



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 01:58 AM UTC

PDB ID : 8AP6 / pdb_00008ap6
EMDB ID : EMD-15559
Title : Trypanosoma brucei mitochondrial F1Fo ATP synthase dimer
Authors : Muehleip, A.; Gahura, O.; Zikova, A.; Amunts, A.
Deposited on : 2022-08-09
Resolution : 3.20 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 : 4-5-2 with Phenix2.0
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 : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

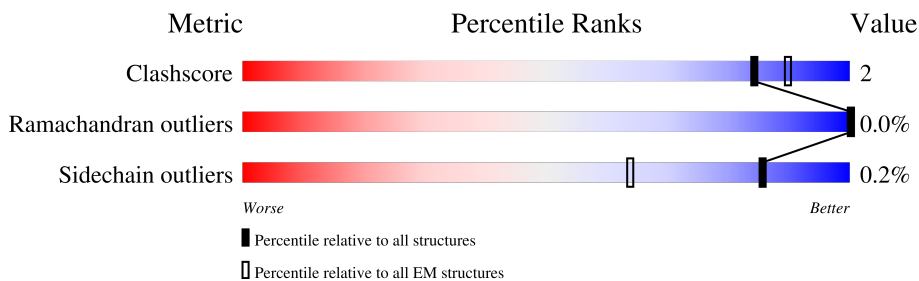
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	231	93% 7%
1	a	231	93% 7%
2	A1	584	86% 5% 9%
2	A2	584	85% 5% 9%
2	B1	584	84% 5% 10%
2	B2	584	84% 5% 10%
2	C1	584	85% 10%
2	C2	584	85% 10%
3	C	114	65% 10% 25%

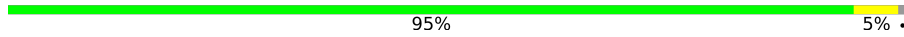
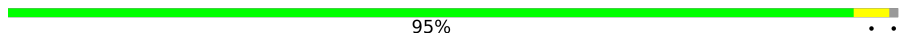








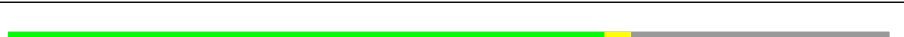


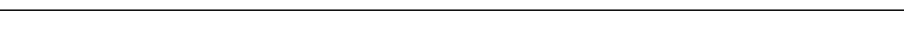
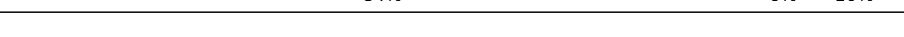
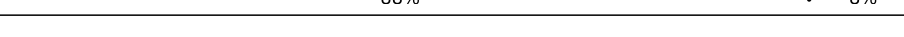



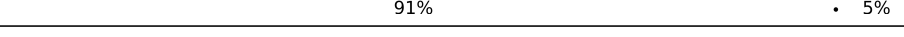





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Mol	Chain	Length	Quality of chain
3	c	114	64% 11% 25%
4	D	370	86% 10%
4	d	370	86% 10%
5	D1	519	87% 7% 6%
5	D2	519	87% 7% 6%
5	E1	519	88% 6% 6%
5	E2	519	87% 6% 6%
5	F1	519	88% 6% 6%
5	F2	519	88% 6% 6%
6	E	396	93%
6	e	396	93%
7	F	145	84% 9% 7%
7	f	145	84% 9% 7%
8	G	269	90% 9%
8	g	269	90% 10%
9	G1	305	90% 8%
9	G2	305	90% 9%
10	H	157	83% 13%
10	h	157	84% 13%
11	H1	182	82% 7% 12%
11	H2	182	81% 7% 12%
12	I	104	91% 8%
12	i	104	91% 8%
13	I1	75	76% 11% 13%
13	I2	75	73% 13% 13%

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Mol	Chain	Length	Quality of chain
14	J	169	 95% 5%
14	j	169	 95%
15	J1	188	 81% 7% 12%
15	J2	188	 80% 9% 12%
15	K1	188	 82% 6% 12%
15	K2	188	 84% 12%
15	L1	188	 85% 12%
15	L2	188	 85% 12%
16	K	124	 82% 15%
16	k	124	 82% 15%
17	L	92	 67% 29%
17	l	92	 65% 5% 29%
18	M	144	 84% 6% 10%
18	m	144	 84% 6% 10%
19	M1	255	 88% 8%
19	M2	255	 88% 8%
20	N	156	 84% 11%
20	n	156	 85% 11%
21	O	101	 91% 5%
21	o	101	 91% 5%
22	O1	118	 54% 12% 34%
22	O2	118	 54% 12% 34%
22	P1	118	 58% 8% 34%
22	P2	118	 58% 8% 34%
22	Q1	118	 60% 6% 34%

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Mol	Chain	Length	Quality of chain		
22	Q2	118	61%	5%	34%
22	R1	118	64%	•	34%
22	R2	118	64%	•	34%
22	S1	118	63%	•	34%
22	S2	118	61%	5%	34%
22	T1	118	64%	•	34%
22	T2	118	64%	•	34%
22	U1	118	64%	•	34%
22	U2	118	65%	•	34%
22	V1	118	64%	•	34%
22	V2	118	64%	•	34%
22	W1	118	66%		34%
22	W2	118	66%		34%
22	X1	118	57%	9%	34%
22	X2	118	57%	9%	34%
23	P	105	73%	•	24%
23	p	105	73%	•	24%
24	Q	98	79%	8%	13%
24	q	98	80%	7%	13%
25	R	62	95%	5%	
25	r	62	95%	5%	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	Q7G	E	402	X	-	-	-
31	Q7G	N	201	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	Q7G	e	407	X	-	-	-
31	Q7G	n	201	X	-	-	-

2 Entry composition [i](#)

There are 34 unique types of molecules in this entry. The entry contains 251552 atoms, of which 126980 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 ATP synthase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	231	4076	1459	2044	261	284	28	0	0
1	a	231	4076	1459	2044	261	284	28	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	TRP	-	insertion	UNP P24499
A	180	TRP	-	insertion	UNP P24499
a	23	TRP	-	insertion	UNP P24499
a	180	TRP	-	insertion	UNP P24499

- Molecule 2 is a protein called ATP synthase subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	A1	530	8280	2612	4196	710	742	20	0	0
2	A2	530	8280	2612	4196	710	742	20	0	0
2	B1	523	8198	2585	4161	702	730	20	0	0
2	B2	523	8198	2585	4161	702	730	20	0	0
2	C1	523	8193	2587	4154	701	731	20	0	0
2	C2	523	8193	2587	4154	701	731	20	0	0

- Molecule 3 is a protein called subunit-8.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	C	86	1460	494	715	116	130	5	0	0
3	c	86	1460	494	715	116	130	5	0	0

- Molecule 4 is a protein called subunit-d.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	D	332	5499	1710	2762	505	514	8	0	0
4	d	332	5499	1710	2762	505	514	8	0	0

- Molecule 5 is a protein called ATP synthase subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	D1	487	7430	2329	3741	631	710	19	0	0
5	D2	487	7430	2329	3741	631	710	19	0	0
5	E1	486	7415	2324	3733	630	709	19	0	0
5	E2	486	7415	2324	3733	630	709	19	0	0
5	F1	489	7461	2339	3758	633	712	19	0	0
5	F2	489	7461	2339	3758	633	712	19	0	0

- Molecule 6 is a protein called ATPTB1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	E	383	6281	2060	3061	558	585	17	0	0
6	e	383	6281	2060	3061	558	585	17	0	0

- Molecule 7 is a protein called subunit-f.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	F	135	2256	744	1111	201	195	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace	
7	f	135	Total	C	H	N	O	S	0	0
			2256	744	1111	201	195	5		

- Molecule 8 is a protein called ATPTB3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
8	G	268	Total	C	H	N	O	S	0	0
			3953	1211	2020	343	378	1		
8	g	268	Total	C	H	N	O	S	0	0
			3953	1211	2020	343	378	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	176	ALA	VAL	conflict	UNP A0A3L6KRX7
g	176	ALA	VAL	conflict	UNP A0A3L6KRX7

- Molecule 9 is a protein called ATP synthase gamma subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace	
9	G1	300	Total	C	H	N	O	S	0	0
			4774	1507	2387	423	448	9		
9	G2	300	Total	C	H	N	O	S	0	0
			4774	1507	2387	423	448	9		

- Molecule 10 is a protein called ATPTB4.

