



wwPDB EM Validation Summary Report ⓘ

Apr 15, 2026 – 01:04 PM UTC

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

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

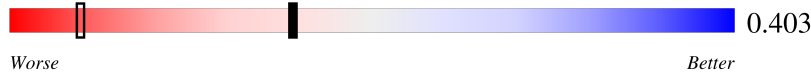
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : **FAILED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

i

ELECTRON MICROSCOPY

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	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	10327 (2.20 - 3.20)

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 285933 atoms, of which 143905 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called subunit a.

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

- Molecule 2 is a protein called subunit b.

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

- Molecule 3 is a protein called subunit d.

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

- Molecule 4 is a protein called subunit f.

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

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

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

- Molecule 6 is a protein called subunit k.

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

- Molecule 7 is a protein called subunit 8.

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

- Molecule 8 is a protein called ATPTT3.

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

- Molecule 9 is a protein called ATPTT4.

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

- Molecule 10 is a protein called ATPTT5.

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

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

- Molecule 11 is a protein called ATPTT6.

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

- Molecule 12 is a protein called ATPTT7.

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

- Molecule 13 is a protein called ATPTT8.

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

- Molecule 14 is a protein called ATPTT9.

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

- Molecule 15 is a protein called ATPTT10.

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

- Molecule 16 is a protein called ATPTT11.

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

- Molecule 17 is a protein called ATPTT12.

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

- Molecule 18 is a protein called ATPTT13.

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

- Molecule 19 is a protein called ATPTT1.

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

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

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

- Molecule 21 is a protein called ATPTT2.

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

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

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

- Molecule 23 is a protein called subunit gamma.

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

- Molecule 24 is a protein called subunit alpha.

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

- Molecule 25 is a protein called subunit beta.

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

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

- Molecule 26 is a protein called subunit c.

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

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

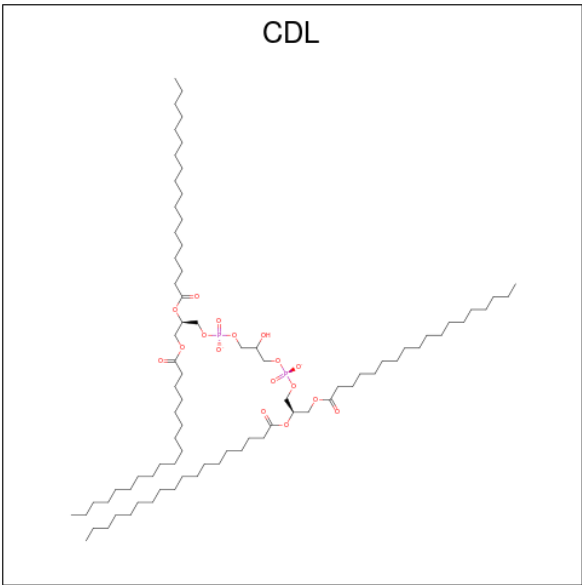
- Molecule 27 is a protein called subunit delta.

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

- Molecule 28 is a protein called subunit epsilon.

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

- Molecule 29 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



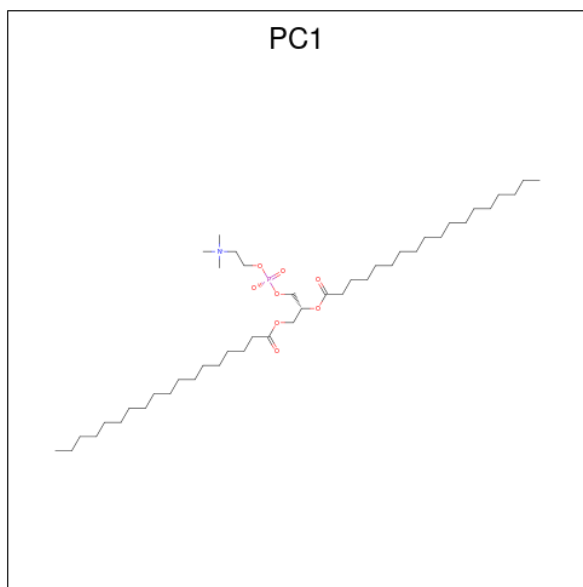
Mol	Chain	Residues	Atoms					AltConf
29	a	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	a	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	f	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	f	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	f	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	f	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	i	1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

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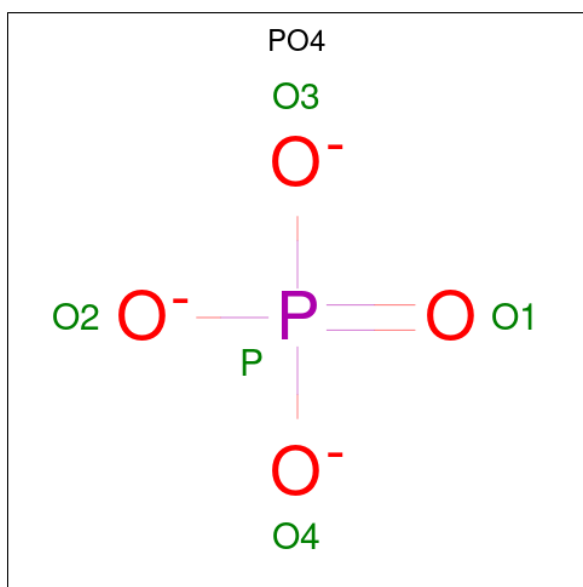
Mol	Chain	Residues	Atoms					AltConf
29	r	1	Total 256	C 81	H 156	O 17	P 2	0
29	A	1	Total 256	C 81	H 156	O 17	P 2	0
29	B	1	Total 256	C 81	H 156	O 17	P 2	0
29	B	1	Total 256	C 81	H 156	O 17	P 2	0
29	B	1	Total 256	C 81	H 156	O 17	P 2	0
29	B	1	Total 256	C 81	H 156	O 17	P 2	0
29	F	1	Total 256	C 81	H 156	O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

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



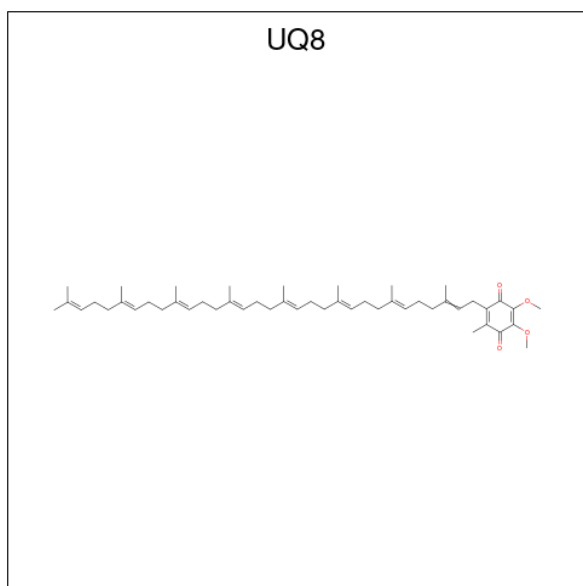
Mol	Chain	Residues	Atoms						AltConf
30	d	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	g	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	g	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	D	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	G	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
30	G	1	Total	C	H	N	O	P	0
			142	44	88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

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



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

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



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

- # ATP

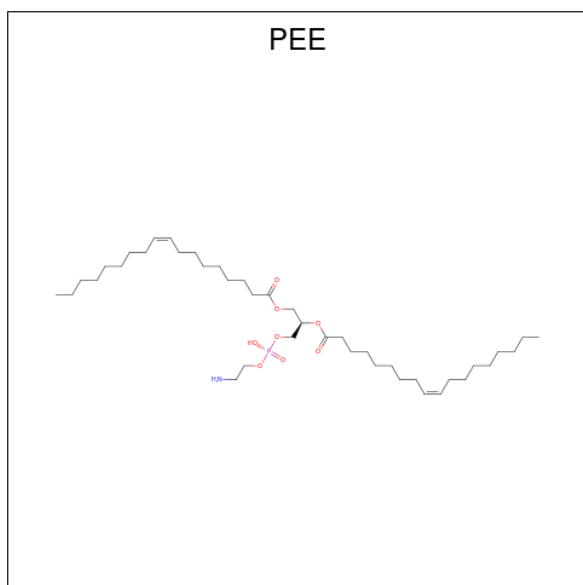
- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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



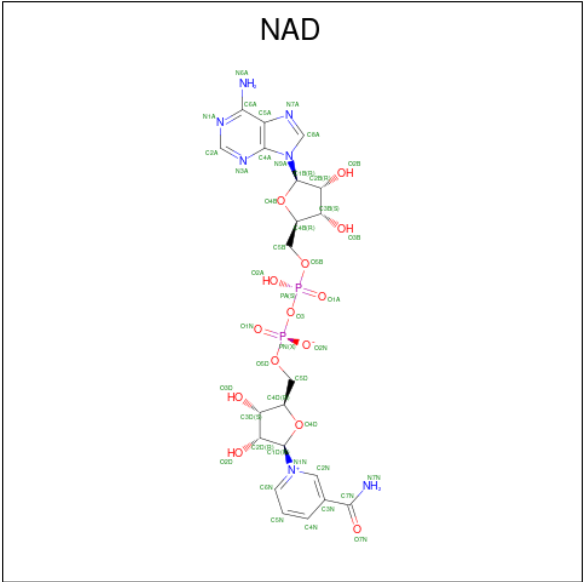
Mol	Chain	Residues	Atoms					AltConf	
35	m	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
35	A	1	Total	C	H	N	O	P	0
			123	38	75	1	8	1	

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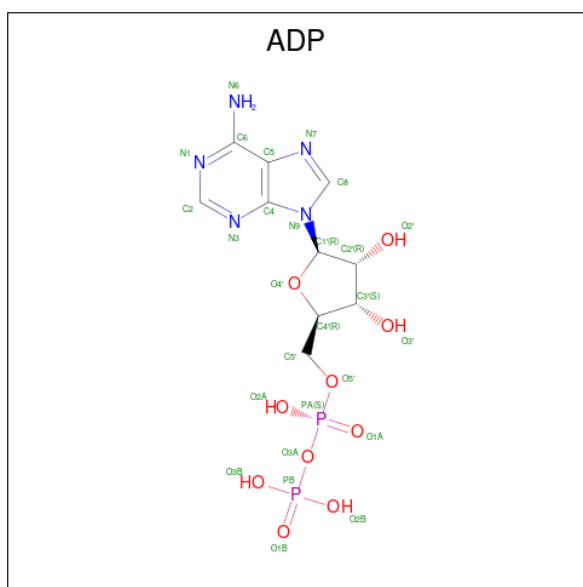
Mol	Chain	Residues	Atoms						AltConf
35	J	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
35	L	1	Total	C	H	N	O	P	0
			123	38	75	1	8	1	

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



Mol	Chain	Residues	Atoms						AltConf
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 (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

MolProbit failed to run properly - this section is therefore empty.

3 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

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 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	f	404	-	99,99,99	0.89	8 (8%)	105,111,111	1.09	5 (4%)
35	PEE	J	303	-	50,50,50	1.17	6 (12%)	53,55,55	1.17	6 (11%)
37	ADP	D1	501	34	28,29,29	3.44	11 (39%)	43,45,45	3.45	14 (32%)
33	ATP	C1	601	34	32,33,33	3.58	13 (40%)	48,52,52	2.19	13 (27%)
33	ATP	A2	601	34	32,33,33	3.60	13 (40%)	48,52,52	2.20	12 (25%)
29	CDL	a	501	-	99,99,99	0.90	7 (7%)	105,111,111	1.05	5 (4%)
33	ATP	G	301	34	32,33,33	3.51	13 (40%)	48,52,52	2.20	12 (25%)
31	PO4	F	301	-	4,4,4	1.08	0	6,6,6	0.47	0
32	UQ8	I	303	-	53,53,53	1.84	7 (13%)	66,67,67	1.66	17 (25%)
30	PC1	G	304	-	53,53,53	0.97	4 (7%)	59,61,61	1.01	2 (3%)
29	CDL	p	201	-	99,99,99	0.89	8 (8%)	105,111,111	1.04	4 (3%)
29	CDL	r	201	-	99,99,99	0.88	8 (8%)	105,111,111	1.03	4 (3%)
33	ATP	g	301	34	32,33,33	3.50	12 (37%)	48,52,52	2.17	13 (27%)
29	CDL	A	502	-	99,99,99	0.89	7 (7%)	105,111,111	1.09	4 (3%)
29	CDL	J	302	-	99,99,99	0.89	8 (8%)	105,111,111	1.01	4 (3%)
29	CDL	F	302	-	99,99,99	0.89	8 (8%)	105,111,111	1.08	4 (3%)
29	CDL	P	201	-	99,99,99	0.89	8 (8%)	105,111,111	1.04	5 (4%)
36	NAD	e	900	-	46,48,48	4.05	22 (47%)	64,73,73	2.11	13 (20%)
29	CDL	j	302	-	99,99,99	0.89	8 (8%)	105,111,111	1.02	4 (3%)
29	CDL	l	301	-	99,99,99	0.89	8 (8%)	105,111,111	1.06	5 (4%)
36	NAD	E	900	-	46,48,48	4.04	22 (47%)	64,73,73	2.11	14 (21%)
29	CDL	i	301	-	99,99,99	0.90	8 (8%)	105,111,111	1.08	4 (3%)
29	CDL	I	301	-	99,99,99	0.88	7 (7%)	105,111,111	1.00	4 (3%)
30	PC1	g	303	-	53,53,53	0.97	4 (7%)	59,61,61	0.98	2 (3%)
33	ATP	B1	601	34	32,33,33	3.58	13 (40%)	48,52,52	2.21	14 (29%)
31	PO4	f	402	-	4,4,4	1.09	0	6,6,6	0.47	0
37	ADP	D2	501	34	28,29,29	3.43	10 (35%)	43,45,45	3.25	15 (34%)
30	PC1	d	301	-	53,53,53	0.95	4 (7%)	59,61,61	1.08	2 (3%)
33	ATP	A1	601	34	32,33,33	3.59	13 (40%)	48,52,52	2.20	12 (25%)
29	CDL	L	301	-	99,99,99	0.90	7 (7%)	105,111,111	1.02	4 (3%)
35	PEE	L	303	-	47,47,50	1.19	6 (12%)	50,52,55	1.18	5 (10%)
37	ADP	B1	603	34	28,29,29	3.42	10 (35%)	43,45,45	3.29	17 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	ATP	C2	601	34	32,33,33	3.57	13 (40%)	48,52,52	2.21	14 (29%)
29	CDL	k	201	-	99,99,99	0.90	8 (8%)	105,111,111	1.02	4 (3%)
35	PEE	A	501	-	47,47,50	1.20	6 (12%)	50,52,55	1.18	3 (6%)
29	CDL	j	301	-	99,99,99	0.89	8 (8%)	105,111,111	1.09	4 (3%)
35	PEE	m	301	-	50,50,50	1.17	6 (12%)	53,55,55	1.09	4 (7%)
29	CDL	a	502	-	99,99,99	0.89	8 (8%)	105,111,111	1.10	6 (5%)
29	CDL	f	401	-	99,99,99	0.88	8 (8%)	105,111,111	1.12	4 (3%)
29	CDL	k	202	-	99,99,99	0.89	7 (7%)	105,111,111	1.13	5 (4%)
37	ADP	B2	603	34	28,29,29	3.43	11 (39%)	43,45,45	3.27	17 (39%)
30	PC1	G	303	-	53,53,53	0.98	4 (7%)	59,61,61	0.99	2 (3%)
29	CDL	f	403	-	99,99,99	0.89	7 (7%)	105,111,111	1.05	4 (3%)
33	ATP	B2	601	34	32,33,33	3.59	13 (40%)	48,52,52	2.22	14 (29%)
30	PC1	D	301	-	53,53,53	0.95	4 (7%)	59,61,61	1.11	2 (3%)
29	CDL	K	202	-	99,99,99	0.89	7 (7%)	105,111,111	1.11	5 (4%)
29	CDL	B	401	-	99,99,99	0.88	8 (8%)	105,111,111	0.99	4 (3%)
30	PC1	g	304	-	53,53,53	0.98	4 (7%)	59,61,61	0.94	2 (3%)
29	CDL	l	302	-	99,99,99	0.90	8 (8%)	105,111,111	1.06	4 (3%)
29	CDL	L	302	-	99,99,99	0.89	7 (7%)	105,111,111	1.04	4 (3%)
29	CDL	I	302	-	99,99,99	0.90	8 (8%)	105,111,111	1.05	4 (3%)
29	CDL	B	403	-	99,99,99	0.89	7 (7%)	105,111,111	1.06	4 (3%)
29	CDL	B	402	-	99,99,99	0.88	8 (8%)	105,111,111	1.13	6 (5%)
29	CDL	K	201	-	99,99,99	0.89	8 (8%)	105,111,111	1.04	4 (3%)
32	UQ8	i	302	-	53,53,53	1.84	7 (13%)	66,67,67	1.64	17 (25%)
29	CDL	J	301	-	99,99,99	0.90	7 (7%)	105,111,111	1.09	5 (4%)
29	CDL	B	404	-	99,99,99	0.89	8 (8%)	105,111,111	1.09	5 (4%)
29	CDL	f	405	-	99,99,99	0.90	8 (8%)	105,111,111	1.06	4 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CDL	f	404	-	-	42/110/110/110	-
35	PEE	J	303	-	-	28/54/54/54	-
37	ADP	D1	501	34	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	ATP	C1	601	34	-	5/22/38/38	0/3/3/3
33	ATP	A2	601	34	-	6/22/38/38	0/3/3/3
29	CDL	a	501	-	-	33/110/110/110	-
33	ATP	G	301	34	-	0/22/38/38	0/3/3/3
32	UQ8	I	303	-	-	9/51/75/75	0/1/1/1
30	PC1	G	304	-	-	19/57/57/57	-
29	CDL	p	201	-	-	43/110/110/110	-
29	CDL	r	201	-	-	36/110/110/110	-
33	ATP	g	301	34	-	0/22/38/38	0/3/3/3
29	CDL	A	502	-	-	45/110/110/110	-
29	CDL	J	302	-	-	41/110/110/110	-
29	CDL	F	302	-	-	47/110/110/110	-
29	CDL	P	201	-	-	36/110/110/110	-
36	NAD	e	900	-	-	8/30/62/62	0/5/5/5
29	CDL	j	302	-	-	41/110/110/110	-
29	CDL	l	301	-	-	39/110/110/110	-
36	NAD	E	900	-	-	6/30/62/62	0/5/5/5
29	CDL	i	301	-	-	37/110/110/110	-
29	CDL	I	301	-	-	44/110/110/110	-
30	PC1	g	303	-	-	21/57/57/57	-
33	ATP	B1	601	34	-	1/22/38/38	0/3/3/3
37	ADP	D2	501	34	-	1/16/32/32	0/3/3/3
30	PC1	d	301	-	-	23/57/57/57	-
33	ATP	A1	601	34	-	5/22/38/38	0/3/3/3
29	CDL	L	301	-	-	37/110/110/110	-
35	PEE	L	303	-	-	21/51/51/54	-
37	ADP	B1	603	34	-	1/16/32/32	0/3/3/3
33	ATP	C2	601	34	-	4/22/38/38	0/3/3/3
29	CDL	k	201	-	-	36/110/110/110	-
35	PEE	A	501	-	-	20/51/51/54	-
29	CDL	j	301	-	-	39/110/110/110	-
35	PEE	m	301	-	-	24/54/54/54	-
29	CDL	a	502	-	-	38/110/110/110	-
29	CDL	f	401	-	-	45/110/110/110	-
29	CDL	k	202	-	-	33/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	ADP	B2	603	34	-	2/16/32/32	0/3/3/3
30	PC1	G	303	-	-	29/57/57/57	-
29	CDL	f	403	-	-	53/110/110/110	-
33	ATP	B2	601	34	-	1/22/38/38	0/3/3/3
30	PC1	D	301	-	-	21/57/57/57	-
29	CDL	K	202	-	-	35/110/110/110	-
29	CDL	B	401	-	-	43/110/110/110	-
30	PC1	g	304	-	-	18/57/57/57	-
29	CDL	l	302	-	-	39/110/110/110	-
29	CDL	L	302	-	-	44/110/110/110	-
29	CDL	I	302	-	-	38/110/110/110	-
29	CDL	B	403	-	-	32/110/110/110	-
29	CDL	B	402	-	-	39/110/110/110	-
29	CDL	K	201	-	-	28/110/110/110	-
32	UQ8	i	302	-	-	8/51/75/75	0/1/1/1
29	CDL	J	301	-	-	40/110/110/110	-
29	CDL	B	404	-	-	45/110/110/110	-
29	CDL	f	405	-	-	47/110/110/110	-

The worst 5 of 481 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	D2	501	ADP	C2'-C3'	-10.59	1.24	1.53
37	B1	603	ADP	C2'-C3'	-10.55	1.24	1.53
37	B2	603	ADP	C2'-C3'	-10.55	1.24	1.53
37	D1	501	ADP	C2'-C3'	-10.53	1.24	1.53
36	e	900	NAD	O4D-C1D	-10.40	1.27	1.40

The worst 5 of 390 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	D1	501	ADP	C1'-N9-C8	-13.43	97.29	127.09
37	B1	603	ADP	C1'-N9-C8	-12.29	99.83	127.09
37	B2	603	ADP	C1'-N9-C8	-12.26	99.88	127.09
37	D1	501	ADP	C4-N9-C1'	12.01	154.72	126.63
37	D2	501	ADP	C1'-N9-C8	-12.00	100.46	127.09

There are no chirality outliers.

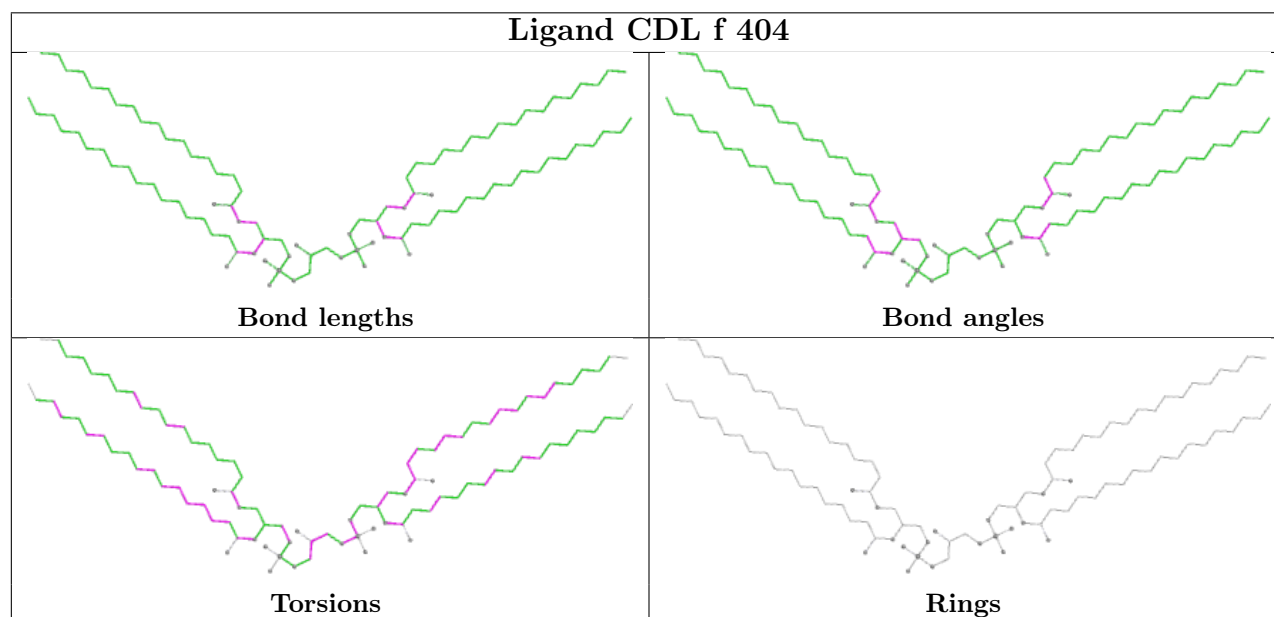
5 of 1479 torsion outliers are listed below:

