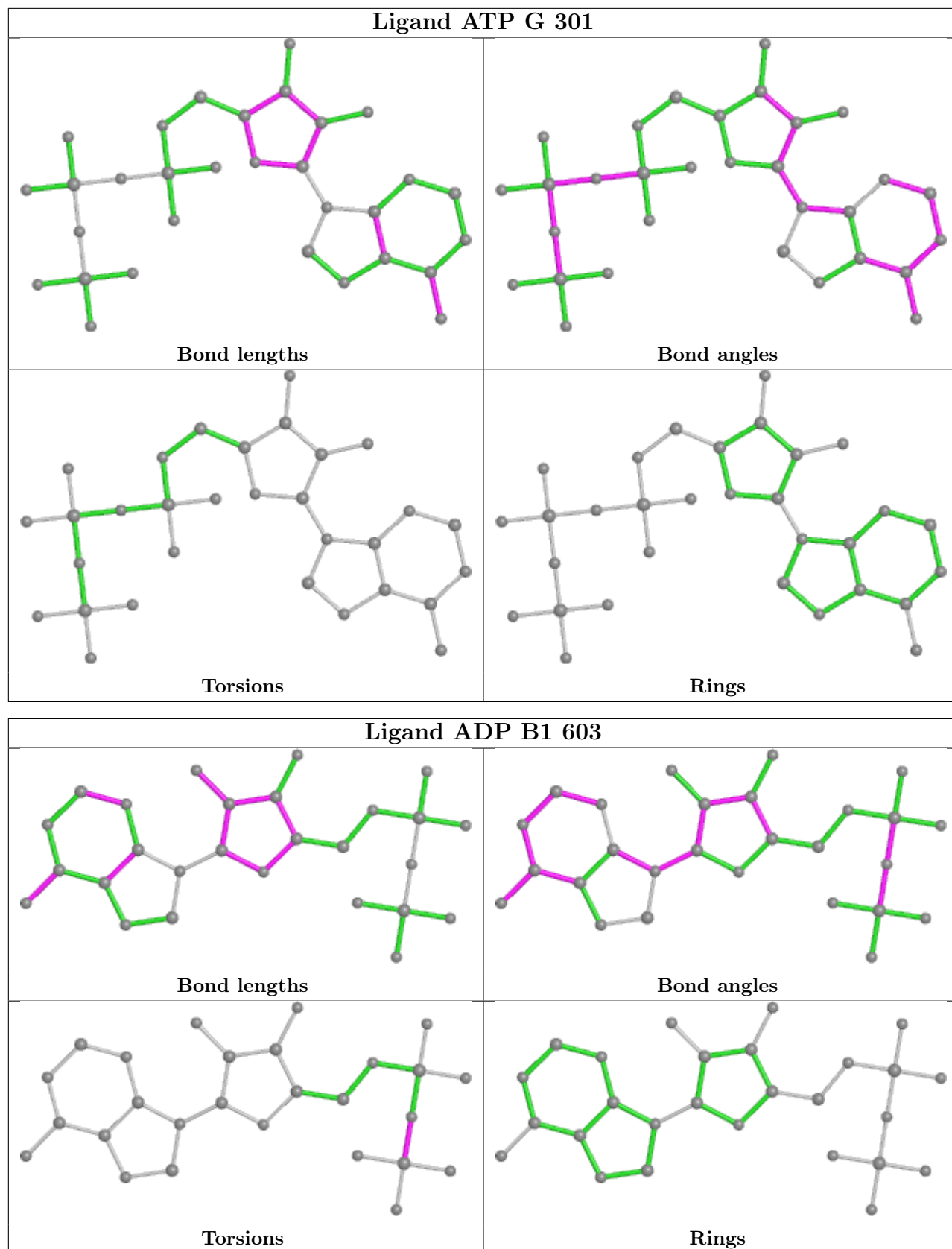


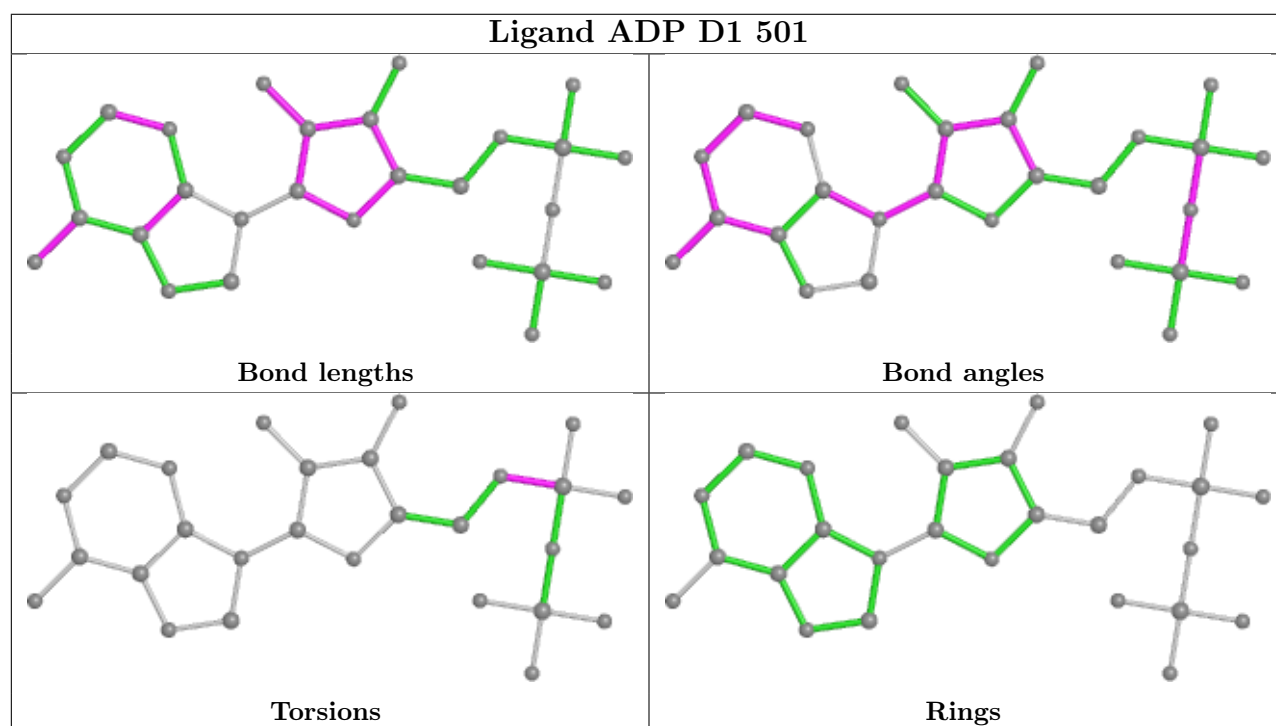
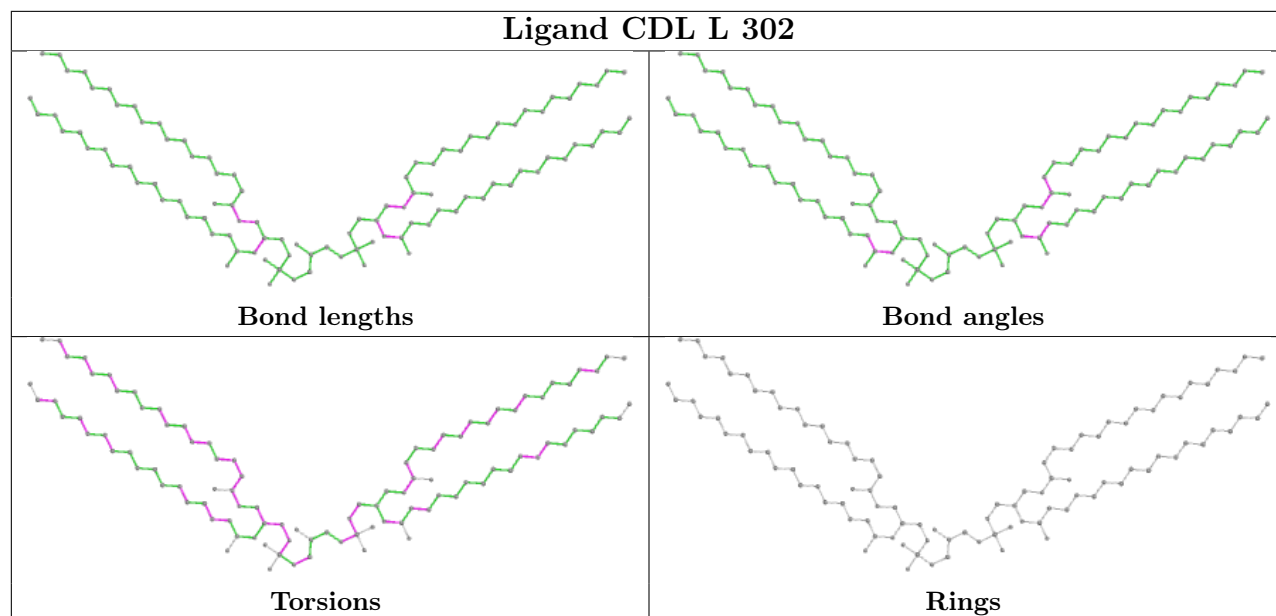


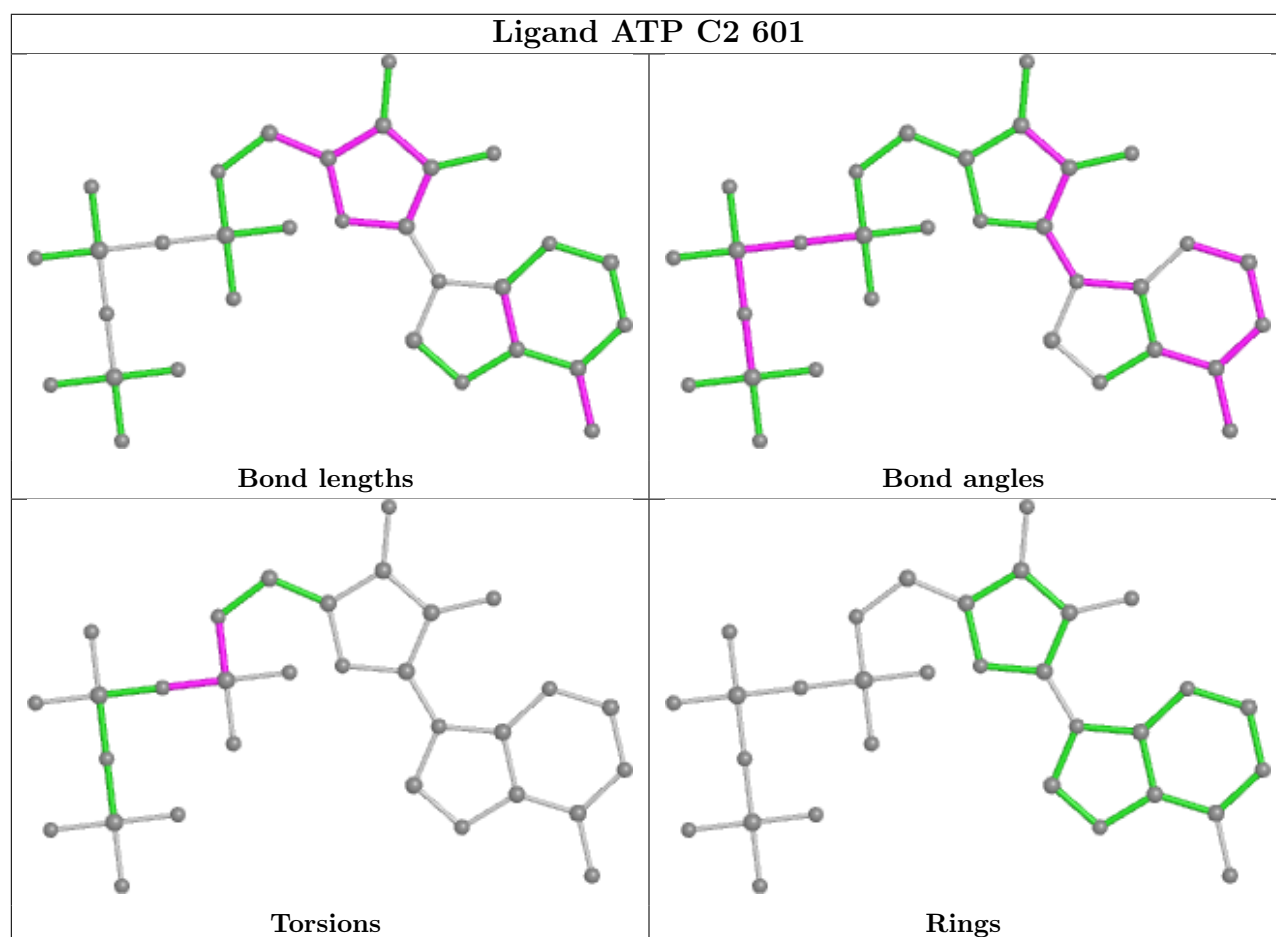
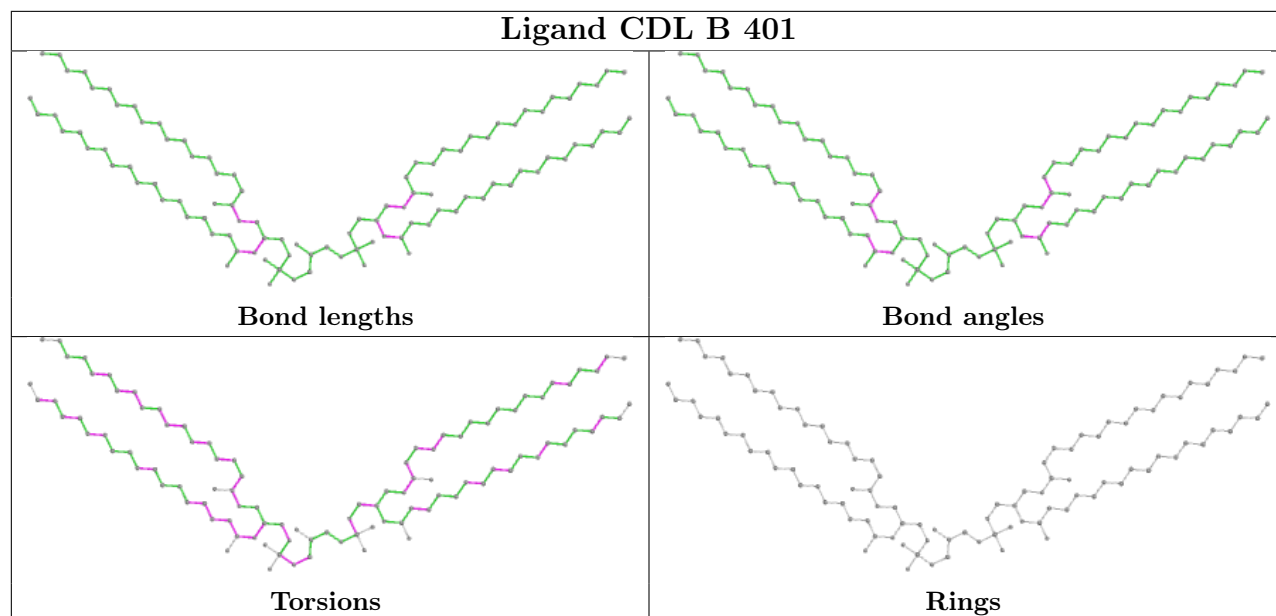