Mol	Chain	Residues	Atoms					AltConf	Trace	
10	H	137	Total	C	H	N	O	S	0	0
			2158	680	1088	184	203	3		
10	h	137	Total	C	H	N	O	S	0	0
			2158	680	1088	184	203	3		

- Molecule 11 is a protein called ATP synthase, epsilon chain, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace	
11	H1	161	Total	C	H	N	O	S	0	0
			2483	788	1232	211	248	4		
11	H2	161	Total	C	H	N	O	S	0	0
			2483	788	1232	211	248	4		

- Molecule 12 is a protein called subunit-i/j.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	I	103	Total	C	H	N	O	S	0	0
			1740	574	857	152	151	6		
12	i	103	Total	C	H	N	O	S	0	0
			1740	574	857	152	151	6		

- Molecule 13 is a protein called ATP synthase subunit epsilon, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	I1	65	Total	C	H	N	O	S	0	0
			1046	332	513	97	102	2		
13	I2	65	Total	C	H	N	O	S	0	0
			1046	332	513	97	102	2		

- Molecule 14 is a protein called ATPTB6.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	J	168	Total	C	H	N	O	S	0	0
			2835	919	1411	249	249	7		
14	j	168	Total	C	H	N	O	S	0	0
			2835	919	1411	249	249	7		

- Molecule 15 is a protein called ATP synthase subunit p18, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	J1	166	Total	C	H	N	O	S	0	0
			2590	822	1276	221	257	14		
15	J2	166	Total	C	H	N	O	S	0	0
			2590	822	1276	221	257	14		
15	K1	166	Total	C	H	N	O	S	0	0
			2591	822	1276	221	258	14		
15	K2	166	Total	C	H	N	O	S	0	0
			2591	822	1276	221	258	14		
15	L1	165	Total	C	H	N	O	S	0	0
			2581	819	1271	220	257	14		
15	L2	165	Total	C	H	N	O	S	0	0
			2581	819	1271	220	257	14		

- Molecule 16 is a protein called subunit-k.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	K	105	Total	C	H	N	O	S	0	0
			1749	577	876	149	141	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
16	k	105	Total	C	H	N	O	S	0	0
			1749	577	876	149	141	6		

- Molecule 17 is a protein called subunit-e.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
17	L	65	Total	C	H	N	O	S	0	0
			1082	340	545	104	92	1		
17	l	65	Total	C	H	N	O	S	0	0
			1082	340	545	104	92	1		

- Molecule 18 is a protein called subunit-g.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
18	M	129	Total	C	H	N	O	S	0	0
			2069	662	1042	177	186	2		
18	m	129	Total	C	H	N	O	S	0	0
			2069	662	1042	177	186	2		

- Molecule 19 is a protein called oligomycin sensitivi y conferring protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
19	M1	234	Total	C	H	N	O	S	0	0
			3750	1212	1873	302	360	3		
19	M2	234	Total	C	H	N	O	S	0	0
			3750	1212	1873	302	360	3		

- Molecule 20 is a protein called ATPTB11.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
20	N	139	Total	C	H	N	O	S	0	0
			2210	730	1082	183	208	7		
20	n	139	Total	C	H	N	O	S	0	0
			2210	730	1082	183	208	7		

- Molecule 21 is a protein called ATPTB12.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
21	O	96	Total	C	H	N	O	S	0	0
			1556	506	767	140	140	3		
21	o	96	Total	C	H	N	O	S	0	0
			1556	506	767	140	140	3		

- Molecule 22 is a protein called ATPase subunit 9, putative.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
22	O1	78	Total 1165	C 376	H 600	N 89	O 96	S 4	0	0
22	O2	78	Total 1165	C 376	H 600	N 89	O 96	S 4	0	0
22	P1	78	Total 1165	C 376	H 600	N 89	O 96	S 4	0	0
22	P2	78	Total 1165	C 376	H 600	N 89	O 96	S 4	0	0
22	Q1	78	Total 1165	C 376	H 600	N 89	O 96	S 4	0	0
22	Q2	78	Total 1165	C 376	H 600	N 89	O 96	S 4	0	0
22	R1	78	Total 1165	C 376	H 600	N 89	O 96	S 4	0	0
22	R2	78	Total 1165	C 376	H 600	N 89	O 96	S 4	0	0
22	S1	78	Total 1166	C 376	H 601	N 89	O 96	S 4	0	0
22	S2	78	Total 1166	C 376	H 601	N 89	O 96	S 4	0	0
22	T1	78	Total 1166	C 376	H 601	N 89	O 96	S 4	0	0
22	T2	78	Total 1166	C 376	H 601	N 89	O 96	S 4	0	0
22	U1	78	Total 1165	C 376	H 600	N 89	O 96	S 4	0	0
22	U2	78	Total 1165	C 376	H 600	N 89	O 96	S 4	0	0
22	V1	78	Total 1165	C 376	H 600	N 89	O 96	S 4	0	0
22	V2	78	Total 1165	C 376	H 600	N 89	O 96	S 4	0	0
22	W1	78	Total 1165	C 376	H 600	N 89	O 96	S 4	0	0
22	W2	78	Total 1165	C 376	H 600	N 89	O 96	S 4	0	0
22	X1	78	Total 1165	C 376	H 600	N 89	O 96	S 4	0	0
22	X2	78	Total 1165	C 376	H 600	N 89	O 96	S 4	0	0

- Molecule 23 is a protein called subunit-b.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
23	P	80	1335	448	651	108	125	3	0	0
23	p	80	1335	448	651	108	125	3	0	0

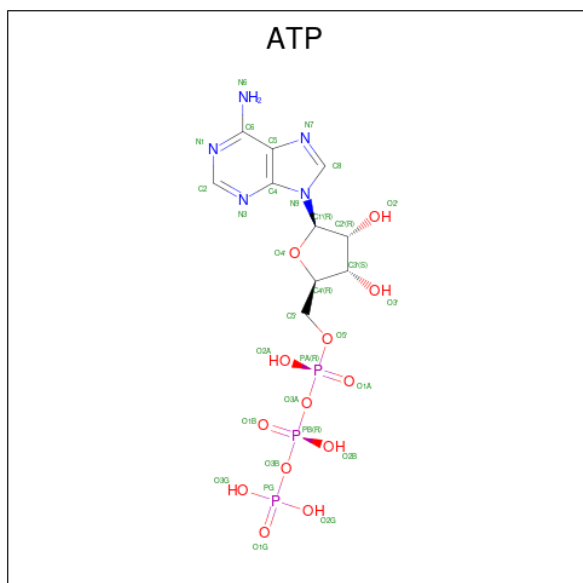
- Molecule 24 is a protein called ATPEG3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
24	Q	85	1486	499	720	142	125	0	0
24	q	85	1486	499	720	142	125	0	0

- Molecule 25 is a protein called ATPEG4.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
25	R	62	1040	358	498	94	85	5	0	0
25	r	62	1040	358	498	94	85	5	0	0

- Molecule 26 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
26	A1	1	43	10	12	5	13	3	0

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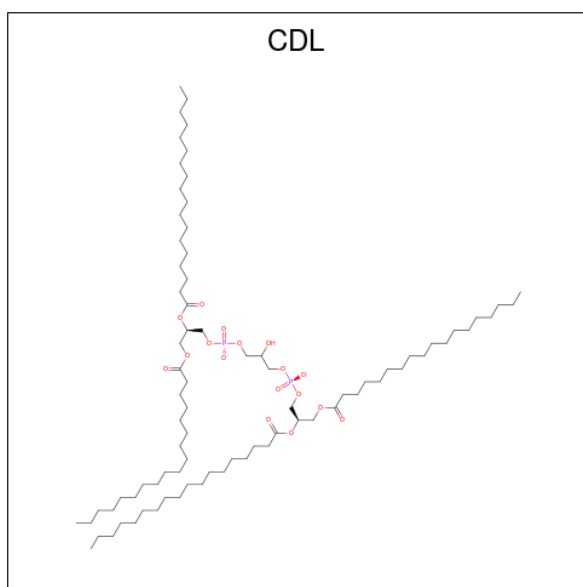
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Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
26	A2	1	43	10	12	5	13	3	0
26	B1	1	43	10	12	5	13	3	0
26	B2	1	43	10	12	5	13	3	0
26	C1	1	43	10	12	5	13	3	0
26	C2	1	43	10	12	5	13	3	0
26	F1	1	43	10	12	5	13	3	0
26	F2	1	43	10	12	5	13	3	0

- Molecule 27 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
27	A1	1	Total 1	Mg 1	0
27	A2	1	Total 1	Mg 1	0
27	B1	1	Total 1	Mg 1	0
27	B2	1	Total 1	Mg 1	0
27	C1	1	Total 1	Mg 1	0
27	C2	1	Total 1	Mg 1	0
27	D1	1	Total 1	Mg 1	0
27	D2	1	Total 1	Mg 1	0
27	F1	1	Total 1	Mg 1	0
27	F2	1	Total 1	Mg 1	0