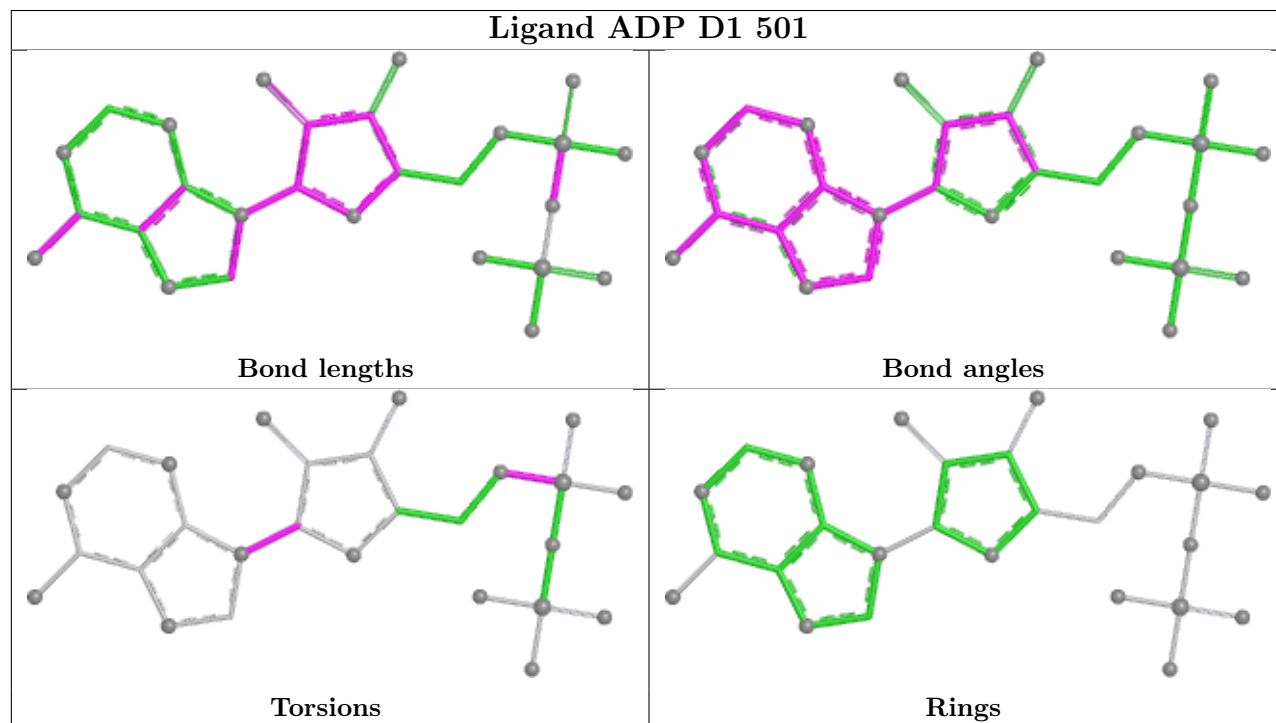
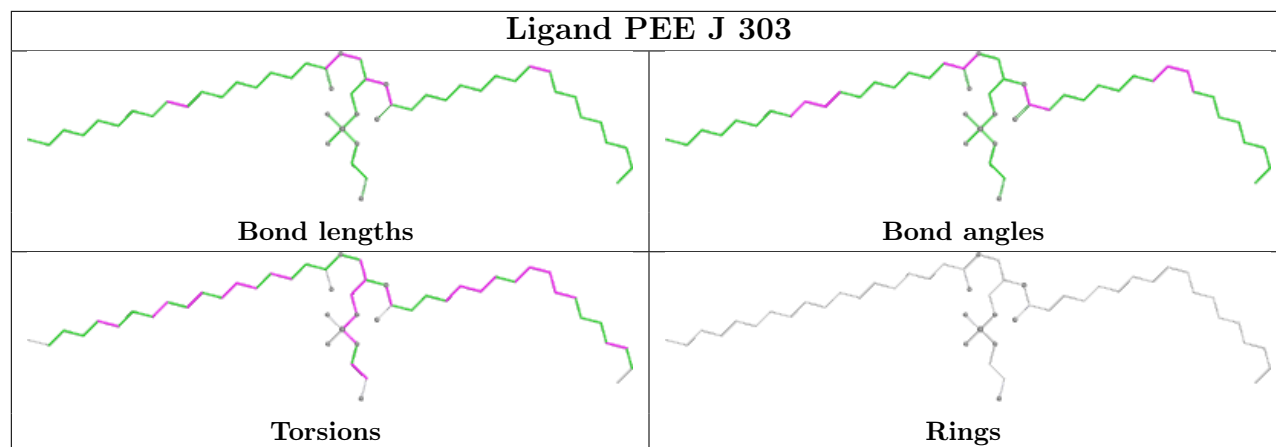
Mol	Chain	Res	Type	Atoms
29	a	501	CDL	OA5-CA3-CA4-OA6
29	a	501	CDL	CB3-OB5-PB2-OB2
29	a	501	CDL	CB3-OB5-PB2-OB4
29	a	501	CDL	OB7-CB5-OB6-CB4
29	a	501	CDL	C51-CB5-OB6-CB4

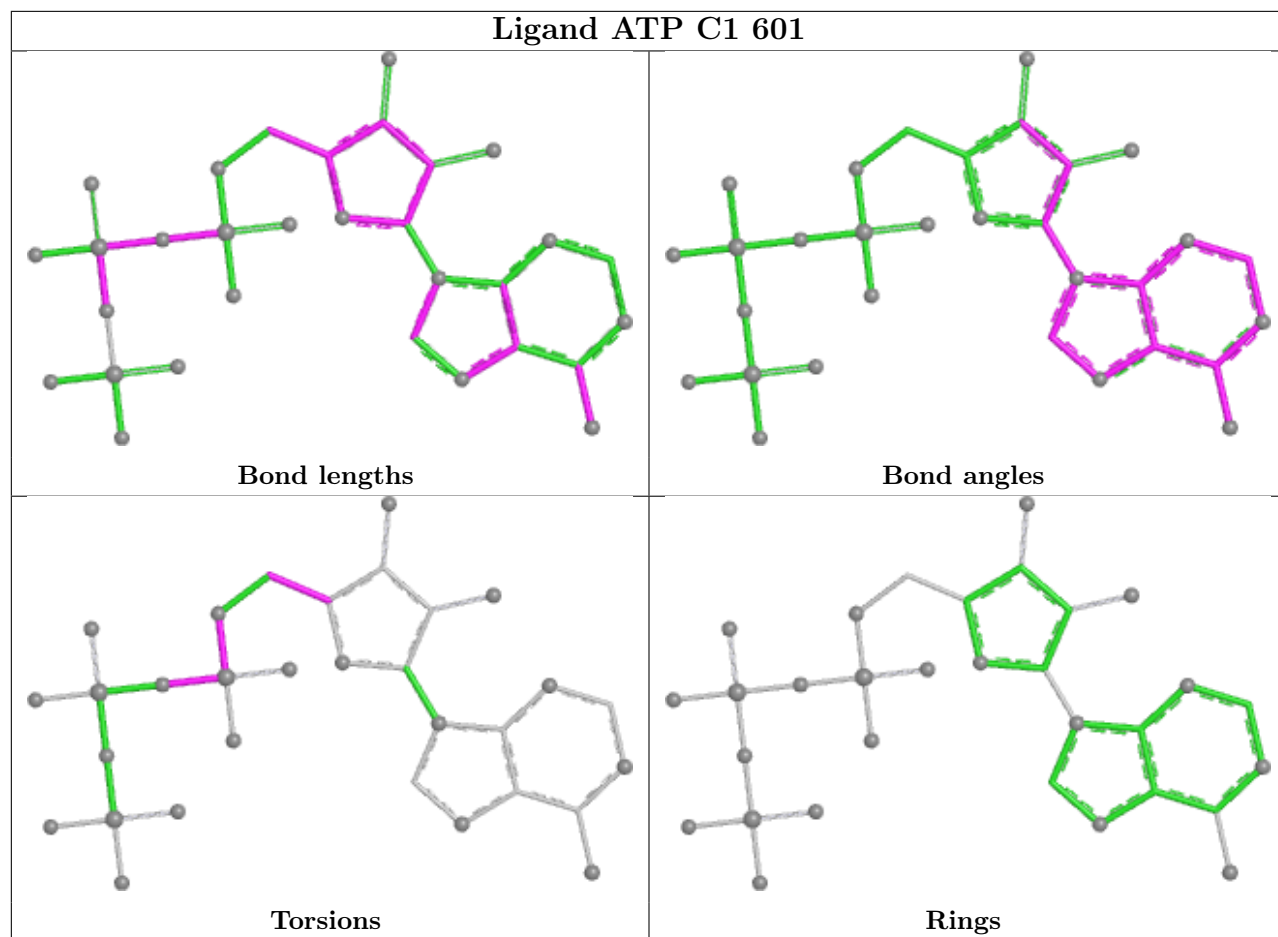
There are no ring outliers.

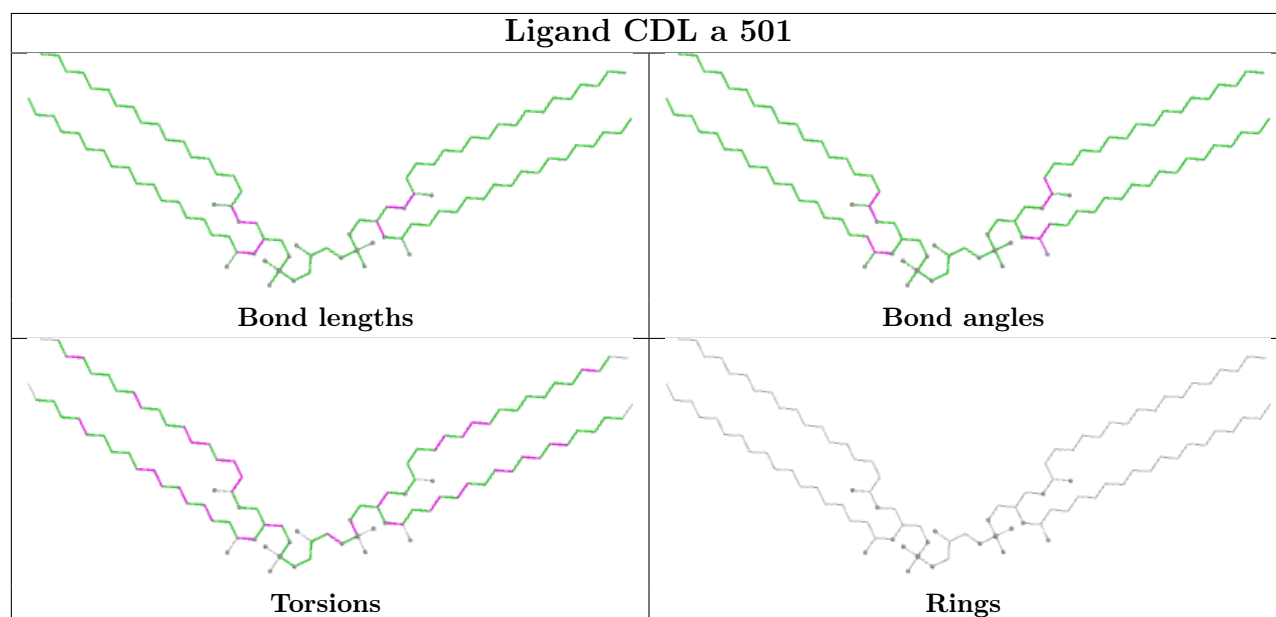
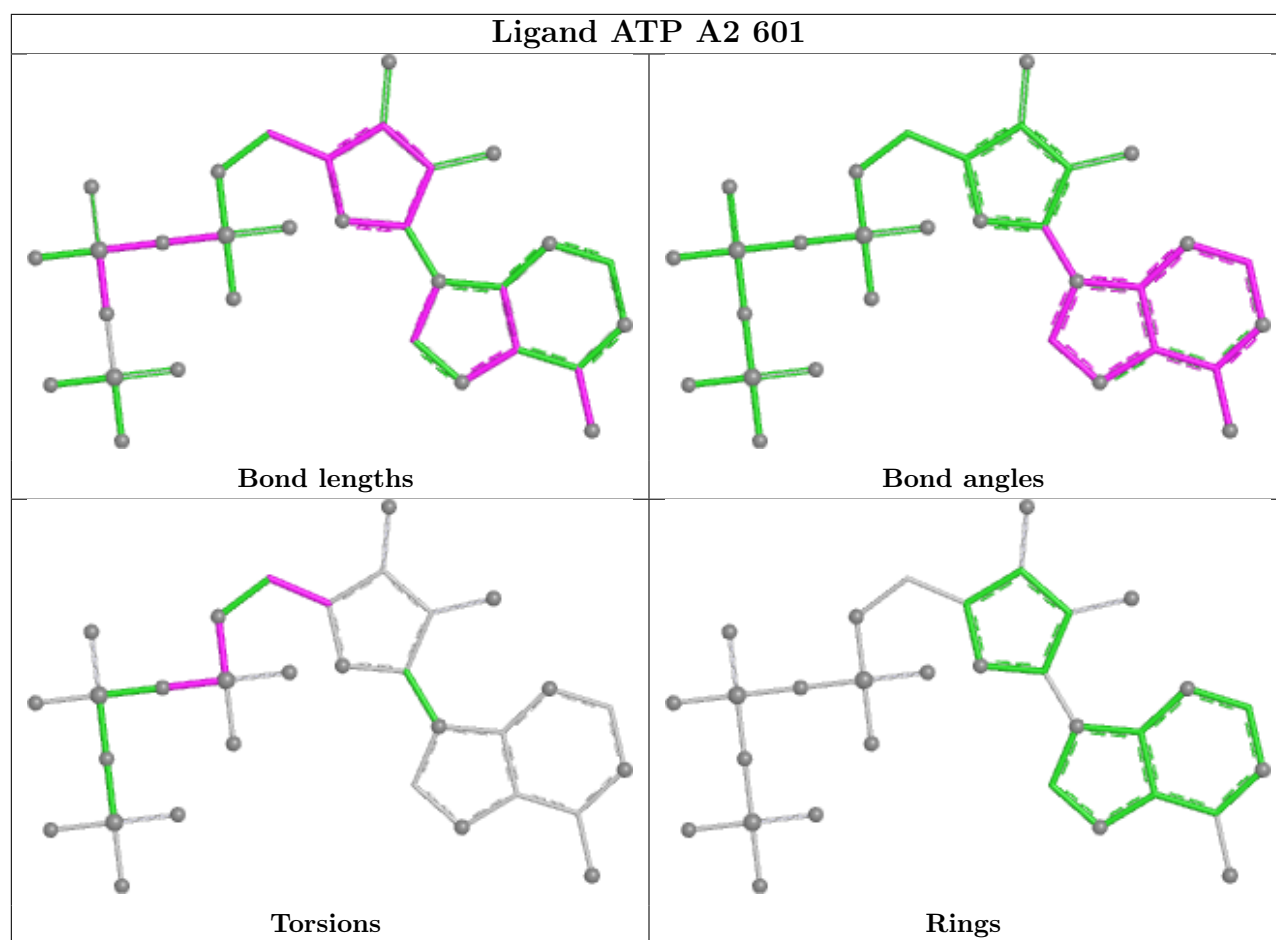
No monomer is involved in short contacts.

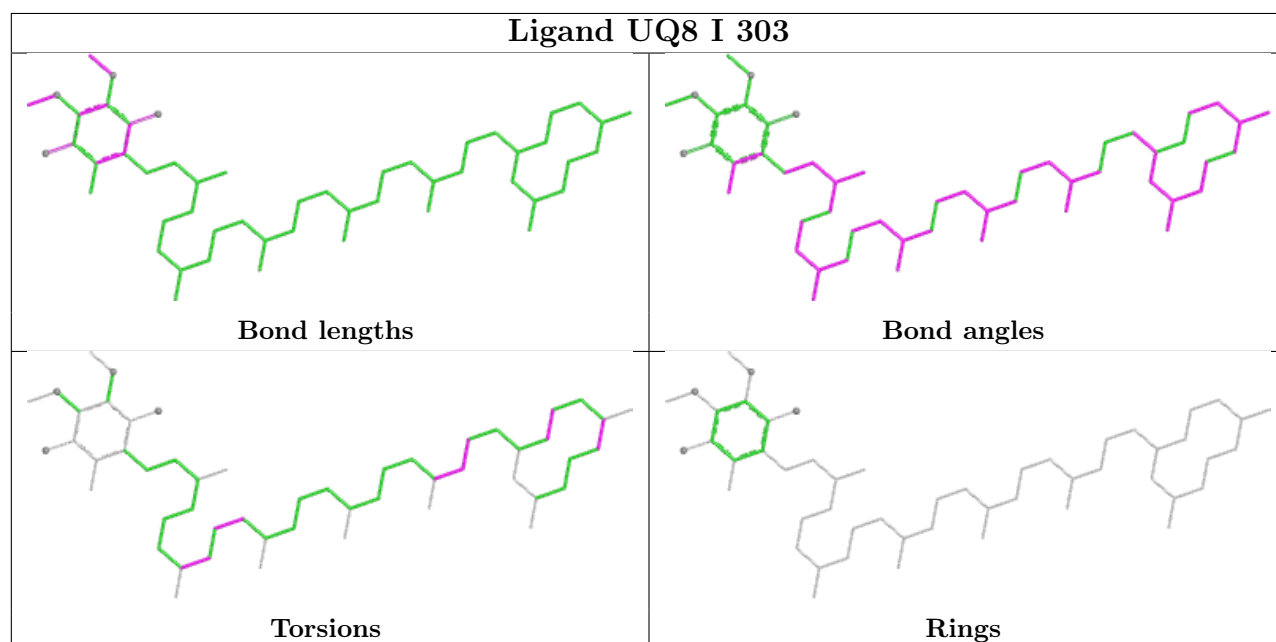
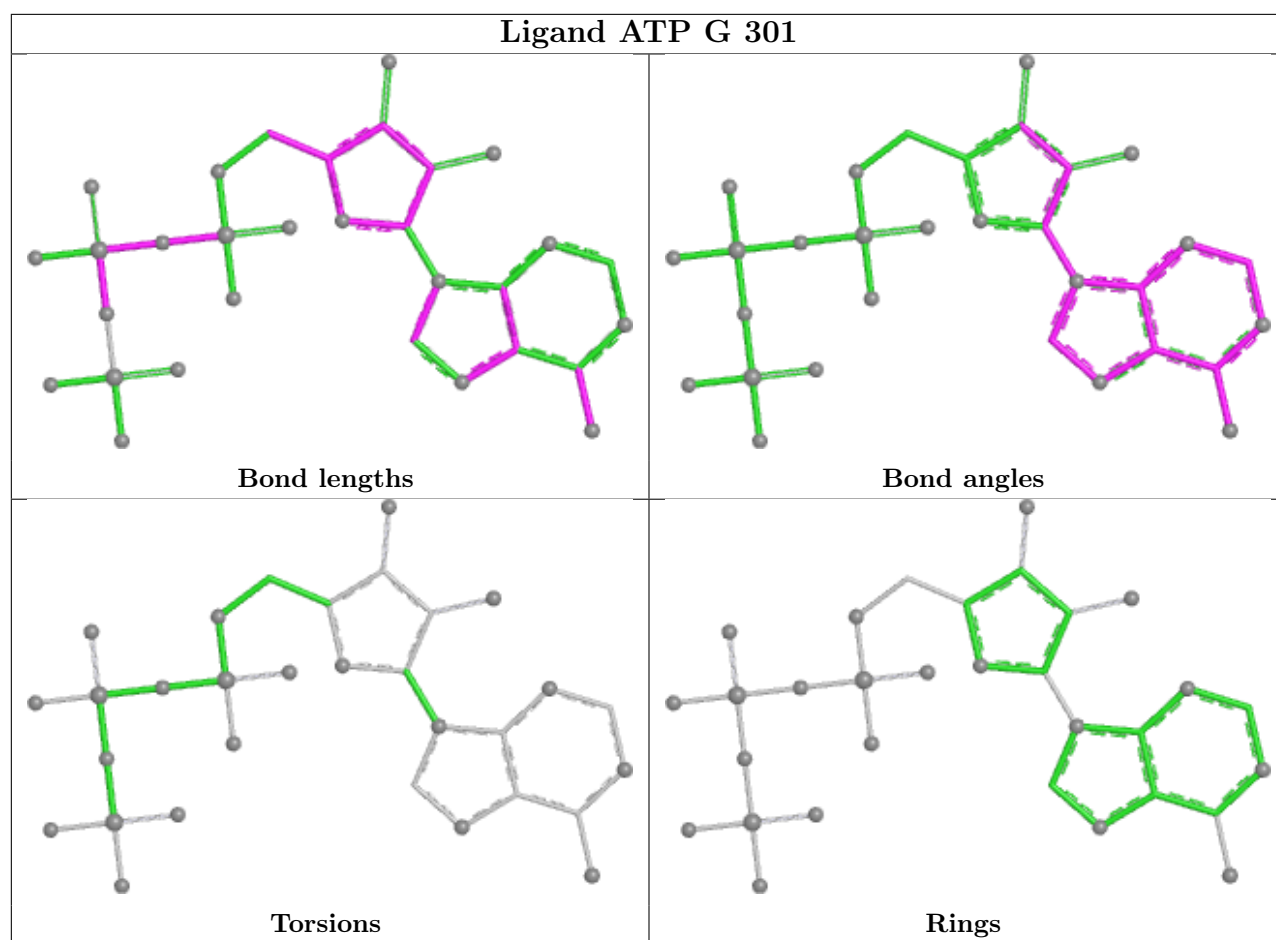
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