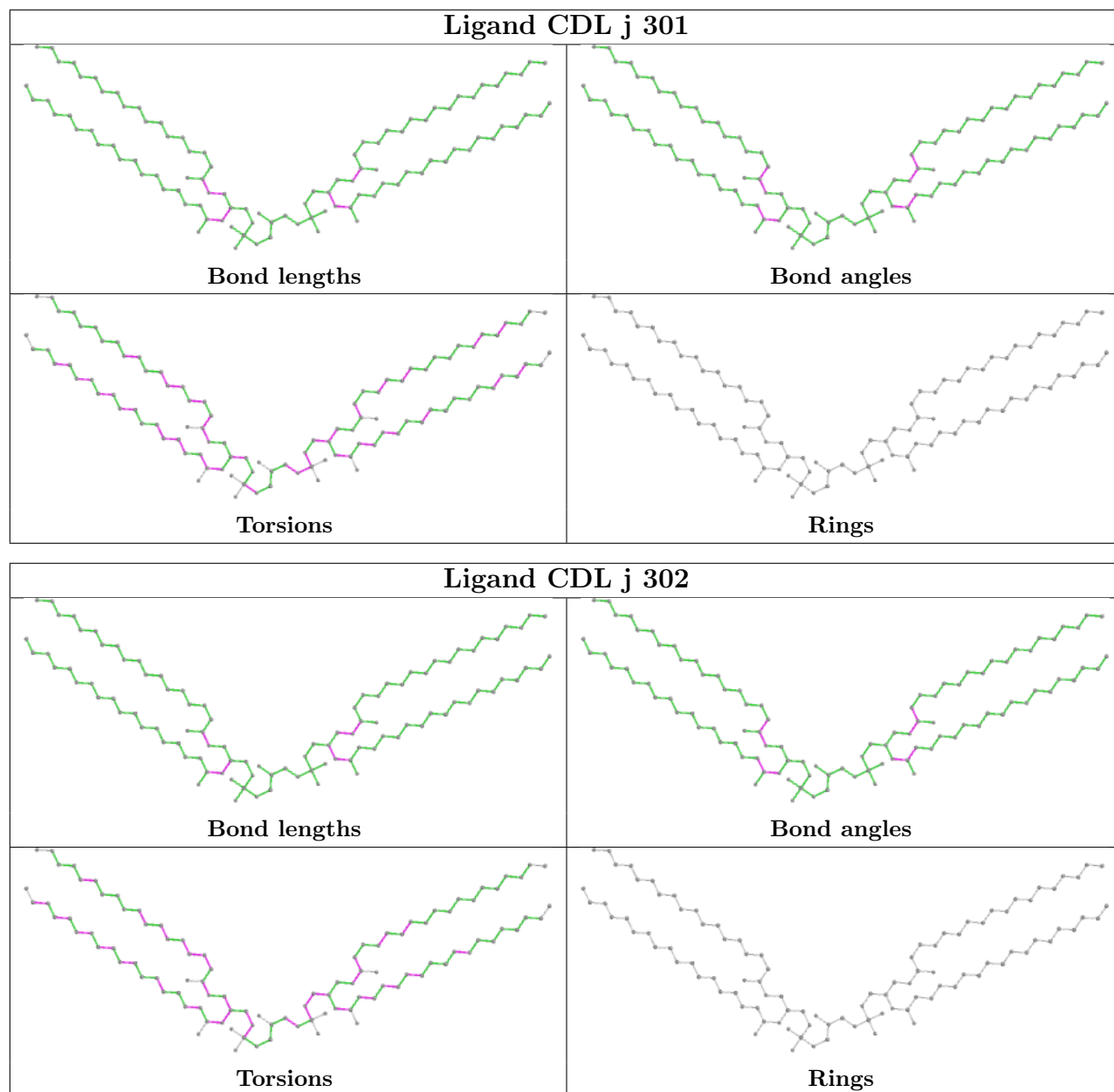


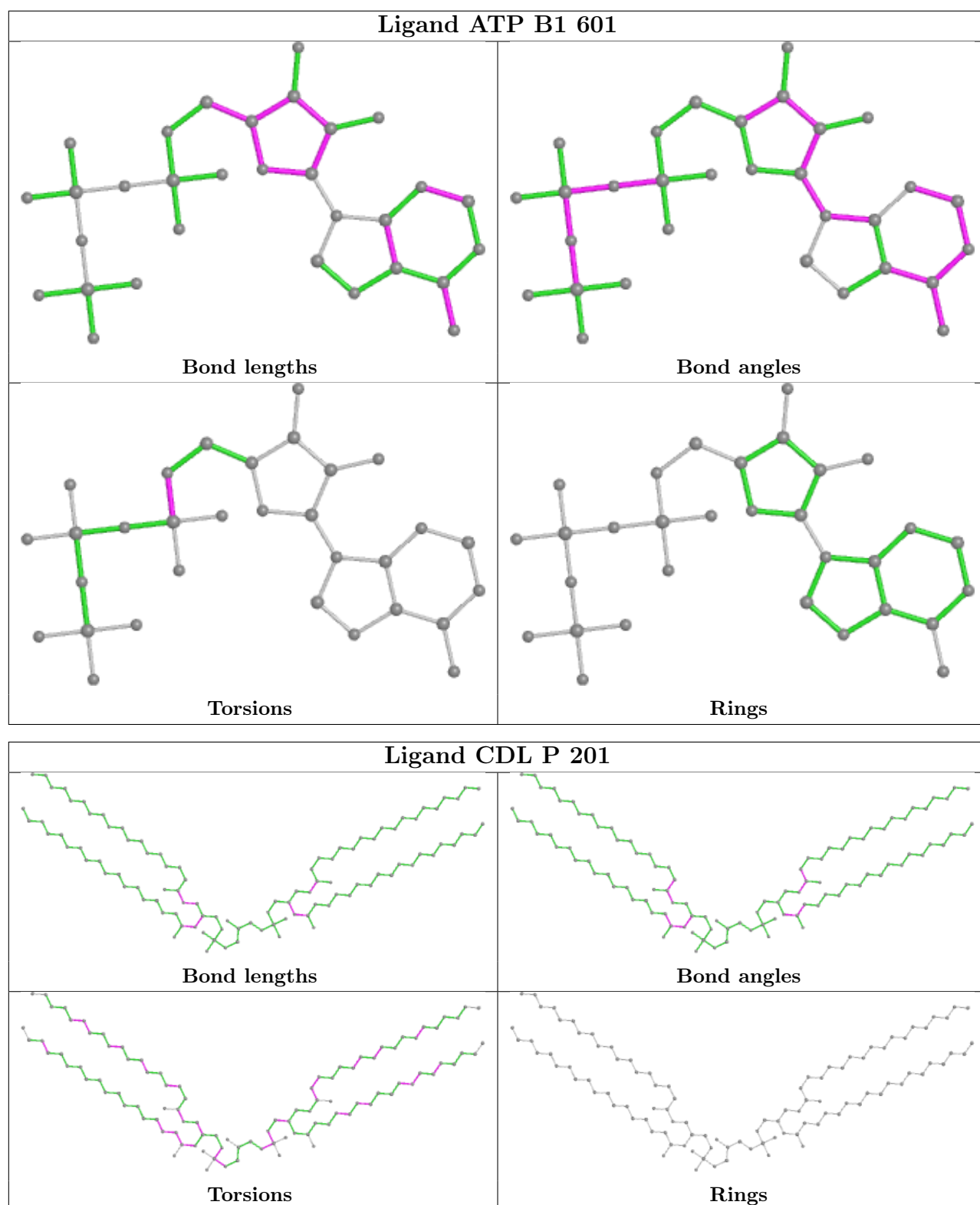


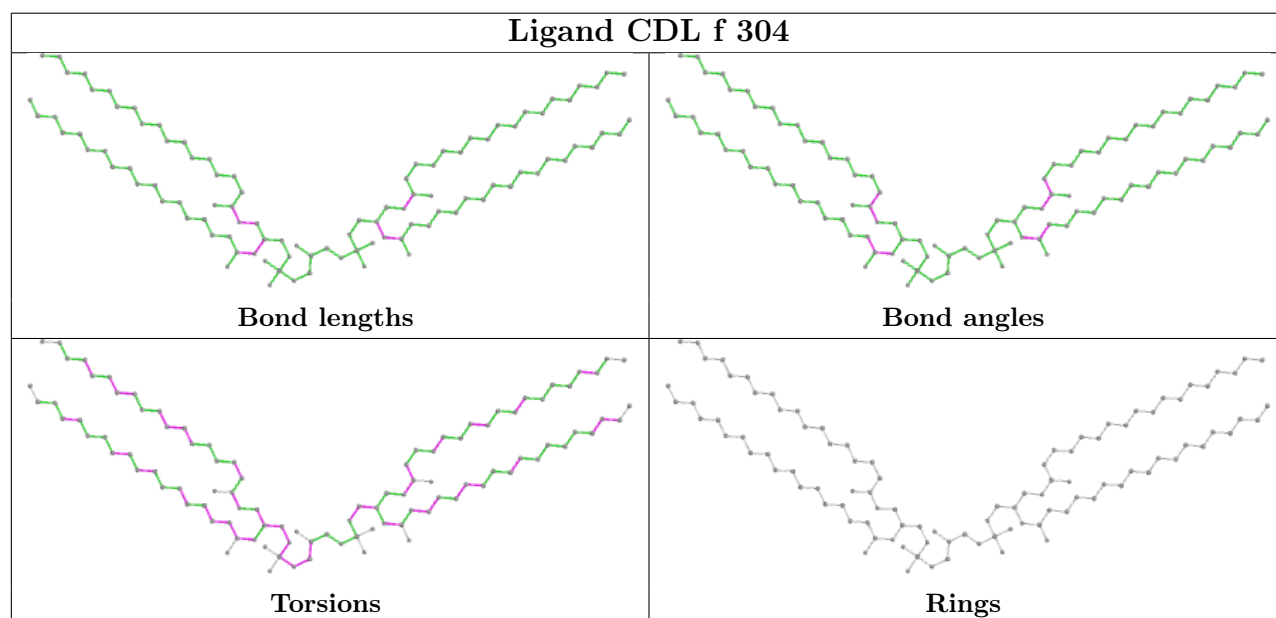
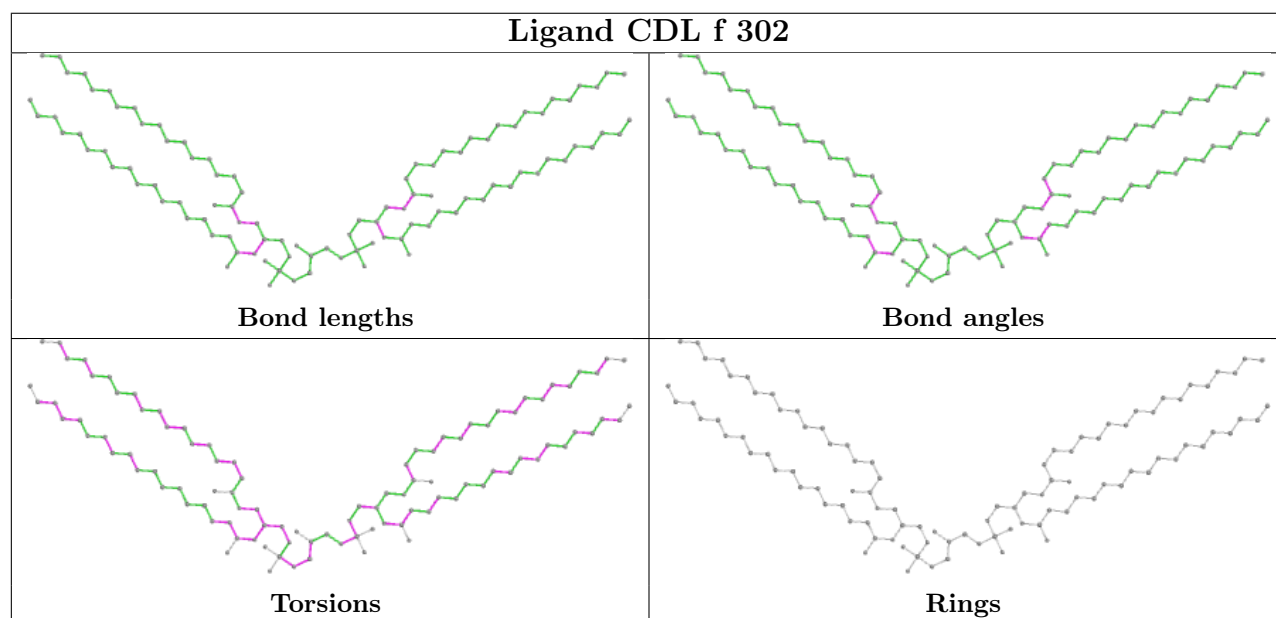
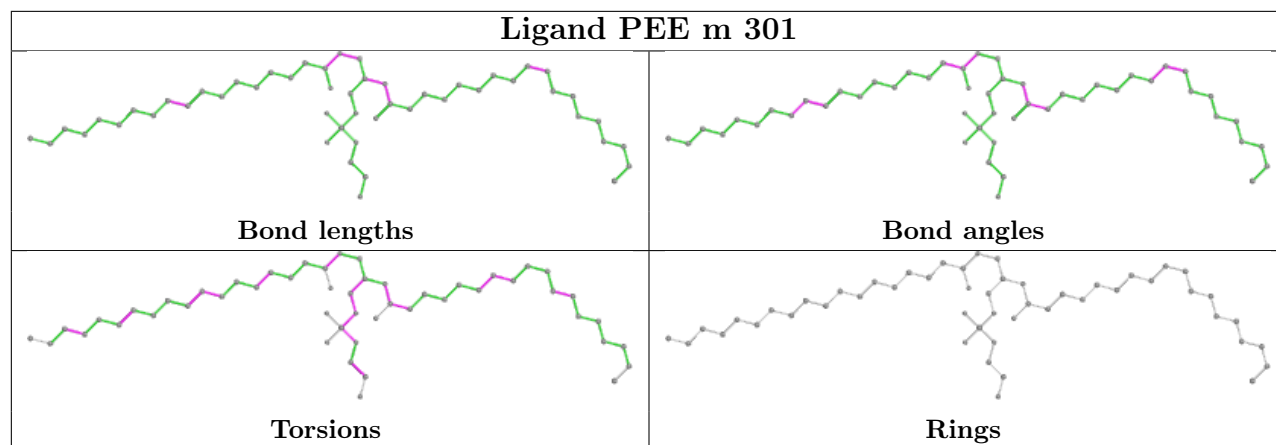