- Molecule 28 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



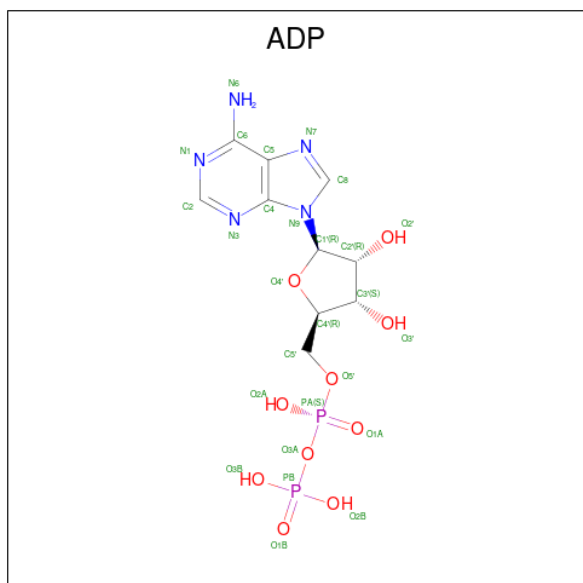
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
28	C	1	256	81	156	17	2	0
28	E	1	256	81	156	17	2	0
28	E	1	256	81	156	17	2	0
28	E	1	256	81	156	17	2	0
28	E	1	256	81	156	17	2	0
28	E	1	256	81	156	17	2	0
28	E	1	256	81	156	17	2	0
28	F	1	256	81	156	17	2	0
28	J	1	256	81	156	17	2	0
28	J	1	256	81	156	17	2	0
28	L	1	256	81	156	17	2	0
28	M	1	256	81	156	17	2	0
28	Q	1	256	81	156	17	2	0
28	c	1	256	81	156	17	2	0
28	e	1	256	81	156	17	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
28	e	1	Total 256	C 81	H 156	O 17	P 2	0
28	e	1	Total 256	C 81	H 156	O 17	P 2	0
28	e	1	Total 256	C 81	H 156	O 17	P 2	0
28	e	1	Total 256	C 81	H 156	O 17	P 2	0
28	f	1	Total 256	C 81	H 156	O 17	P 2	0
28	j	1	Total 256	C 81	H 156	O 17	P 2	0
28	j	1	Total 256	C 81	H 156	O 17	P 2	0
28	l	1	Total 256	C 81	H 156	O 17	P 2	0
28	m	1	Total 256	C 81	H 156	O 17	P 2	0
28	q	1	Total 256	C 81	H 156	O 17	P 2	0

- Molecule 29 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



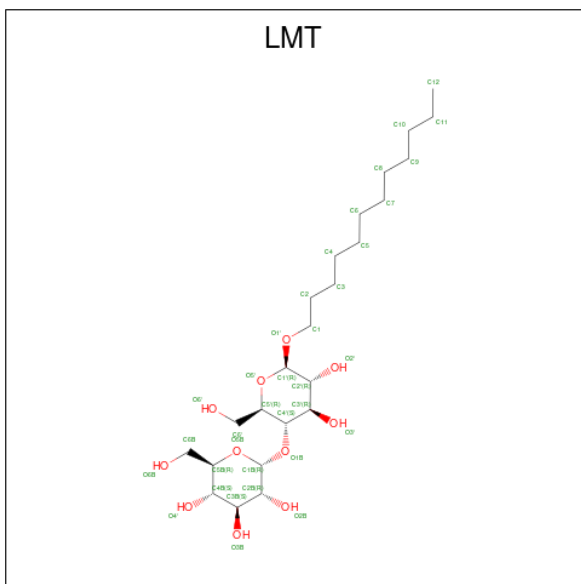
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
29	D1	1	Total 39	C 10	H 12	N 5	O 10	P 2	0

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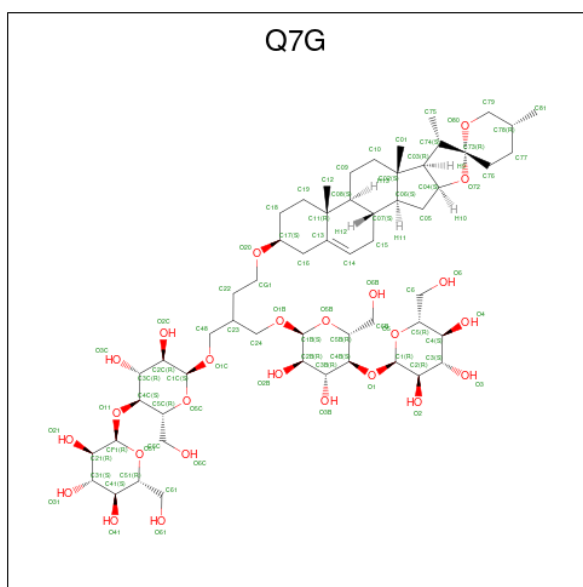
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
29	D2	1	39	10	12	5	10	2	0

- Molecule 30 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



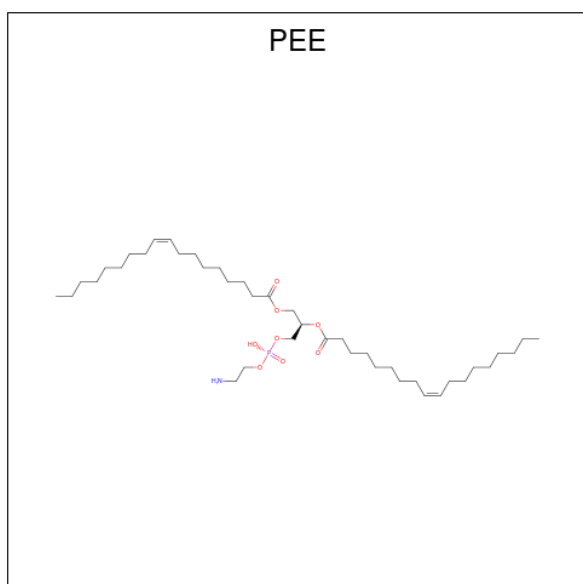
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
30	E	1	74	24	39	11	0
30	J	1	74	24	39	11	0
30	e	1	74	24	39	11	0
30	j	1	74	24	39	11	0

- Molecule 31 is 2-[[[4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranosyl]oxy]methyl]-4-[[[(3 beta,9beta,14beta,17beta,25R)-spirost-5-en-3-yl]oxy]butyl 4-O-alpha-D-glucopyranosyl-alpha-D-glucopyranoside (CCD ID: Q7G) (formula: C₅₆H₉₂O₂₅).



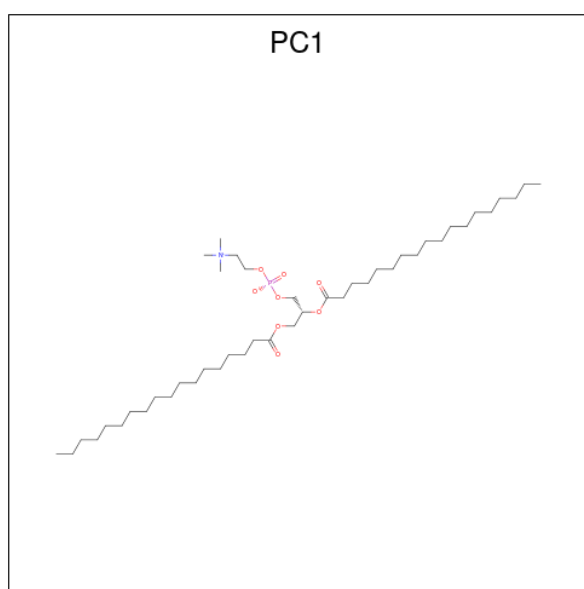
Mol	Chain	Residues	Atoms			AltConf	
			Total	C	H		O
31	E	1	108	38	60	10	0
31	N	1	129	44	70	15	0
31	e	1	108	38	60	10	0
31	n	1	129	44	70	15	0

- Molecule 32 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
32	F	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
32	R	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
32	f	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
32	r	1	Total 133	C 41	H 82	N 1	O 8	P 1	0

- Molecule 33 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P) (labeled as "Ligand of Interest" by depositor).