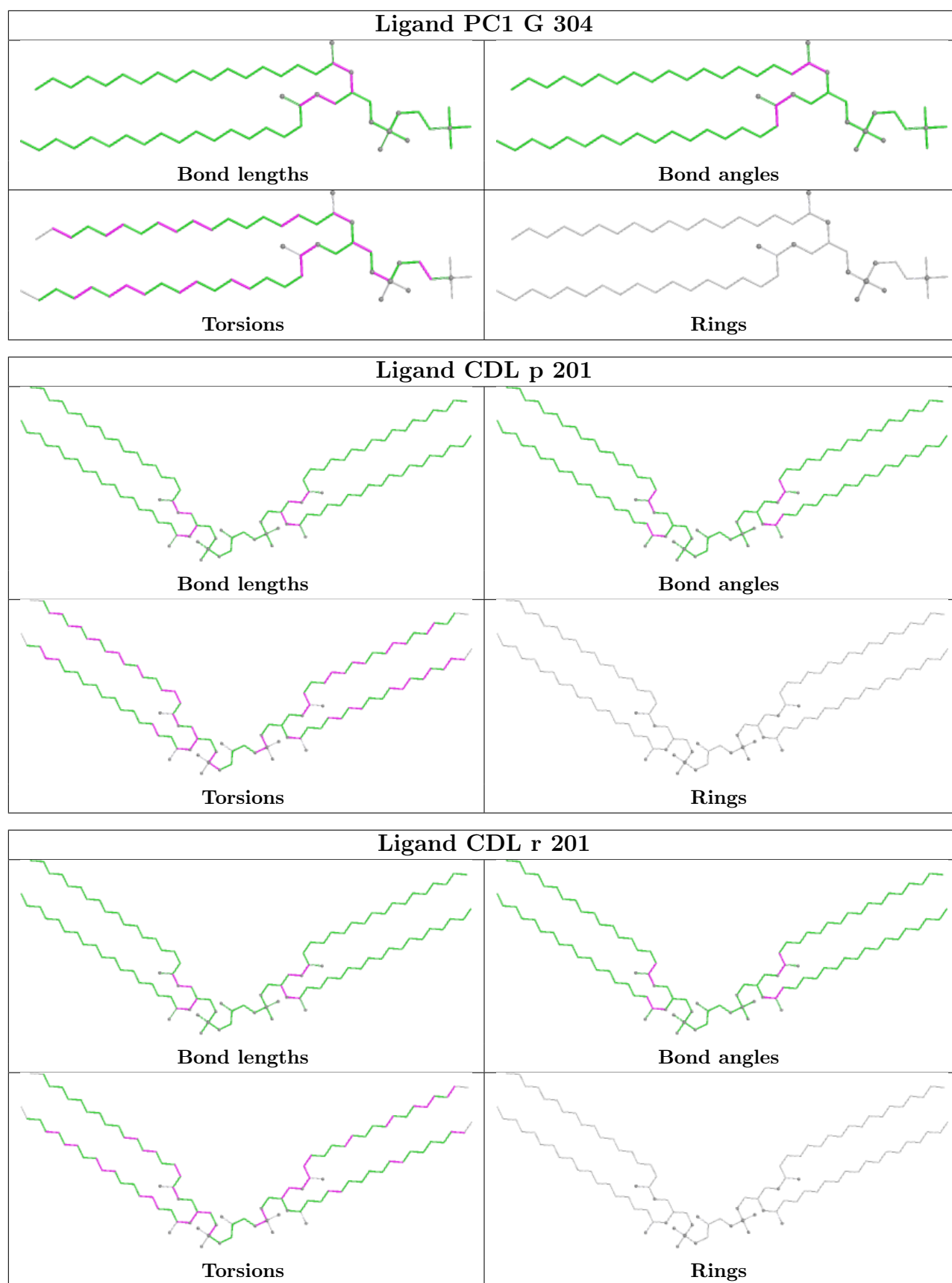


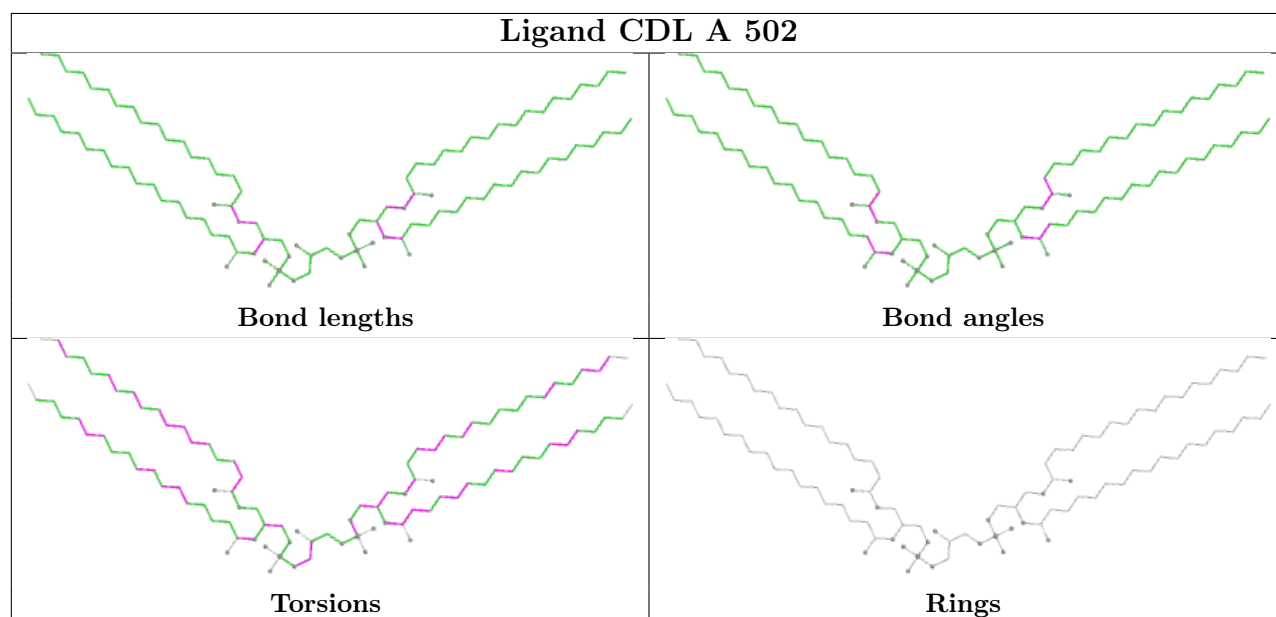
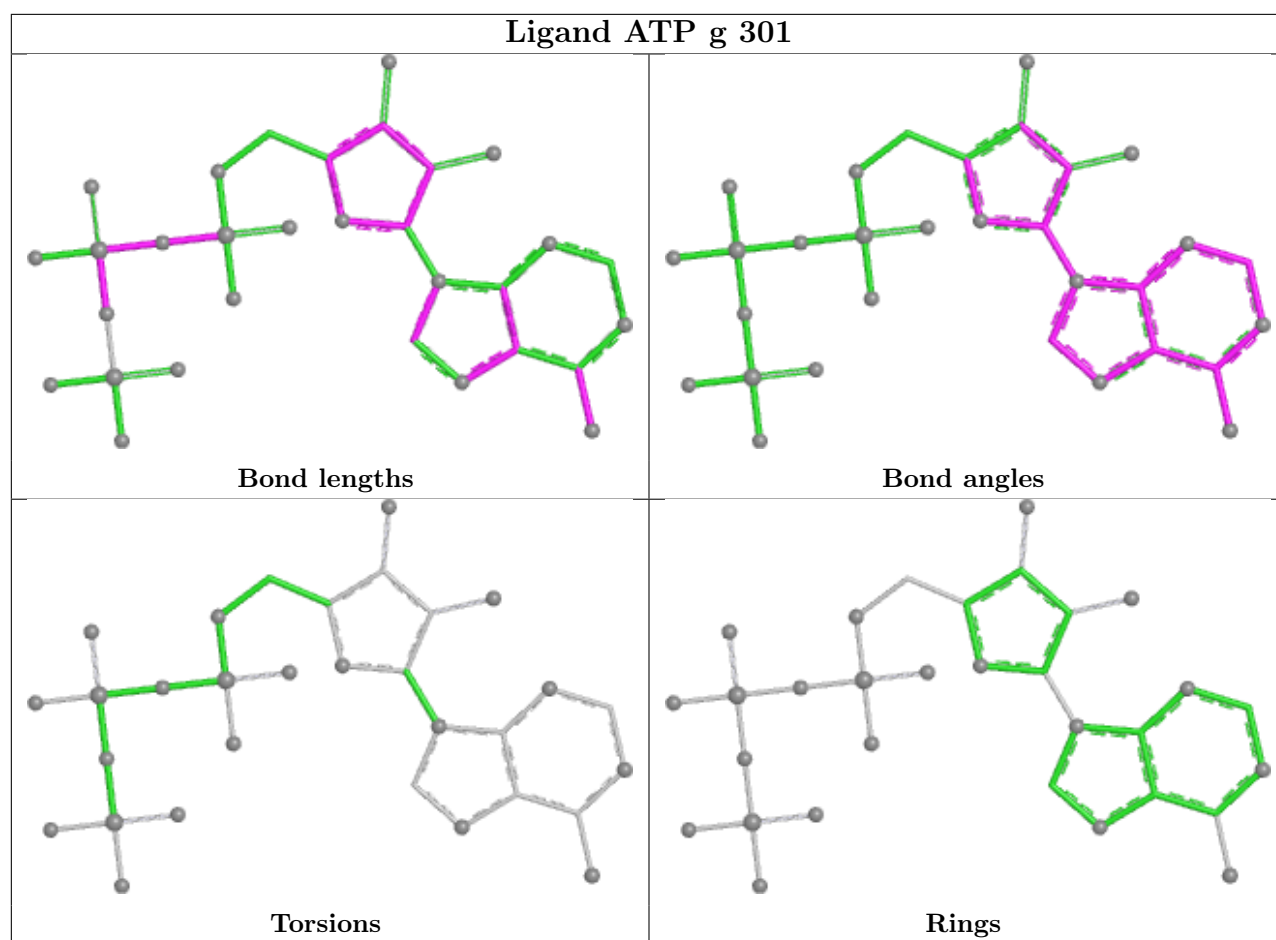


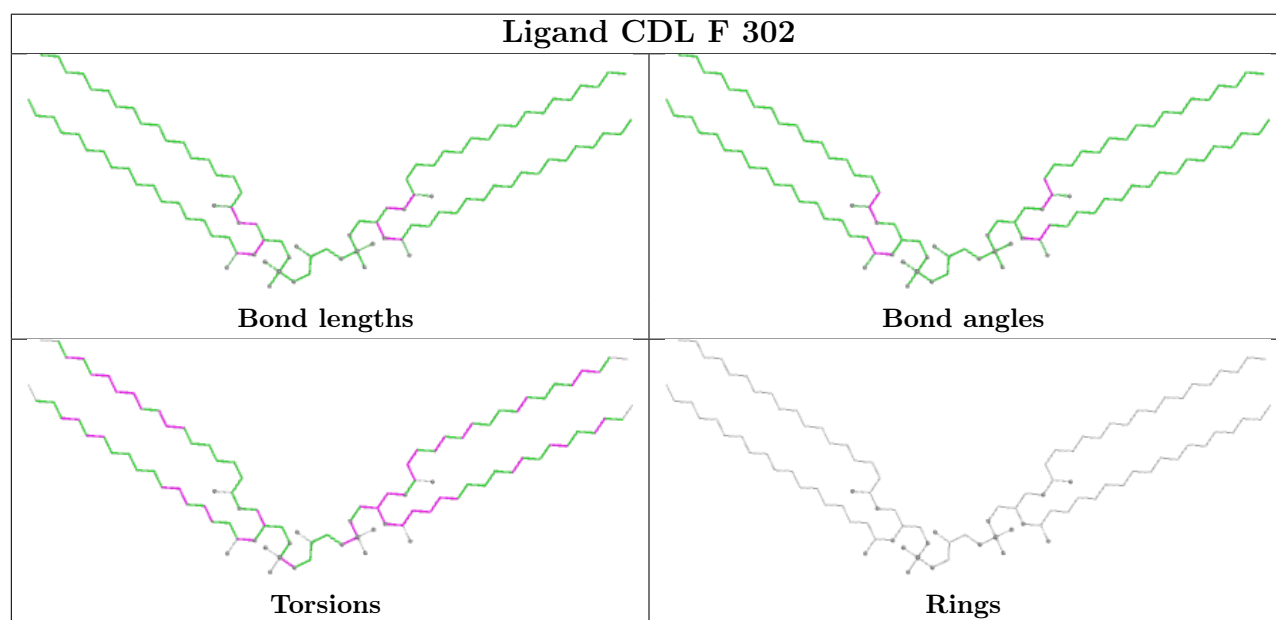
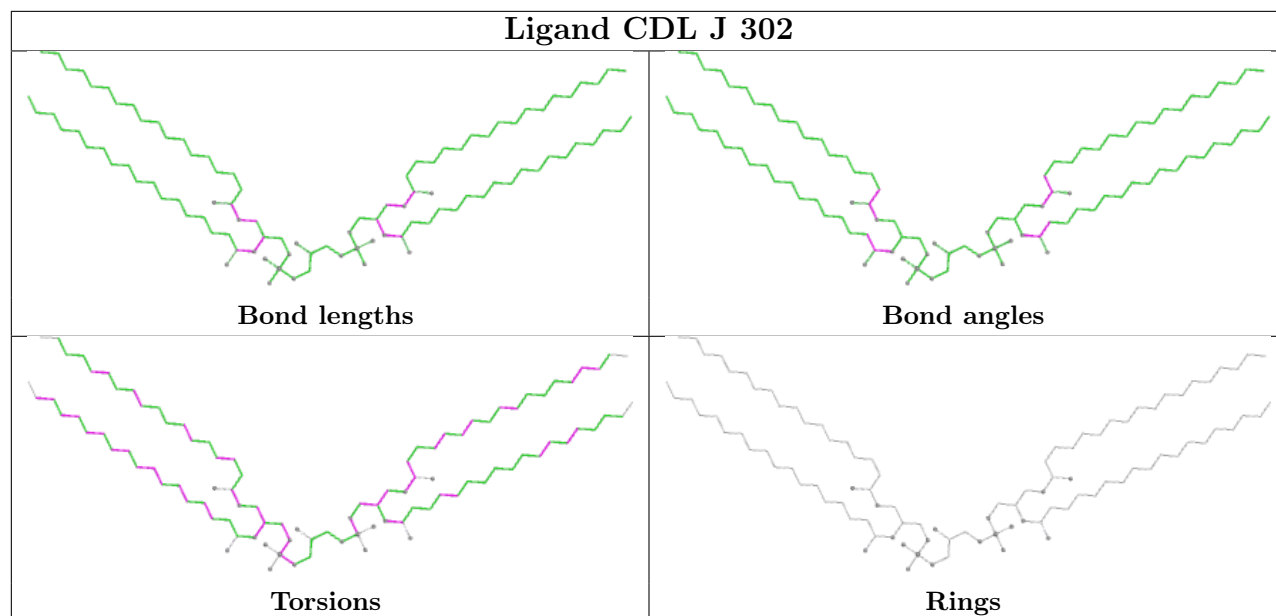


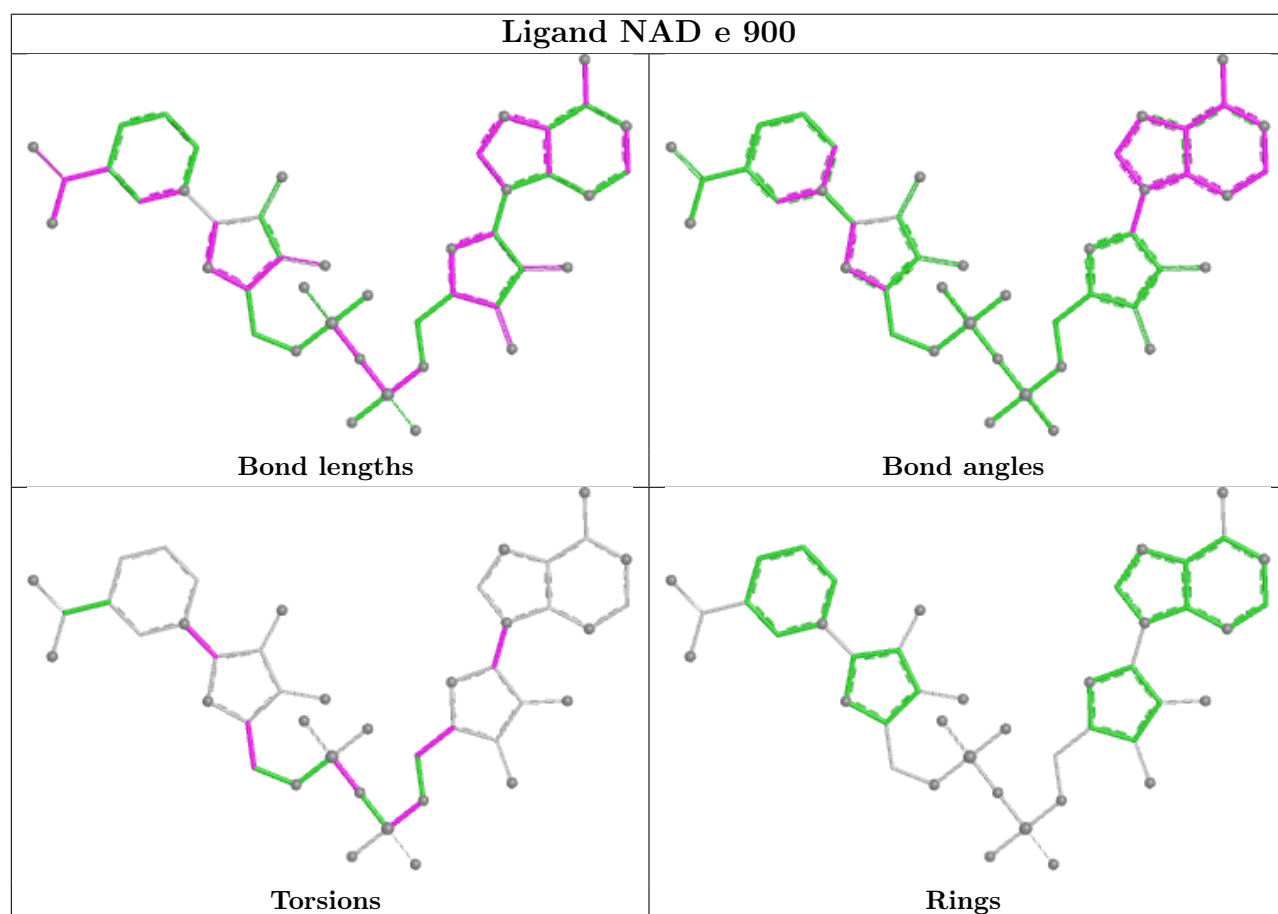
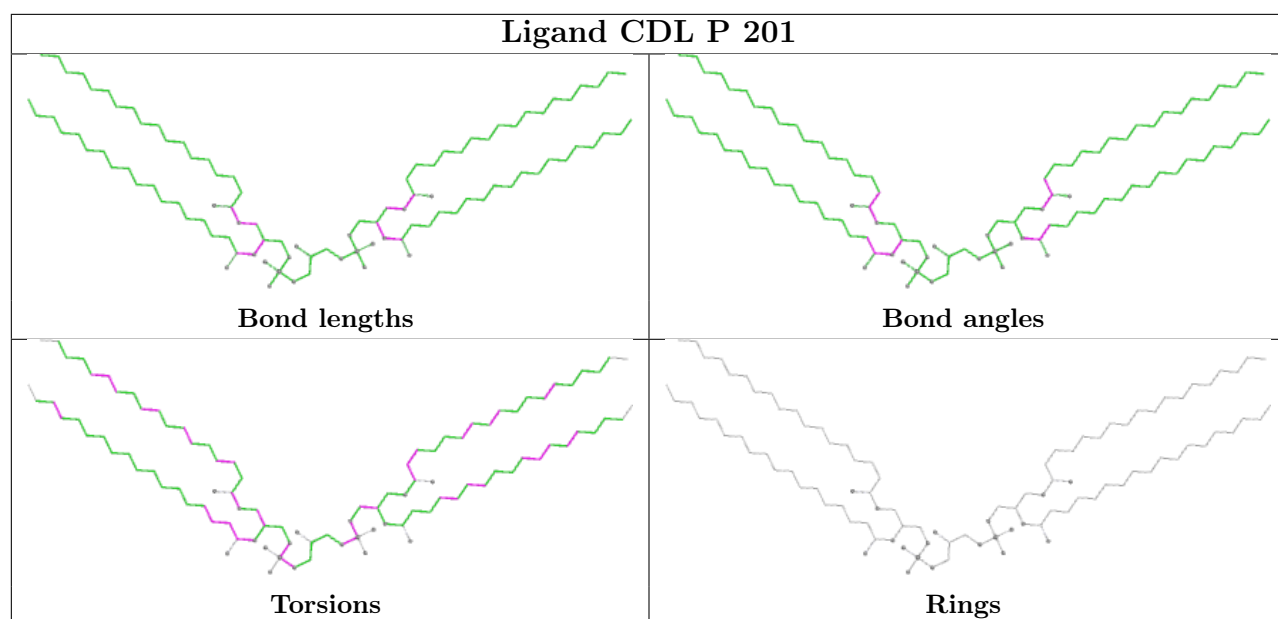


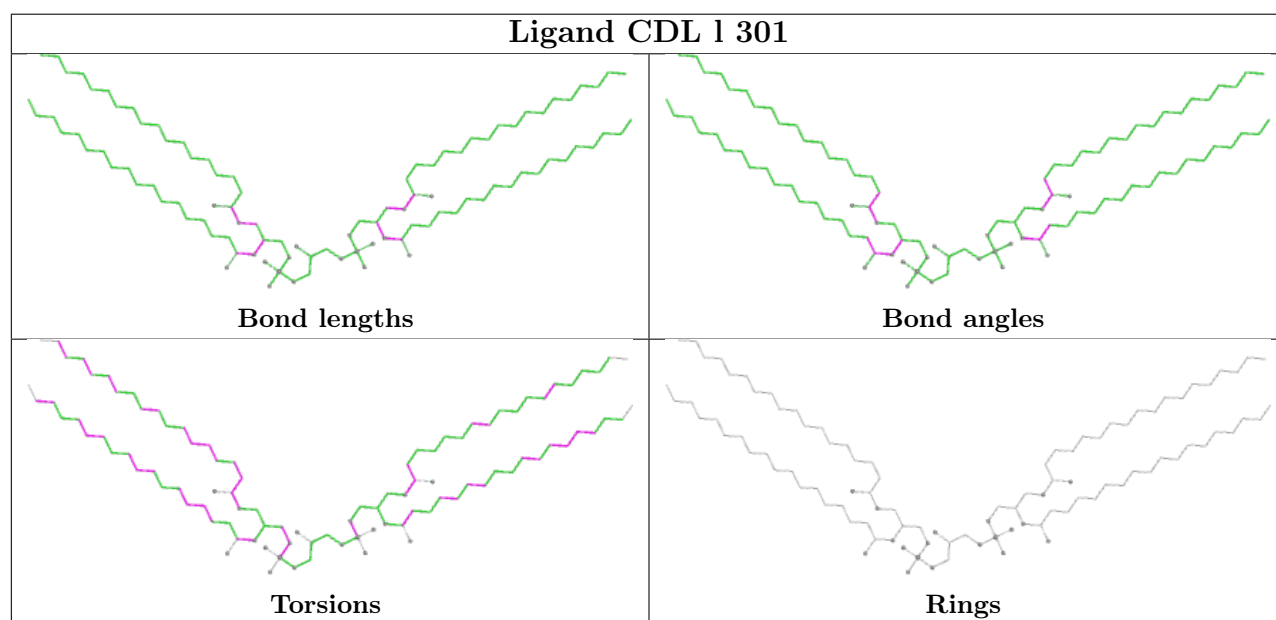
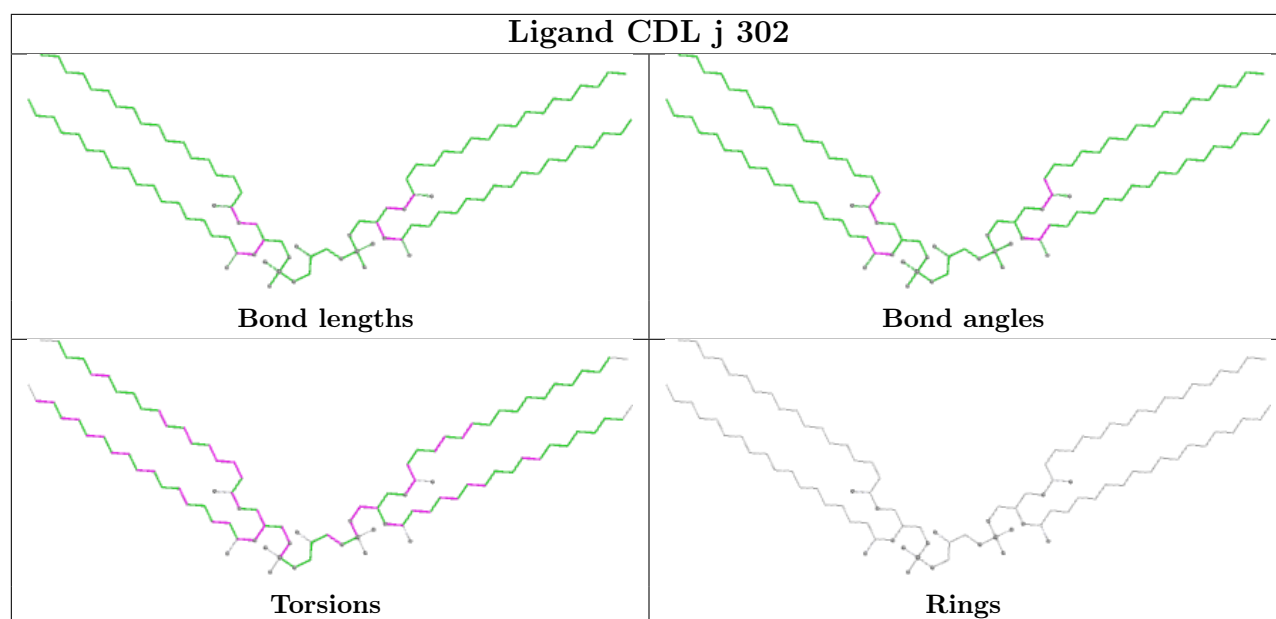


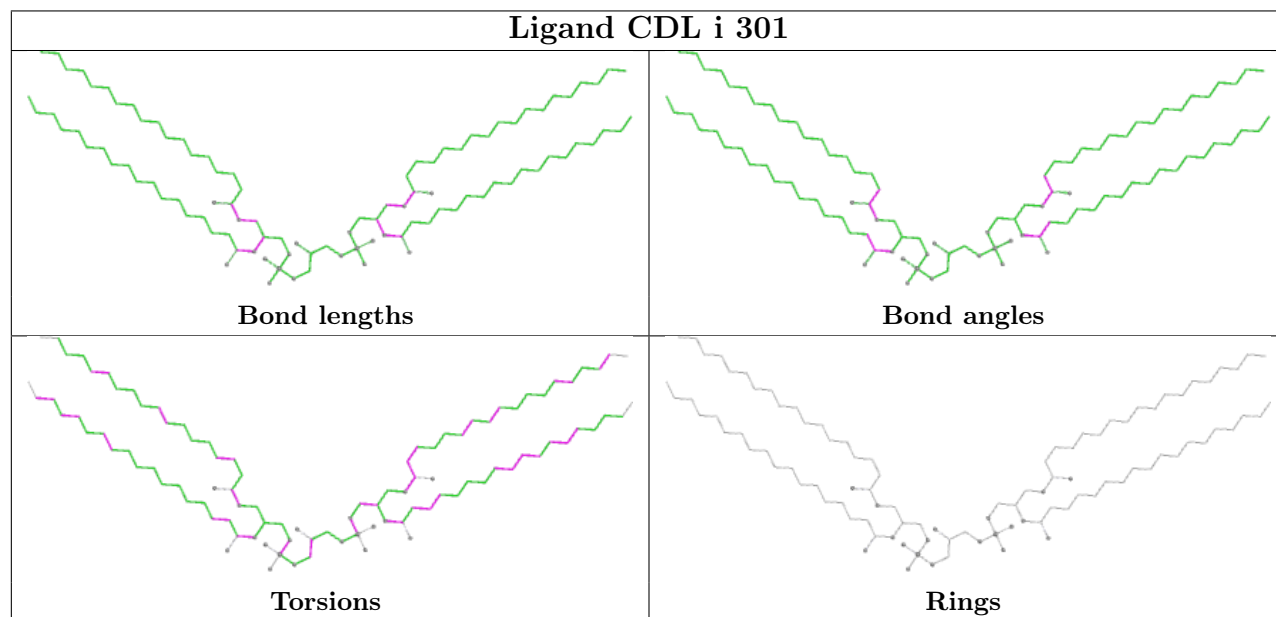
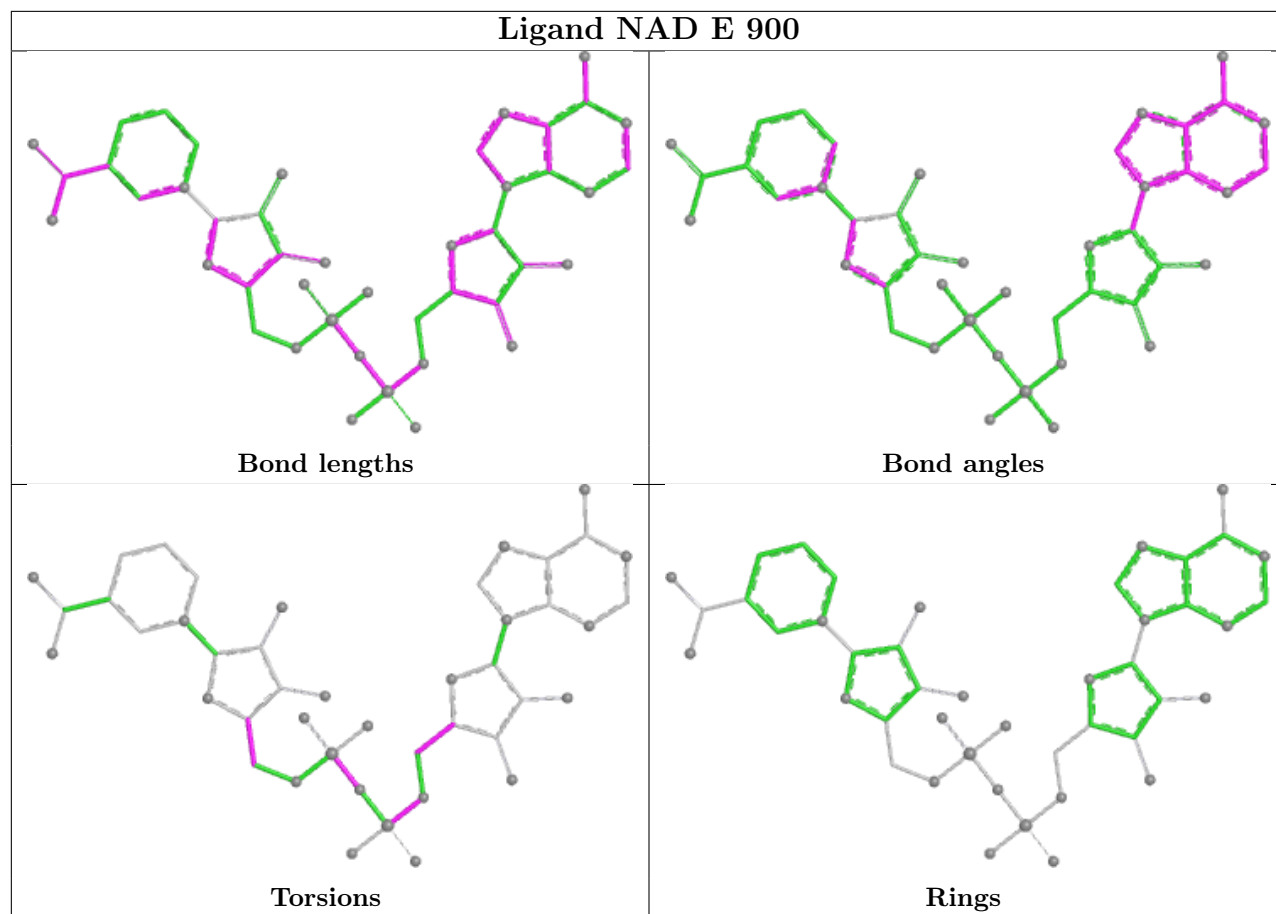