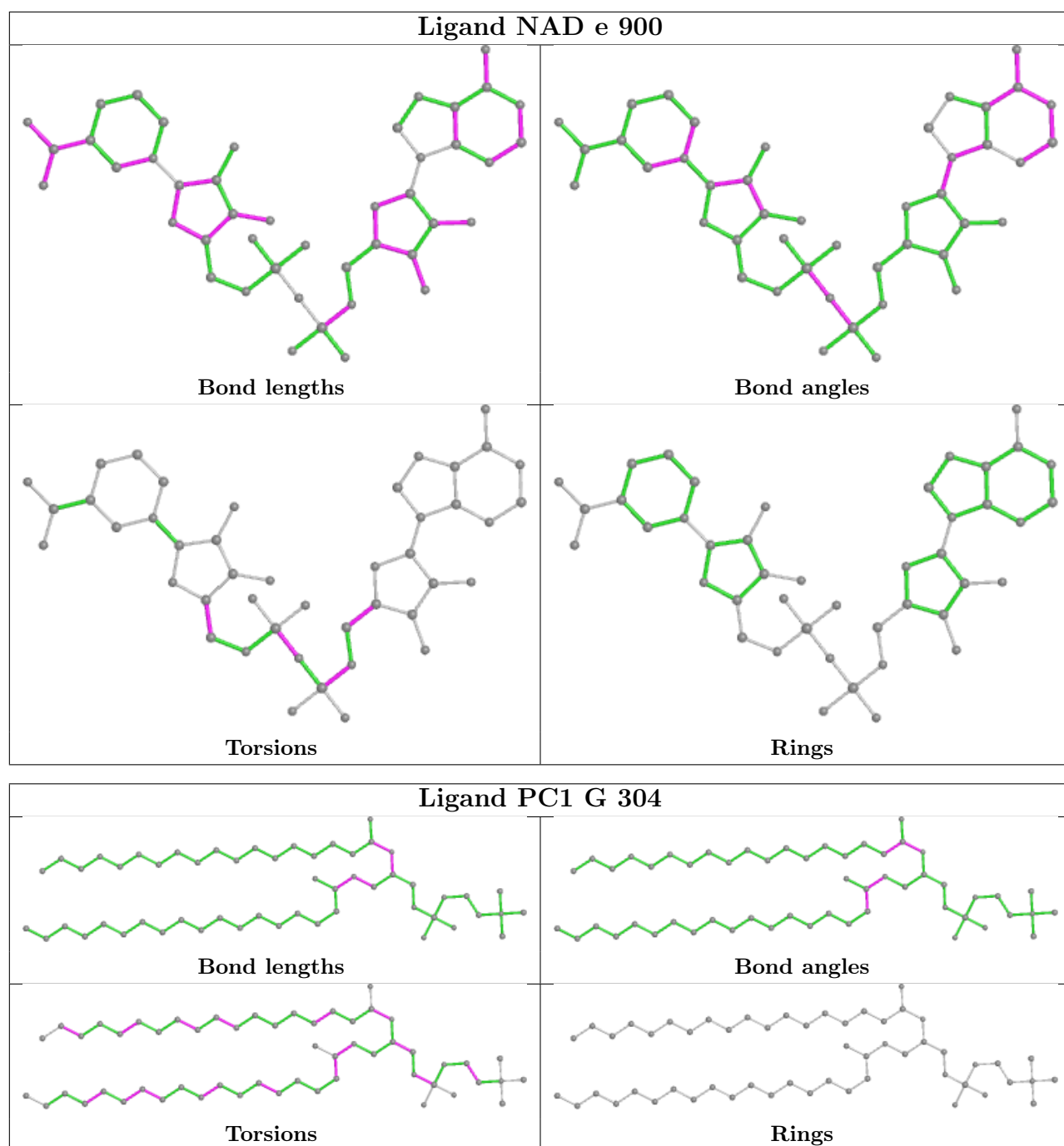


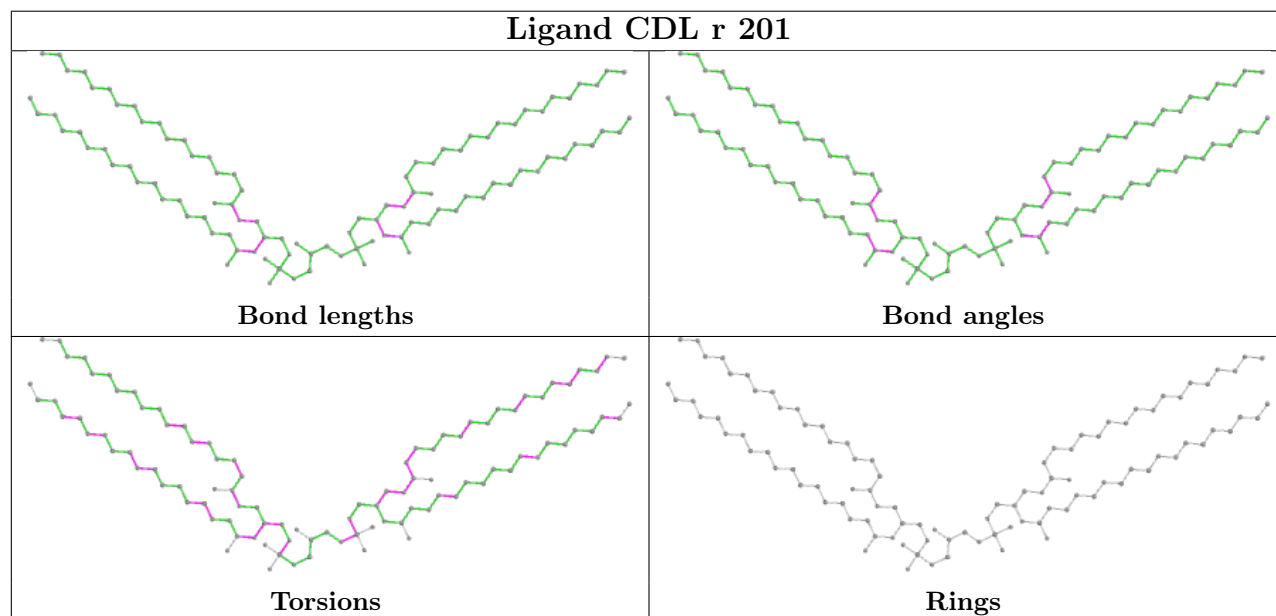
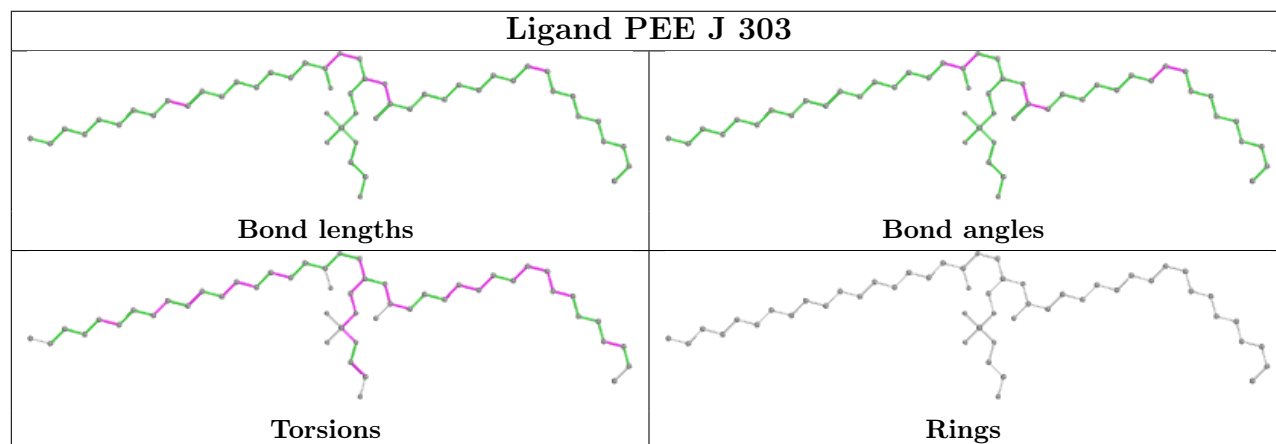
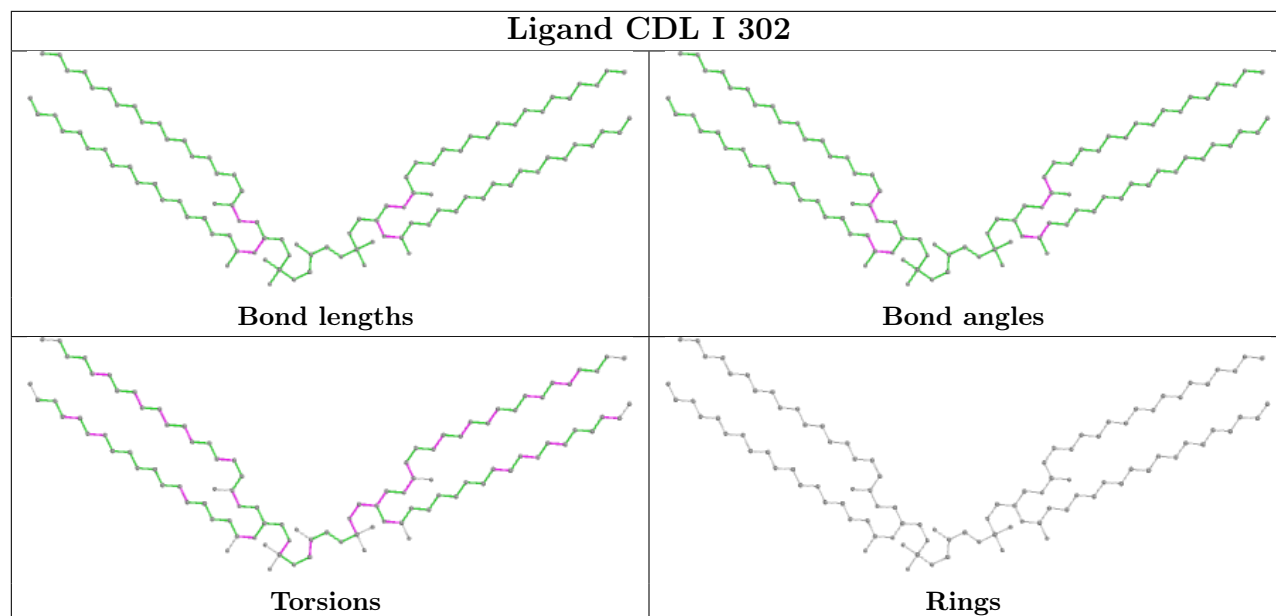




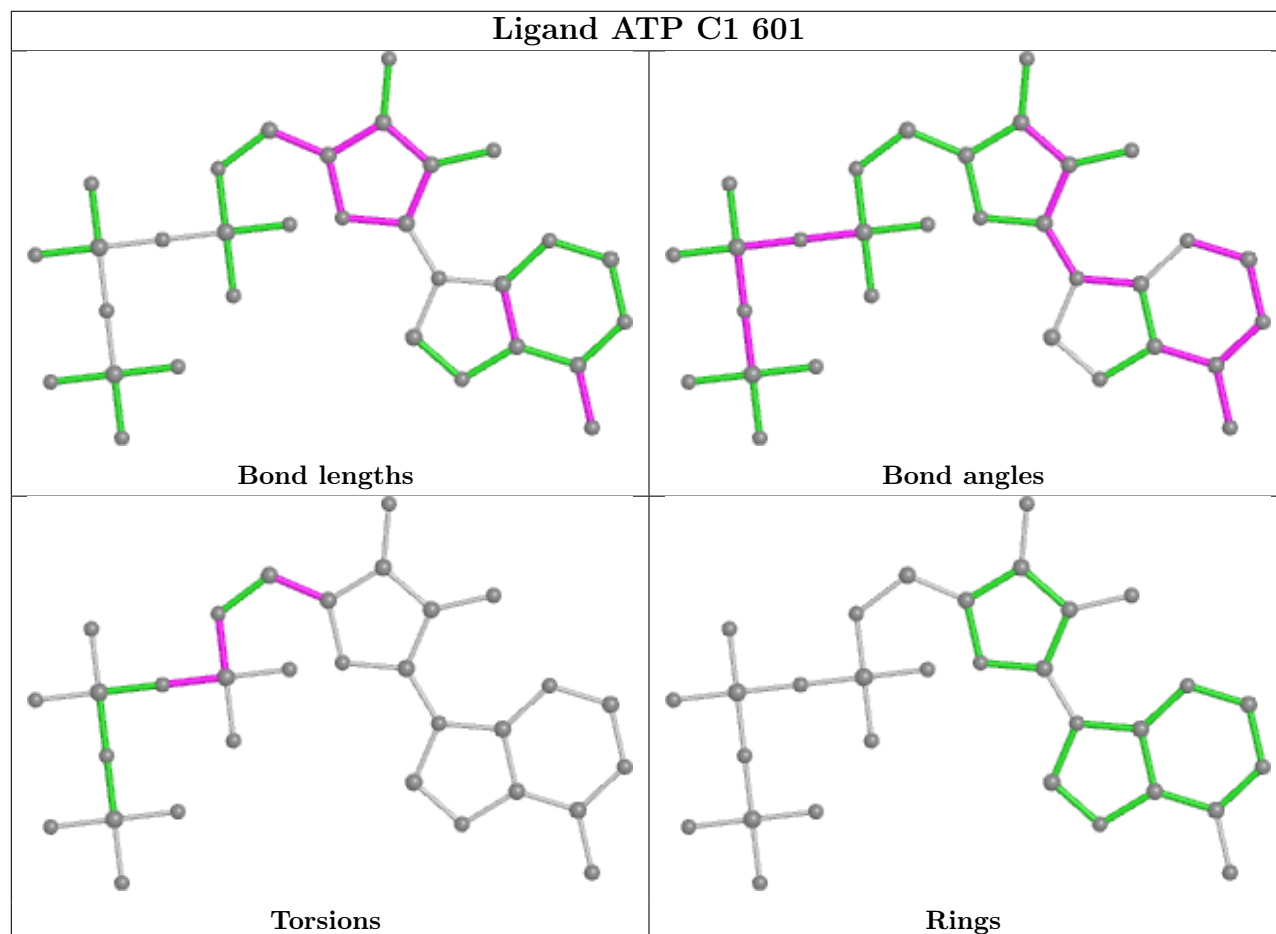
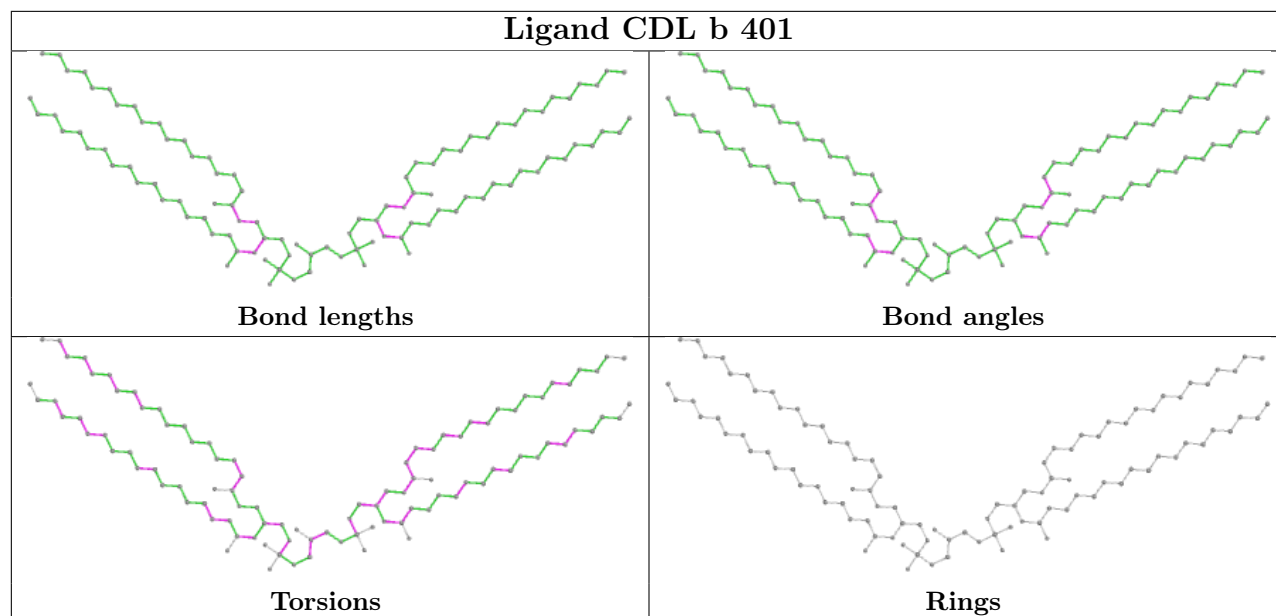