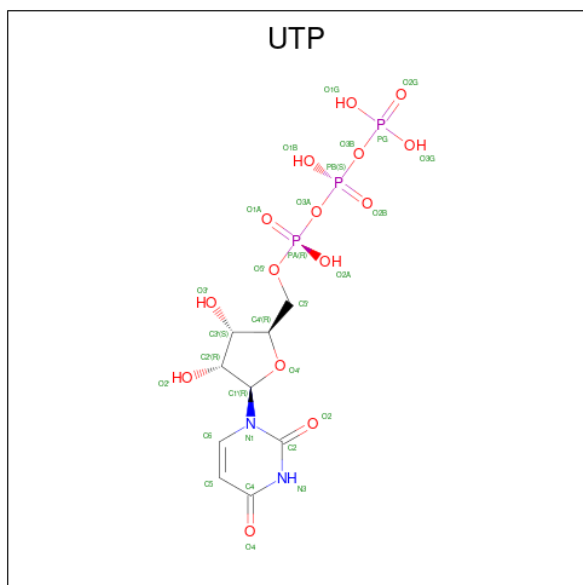
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
33	F	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
33	F	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
33	I	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
33	J	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
33	f	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
33	f	1	Total 142	C 44	H 88	N 1	O 8	P 1	0
33	i	1	Total 142	C 44	H 88	N 1	O 8	P 1	0

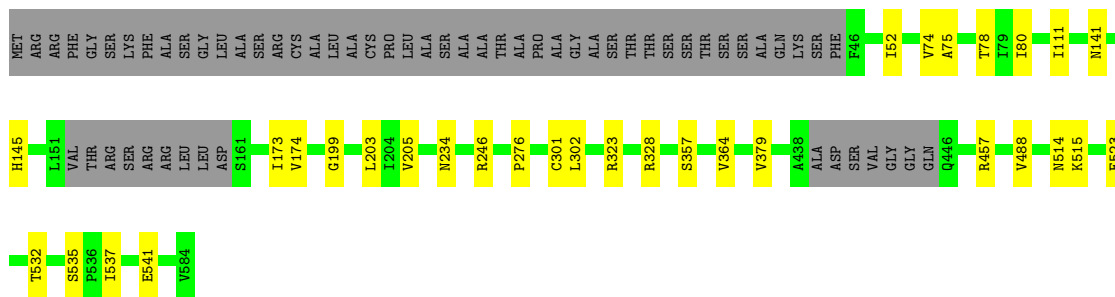
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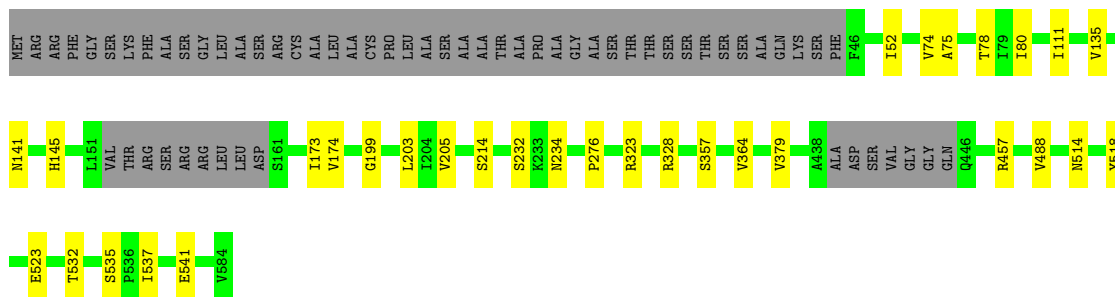
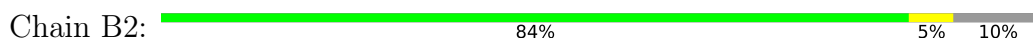
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
33	j	1	142	44	88	1	8	1	0

- Molecule 34 is URIDINE 5'-TRIPHOSPHATE (CCD ID: UTP) (formula: $C_9H_{15}N_2O_{15}P_3$) (labeled as "Ligand of Interest" by depositor).

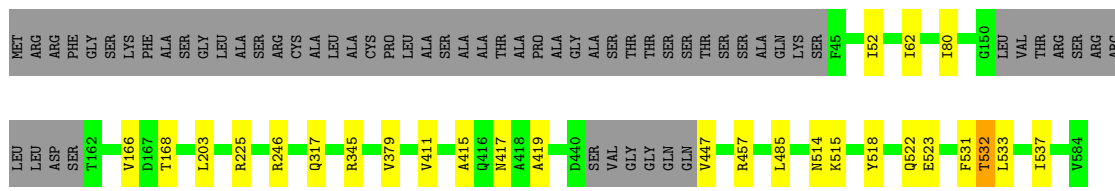
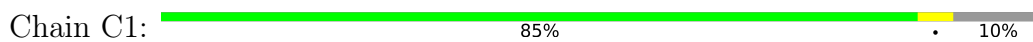




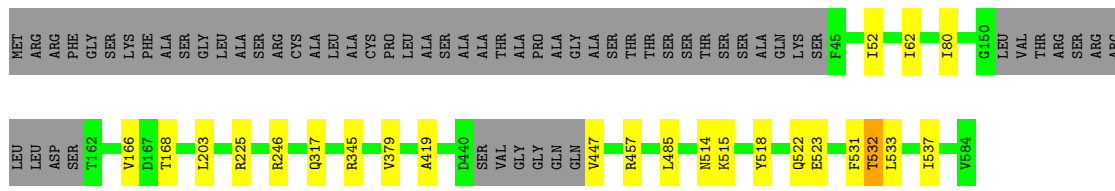
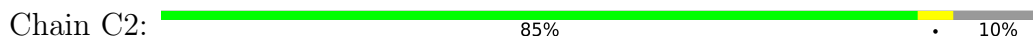
• Molecule 2: ATP synthase subunit alpha, mitochondrial



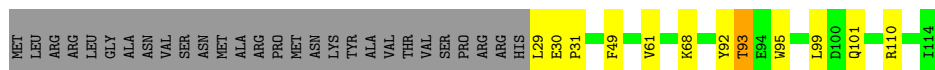
• Molecule 2: ATP synthase subunit alpha, mitochondrial



• Molecule 2: ATP synthase subunit alpha, mitochondrial

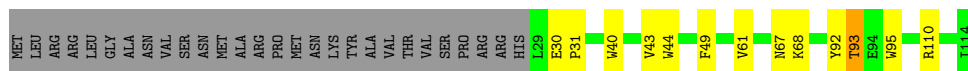


• Molecule 3: subunit-8




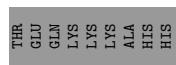
• Molecule 3: subunit-8

Chain c:  64% 11% 25%




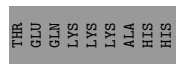
• Molecule 4: subunit-d

Chain D:  86% 10%



• Molecule 4: subunit-d

Chain d:  86% 10%




• Molecule 5: ATP synthase subunit beta, mitochondrial

Chain D1:  87% 7% 6%




• Molecule 5: ATP synthase subunit beta, mitochondrial

Chain D2:  87% 7% 6%

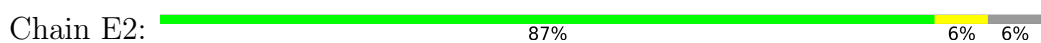


• Molecule 5: ATP synthase subunit beta, mitochondrial

Chain E1:  88% 6% 6%



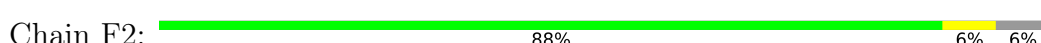
• Molecule 5: ATP synthase subunit beta, mitochondrial



• Molecule 5: ATP synthase subunit beta, mitochondrial



• Molecule 5: ATP synthase subunit beta, mitochondrial




• Molecule 6: ATPTB1



• Molecule 6: ATPTB1




- Molecule 7: subunit-f

Chain F:  84% 9% 7%



- Molecule 7: subunit-f

Chain f:  84% 9% 7%




- Molecule 8: ATPTB3

Chain G:  90% 9%



- Molecule 8: ATPTB3

Chain g:  90% 10%




- Molecule 9: ATP synthase gamma subunit

Chain G1:  90% 8%




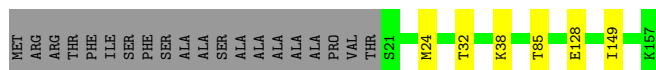
- Molecule 9: ATP synthase gamma subunit

Chain G2:  90% 9%

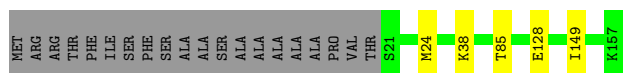
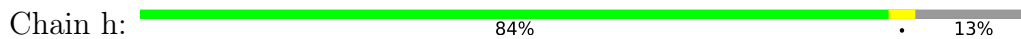