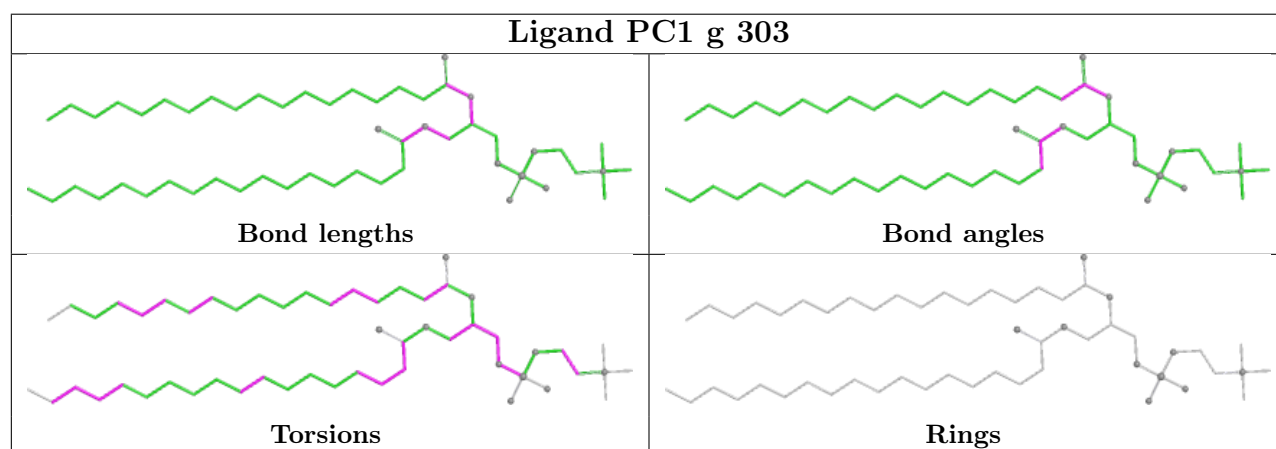
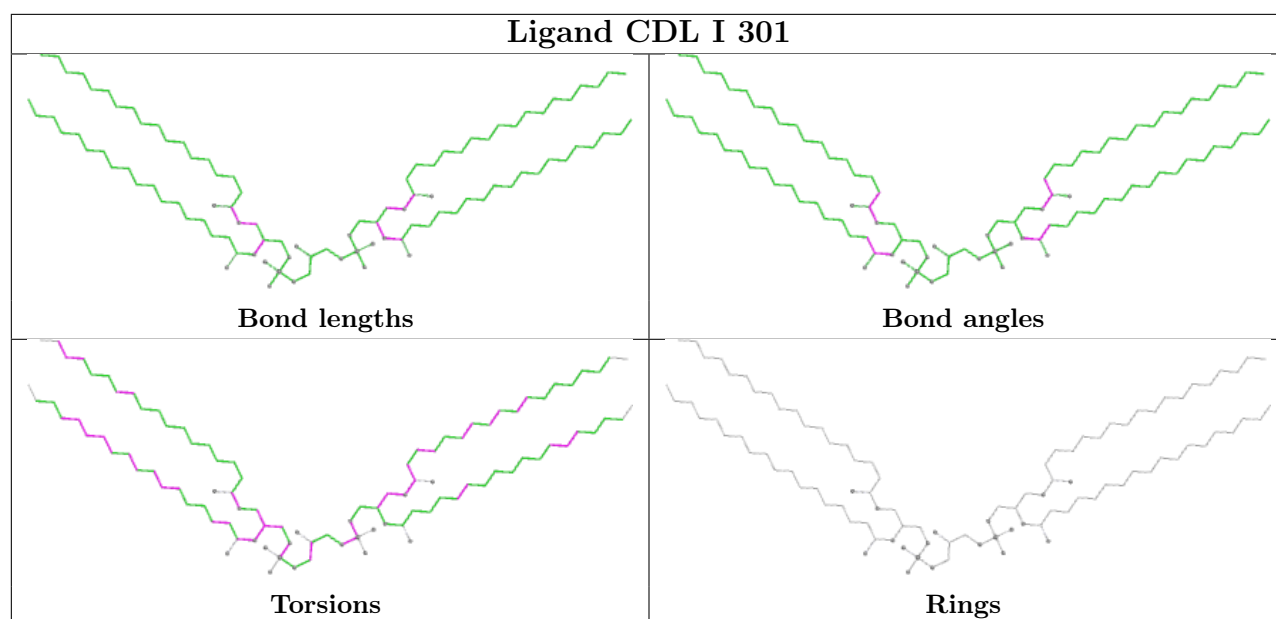


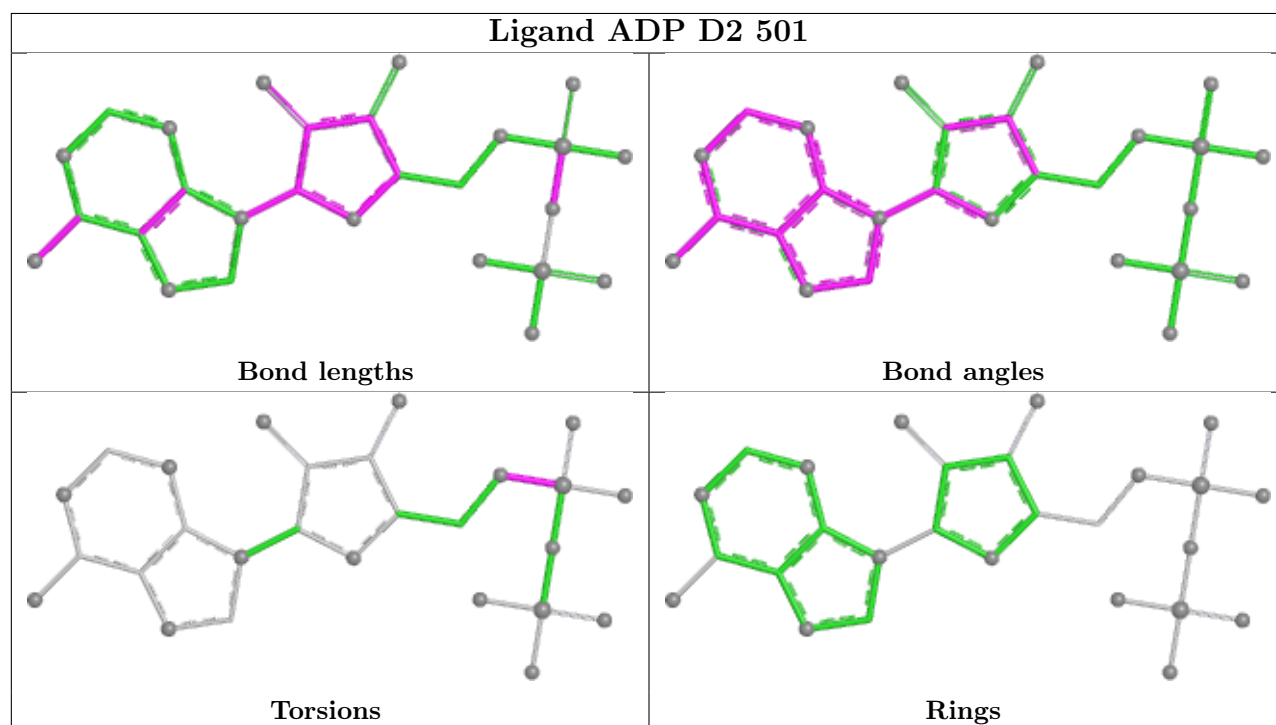
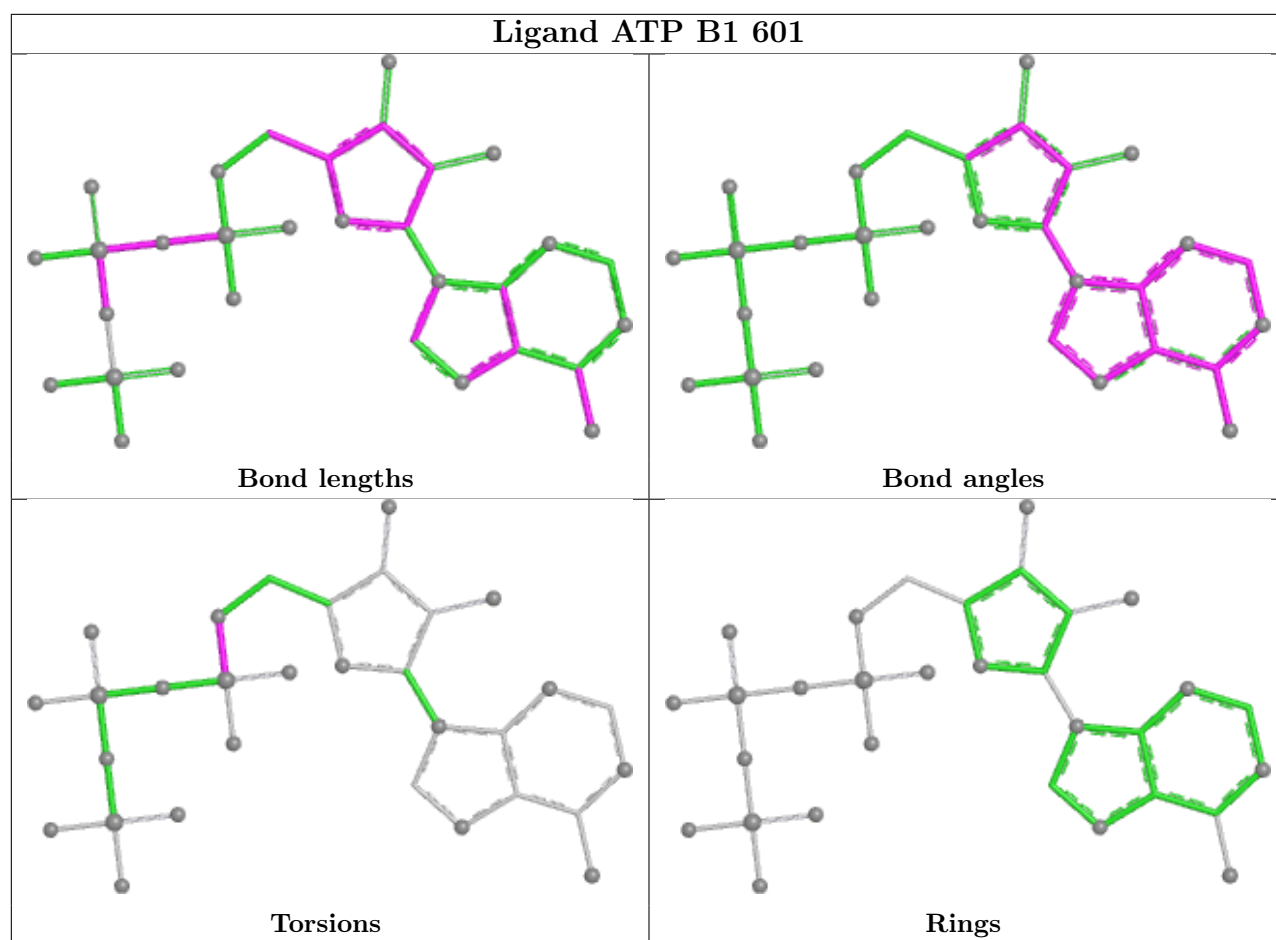


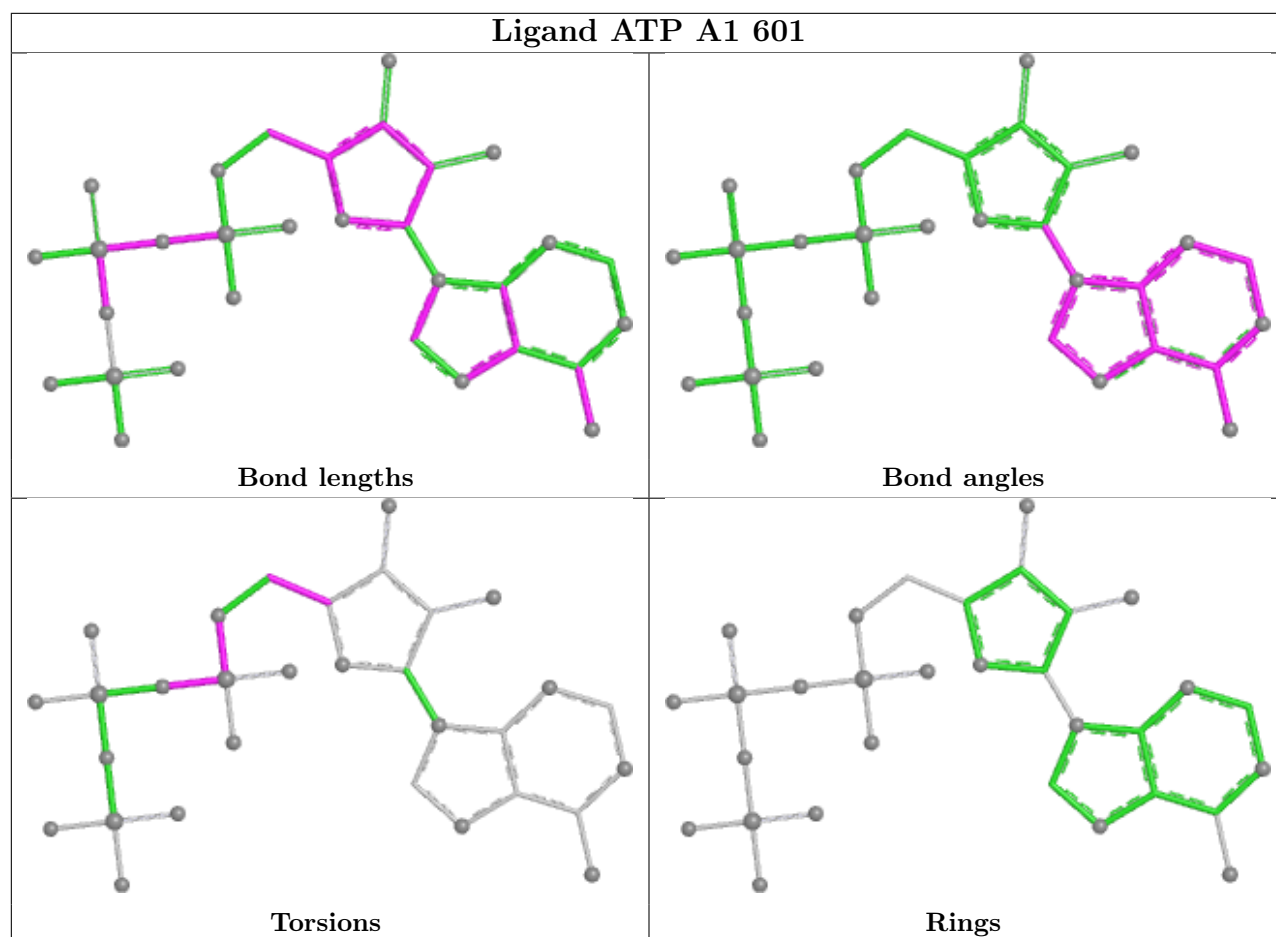
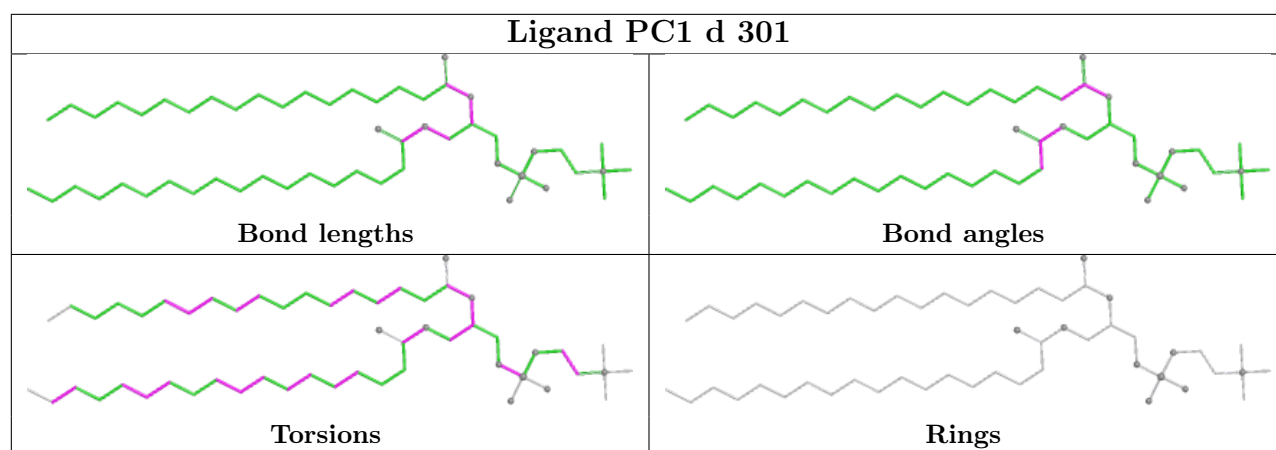


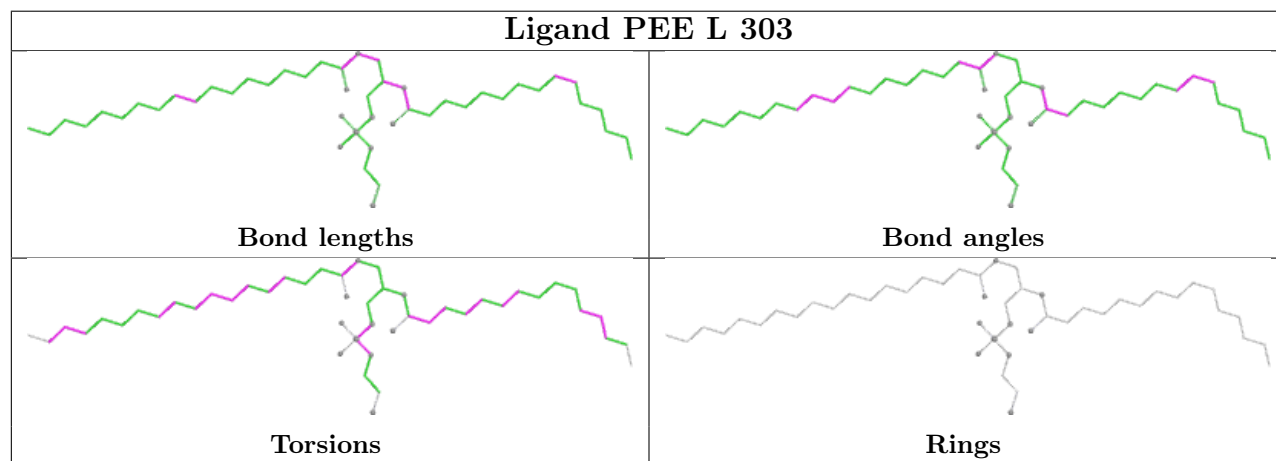
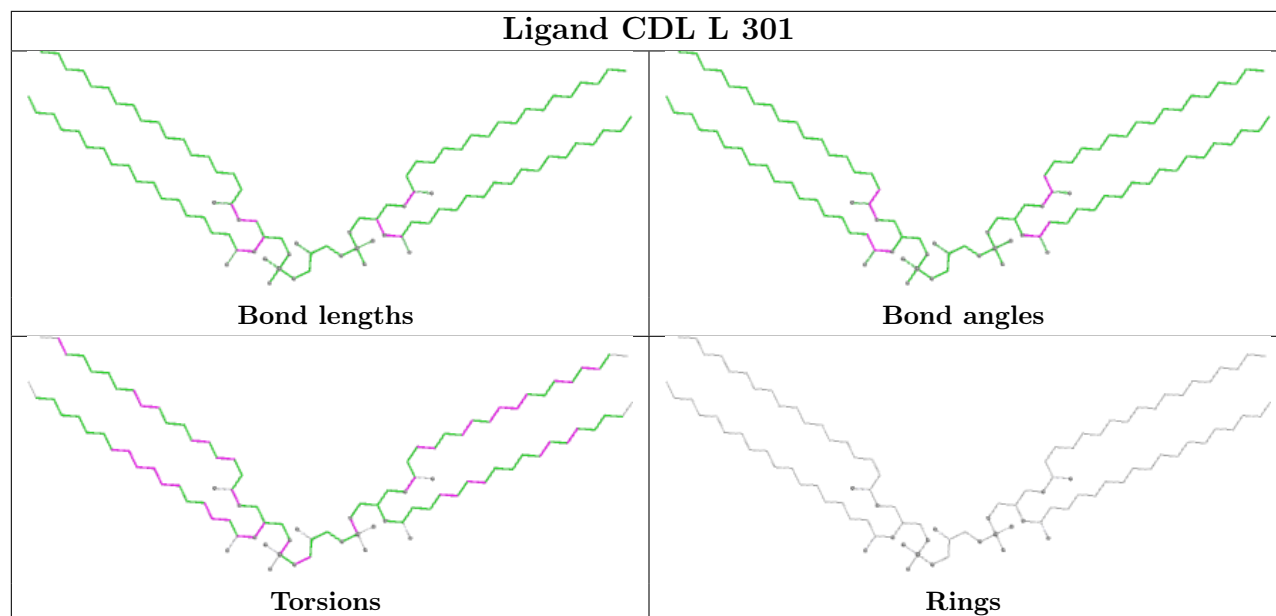


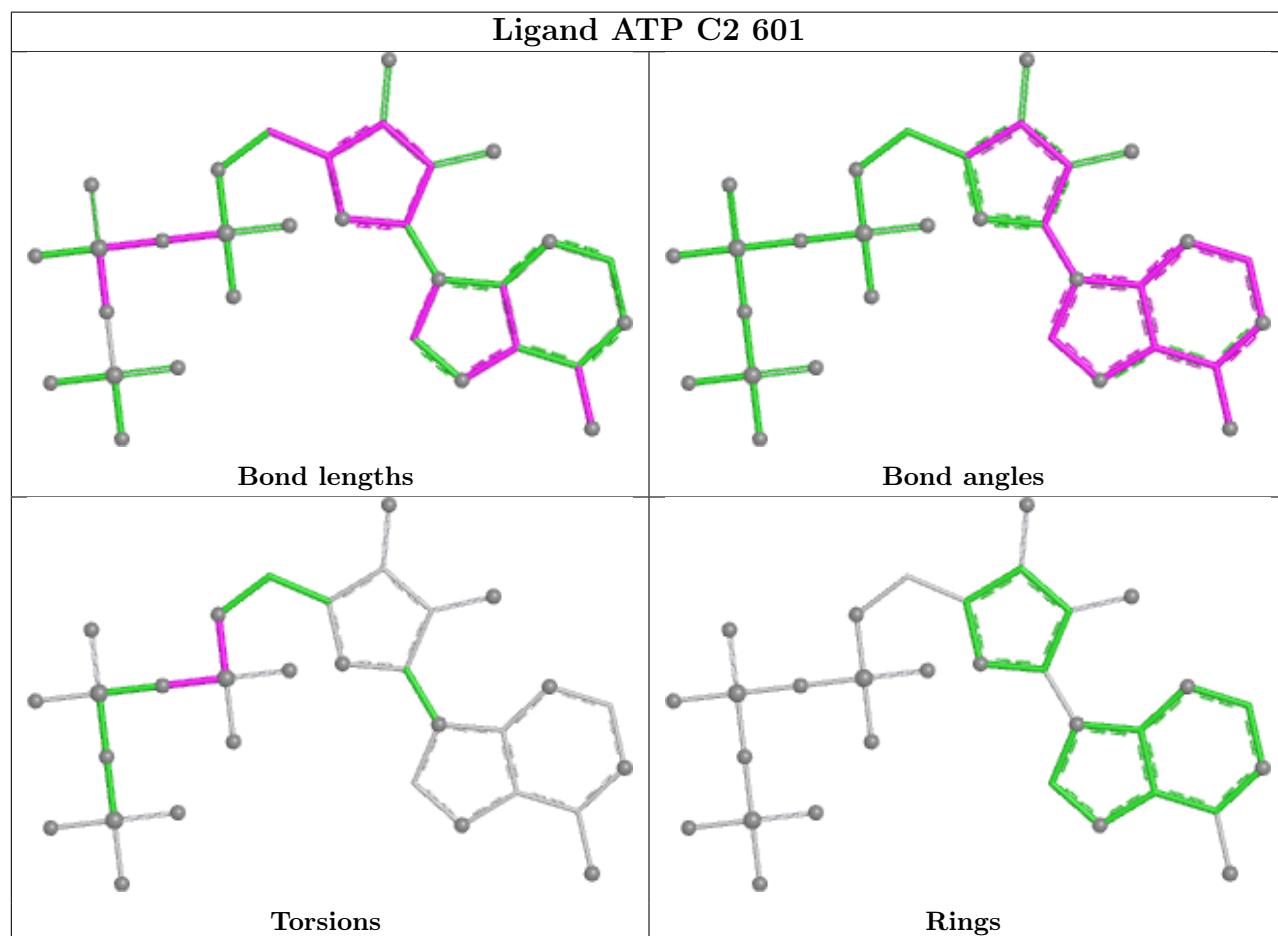
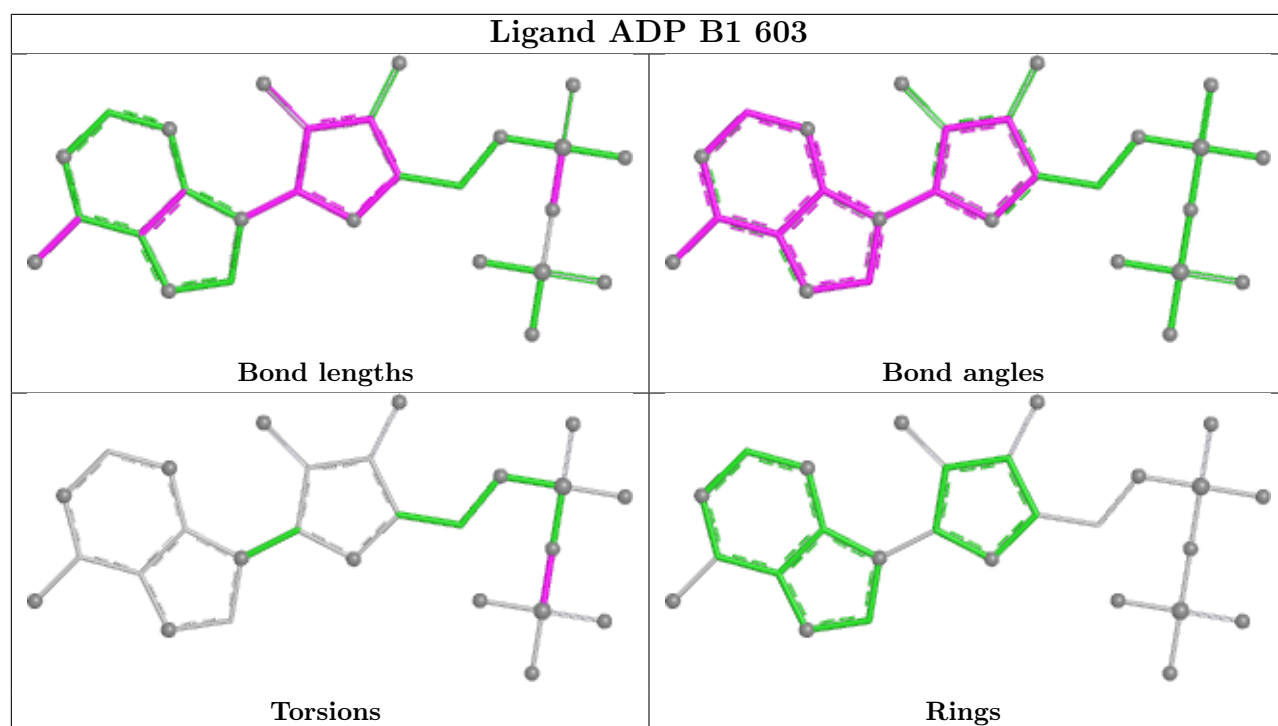