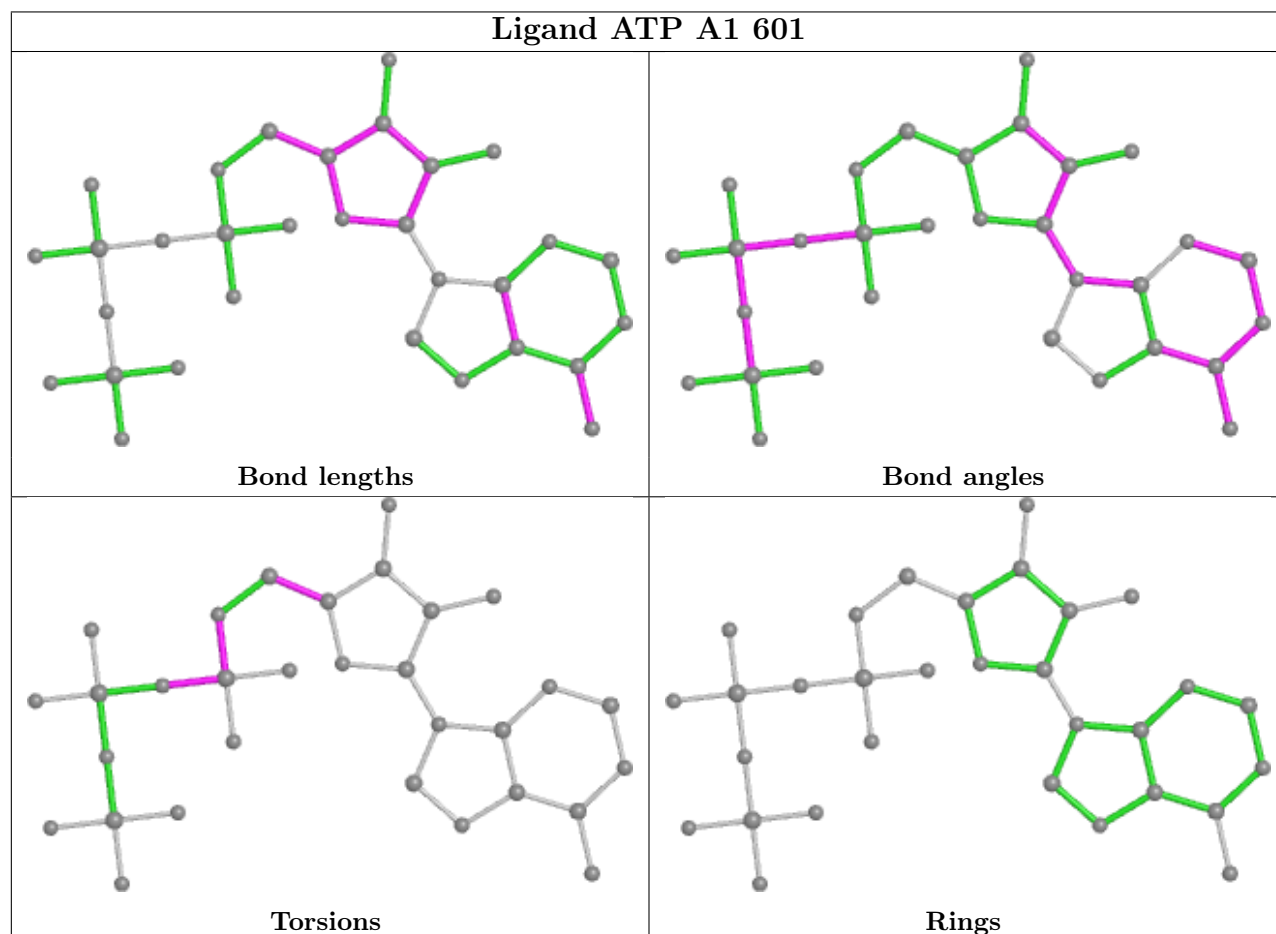
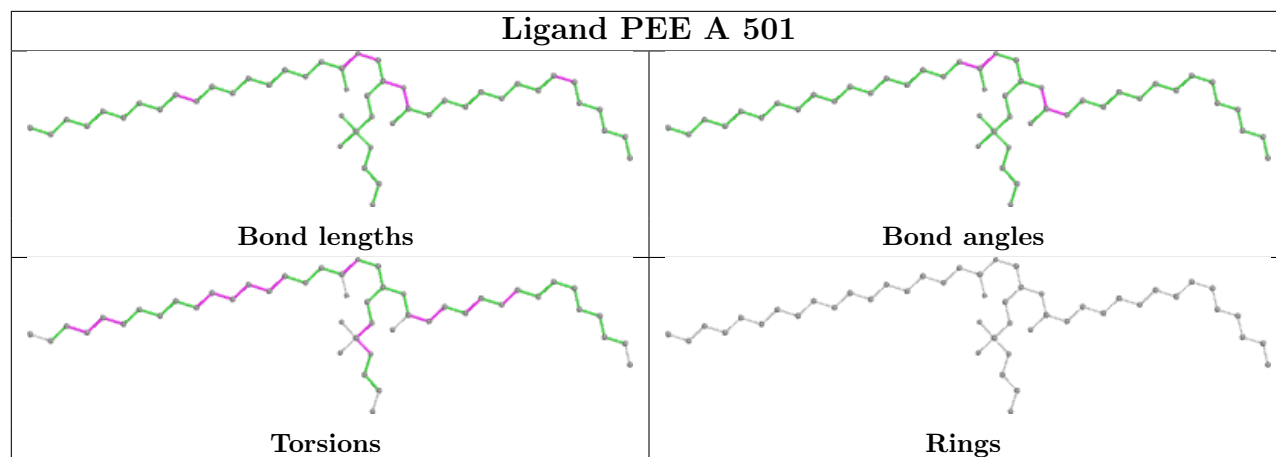


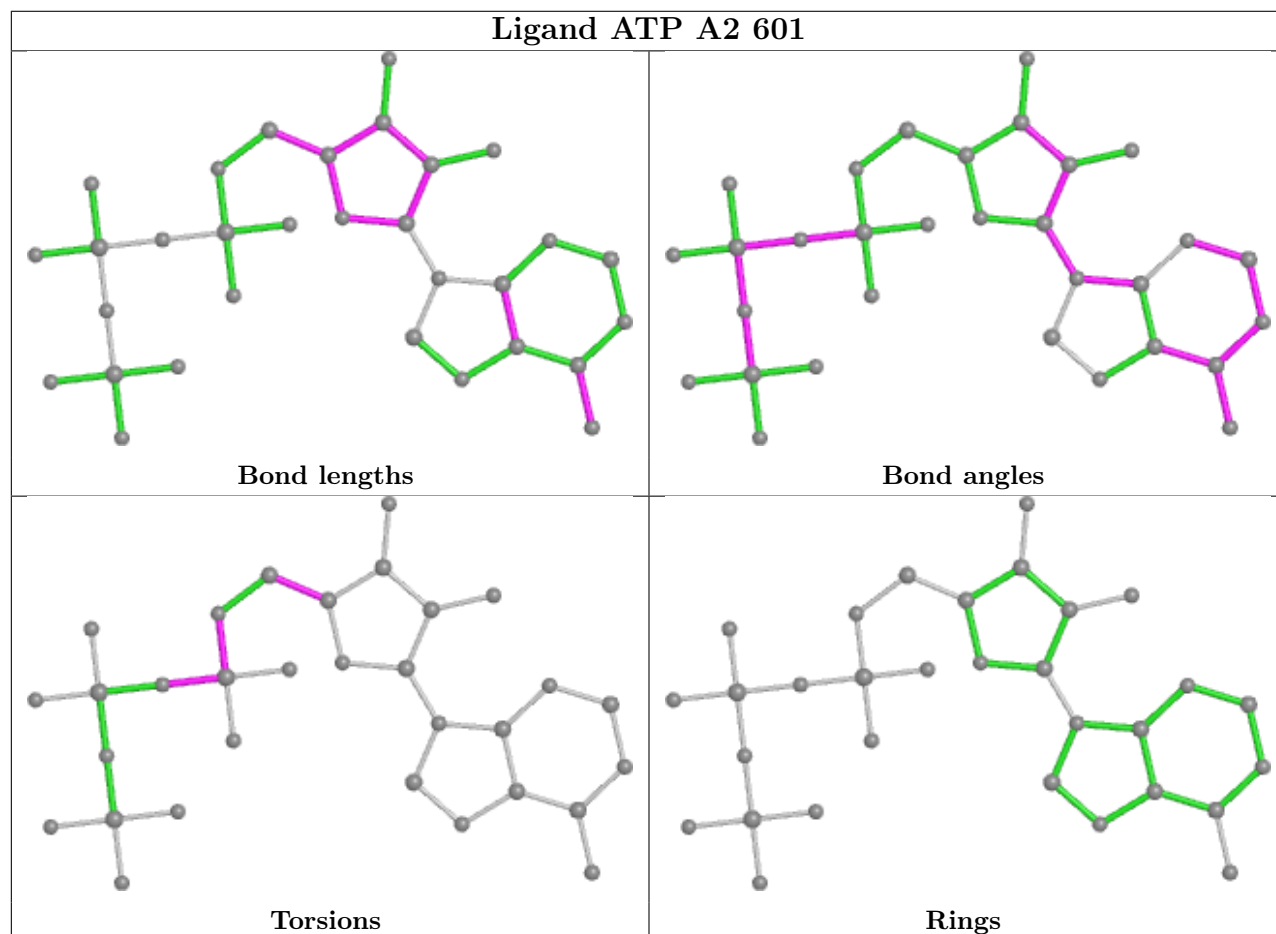
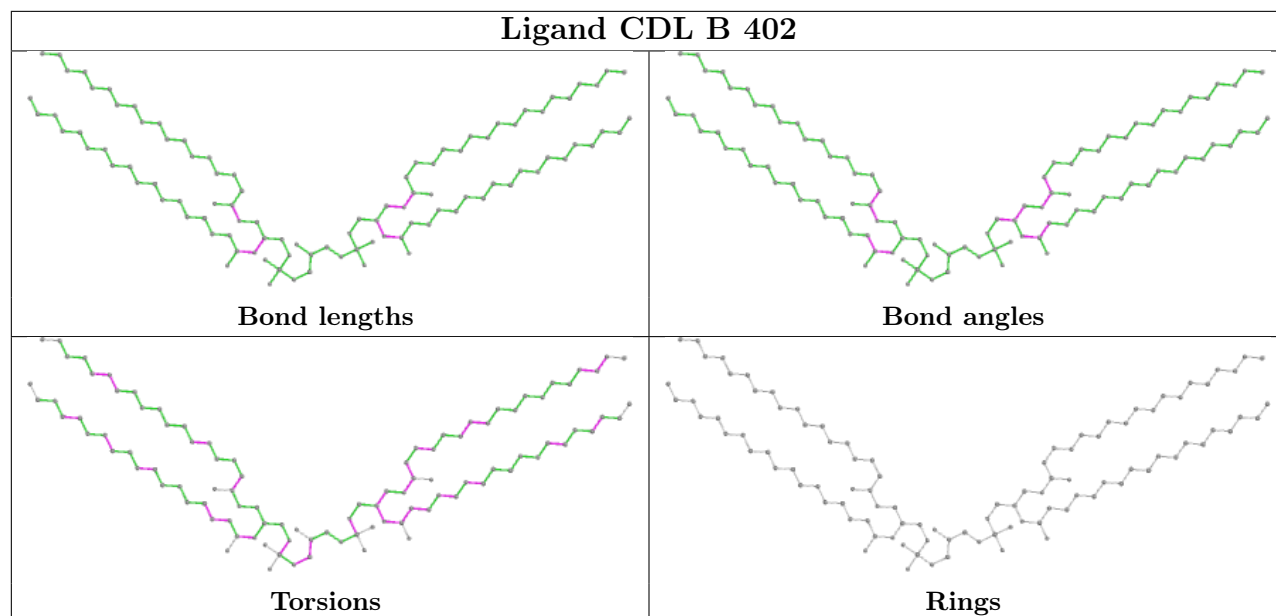