- Molecule 10: ATPTB4

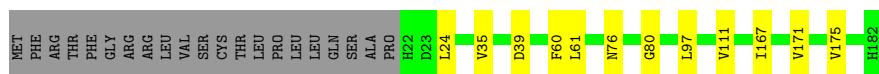
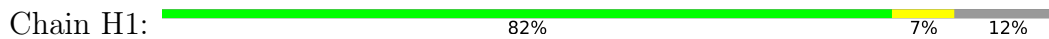
Chain H:  83% 13%



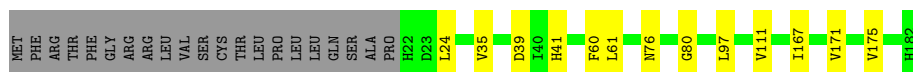
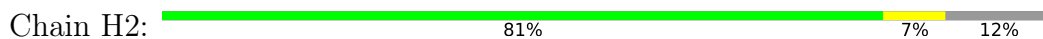
- Molecule 10: ATPTB4



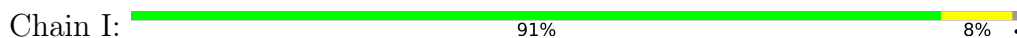
- Molecule 11: ATP synthase, epsilon chain, putative



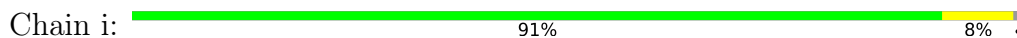
- Molecule 11: ATP synthase, epsilon chain, putative



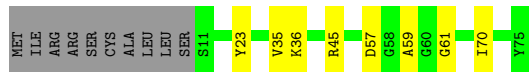
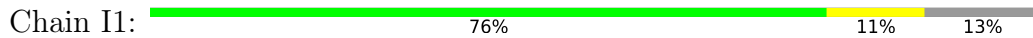
- Molecule 12: subunit-i/j



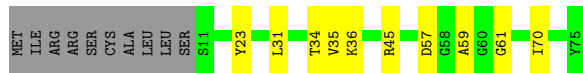
- Molecule 12: subunit-i/j



- Molecule 13: ATP synthase subunit epsilon, mitochondrial



- Molecule 13: ATP synthase subunit epsilon, mitochondrial



- Molecule 14: ATPTB6

Chain J:  95% 5%




- Molecule 14: ATPTB6

Chain j:  95%




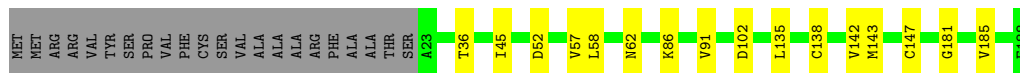
- Molecule 15: ATP synthase subunit p18, mitochondrial

Chain J1:  81% 7% 12%




- Molecule 15: ATP synthase subunit p18, mitochondrial

Chain J2:  80% 9% 12%




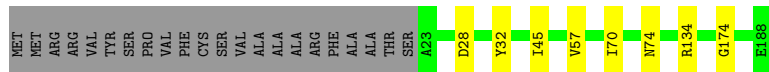
- Molecule 15: ATP synthase subunit p18, mitochondrial

Chain K1:  82% 6% 12%




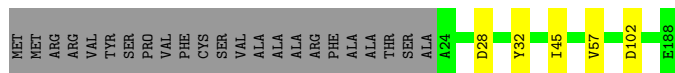
- Molecule 15: ATP synthase subunit p18, mitochondrial

Chain K2:  84% 12%

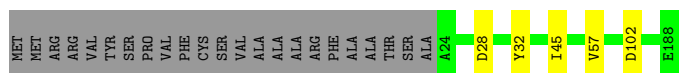
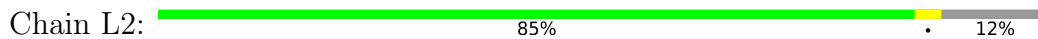


- Molecule 15: ATP synthase subunit p18, mitochondrial

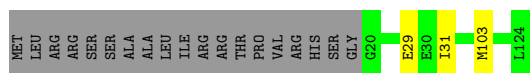
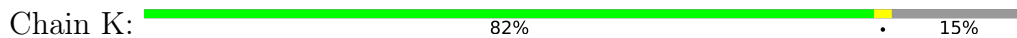
Chain L1:  85% 12%



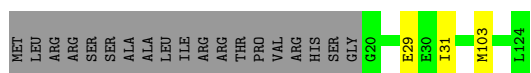
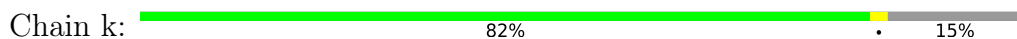
- Molecule 15: ATP synthase subunit p18, mitochondrial



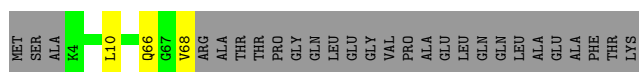
• Molecule 16: subunit-k



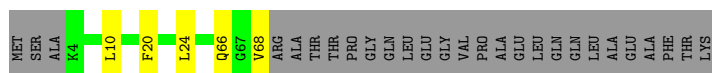
• Molecule 16: subunit-k



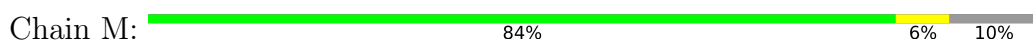
• Molecule 17: subunit-e



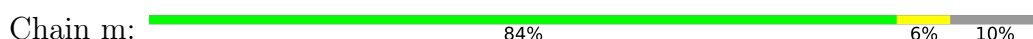
• Molecule 17: subunit-e



• Molecule 18: subunit-g



• Molecule 18: subunit-g



• Molecule 19: oligomycin sensitivy conferring protein





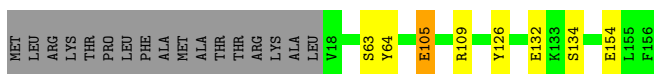
- Molecule 19: oligomycin sensitivity conferring protein

Chain M2: 88% 8%



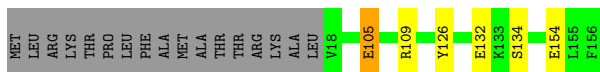
- Molecule 20: ATPTB11

Chain N: 84% 11%



- Molecule 20: ATPTB11

Chain n: 85% 11%



- Molecule 21: ATPTB12

Chain O: 91% 5%



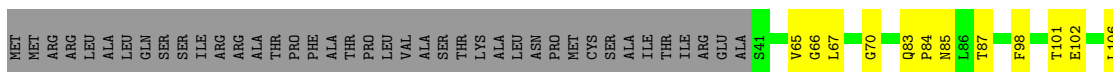
- Molecule 21: ATPTB12

Chain o: 91% 5%



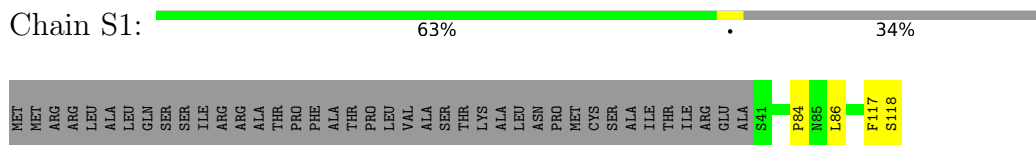
- Molecule 22: ATPase subunit 9, putative

Chain O1: 54% 12% 34%

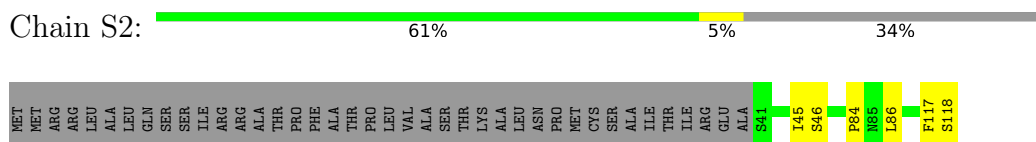


- Molecule 22: ATPase subunit 9, putative

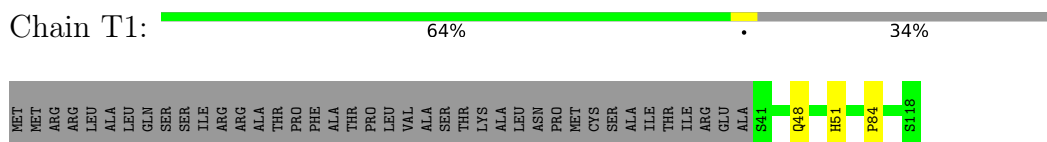
- Molecule 22: ATPase subunit 9, putative