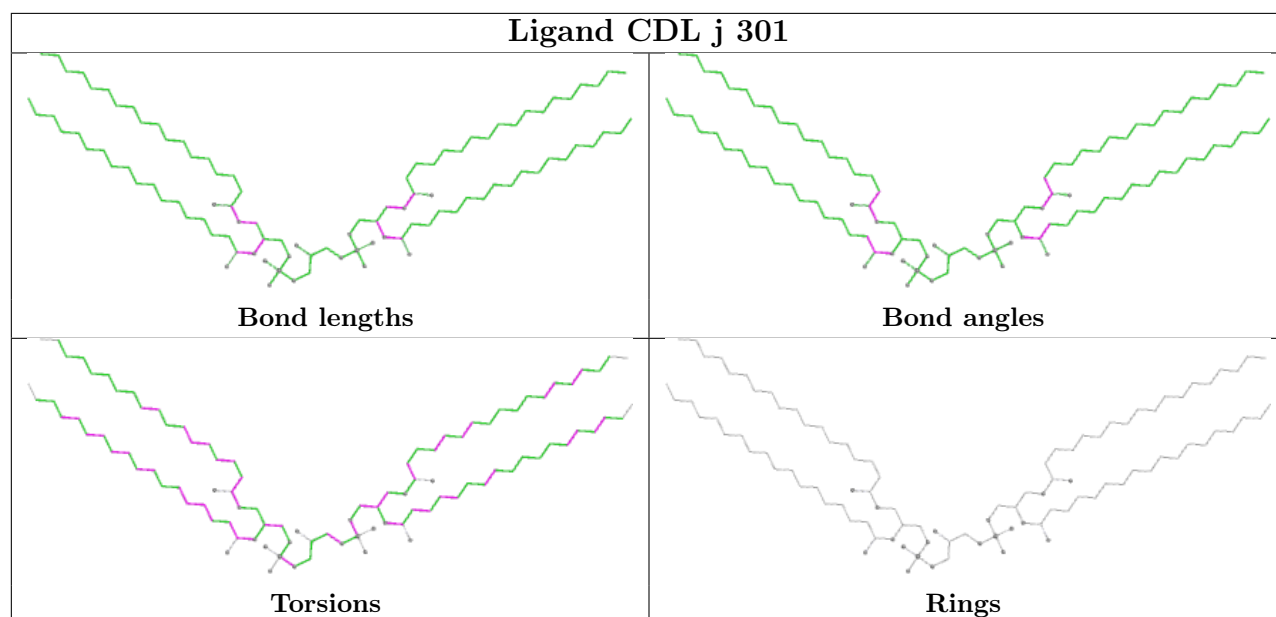
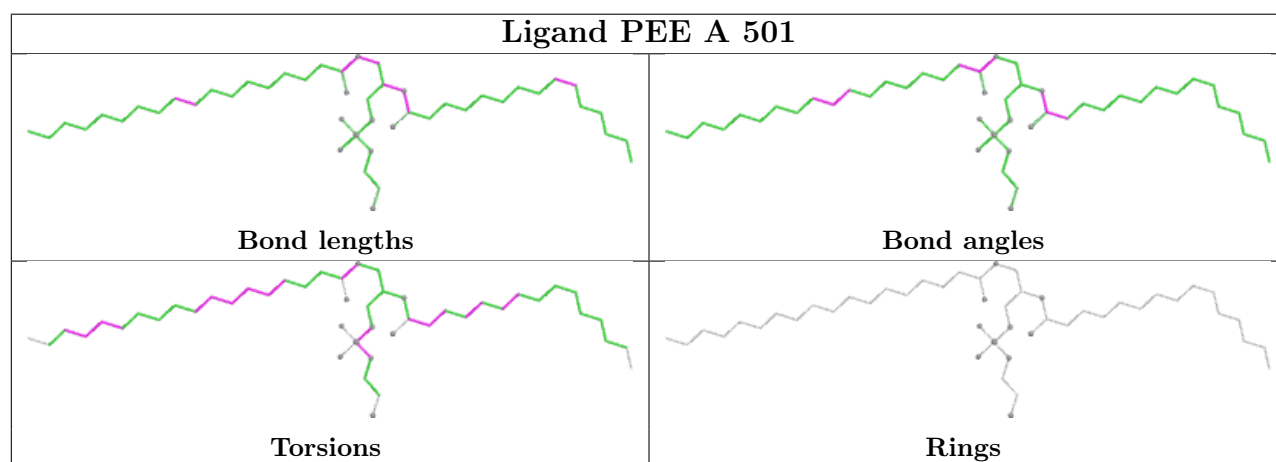
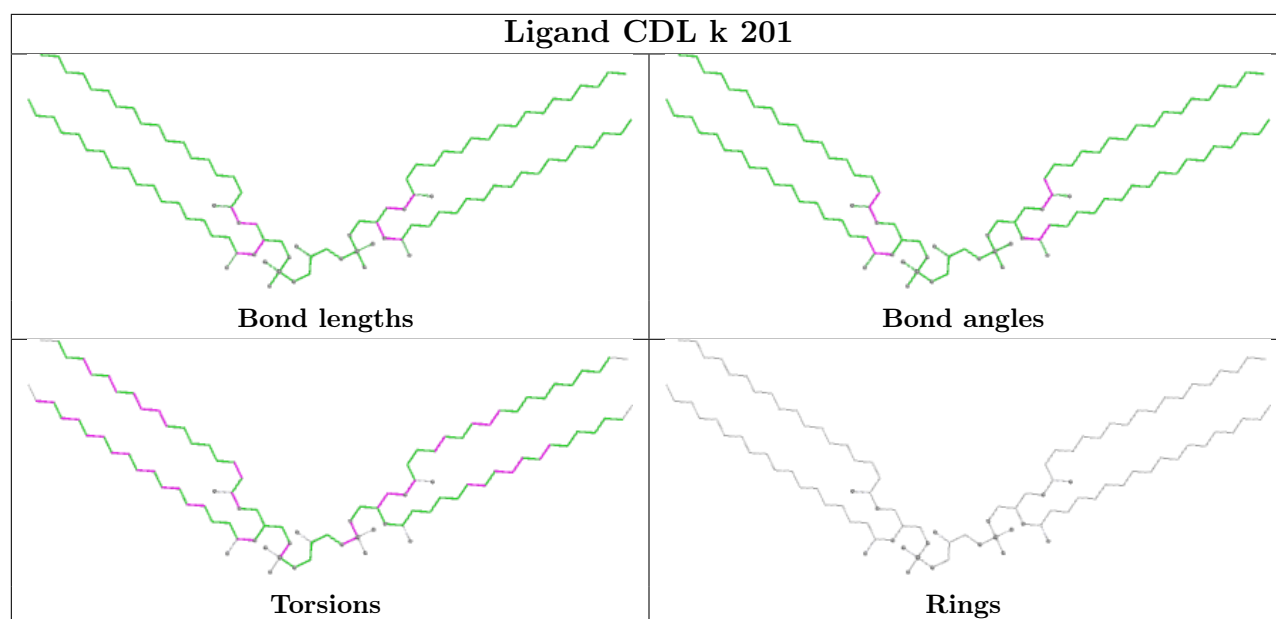


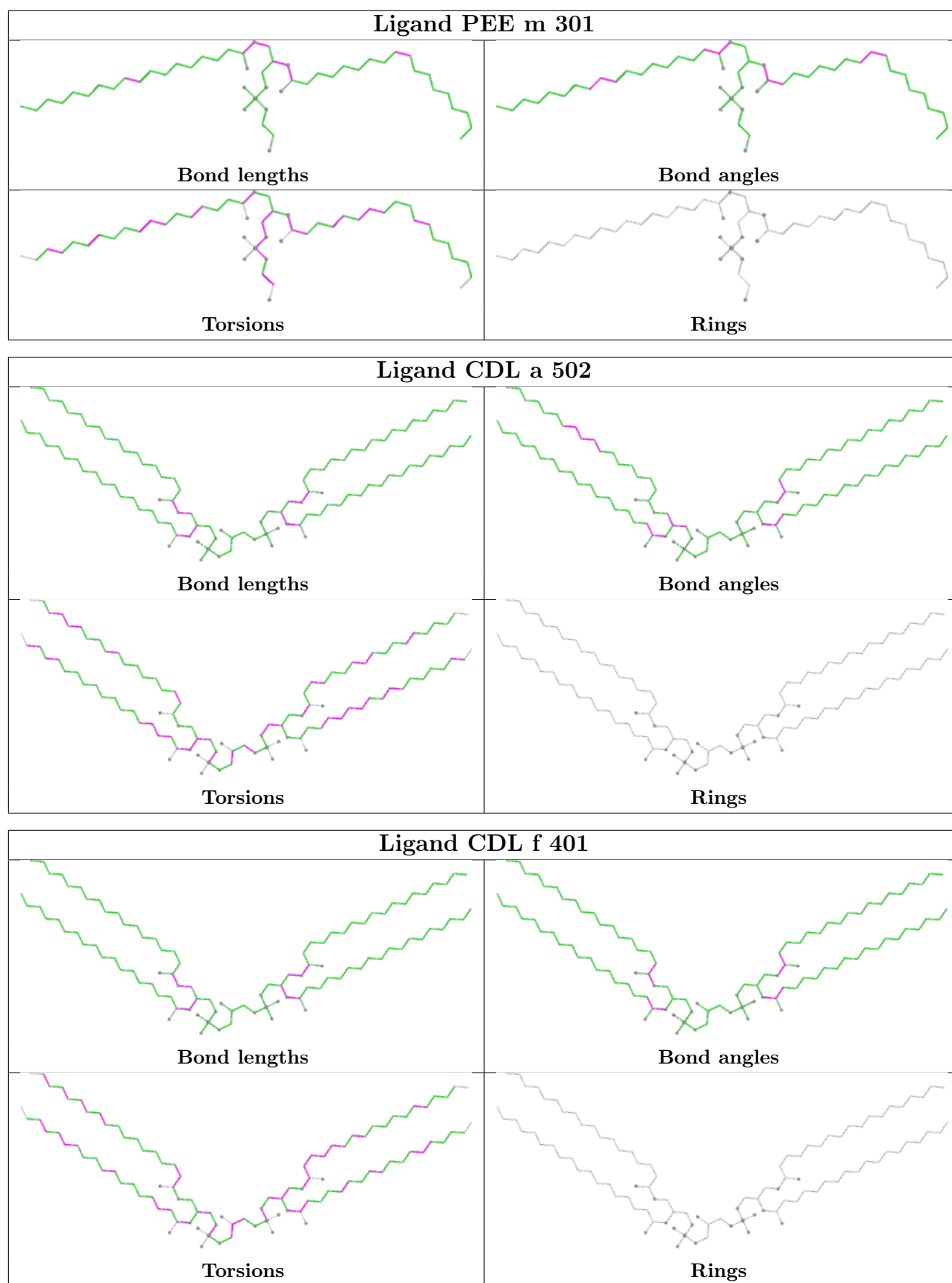


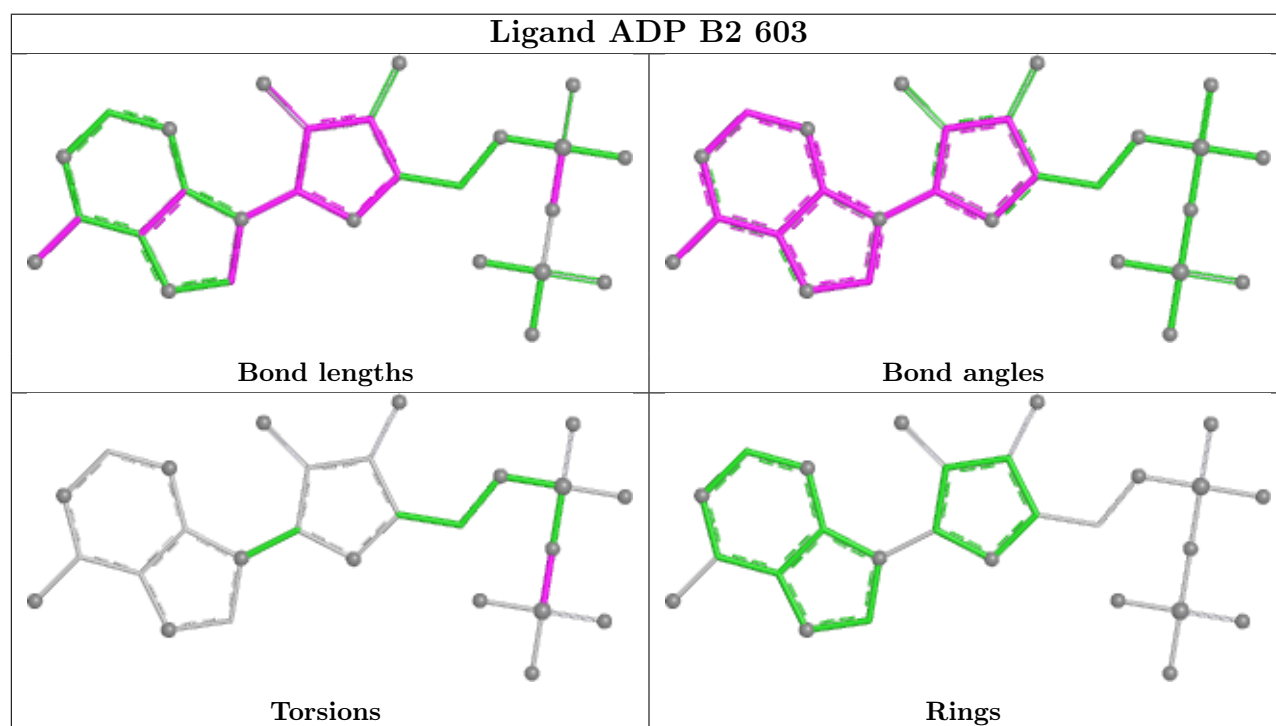
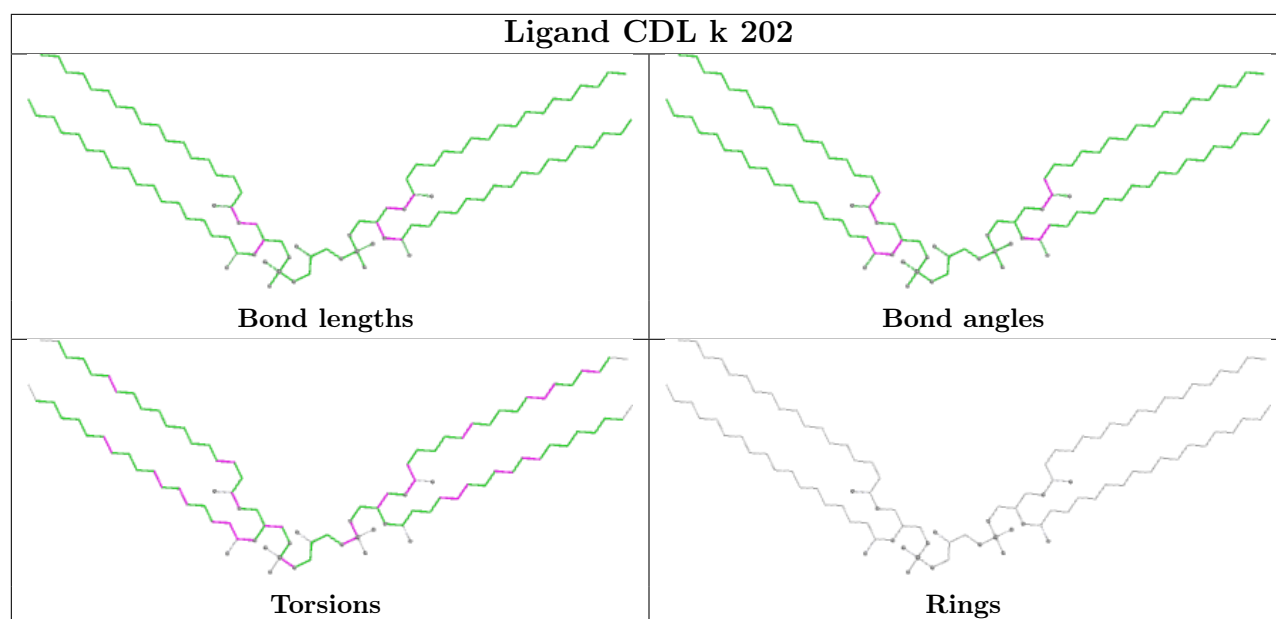


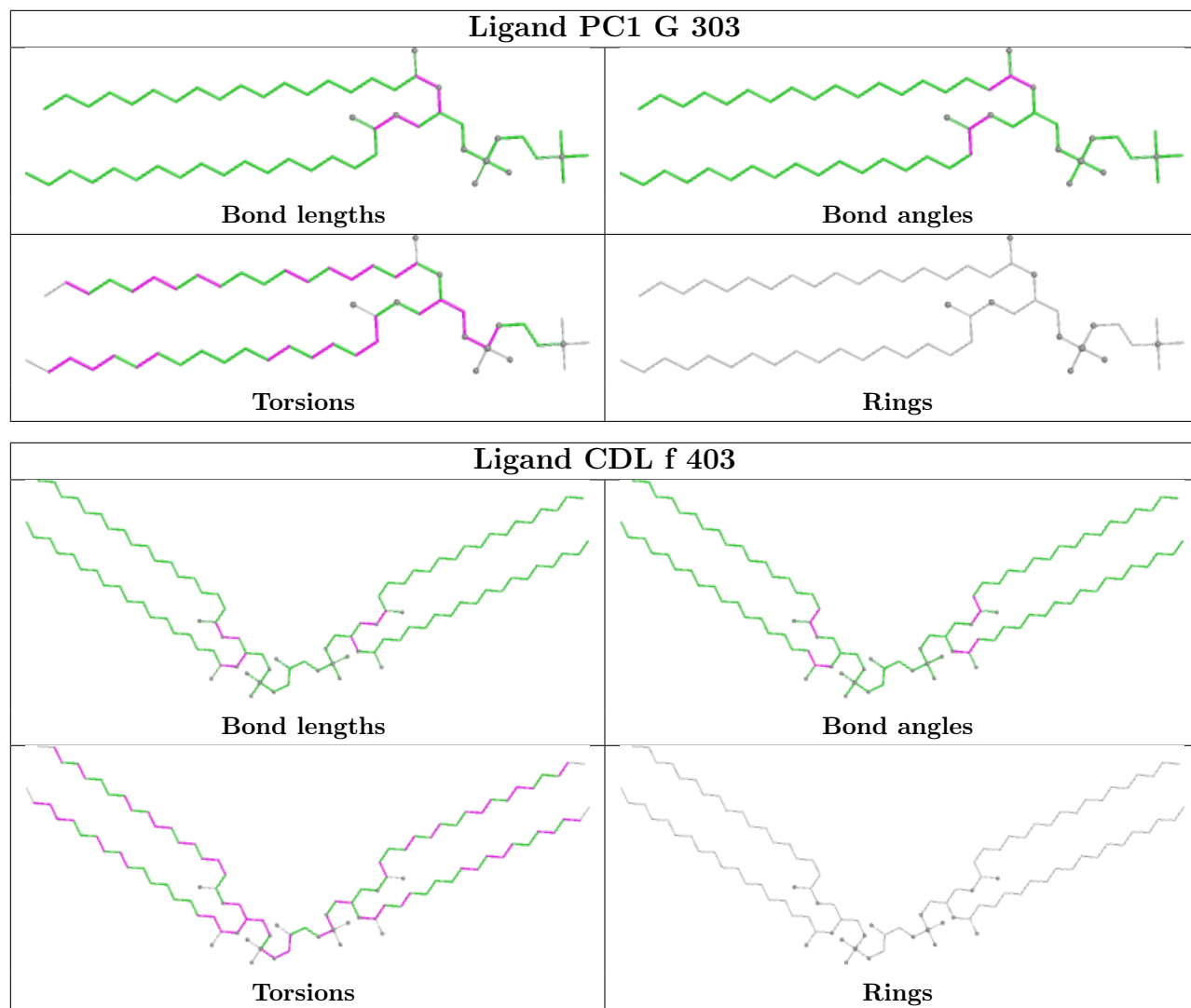


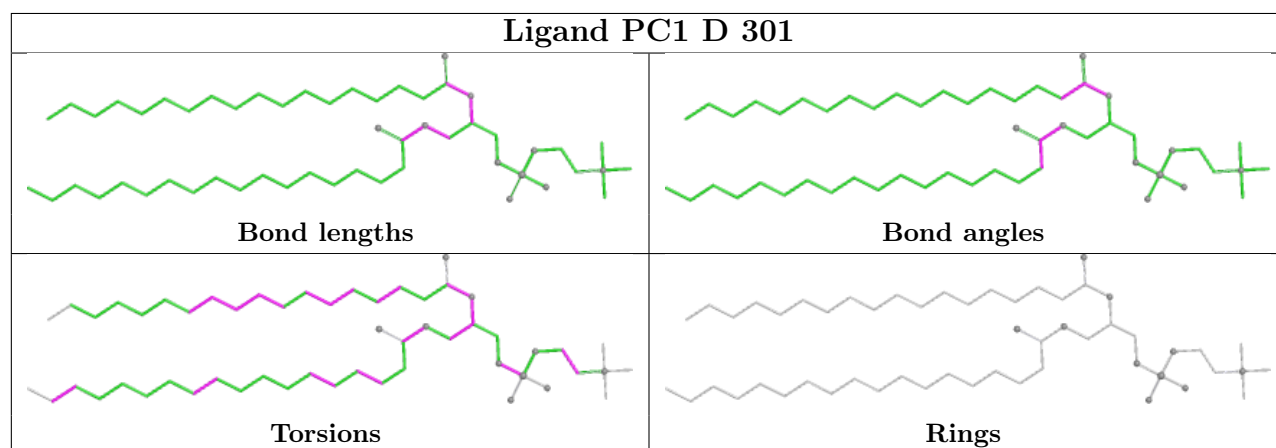
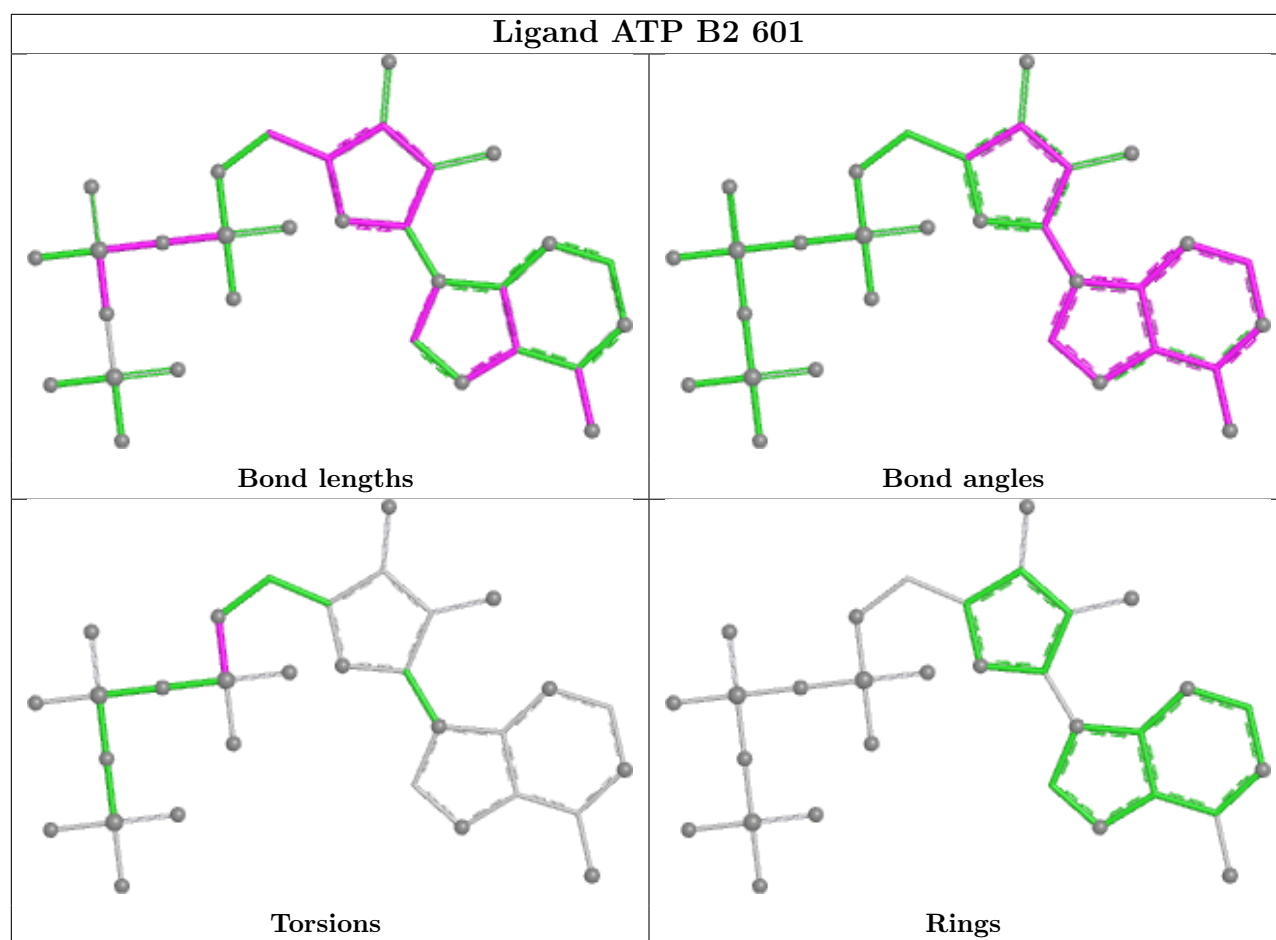