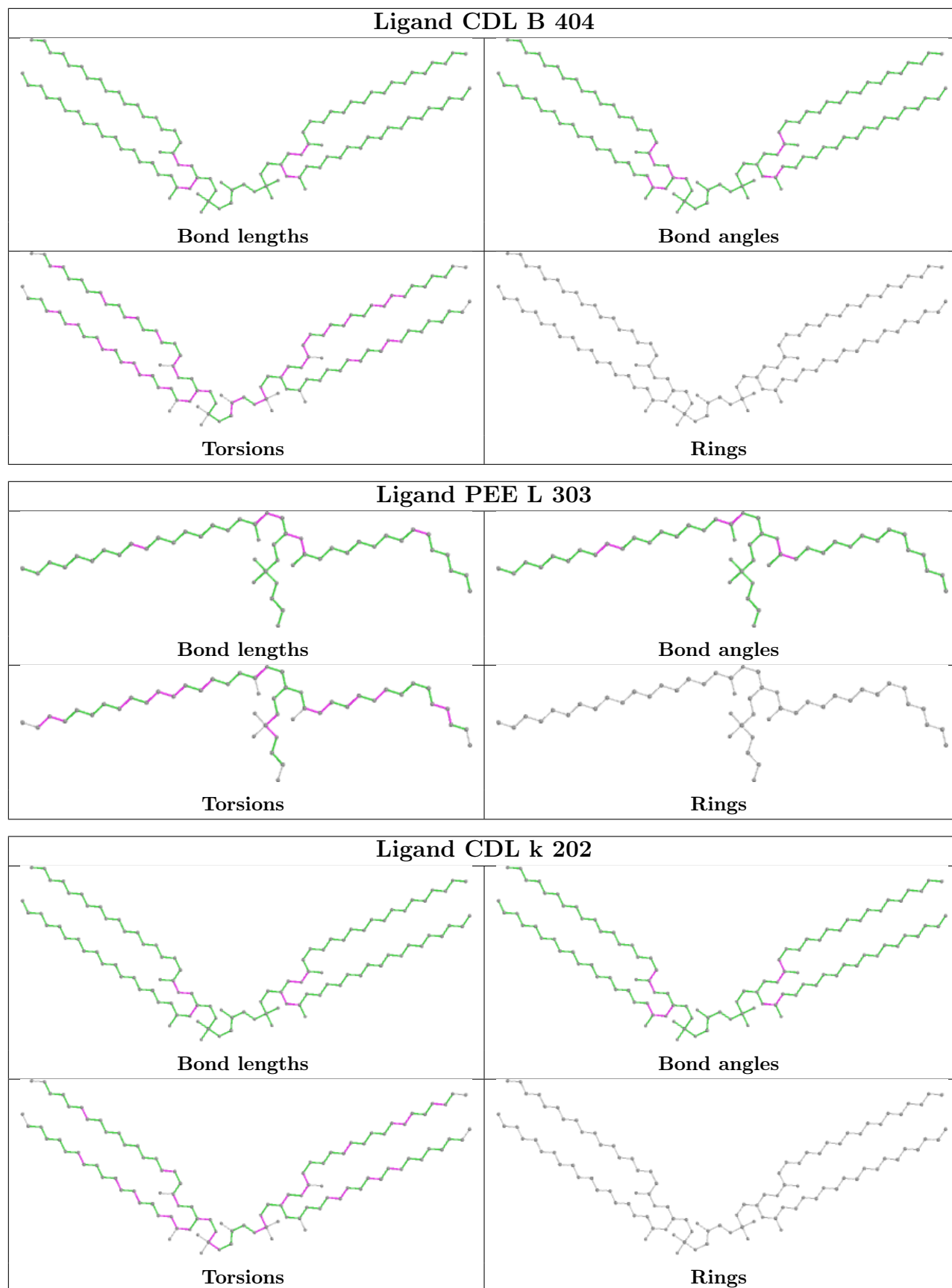


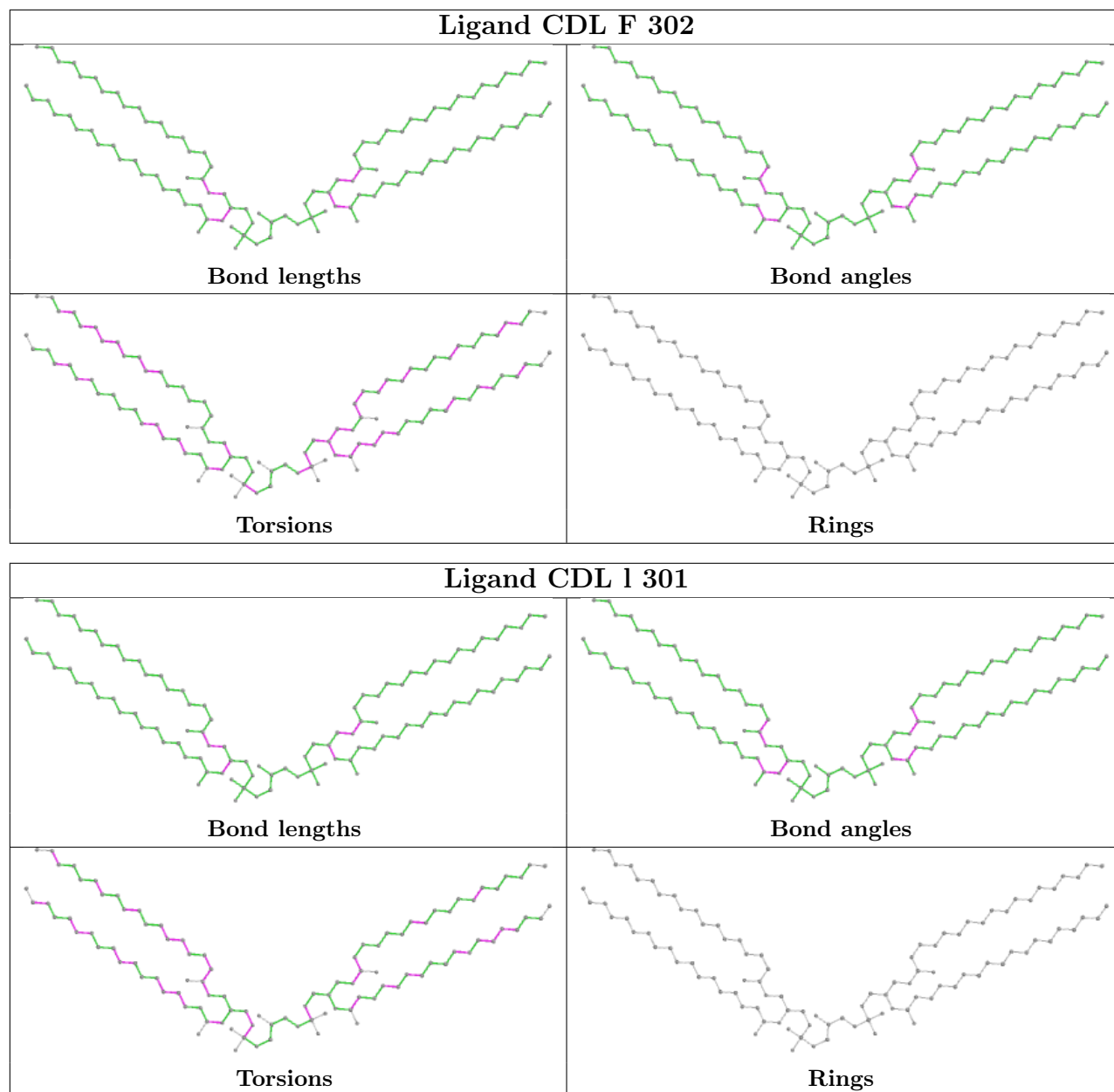


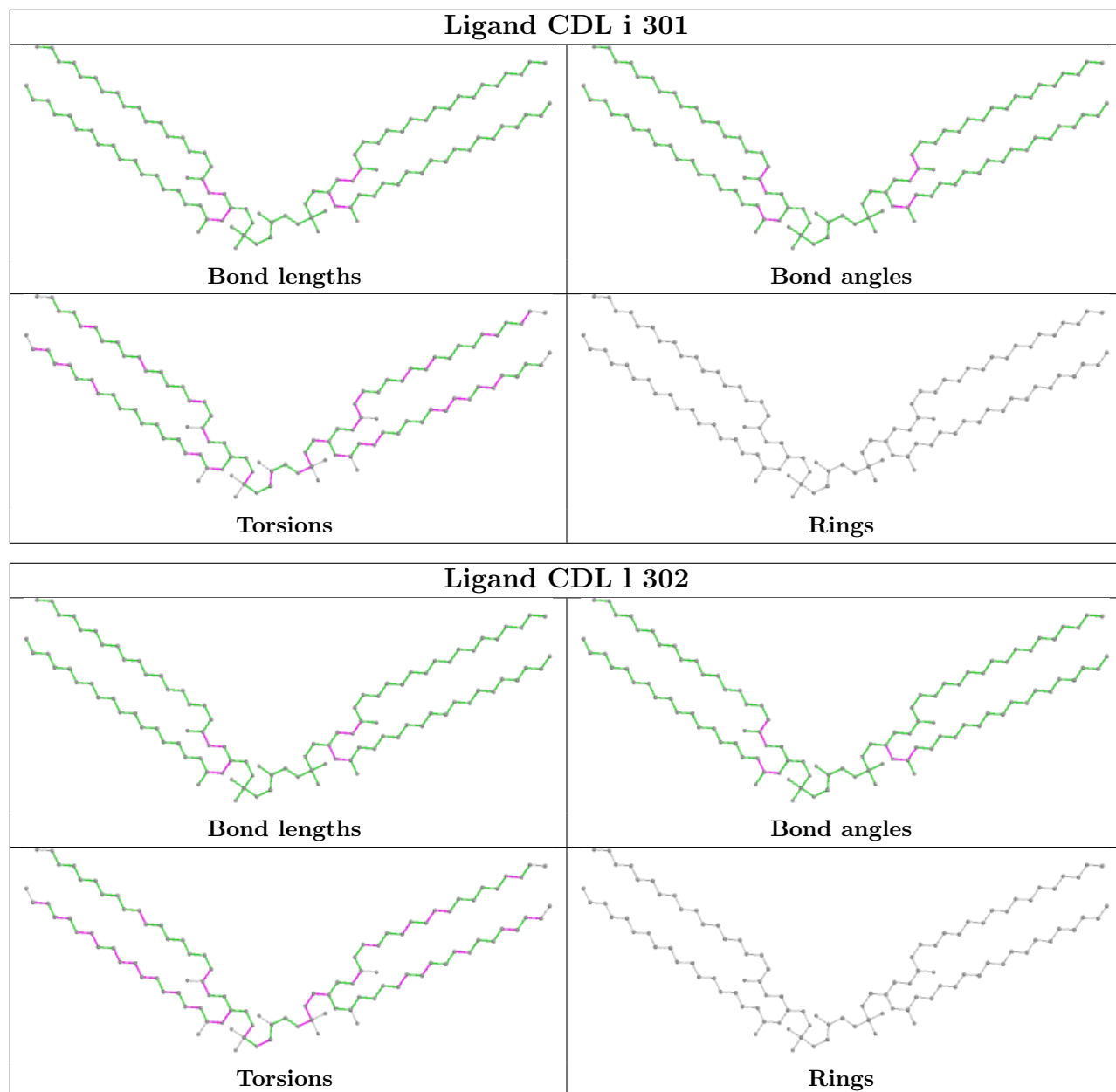


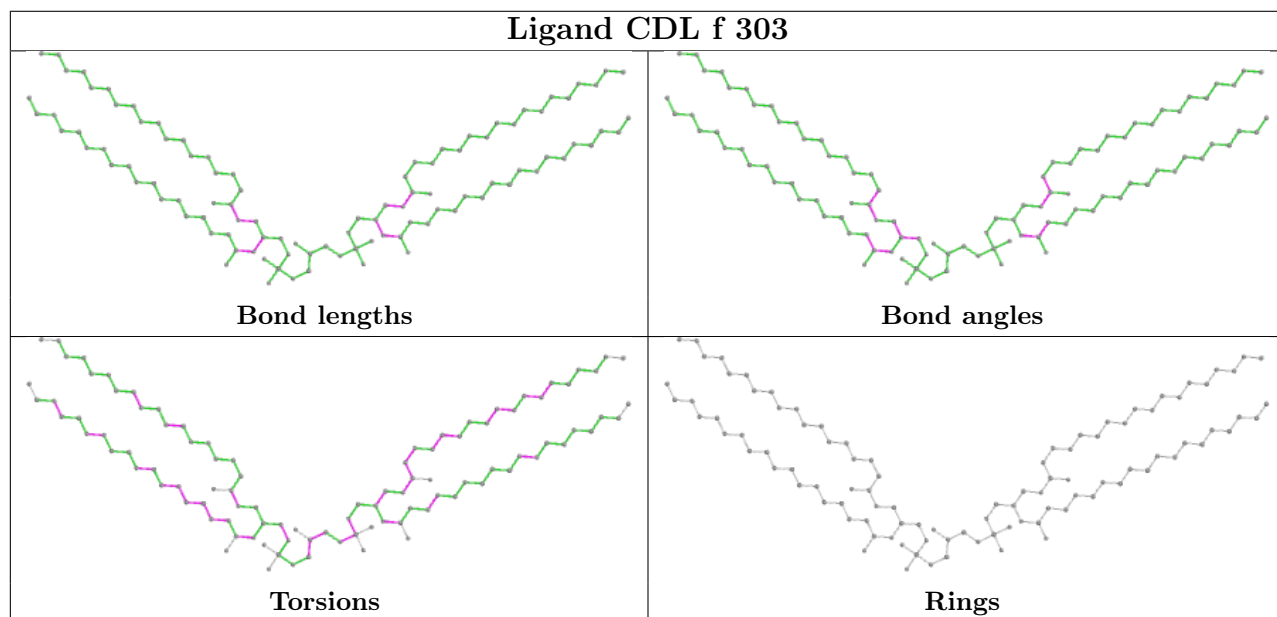
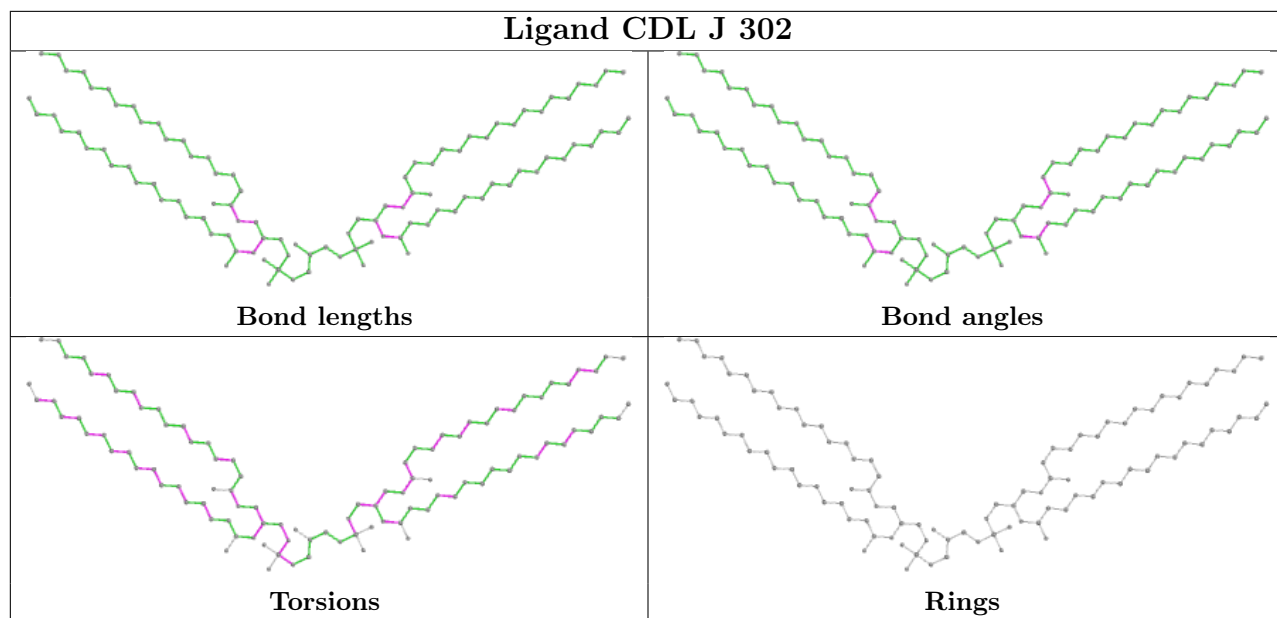