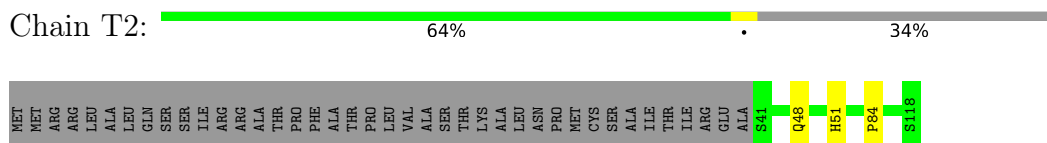
- Molecule 22: ATPase subunit 9, putative



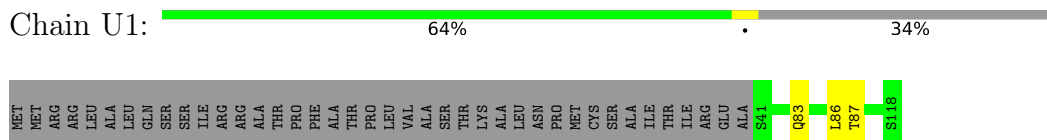
- Molecule 22: ATPase subunit 9, putative



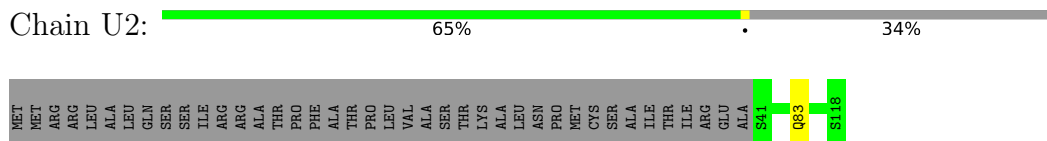
- Molecule 22: ATPase subunit 9, putative



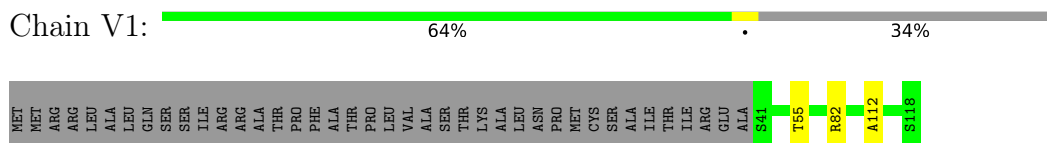
- Molecule 22: ATPase subunit 9, putative



- Molecule 22: ATPase subunit 9, putative

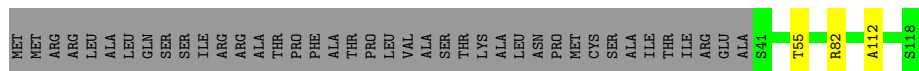


- Molecule 22: ATPase subunit 9, putative



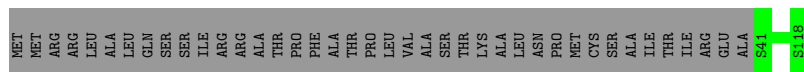
- Molecule 22: ATPase subunit 9, putative

Chain V2:  64% 34%



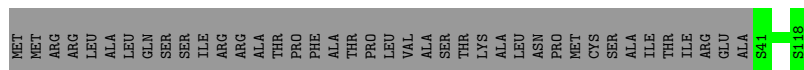
• Molecule 22: ATPase subunit 9, putative

Chain W1:  66% 34%



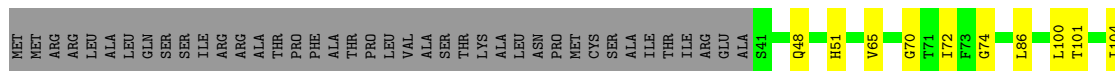
• Molecule 22: ATPase subunit 9, putative

Chain W2:  66% 34%



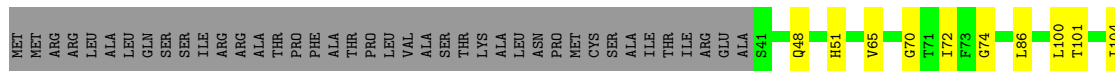
• Molecule 22: ATPase subunit 9, putative

Chain X1:  57% 9% 34%



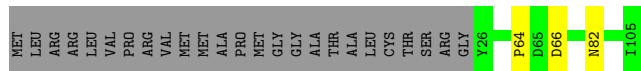
• Molecule 22: ATPase subunit 9, putative

Chain X2:  57% 9% 34%



• Molecule 23: subunit-b

Chain P:  73% 24%



• Molecule 23: subunit-b

Chain p:  73% 24%

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36925	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 ($e^-/\text{\AA}^2$)	33	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, CDL, ATP, Q7G, PC1, LMT, UTP, PEE, AME

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	0.20	0/2111	0.26	0/2861
1	a	0.20	0/2111	0.26	0/2861
2	A1	0.07	0/4159	0.22	0/5632
2	A2	0.07	0/4159	0.22	0/5632
2	B1	0.07	0/4110	0.22	0/5566
2	B2	0.07	0/4110	0.22	0/5566
2	C1	0.07	0/4113	0.22	0/5569
2	C2	0.07	0/4113	0.22	0/5569
3	C	0.18	0/772	0.28	0/1054
3	c	0.18	0/772	0.32	0/1054
4	D	0.12	0/2786	0.25	0/3760
4	d	0.12	0/2786	0.25	0/3760
5	D1	0.08	0/3745	0.23	0/5077
5	D2	0.08	0/3745	0.23	0/5077
5	E1	0.07	0/3738	0.22	0/5067
5	E2	0.07	0/3738	0.22	0/5067
5	F1	0.08	0/3760	0.24	0/5098
5	F2	0.08	0/3760	0.24	0/5098
6	E	0.16	0/3305	0.21	0/4482
6	e	0.16	0/3305	0.21	0/4482
7	F	0.18	0/1183	0.28	0/1601
7	f	0.18	0/1183	0.28	0/1601
8	G	0.07	0/1953	0.20	0/2650
8	g	0.07	0/1953	0.20	0/2650
9	G1	0.07	0/2427	0.20	0/3268
9	G2	0.07	0/2427	0.20	0/3268
10	H	0.05	0/1088	0.16	0/1466
10	h	0.05	0/1088	0.16	0/1466
11	H1	0.13	0/1274	0.22	0/1728
11	H2	0.13	0/1274	0.22	0/1728
12	I	0.17	0/913	0.22	0/1240
12	i	0.17	0/913	0.22	0/1240

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
13	I1	0.06	0/547	0.18	0/738
13	I2	0.06	0/547	0.18	0/738
14	J	0.14	0/1462	0.20	0/1973
14	j	0.14	0/1462	0.20	0/1973
15	J1	0.05	0/1341	0.16	0/1810
15	J2	0.05	0/1341	0.17	0/1810
15	K1	0.05	0/1342	0.18	0/1810
15	K2	0.05	0/1342	0.18	0/1810
15	L1	0.05	0/1337	0.17	0/1803
15	L2	0.05	0/1337	0.17	0/1803
16	K	0.13	0/904	0.22	0/1228
16	k	0.13	0/904	0.22	0/1228
17	L	0.14	0/547	0.18	0/735
17	l	0.14	0/547	0.18	0/735
18	M	0.15	0/1049	0.21	0/1423
18	m	0.15	0/1049	0.21	0/1423
19	M1	0.08	0/1916	0.21	0/2591
19	M2	0.08	0/1916	0.21	0/2591
20	N	0.17	0/1166	0.23	0/1581
20	n	0.17	0/1166	0.23	0/1581
21	O	0.13	0/814	0.20	0/1100
21	o	0.13	0/814	0.19	0/1100
22	O1	0.10	0/574	0.28	0/777
22	O2	0.10	0/574	0.28	0/777
22	P1	0.15	0/574	0.29	0/777
22	P2	0.15	0/574	0.29	0/777
22	Q1	0.09	0/574	0.19	0/777
22	Q2	0.09	0/574	0.19	0/777
22	R1	0.09	0/574	0.20	0/777
22	R2	0.09	0/574	0.20	0/777
22	S1	0.08	0/574	0.19	0/777
22	S2	0.08	0/574	0.19	0/777
22	T1	0.07	0/574	0.20	0/777
22	T2	0.08	0/574	0.20	0/777
22	U1	0.08	0/574	0.20	0/777
22	U2	0.08	0/574	0.20	0/777
22	V1	0.08	0/574	0.19	0/777
22	V2	0.08	0/574	0.19	0/777
22	W1	0.07	0/574	0.18	0/777
22	W2	0.07	0/574	0.18	0/777
22	X1	0.08	0/574	0.25	0/777
22	X2	0.08	0/574	0.25	0/777
23	P	0.15	0/707	0.23	0/957