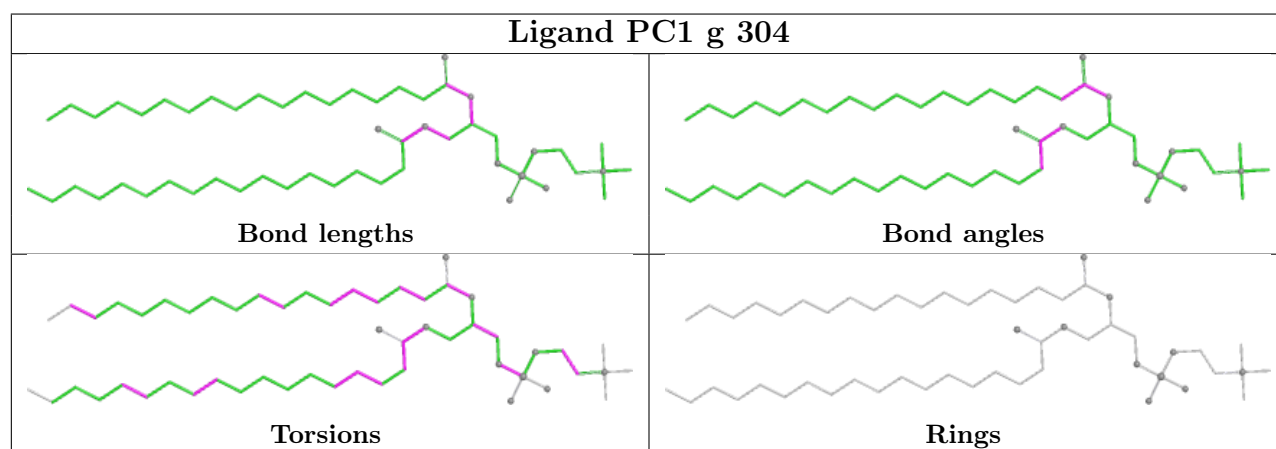
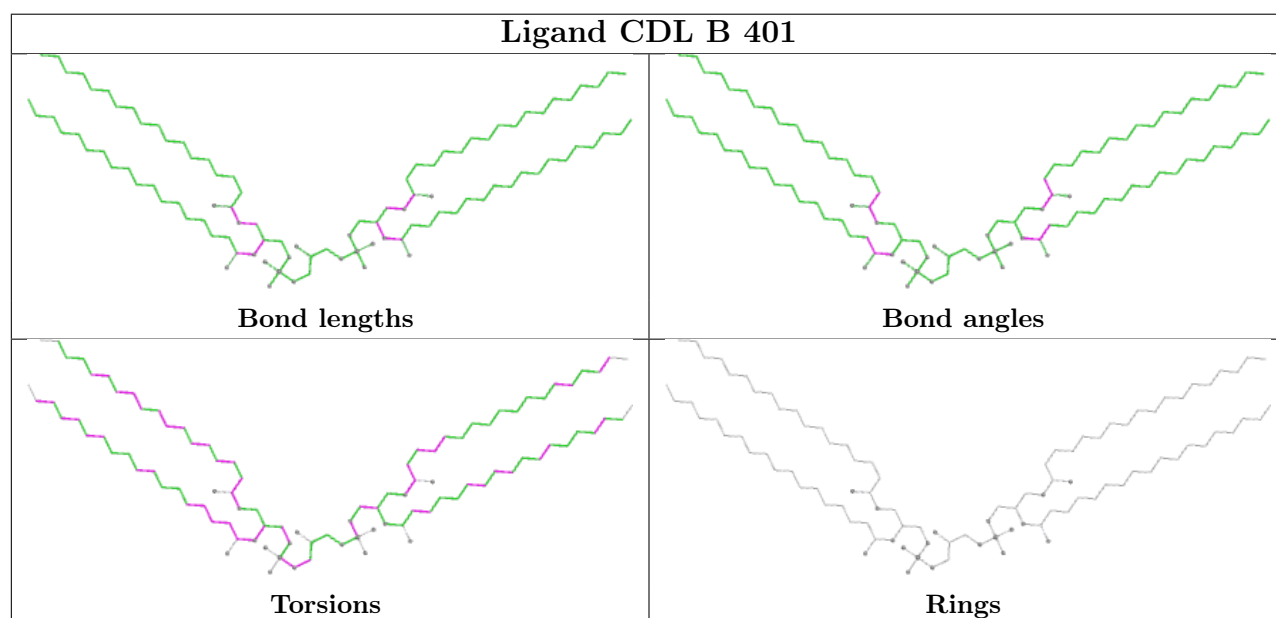
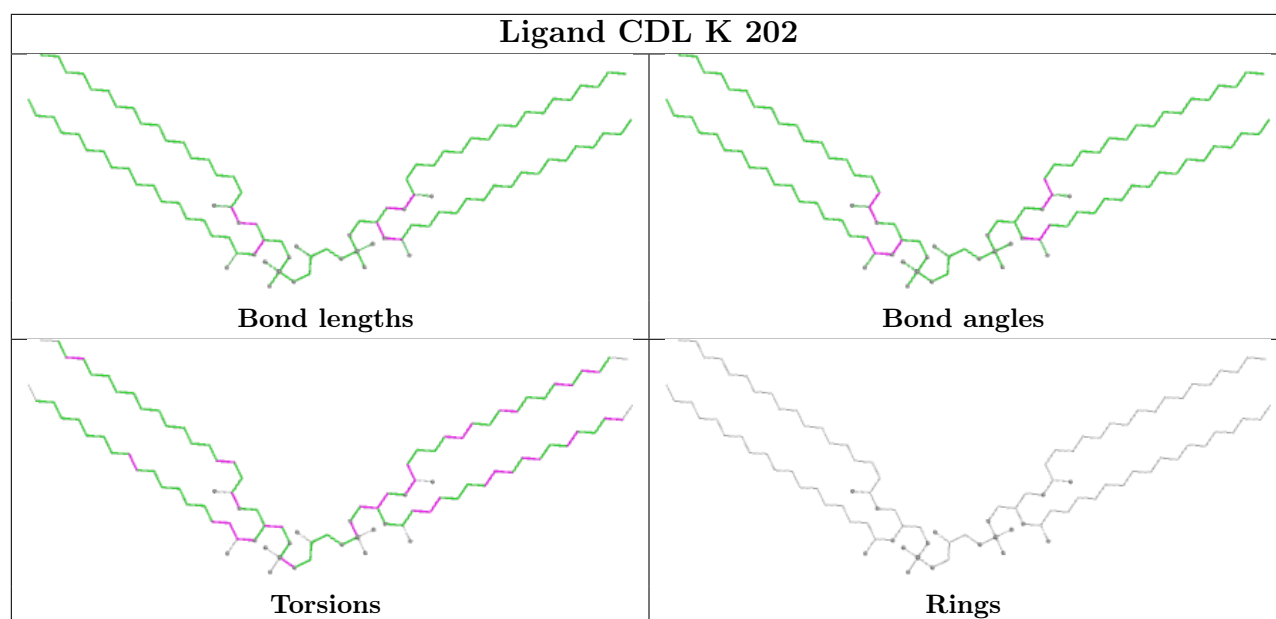


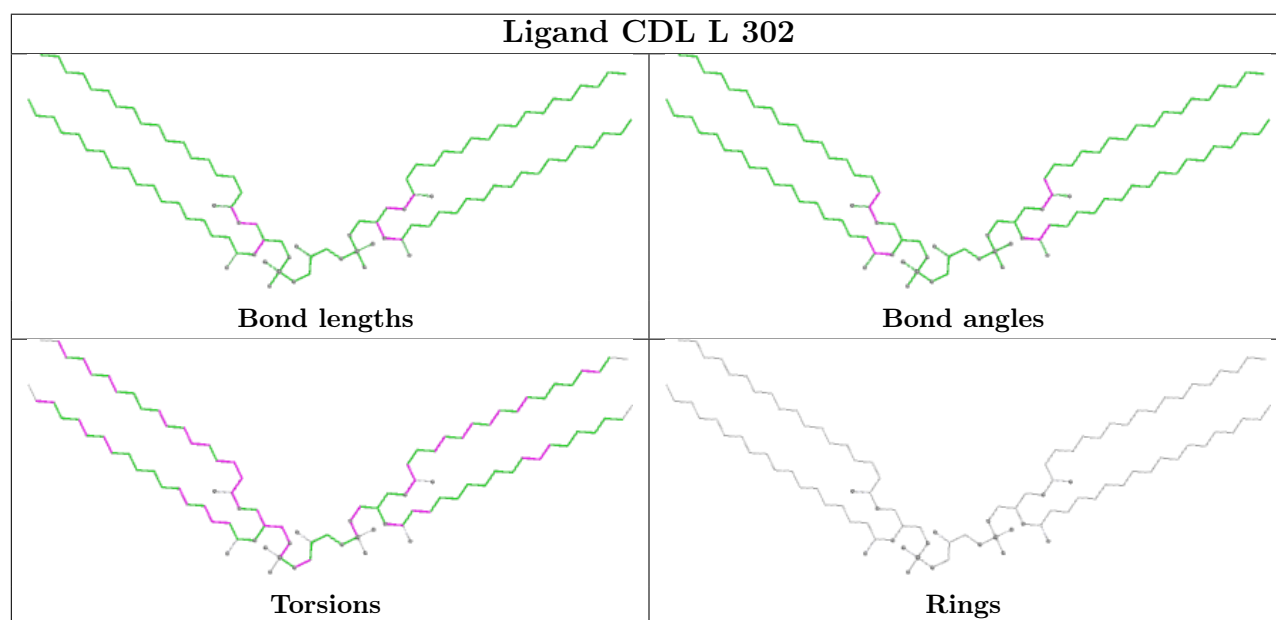
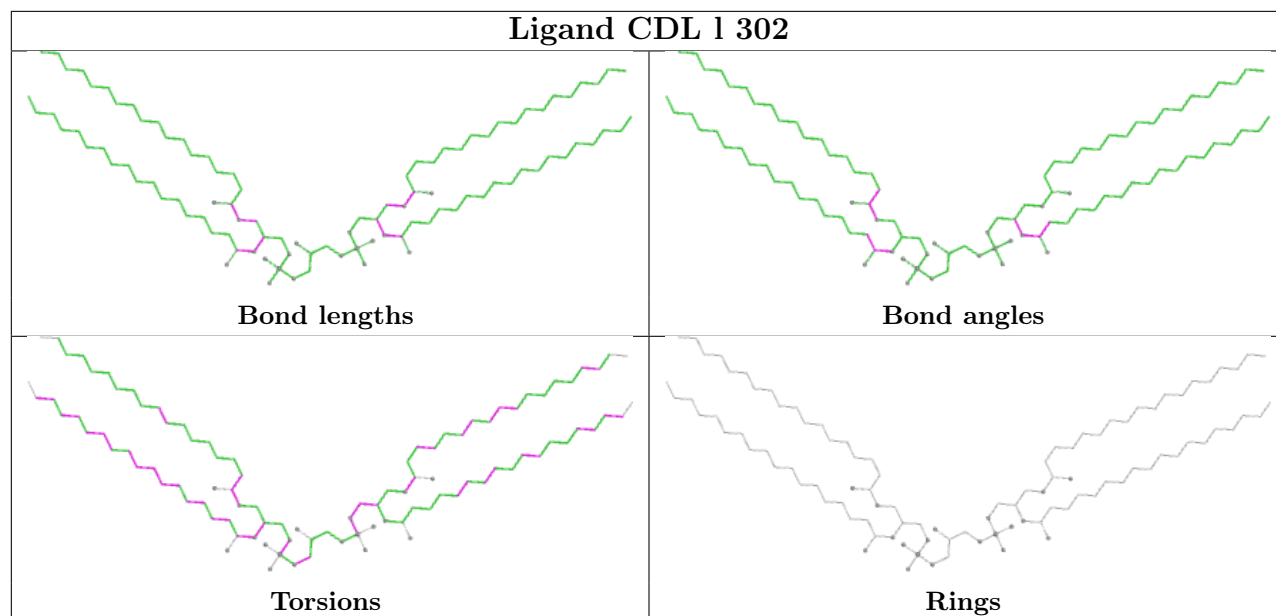


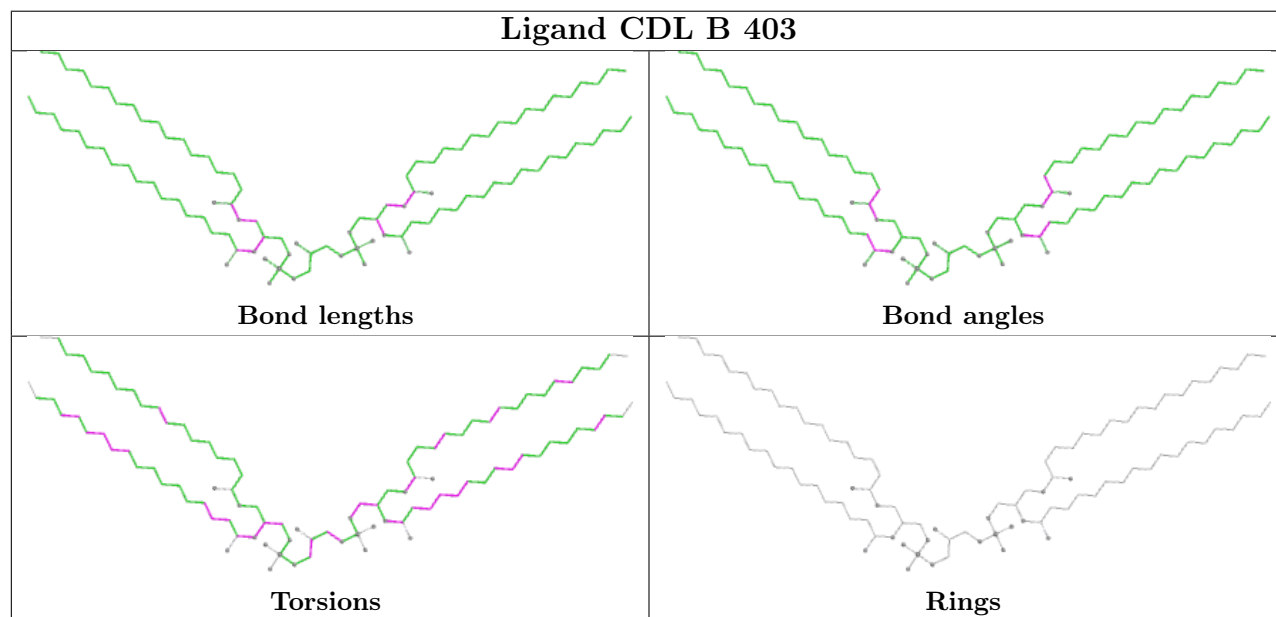
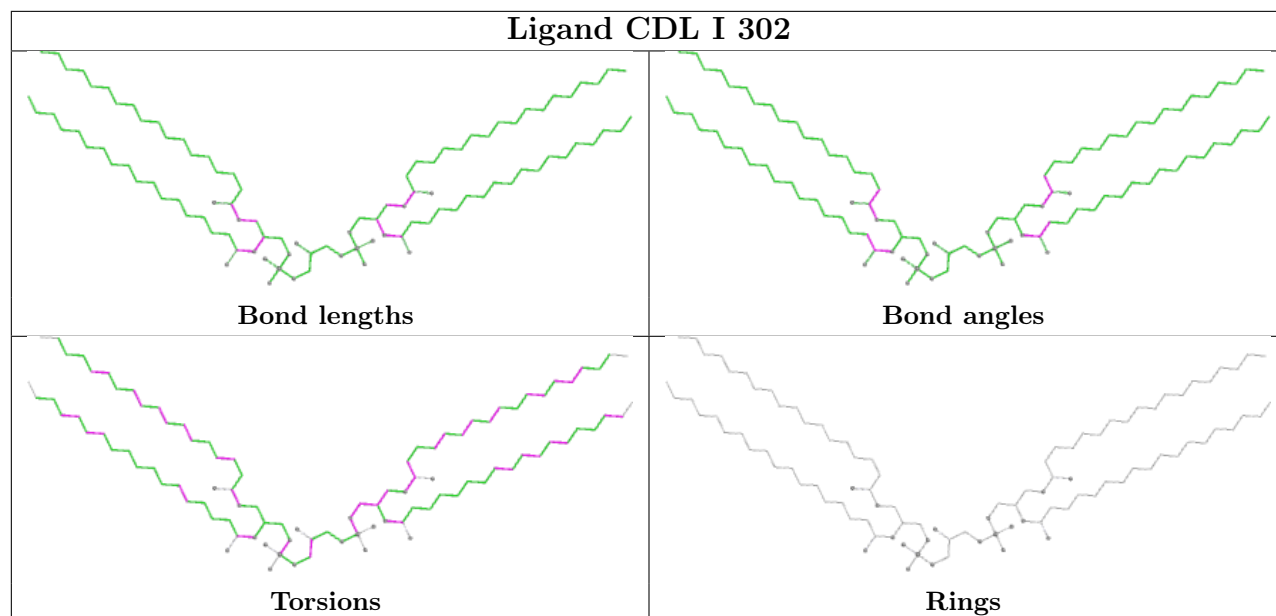


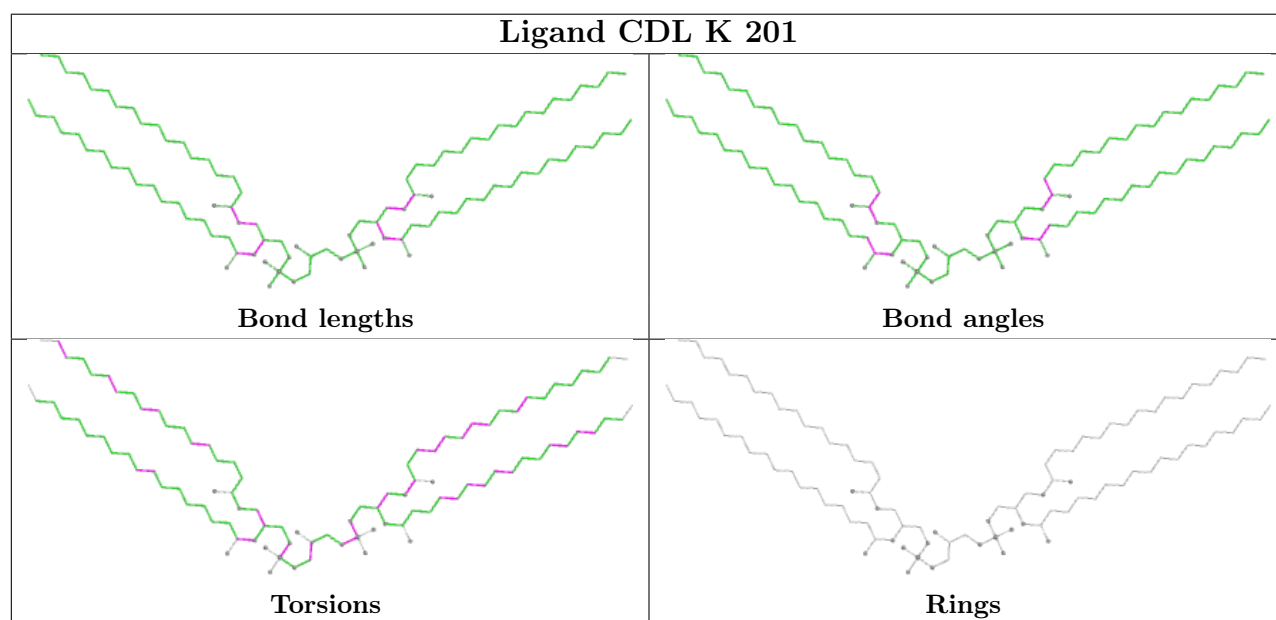
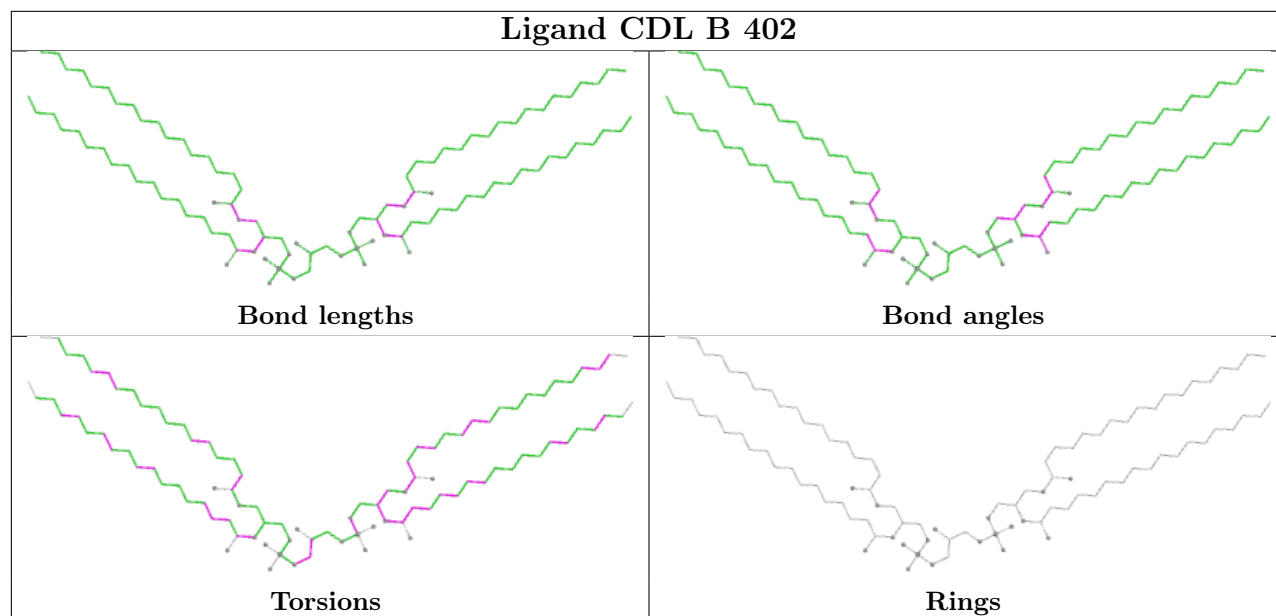