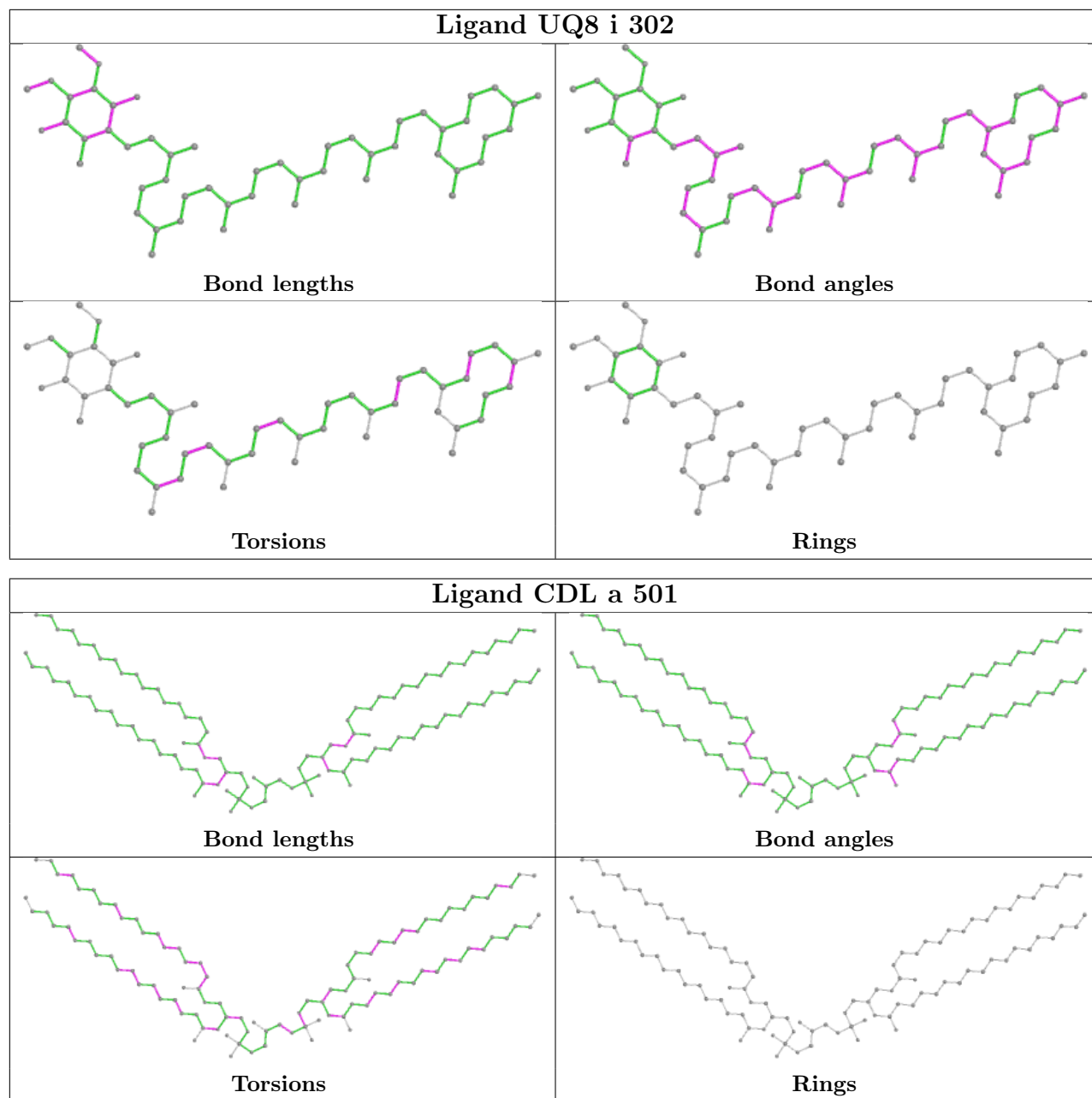




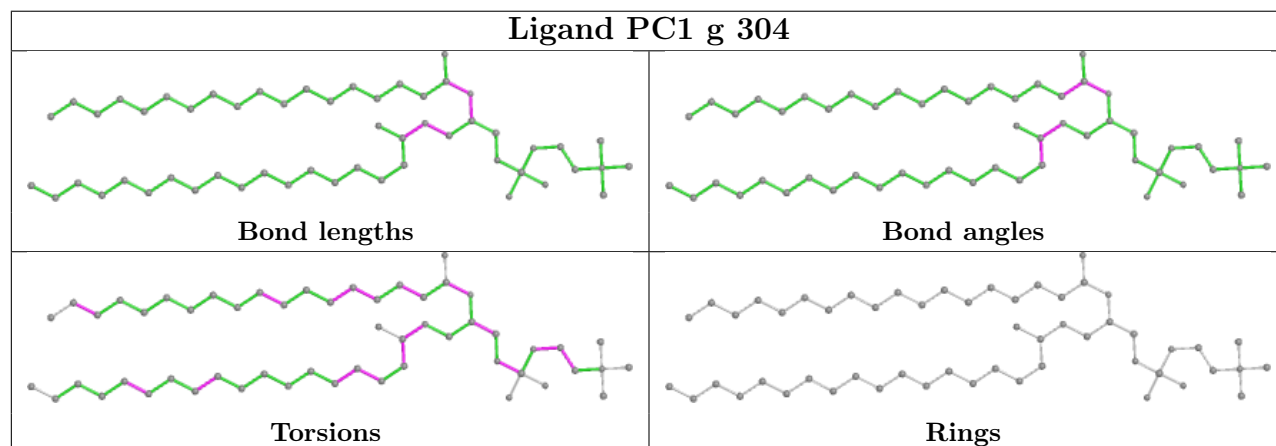
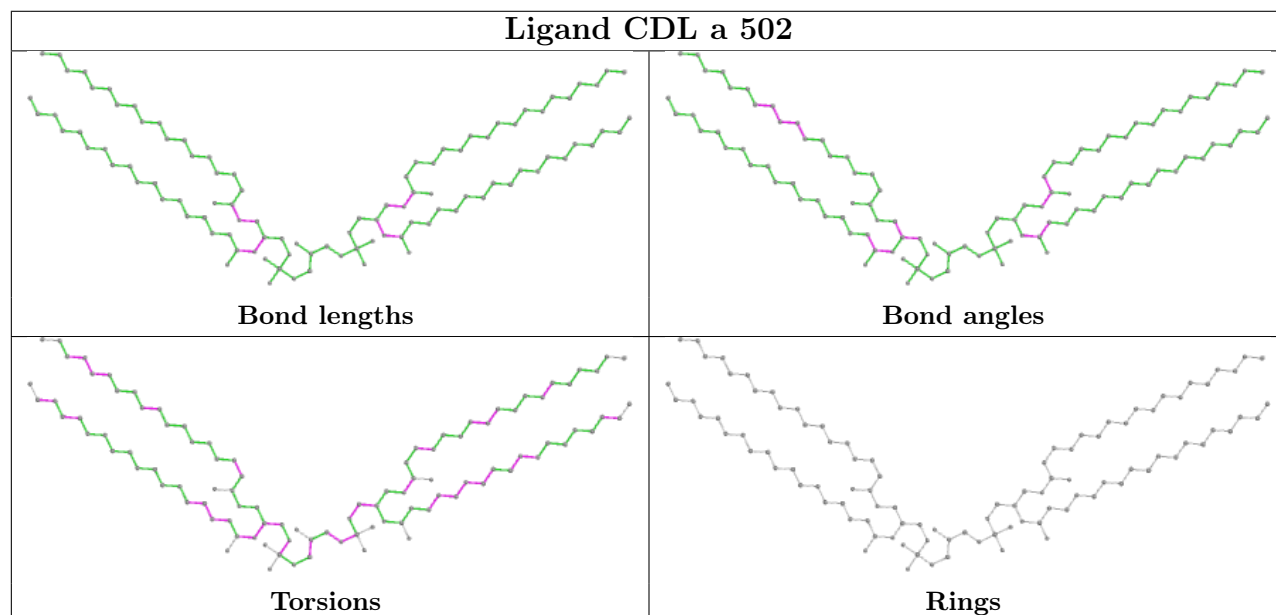
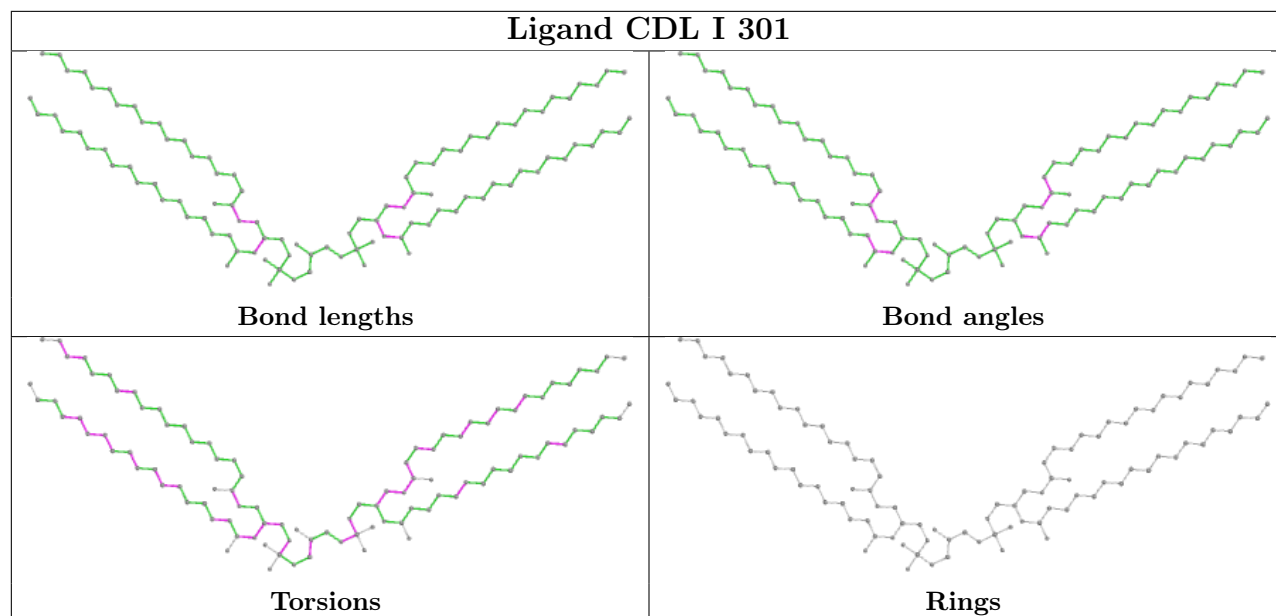












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

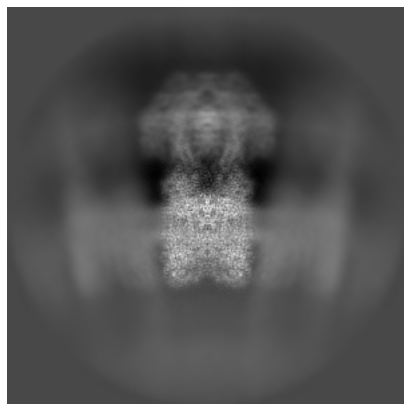
## 6 Map visualisation [i](#)

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.

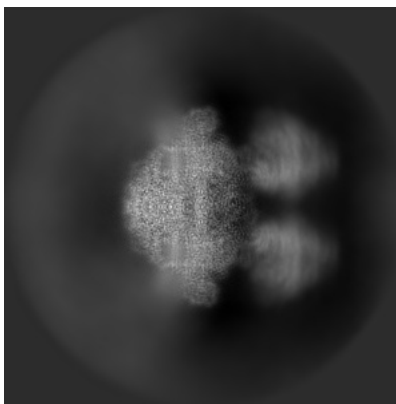
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

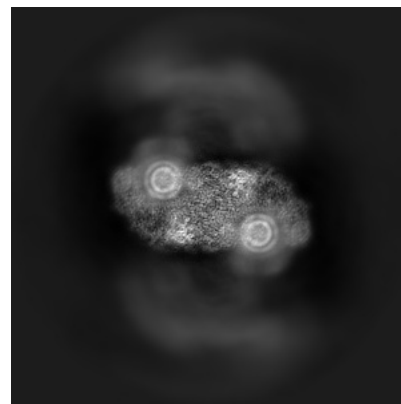
#### 6.1.1 Primary map



X

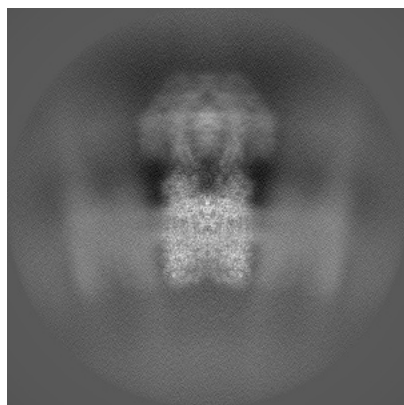


Y

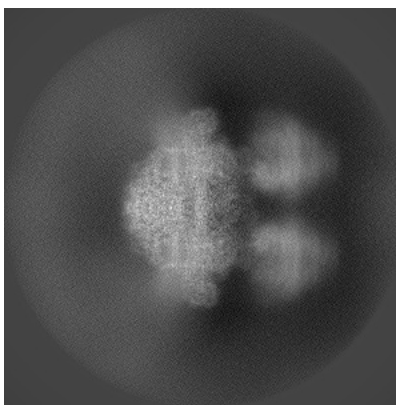


Z

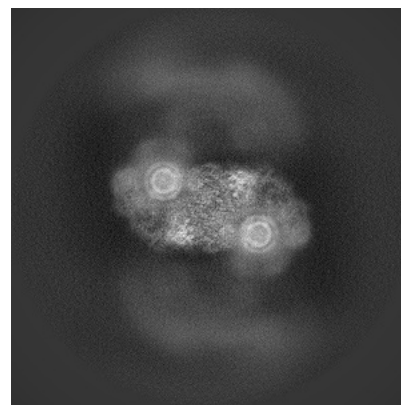
#### 6.1.2 Raw map



X



Y

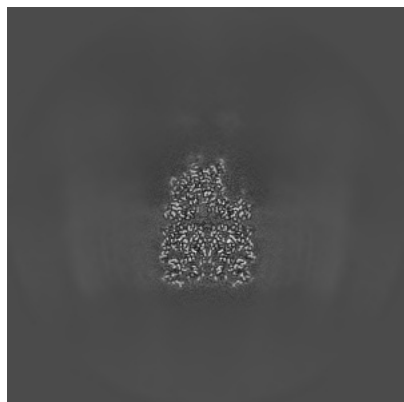


Z

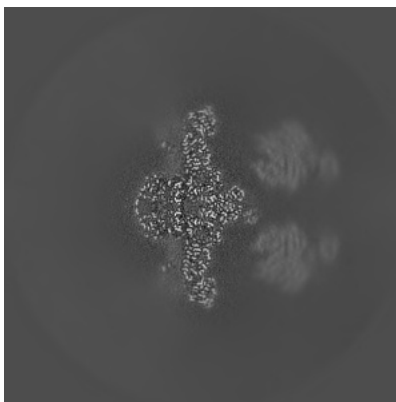
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 300

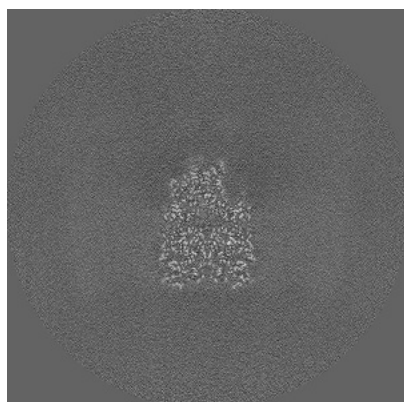


Y Index: 300

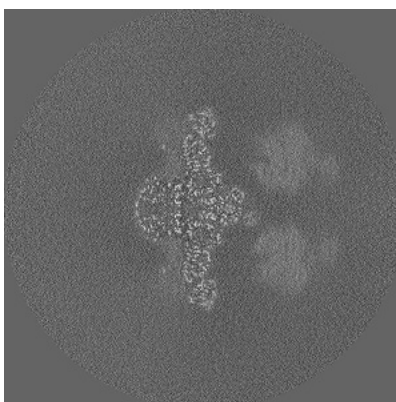


Z Index: 300

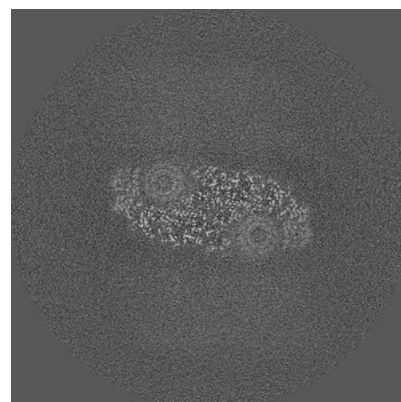
### 6.2.2 Raw map



X Index: 300



Y Index: 300

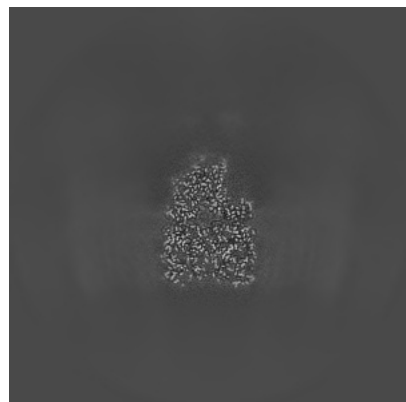


Z Index: 300

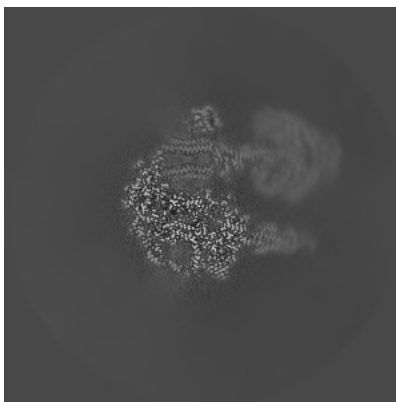
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