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
23	p	0.15	0/707	0.23	0/957
24	Q	0.17	0/799	0.24	0/1091
24	q	0.17	0/799	0.24	0/1091
25	R	0.18	0/567	0.23	0/767
25	r	0.18	0/567	0.23	0/767
All	All	0.11	0/123350	0.22	0/166992

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2032	2044	2044	17	0
1	a	2032	2044	2044	17	0
2	A1	4084	4196	4196	19	0
2	A2	4084	4196	4196	20	0
2	B1	4037	4161	4160	22	0
2	B2	4037	4161	4160	23	0
2	C1	4039	4154	4154	21	0
2	C2	4039	4154	4154	19	0
3	C	745	715	715	10	0
3	c	745	715	715	11	0
4	D	2737	2762	2763	15	0
4	d	2737	2762	2763	15	0
5	D1	3689	3741	3741	21	0
5	D2	3689	3741	3741	23	0
5	E1	3682	3733	3733	23	0
5	E2	3682	3733	3733	22	0
5	F1	3703	3758	3758	21	0
5	F2	3703	3758	3758	22	0
6	E	3220	3061	3061	10	0
6	e	3220	3061	3061	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	F	1145	1111	1111	11	0
7	f	1145	1111	1111	10	0
8	G	1933	2020	2020	14	0
8	g	1933	2020	2020	15	0
9	G1	2387	2387	2387	19	0
9	G2	2387	2387	2387	23	0
10	H	1070	1088	1088	5	0
10	h	1070	1088	1088	4	0
11	H1	1251	1232	1231	10	0
11	H2	1251	1232	1231	10	0
12	I	883	857	857	6	0
12	i	883	857	857	6	0
13	I1	533	513	513	6	0
13	I2	533	513	513	8	0
14	J	1424	1411	1411	6	0
14	j	1424	1411	1411	5	0
15	J1	1314	1276	1276	10	0
15	J2	1314	1276	1276	11	0
15	K1	1315	1276	1276	8	0
15	K2	1315	1276	1276	6	0
15	L1	1310	1271	1271	4	0
15	L2	1310	1271	1271	4	0
16	K	873	876	876	3	0
16	k	873	876	876	3	0
17	L	537	545	545	2	0
17	l	537	545	545	3	0
18	M	1027	1042	1042	5	0
18	m	1027	1042	1042	5	0
19	M1	1877	1873	1873	7	0
19	M2	1877	1873	1873	6	0
20	N	1128	1082	1082	5	0
20	n	1128	1082	1082	4	0
21	O	789	767	767	3	0
21	o	789	767	767	3	0
22	O1	565	600	599	12	0
22	O2	565	600	599	12	0
22	P1	565	600	599	10	0
22	P2	565	600	599	10	0
22	Q1	565	600	599	5	0
22	Q2	565	600	599	4	0
22	R1	565	600	599	3	0
22	R2	565	600	599	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	S1	565	601	599	3	0
22	S2	565	601	599	4	0
22	T1	565	601	599	2	0
22	T2	565	601	599	2	0
22	U1	565	600	599	2	0
22	U2	565	600	599	1	0
22	V1	565	600	599	2	0
22	V2	565	600	599	2	0
22	W1	565	600	599	0	0
22	W2	565	600	599	0	0
22	X1	565	600	599	6	0
22	X2	565	600	599	6	0
23	P	684	651	651	4	0
23	p	684	651	651	4	0
24	Q	766	720	720	7	0
24	q	766	720	720	6	0
25	R	542	498	498	4	0
25	r	542	498	498	3	0
26	A1	31	12	12	0	0
26	A2	31	12	12	0	0
26	B1	31	12	12	0	0
26	B2	31	12	12	1	0
26	C1	31	12	12	0	0
26	C2	31	12	12	0	0
26	F1	31	12	12	0	0
26	F2	31	12	12	0	0
27	A1	1	0	0	0	0
27	A2	1	0	0	0	0
27	B1	1	0	0	0	0
27	B2	1	0	0	0	0
27	C1	1	0	0	0	0
27	C2	1	0	0	0	0
27	D1	1	0	0	0	0
27	D2	1	0	0	0	0
27	F1	1	0	0	0	0
27	F2	1	0	0	0	0
28	C	100	156	156	1	0
28	E	500	780	780	4	0
28	F	100	156	156	0	0
28	J	200	312	312	1	0
28	L	100	156	156	0	0
28	M	100	156	156	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	Q	100	156	156	1	0
28	c	100	156	156	1	0
28	e	500	780	780	4	0
28	f	100	156	156	0	0
28	j	200	312	312	1	0
28	l	100	156	156	0	0
28	m	100	156	156	0	0
28	q	100	156	156	0	0
29	D1	27	12	12	0	0
29	D2	27	12	12	0	0
30	E	35	39	46	0	0
30	J	35	39	46	0	0
30	e	35	39	46	0	0
30	j	35	39	46	0	0
31	E	48	60	0	0	0
31	N	59	70	0	0	0
31	e	48	60	0	0	0
31	n	59	70	0	0	0
32	F	51	82	82	0	0
32	R	51	82	82	0	0
32	f	51	82	82	0	0
32	r	51	82	82	1	0
33	F	108	176	176	1	0
33	I	54	88	88	0	0
33	J	54	88	88	0	0
33	f	108	176	176	1	0
33	i	54	88	88	0	0
33	j	54	88	88	0	0
34	H1	29	11	11	2	0
34	H2	29	11	11	2	0
All	All	124572	126980	126722	585	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 585 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:93:THR:HG21	4:D:136:ASP:OD2	1.72	0.89
5:F2:421:GLU:OE2	9:G2:82:SER:N	2.16	0.79
5:F1:421:GLU:OE2	9:G1:82:SER:N	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H1:80:GLY:O	22:U1:83:GLN:NE2	2.19	0.76
11:H2:80:GLY:O	22:U2:83:GLN:NE2	2.19	0.75