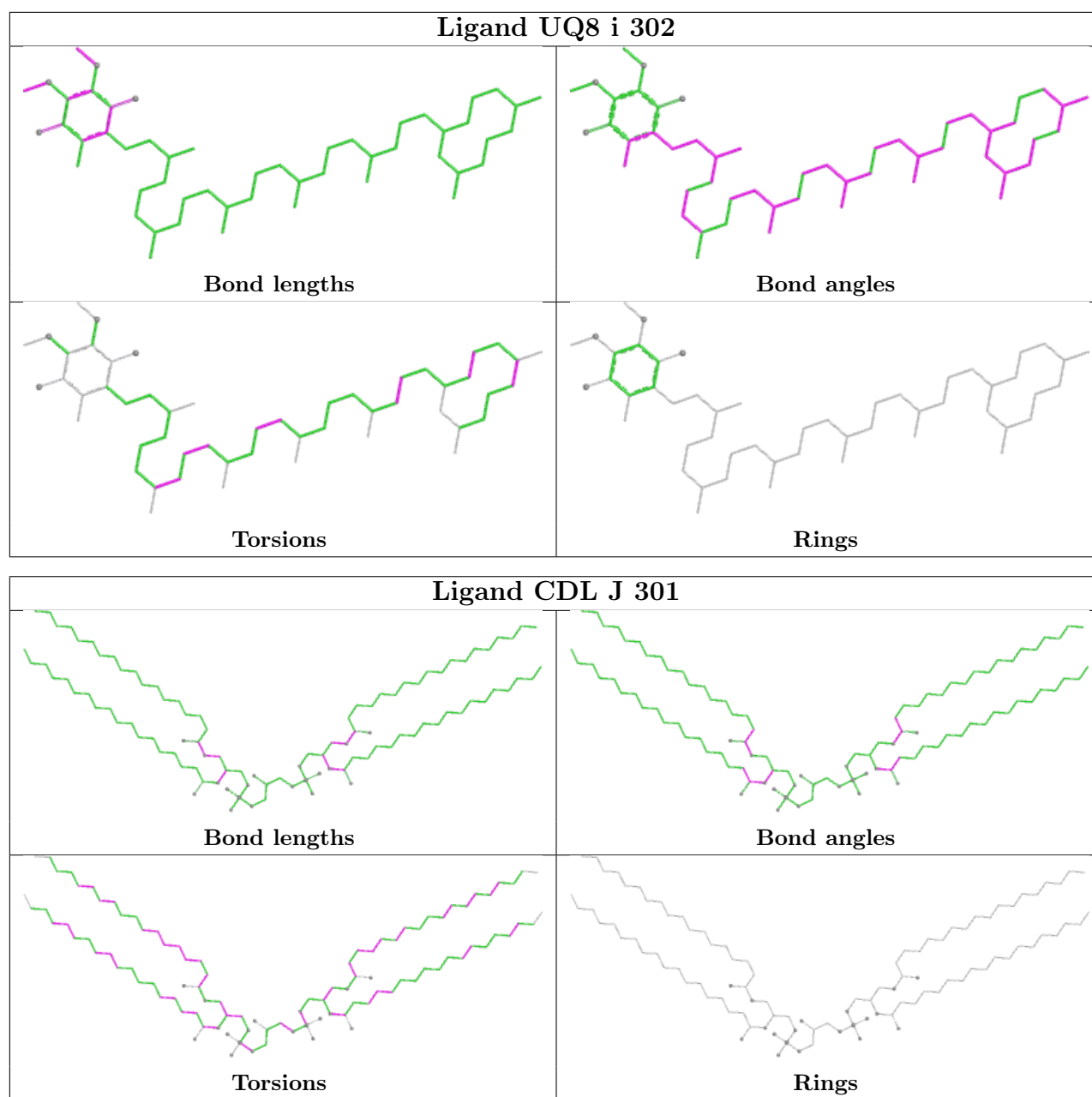


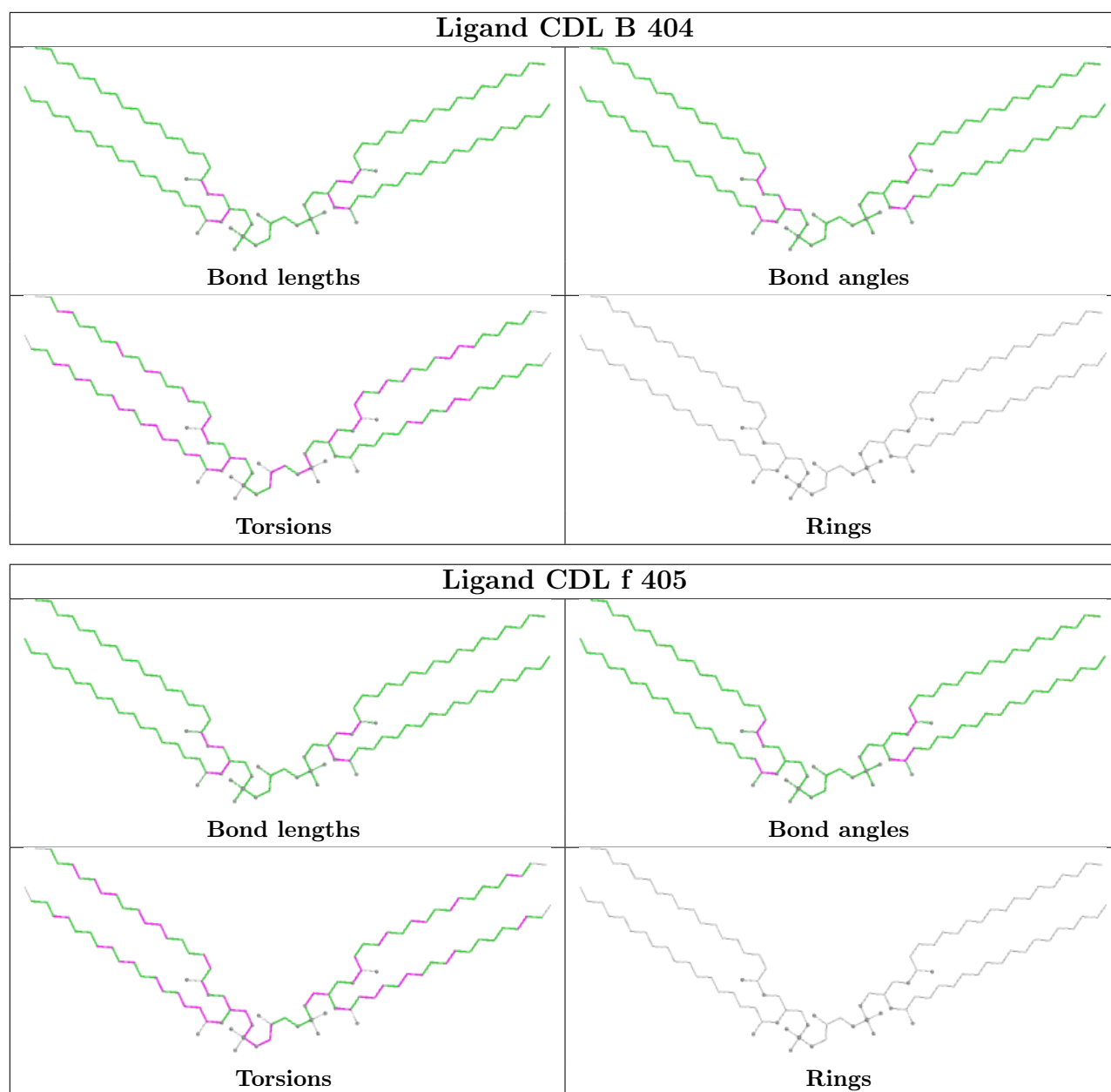












4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

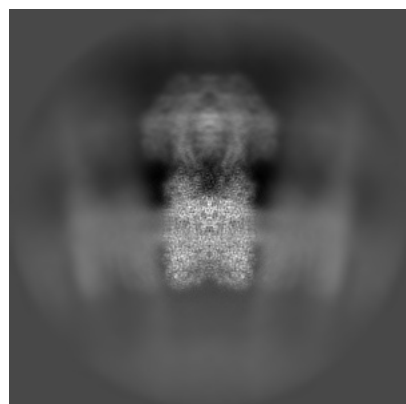
5 Map visualisation [i](#)

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.

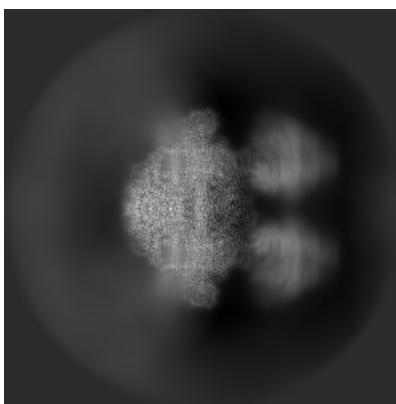
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

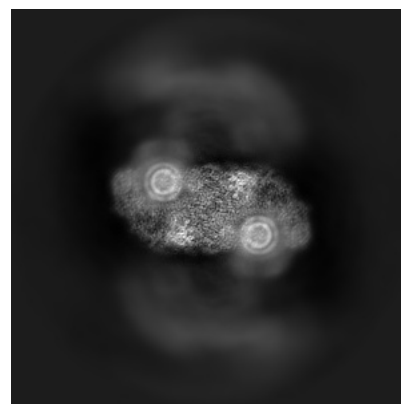
5.1.1 Primary map



X

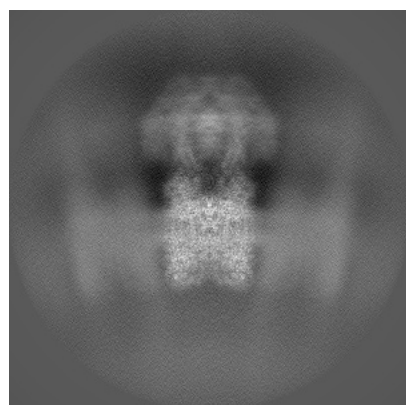


Y

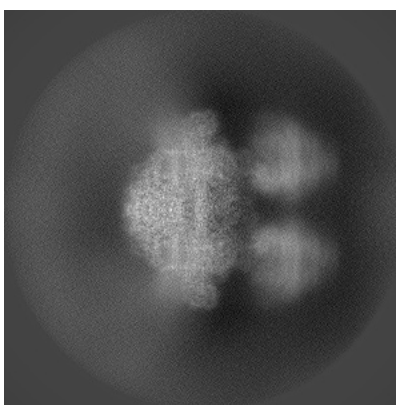


Z

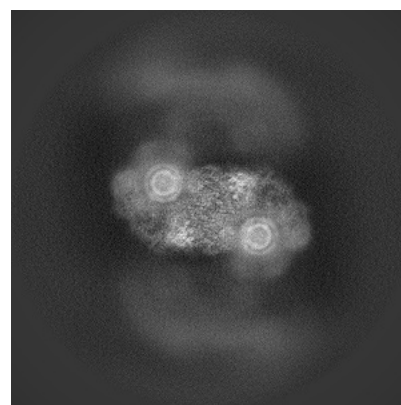
5.1.2 Raw map



X



Y

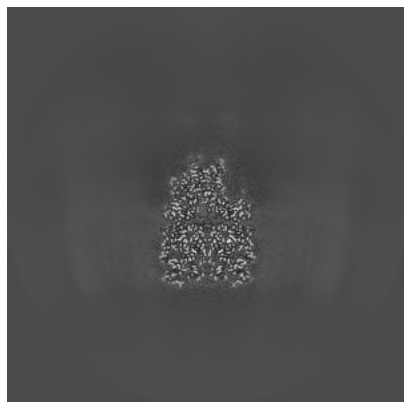


Z

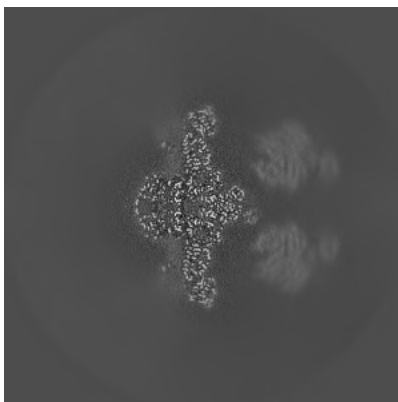
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

5.2.1 Primary map



X Index: 300

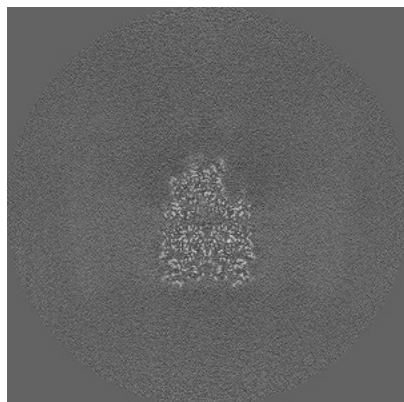


Y Index: 300

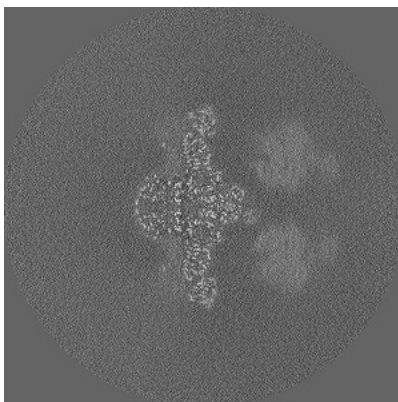


Z Index: 300

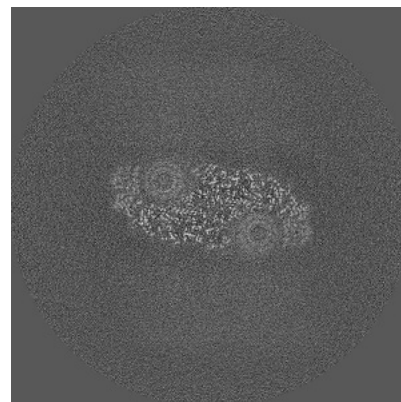
5.2.2 Raw map



X Index: 300



Y Index: 300

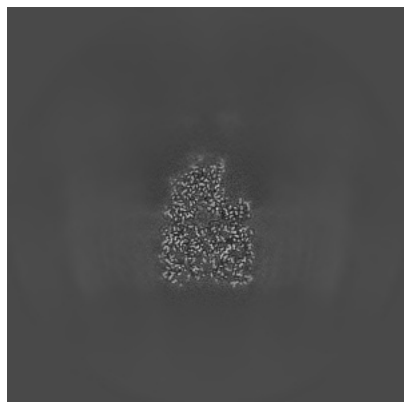


Z Index: 300

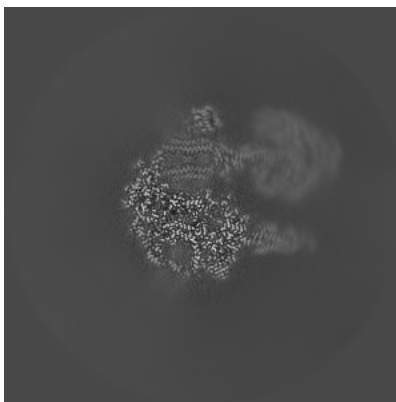
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

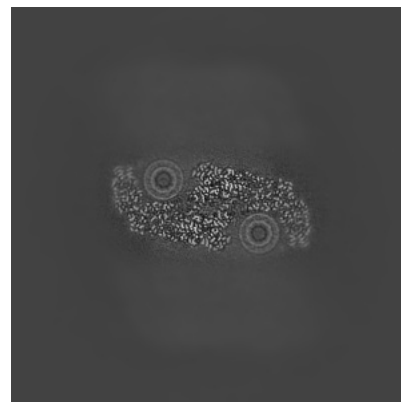
5.3.1 Primary map



X Index: 298

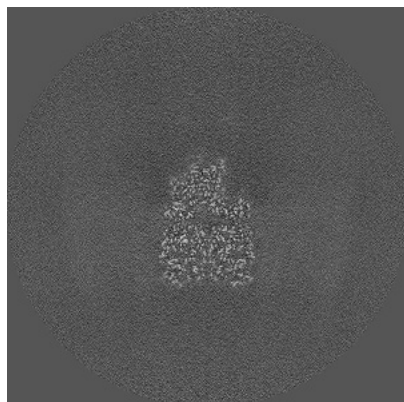


Y Index: 258

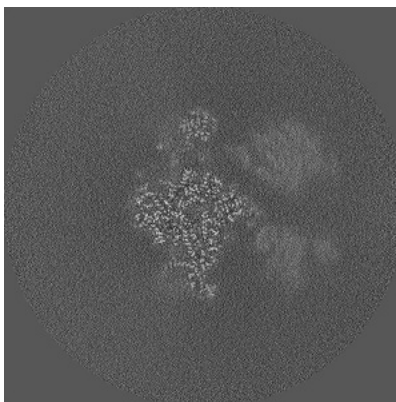


Z Index: 292

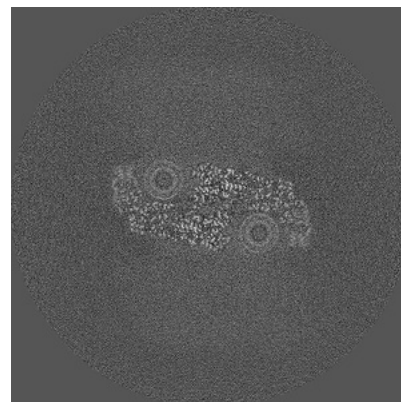
5.3.2 Raw map



X Index: 299



Y Index: 290

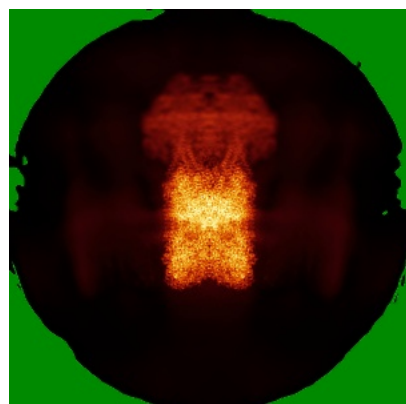


Z Index: 292

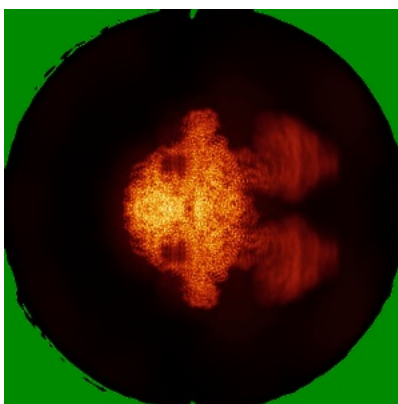
The images above show the largest variance slices of the map in three orthogonal directions.

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

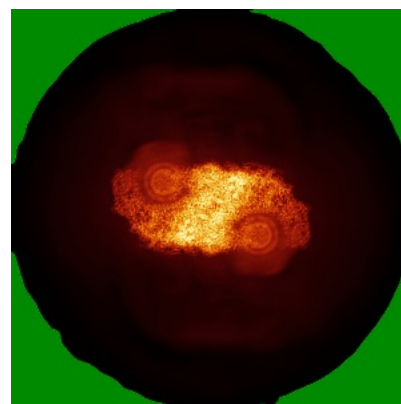
5.4.1 Primary map



X

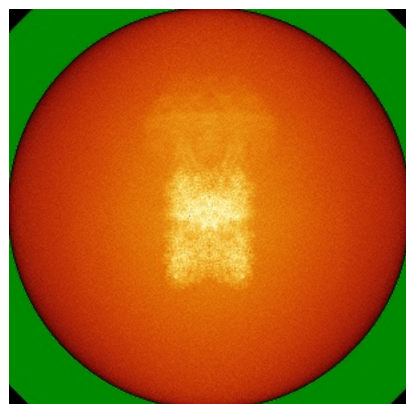


Y

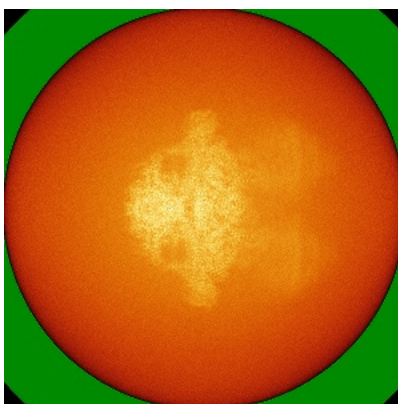


Z

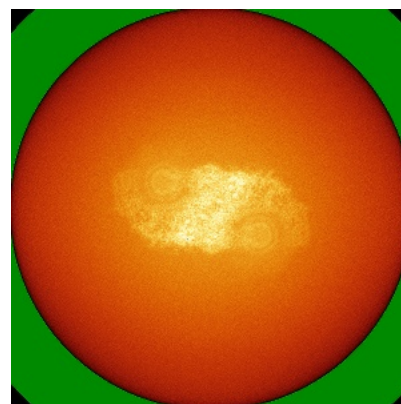
5.4.2 Raw map



X



Y

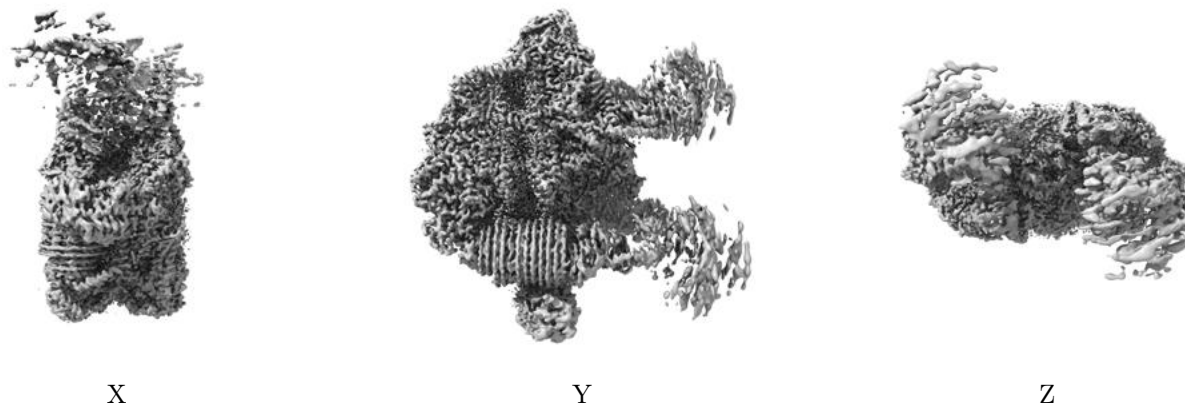


Z

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

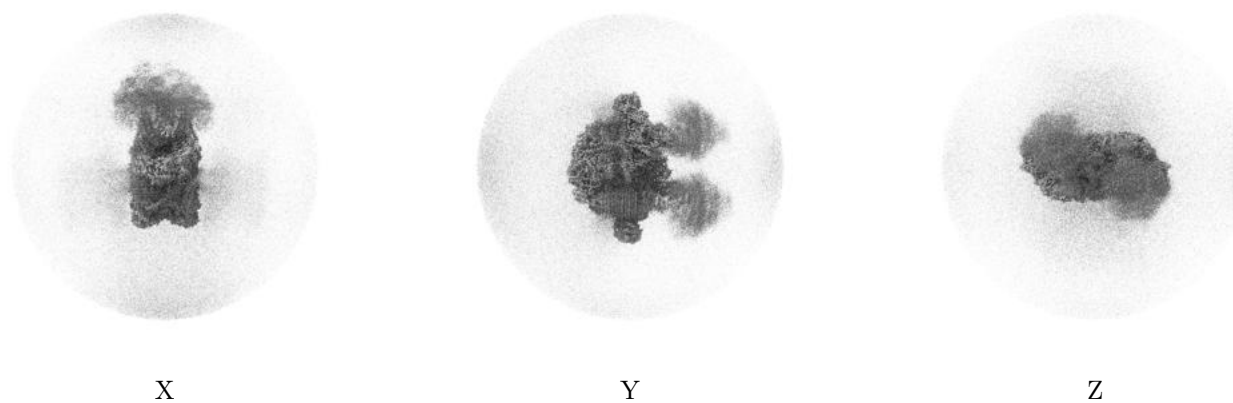
5.5 Orthogonal surface views [i](#)

5.5.1 Primary map



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

5.5.2 Raw map



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

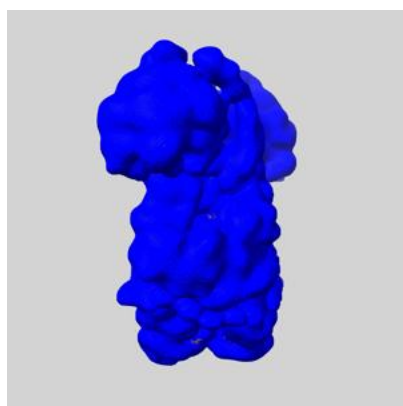
5.6 Mask visualisation [i](#)

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

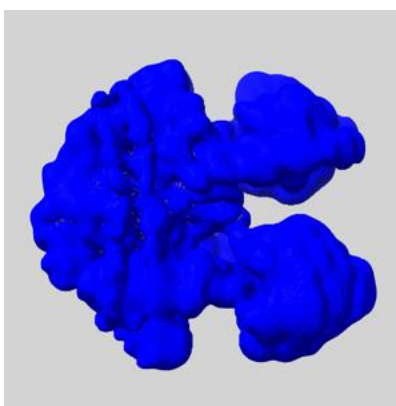
A mask typically either:

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

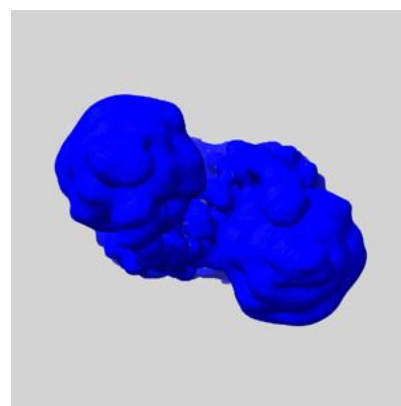
5.6.1 emd_10860_msk_1.map [i](#)