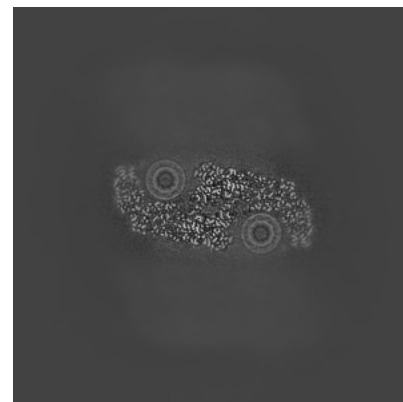
### 6.3.1 Primary map



X Index: 298

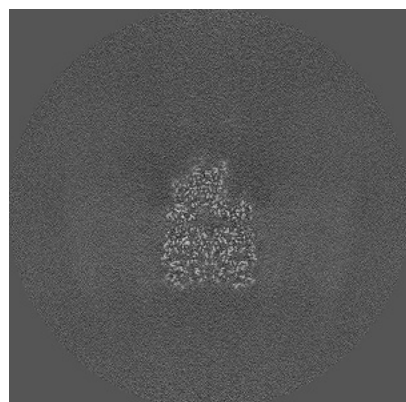


Y Index: 258

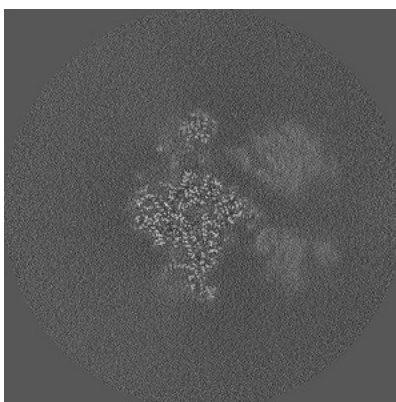


Z Index: 292

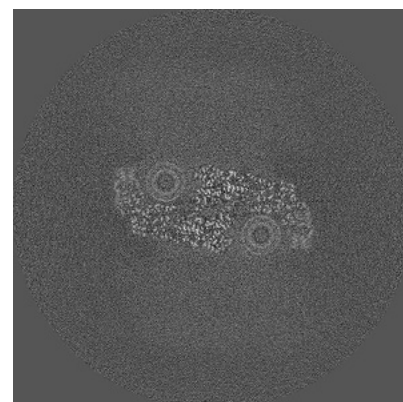
### 6.3.2 Raw map



X Index: 299



Y Index: 290

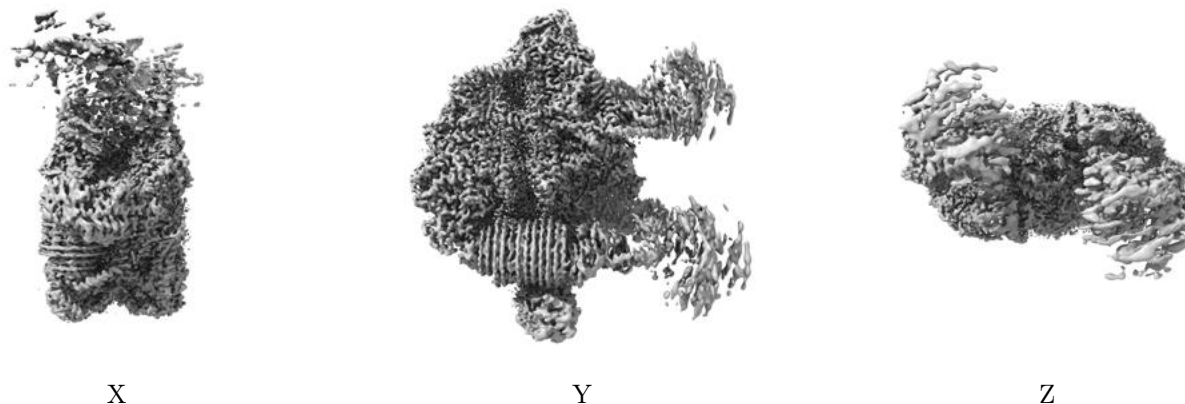


Z Index: 292

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

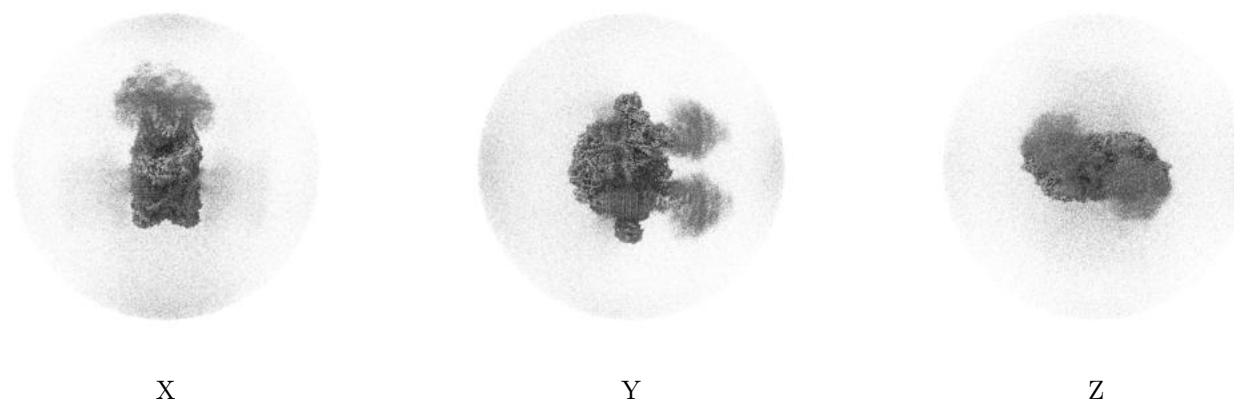
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



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

### 6.4.2 Raw map



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

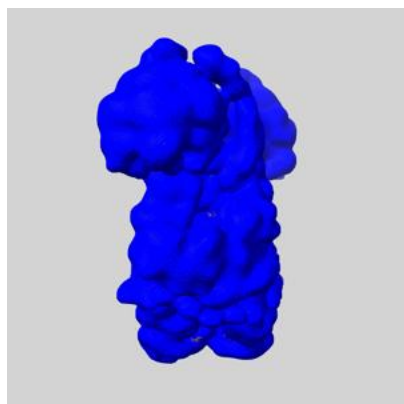
## 6.5 Mask visualisation [i](#)

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

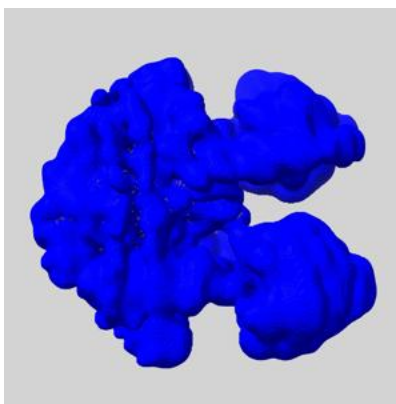
A mask typically either:

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

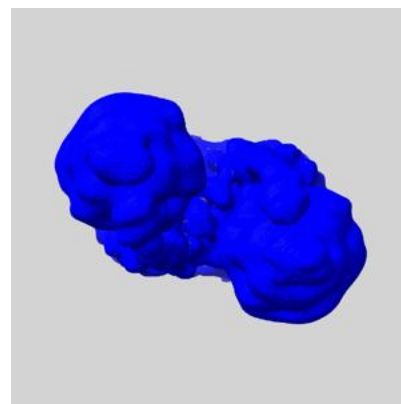
### 6.5.1 emd\_10860\_msk\_1.map [i](#)



X



Y

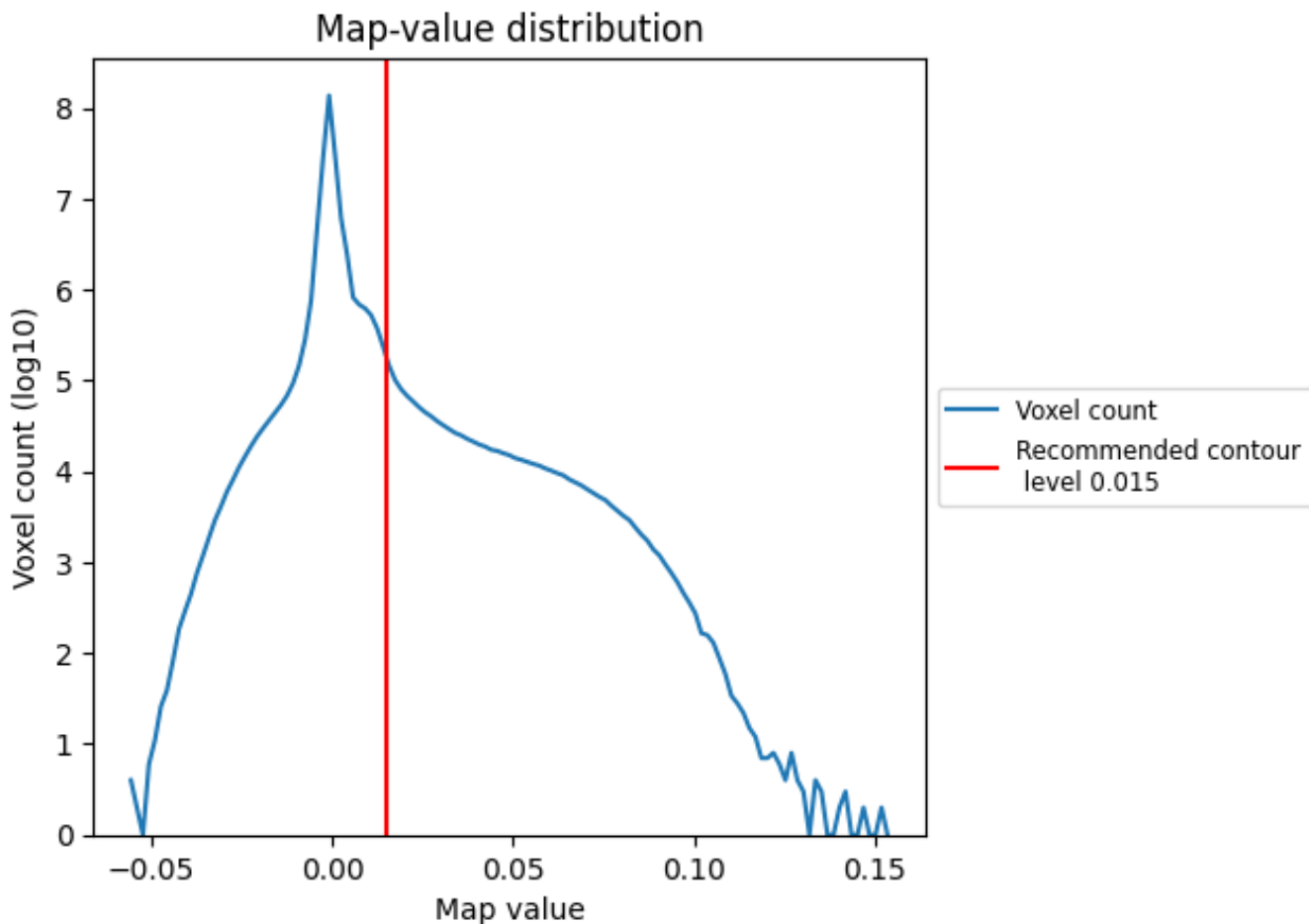


Z

## 7 Map analysis [i](#)

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

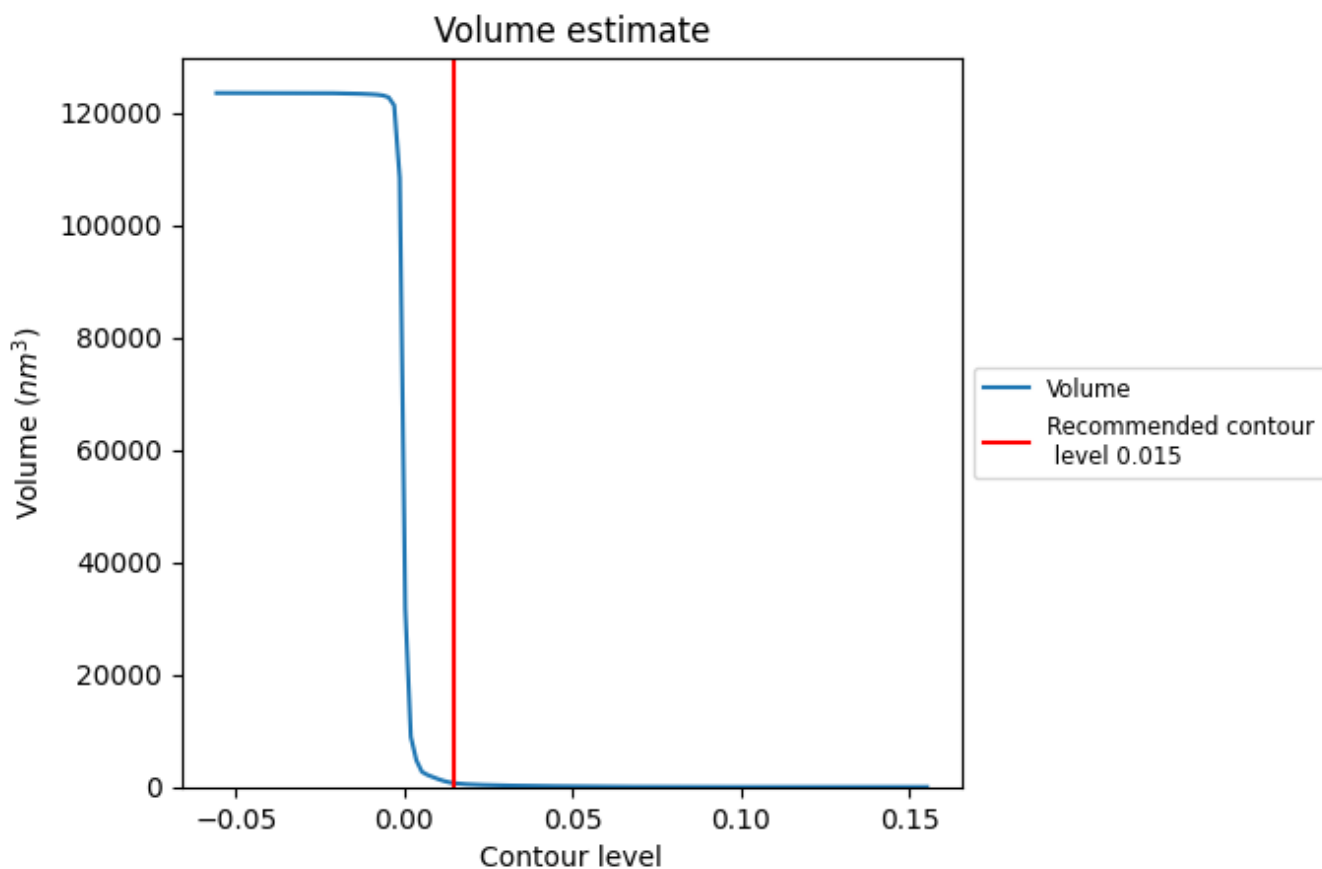
### 7.1 Map-value distribution [i](#)



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.



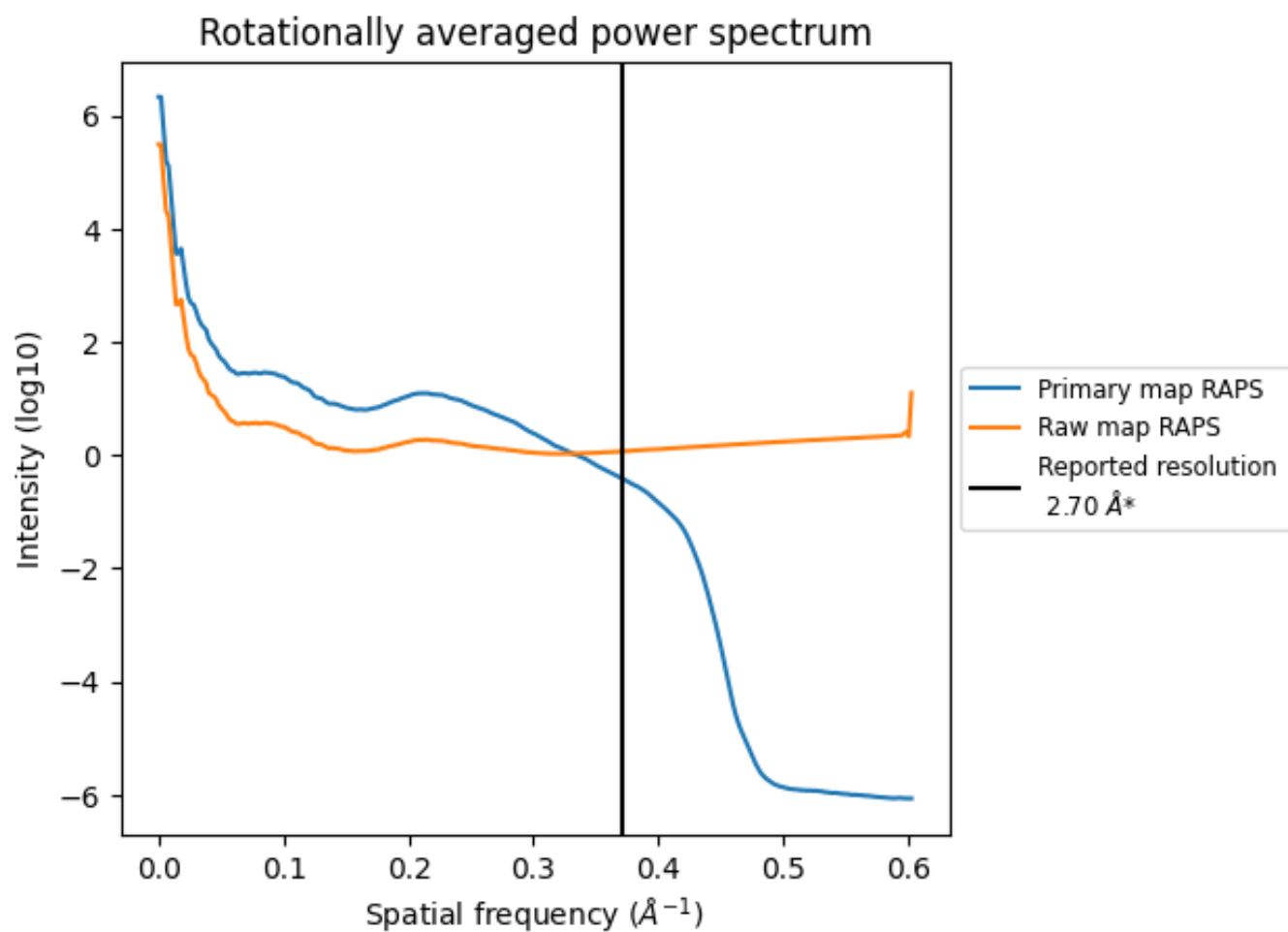
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 665 nm<sup>3</sup>; 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 i

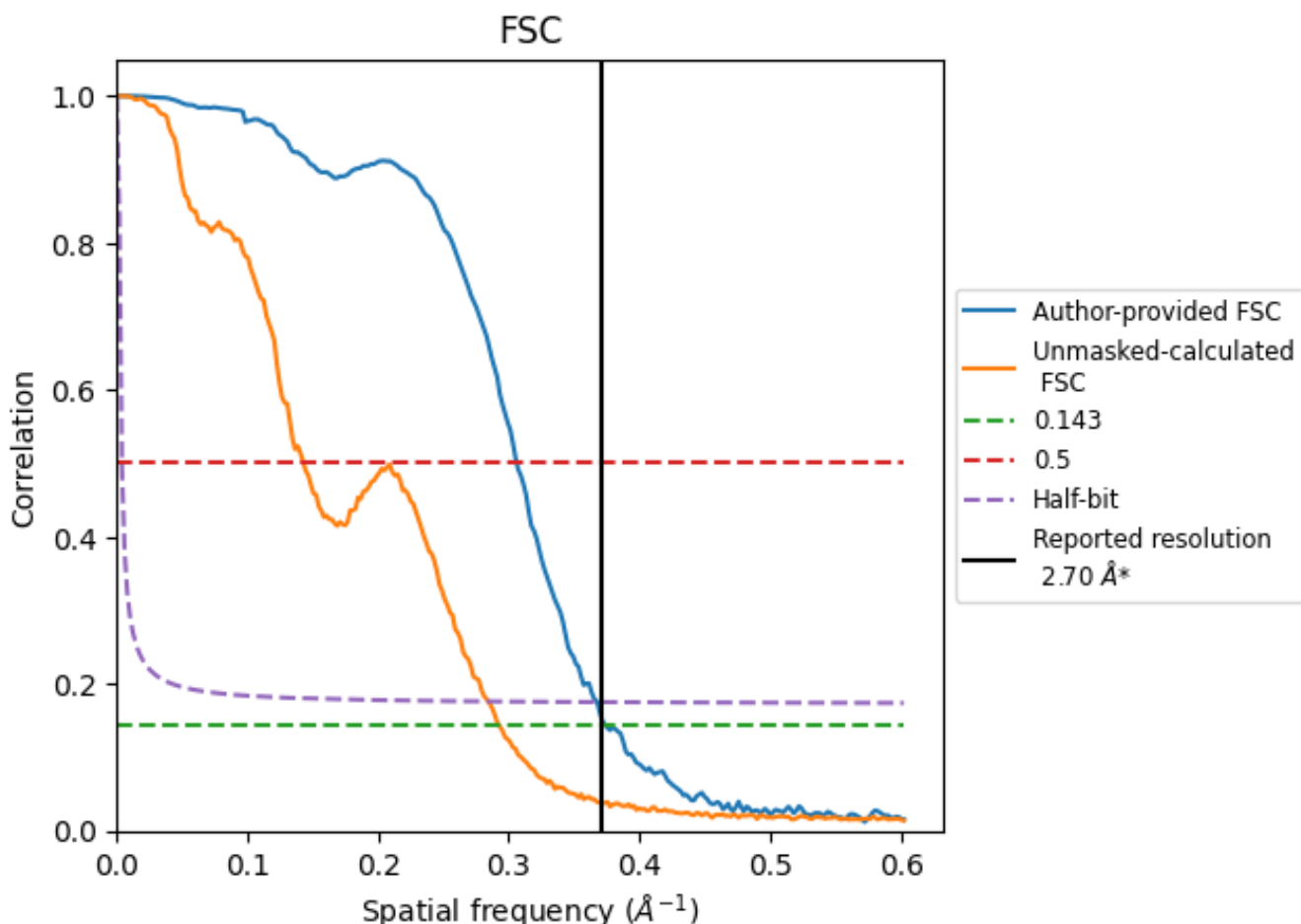


\*Reported resolution corresponds to spatial frequency of 0.370 Å<sup>-1</sup>

## 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 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

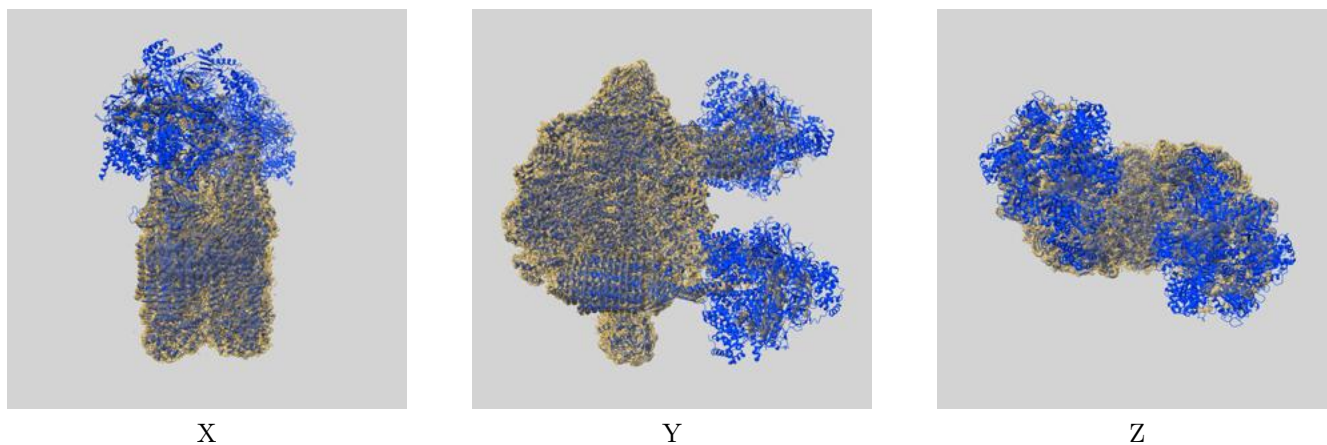
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.67	3.27	2.72
Unmasked-calculated*	3.42	7.00	3.52

\*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](#)

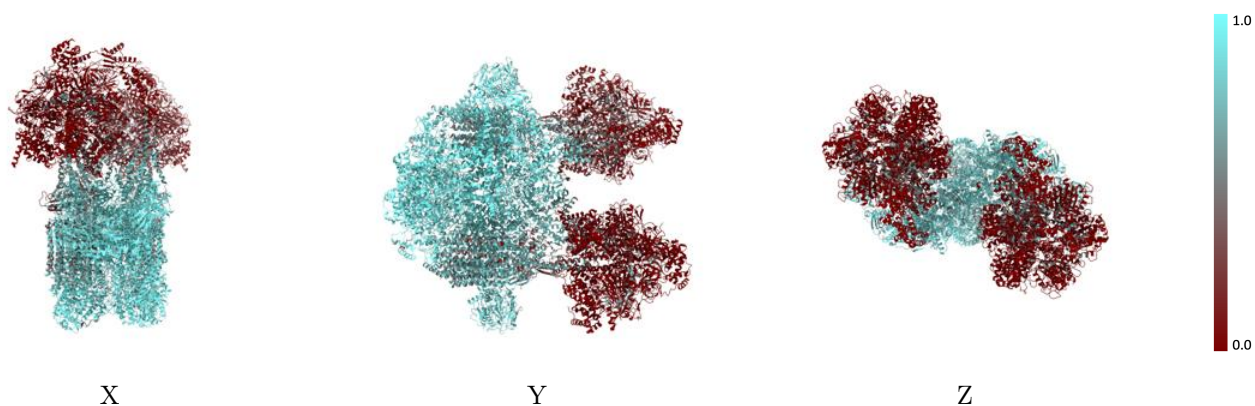


The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

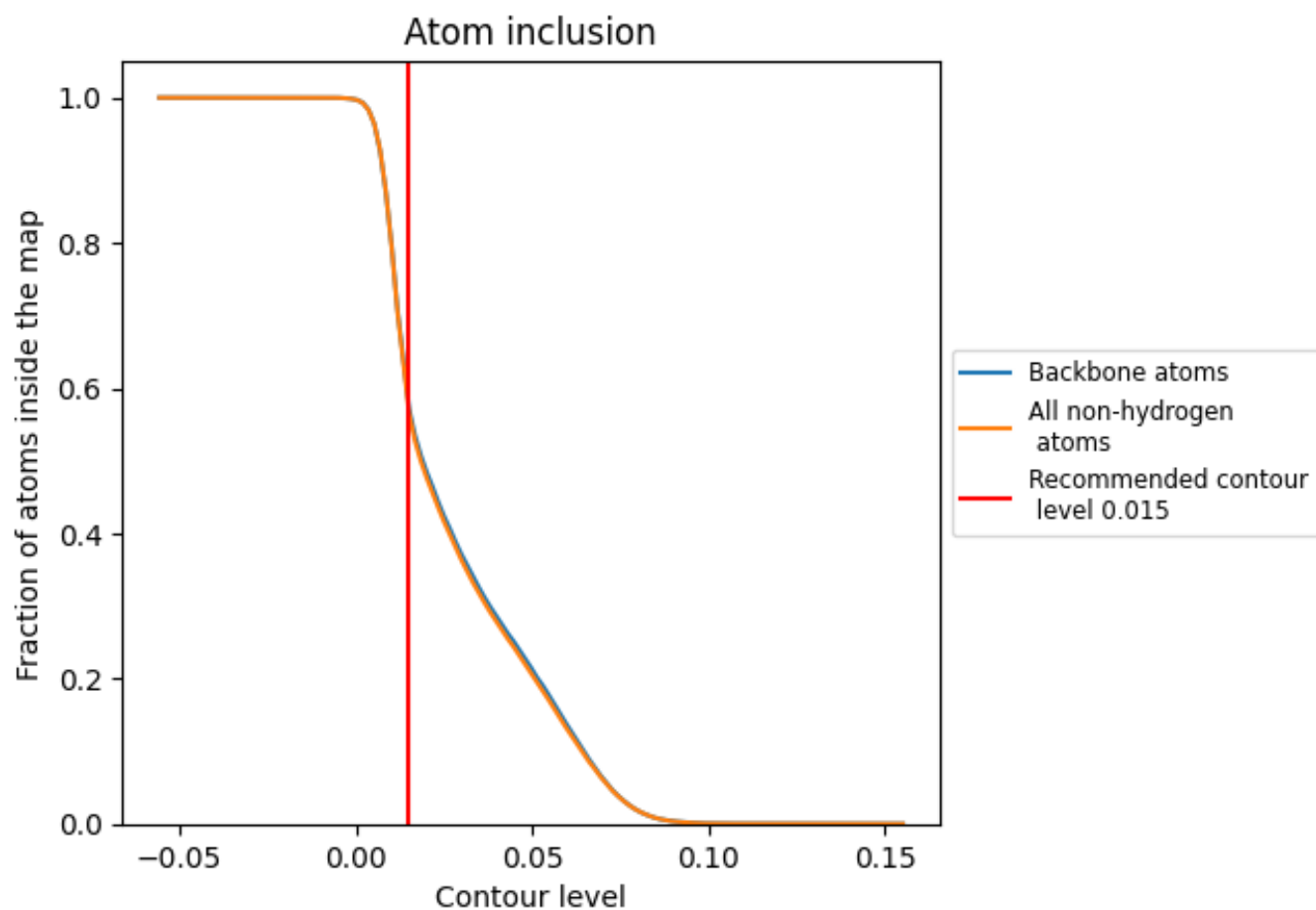
This section was not generated.

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



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




































## 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
All	 0.5700
A	 0.9538
A1	 0.2439
A2	 0.2049
B	 0.6040
B1	 0.0903
B2	 0.0880
C	 0.9744
C1	 0.0270
C2	 0.0247
D	 0.7475
D1	 0.0542
D2	 0.0468
E	 0.8523
E1	 0.1001
E2	 0.0830
F	 0.9581
F1	 0.0494
F2	 0.0605
G	 0.9161
G1	 0.0000
G2	 0.0000
H	 0.9272
H1	 0.7567
H2	 0.7102
I	 0.9041
I1	 0.6834
I2	 0.6744
J	 0.8814
J1	 0.6959
J2	 0.6762
K	 0.8497
K1	 0.6673
K2	 0.6154
L	 0.9209



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Chain	Atom inclusion
L1	0.6494
L2	0.6261
M	0.9686
M1	0.6941
M2	0.6637
N	0.9663
N1	0.7030
N2	0.6905
O	0.9431
O1	0.6923
O2	0.6816
P	0.8318
P1	0.7013
P2	0.6959
Q	0.9259
Q1	0.7317
Q2	0.7174
R	0.9469
S	0.8484
a	0.9430
b	0.6106
c	0.9793
d	0.7493
d1	0.4871
d2	0.4573
e	0.8564
e1	0.5152
e2	0.4527
f	0.9222
g	0.9183
g1	0.4623
g2	0.4179
h	0.9399
i	0.9136
i1	0.4316
i2	0.3789
j	0.8836
k	0.8442
l	0.9269
m	0.9652
n	0.9612
o	0.9368

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Chain	Atom inclusion
p	 0.8326
q	 0.9294
r	 0.9377
s	 0.8443
t	 0.9282