X



Y

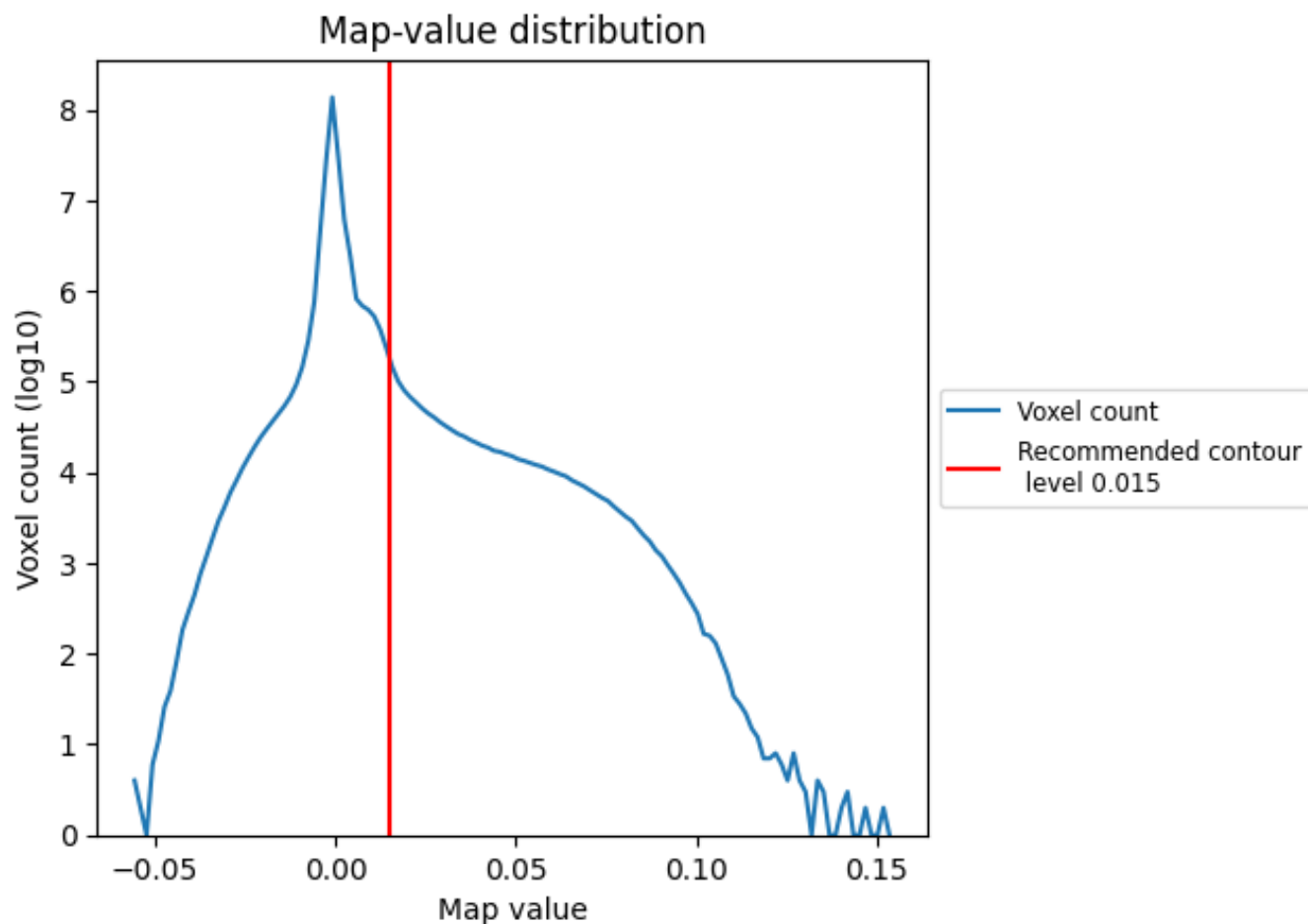


Z

6 Map analysis [i](#)

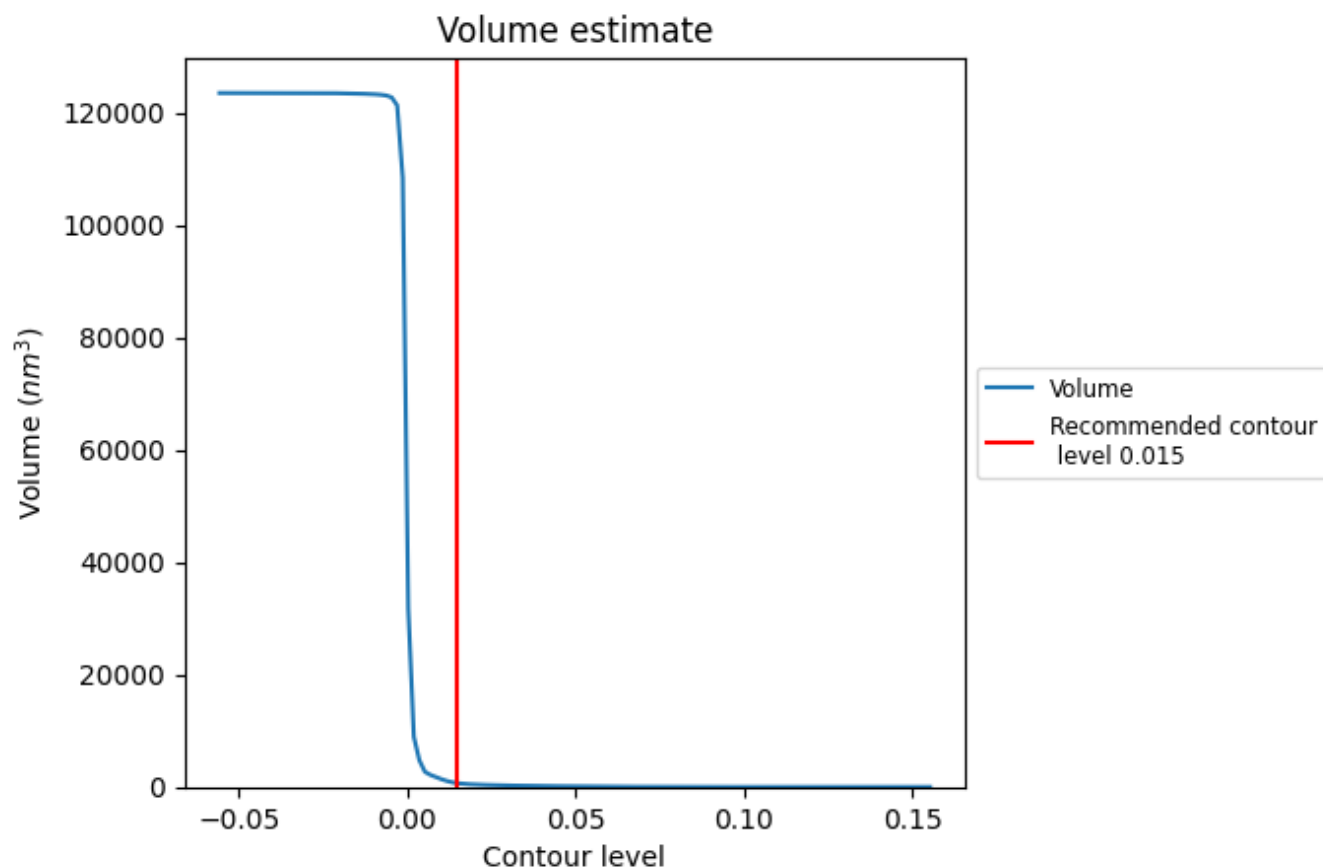
This section contains the results of statistical analysis of the map.

6.1 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.

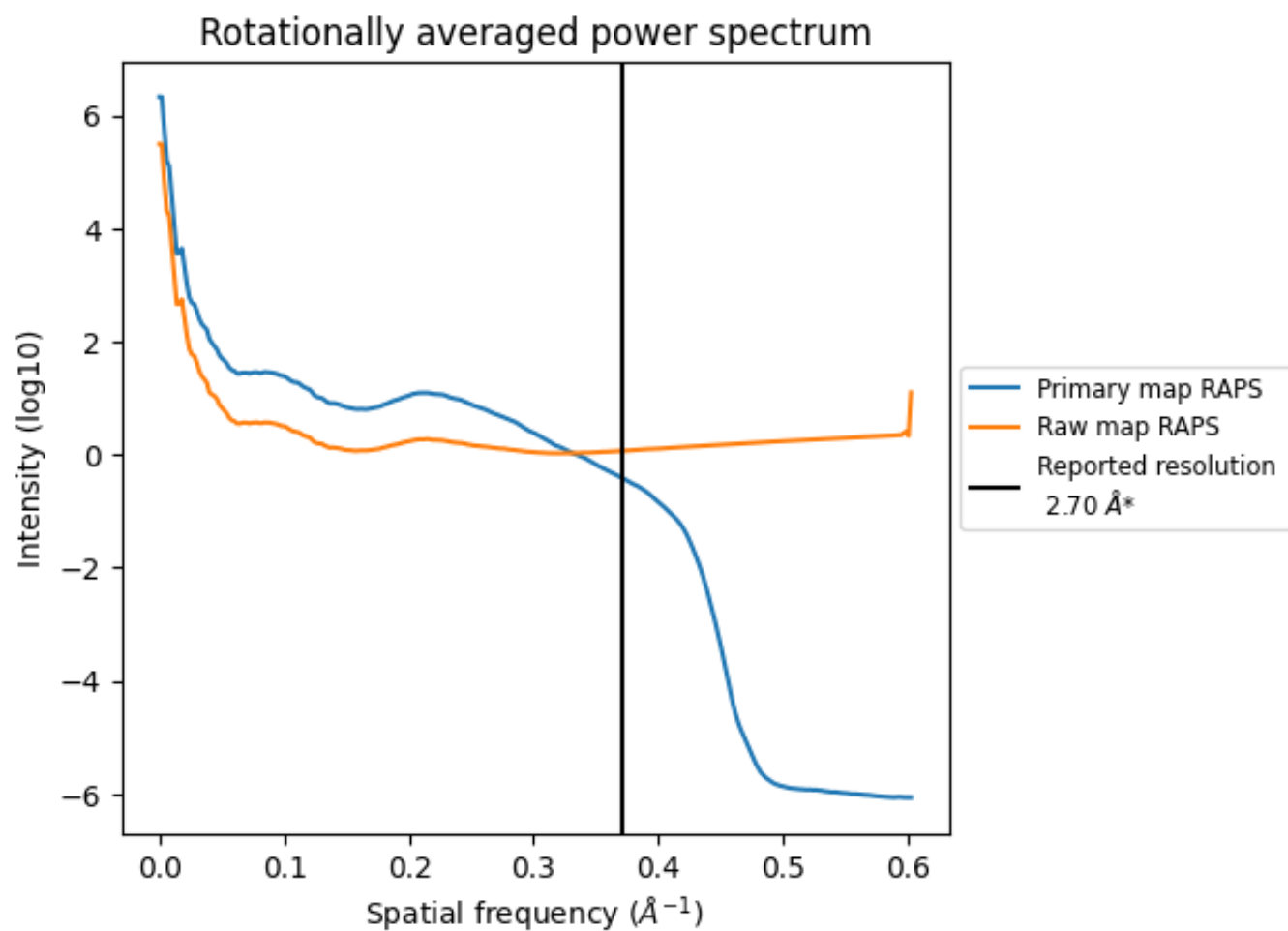
6.2 Volume estimate [i](#)



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

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

6.3 Rotationally averaged power spectrum ⓘ

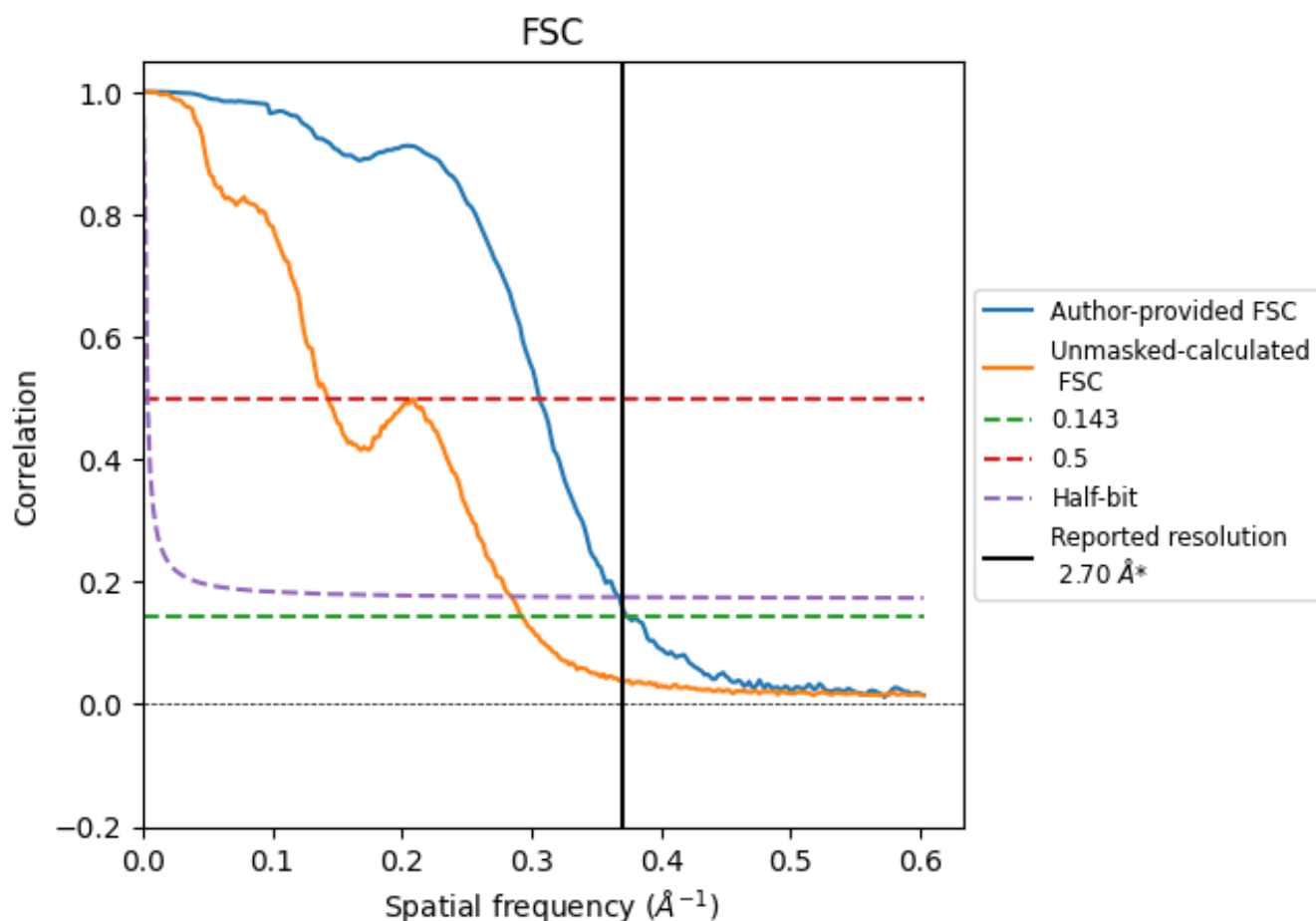


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

7 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.

7.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 $\text{\AA}^{-1}$

7.2 Resolution estimates [i](#)

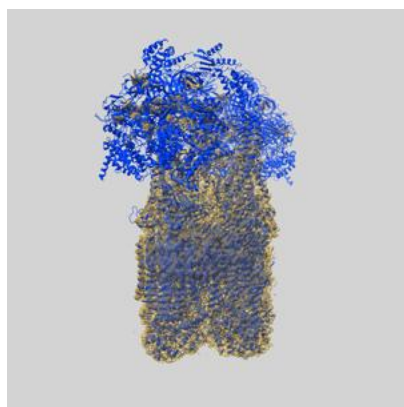
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.67	3.27	2.72
Unmasked-calculated*	3.42	7.00	3.52

*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 %

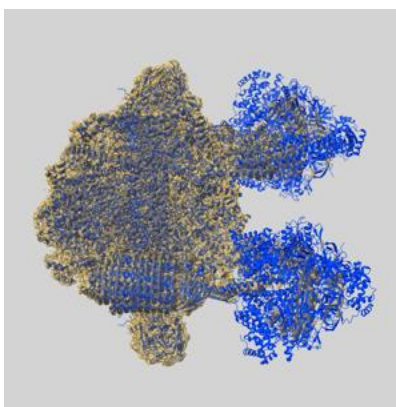
8 Map-model fit [i](#)

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 ?? on page ??.

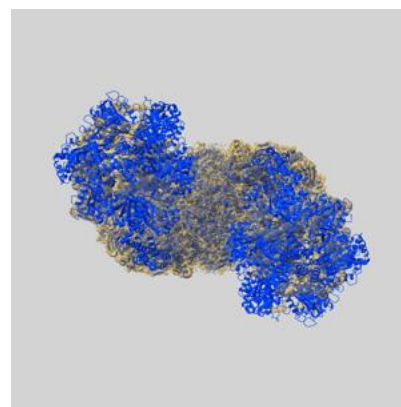
8.1 Map-model overlay [i](#)



X



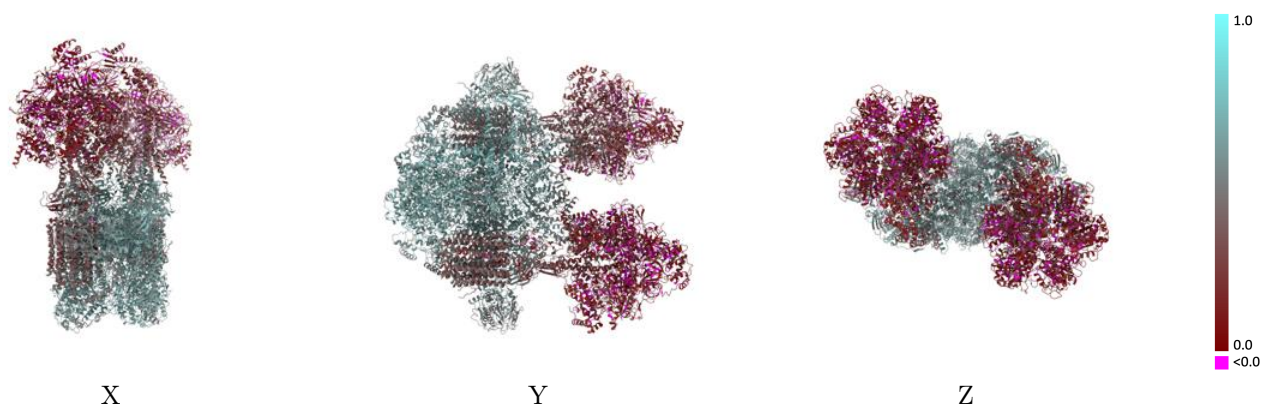
Y



Z

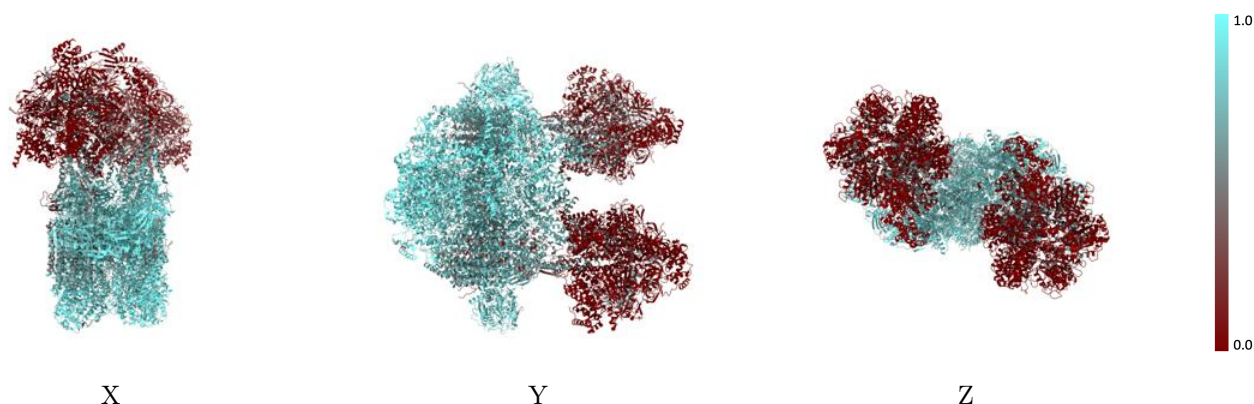
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



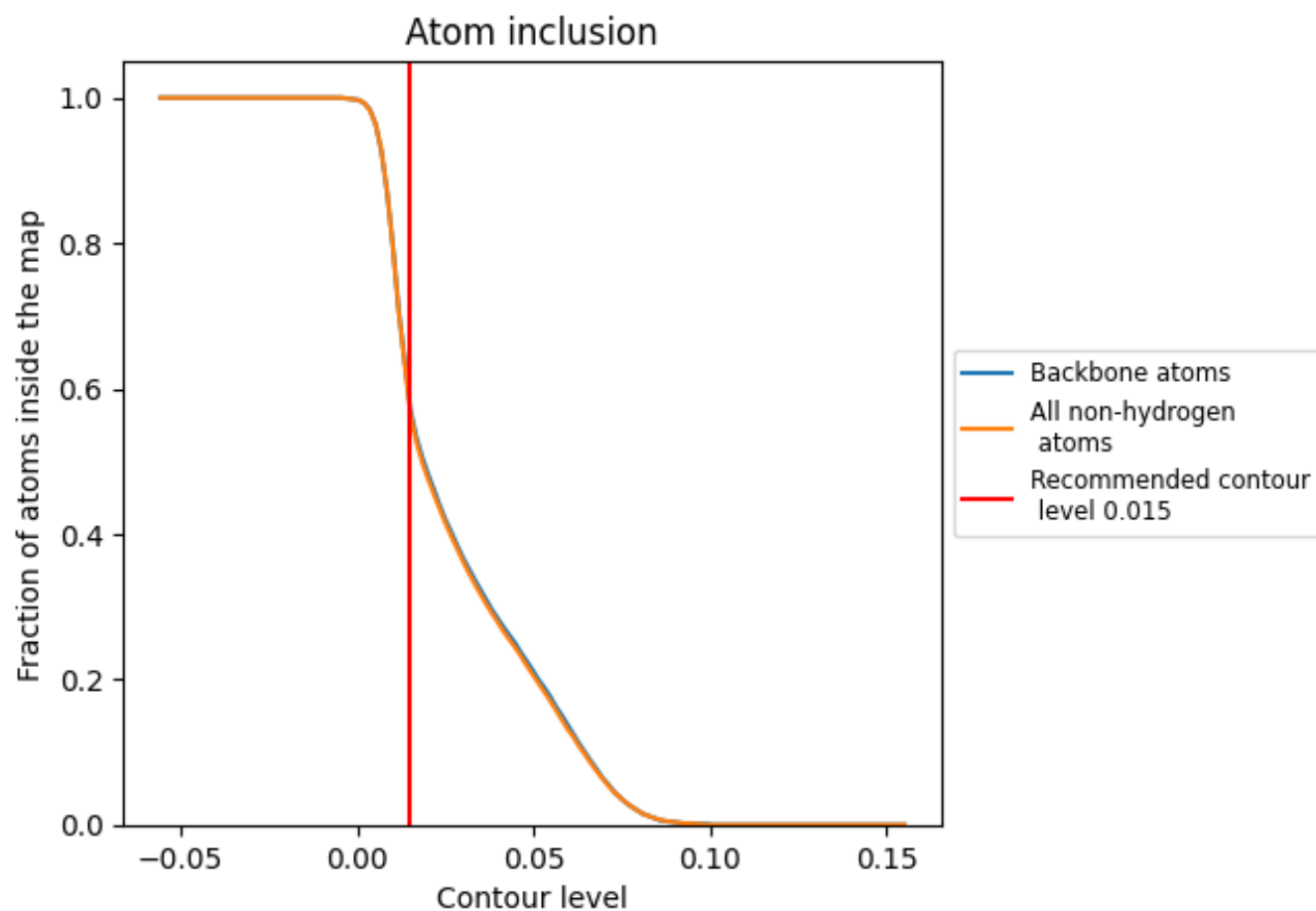
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

8.3 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).

8.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5690	 0.4030
A	 0.9540	 0.6410
A1	 0.2440	 0.2160
A2	 0.2050	 0.2000
B	 0.6040	 0.4500
B1	 0.0900	 0.1260
B2	 0.0880	 0.1250
C	 0.9740	 0.6530
C1	 0.0270	 0.1220
C2	 0.0250	 0.1070
D	 0.7480	 0.5130
D1	 0.0540	 0.1330
D2	 0.0470	 0.1300
E	 0.8520	 0.5130
E1	 0.1000	 0.1640
E2	 0.0830	 0.1510
F	 0.9580	 0.6580
F1	 0.0490	 0.1230
F2	 0.0600	 0.1210
G	 0.9160	 0.6040
G1	 0.0000	 0.1260
G2	 0.0000	 0.1340
H	 0.9270	 0.6200
H1	 0.7570	 0.4040
H2	 0.7100	 0.3980
I	 0.9040	 0.6100
I1	 0.6830	 0.3880
I2	 0.6740	 0.3670
J	 0.8810	 0.5980
J1	 0.6960	 0.3790
J2	 0.6760	 0.3790
K	 0.8500	 0.5560
K1	 0.6670	 0.3780
K2	 0.6150	 0.3680
L	 0.9210	 0.6280



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Chain	Atom inclusion	Q-score
L1	 0.6490	 0.3630
L2	 0.6260	 0.3660
M	 0.9690	 0.6440
M1	 0.6940	 0.3700
M2	 0.6640	 0.3670
N	 0.9660	 0.6470
N1	 0.7030	 0.3780
N2	 0.6910	 0.3690
O	 0.9430	 0.6110
O1	 0.6920	 0.3810
O2	 0.6820	 0.3750
P	 0.8320	 0.5540
P1	 0.7010	 0.3740
P2	 0.6960	 0.3710
Q	 0.9260	 0.6100
Q1	 0.7320	 0.3910
Q2	 0.7170	 0.3900
R	 0.9470	 0.6320
S	 0.8480	 0.5740
a	 0.9430	 0.6340
b	 0.6020	 0.4470
c	 0.9790	 0.6570
d	 0.7490	 0.5210
d1	 0.4870	 0.3030
d2	 0.4570	 0.2940
e	 0.8560	 0.5170
e1	 0.5150	 0.3110
e2	 0.4530	 0.2710
f	 0.9190	 0.6280
g	 0.9180	 0.6060
g1	 0.4620	 0.3030
g2	 0.4180	 0.2790
h	 0.9400	 0.6270
i	 0.9140	 0.6180
i1	 0.4320	 0.3210
i2	 0.3790	 0.3130
j	 0.8840	 0.6010
k	 0.8440	 0.5500
l	 0.9270	 0.6260
m	 0.9650	 0.6410
n	 0.9610	 0.6460
o	 0.9370	 0.6100

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