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	229/231 (99%)	227 (99%)	2 (1%)	0	100	100
1	a	229/231 (99%)	227 (99%)	2 (1%)	0	100	100
2	A1	526/584 (90%)	523 (99%)	3 (1%)	0	100	100
2	A2	526/584 (90%)	523 (99%)	3 (1%)	0	100	100
2	B1	517/584 (88%)	510 (99%)	7 (1%)	0	100	100
2	B2	517/584 (88%)	510 (99%)	7 (1%)	0	100	100
2	C1	517/584 (88%)	512 (99%)	4 (1%)	1 (0%)	43	73
2	C2	517/584 (88%)	512 (99%)	4 (1%)	1 (0%)	43	73
3	C	84/114 (74%)	83 (99%)	1 (1%)	0	100	100
3	c	84/114 (74%)	84 (100%)	0	0	100	100
4	D	328/370 (89%)	321 (98%)	7 (2%)	0	100	100
4	d	328/370 (89%)	321 (98%)	7 (2%)	0	100	100
5	D1	485/519 (93%)	478 (99%)	7 (1%)	0	100	100
5	D2	485/519 (93%)	478 (99%)	7 (1%)	0	100	100
5	E1	484/519 (93%)	471 (97%)	13 (3%)	0	100	100
5	E2	484/519 (93%)	471 (97%)	13 (3%)	0	100	100
5	F1	487/519 (94%)	479 (98%)	8 (2%)	0	100	100
5	F2	487/519 (94%)	479 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	E	381/396 (96%)	375 (98%)	6 (2%)	0	100	100
6	e	381/396 (96%)	376 (99%)	5 (1%)	0	100	100
7	F	133/145 (92%)	131 (98%)	2 (2%)	0	100	100
7	f	133/145 (92%)	131 (98%)	2 (2%)	0	100	100
8	G	266/269 (99%)	263 (99%)	3 (1%)	0	100	100
8	g	266/269 (99%)	263 (99%)	3 (1%)	0	100	100
9	G1	298/305 (98%)	296 (99%)	2 (1%)	0	100	100
9	G2	298/305 (98%)	296 (99%)	2 (1%)	0	100	100
10	H	135/157 (86%)	133 (98%)	2 (2%)	0	100	100
10	h	135/157 (86%)	133 (98%)	2 (2%)	0	100	100
11	H1	159/182 (87%)	158 (99%)	1 (1%)	0	100	100
11	H2	159/182 (87%)	158 (99%)	1 (1%)	0	100	100
12	I	101/104 (97%)	100 (99%)	1 (1%)	0	100	100
12	i	101/104 (97%)	100 (99%)	1 (1%)	0	100	100
13	I1	63/75 (84%)	63 (100%)	0	0	100	100
13	I2	63/75 (84%)	63 (100%)	0	0	100	100
14	J	166/169 (98%)	163 (98%)	3 (2%)	0	100	100
14	j	166/169 (98%)	163 (98%)	3 (2%)	0	100	100
15	J1	164/188 (87%)	161 (98%)	3 (2%)	0	100	100
15	J2	164/188 (87%)	161 (98%)	3 (2%)	0	100	100
15	K1	164/188 (87%)	159 (97%)	5 (3%)	0	100	100
15	K2	164/188 (87%)	159 (97%)	5 (3%)	0	100	100
15	L1	163/188 (87%)	163 (100%)	0	0	100	100
15	L2	163/188 (87%)	162 (99%)	1 (1%)	0	100	100
16	K	103/124 (83%)	99 (96%)	4 (4%)	0	100	100
16	k	103/124 (83%)	99 (96%)	4 (4%)	0	100	100
17	L	63/92 (68%)	63 (100%)	0	0	100	100
17	l	63/92 (68%)	63 (100%)	0	0	100	100
18	M	127/144 (88%)	127 (100%)	0	0	100	100
18	m	127/144 (88%)	127 (100%)	0	0	100	100
19	M1	230/255 (90%)	226 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	M2	230/255 (90%)	226 (98%)	4 (2%)	0	100	100
20	N	137/156 (88%)	131 (96%)	6 (4%)	0	100	100
20	n	137/156 (88%)	131 (96%)	6 (4%)	0	100	100
21	O	94/101 (93%)	94 (100%)	0	0	100	100
21	o	94/101 (93%)	94 (100%)	0	0	100	100
22	O1	76/118 (64%)	71 (93%)	5 (7%)	0	100	100
22	O2	76/118 (64%)	71 (93%)	5 (7%)	0	100	100
22	P1	76/118 (64%)	73 (96%)	3 (4%)	0	100	100
22	P2	76/118 (64%)	73 (96%)	3 (4%)	0	100	100
22	Q1	76/118 (64%)	76 (100%)	0	0	100	100
22	Q2	76/118 (64%)	76 (100%)	0	0	100	100
22	R1	76/118 (64%)	76 (100%)	0	0	100	100
22	R2	76/118 (64%)	76 (100%)	0	0	100	100
22	S1	76/118 (64%)	74 (97%)	2 (3%)	0	100	100
22	S2	76/118 (64%)	74 (97%)	2 (3%)	0	100	100
22	T1	76/118 (64%)	75 (99%)	1 (1%)	0	100	100
22	T2	76/118 (64%)	75 (99%)	1 (1%)	0	100	100
22	U1	76/118 (64%)	72 (95%)	4 (5%)	0	100	100
22	U2	76/118 (64%)	72 (95%)	4 (5%)	0	100	100
22	V1	76/118 (64%)	74 (97%)	2 (3%)	0	100	100
22	V2	76/118 (64%)	74 (97%)	2 (3%)	0	100	100
22	W1	76/118 (64%)	74 (97%)	2 (3%)	0	100	100
22	W2	76/118 (64%)	74 (97%)	2 (3%)	0	100	100
22	X1	76/118 (64%)	75 (99%)	1 (1%)	0	100	100
22	X2	76/118 (64%)	75 (99%)	1 (1%)	0	100	100
23	P	78/105 (74%)	77 (99%)	1 (1%)	0	100	100
23	p	78/105 (74%)	77 (99%)	1 (1%)	0	100	100
24	Q	83/98 (85%)	80 (96%)	3 (4%)	0	100	100
24	q	83/98 (85%)	80 (96%)	3 (4%)	0	100	100
25	R	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
25	r	60/62 (97%)	59 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	15170/17414 (87%)	14931 (98%)	237 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C2	532	THR
2	C1	532	THR

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	225/225 (100%)	224 (100%)	1 (0%)	84	86
1	a	225/225 (100%)	224 (100%)	1 (0%)	84	86
2	A1	439/479 (92%)	439 (100%)	0	100	100
2	A2	439/479 (92%)	439 (100%)	0	100	100
2	B1	435/479 (91%)	435 (100%)	0	100	100
2	B2	435/479 (91%)	435 (100%)	0	100	100
2	C1	434/479 (91%)	434 (100%)	0	100	100
2	C2	434/479 (91%)	434 (100%)	0	100	100
3	C	80/104 (77%)	79 (99%)	1 (1%)	61	78
3	c	80/104 (77%)	79 (99%)	1 (1%)	61	78
4	D	297/334 (89%)	296 (100%)	1 (0%)	86	88
4	d	297/334 (89%)	296 (100%)	1 (0%)	86	88
5	D1	398/420 (95%)	397 (100%)	1 (0%)	86	88
5	D2	398/420 (95%)	398 (100%)	0	100	100
5	E1	397/420 (94%)	397 (100%)	0	100	100
5	E2	397/420 (94%)	397 (100%)	0	100	100
5	F1	400/420 (95%)	400 (100%)	0	100	100
5	F2	400/420 (95%)	400 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	E	334/341 (98%)	333 (100%)	1 (0%)	86	88
6	e	334/341 (98%)	333 (100%)	1 (0%)	86	88
7	F	119/124 (96%)	118 (99%)	1 (1%)	73	82
7	f	119/124 (96%)	118 (99%)	1 (1%)	73	82
8	G	205/206 (100%)	205 (100%)	0	100	100
8	g	205/206 (100%)	205 (100%)	0	100	100
9	G1	253/257 (98%)	252 (100%)	1 (0%)	84	86
9	G2	253/257 (98%)	252 (100%)	1 (0%)	84	86
10	H	110/123 (89%)	110 (100%)	0	100	100
10	h	110/123 (89%)	110 (100%)	0	100	100
11	H1	137/156 (88%)	136 (99%)	1 (1%)	76	83
11	H2	137/156 (88%)	135 (98%)	2 (2%)	57	76
12	I	95/96 (99%)	95 (100%)	0	100	100
12	i	95/96 (99%)	95 (100%)	0	100	100
13	I1	58/67 (87%)	58 (100%)	0	100	100
13	I2	58/67 (87%)	58 (100%)	0	100	100
14	J	149/150 (99%)	149 (100%)	0	100	100
14	j	149/150 (99%)	149 (100%)	0	100	100
15	J1	145/162 (90%)	145 (100%)	0	100	100
15	J2	145/162 (90%)	145 (100%)	0	100	100
15	K1	145/162 (90%)	145 (100%)	0	100	100
15	K2	145/162 (90%)	145 (100%)	0	100	100
15	L1	145/162 (90%)	145 (100%)	0	100	100
15	L2	145/162 (90%)	145 (100%)	0	100	100
16	K	91/107 (85%)	91 (100%)	0	100	100
16	k	91/107 (85%)	91 (100%)	0	100	100
17	L	55/75 (73%)	55 (100%)	0	100	100
17	l	55/75 (73%)	55 (100%)	0	100	100
18	M	111/124 (90%)	110 (99%)	1 (1%)	70	81
18	m	111/124 (90%)	110 (99%)	1 (1%)	70	81
19	M1	200/215 (93%)	199 (100%)	1 (0%)	81	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	M2	200/215 (93%)	199 (100%)	1 (0%)	81	85
20	N	123/137 (90%)	121 (98%)	2 (2%)	55	75
20	n	123/137 (90%)	121 (98%)	2 (2%)	55	75
21	O	82/86 (95%)	82 (100%)	0	100	100
21	o	82/86 (95%)	82 (100%)	0	100	100
22	O1	56/89 (63%)	56 (100%)	0	100	100
22	O2	56/89 (63%)	56 (100%)	0	100	100
22	P1	56/89 (63%)	56 (100%)	0	100	100
22	P2	56/89 (63%)	56 (100%)	0	100	100
22	Q1	56/89 (63%)	56 (100%)	0	100	100
22	Q2	56/89 (63%)	56 (100%)	0	100	100
22	R1	56/89 (63%)	56 (100%)	0	100	100
22	R2	56/89 (63%)	56 (100%)	0	100	100
22	S1	56/89 (63%)	56 (100%)	0	100	100
22	S2	56/89 (63%)	56 (100%)	0	100	100
22	T1	56/89 (63%)	56 (100%)	0	100	100
22	T2	56/89 (63%)	56 (100%)	0	100	100
22	U1	56/89 (63%)	56 (100%)	0	100	100
22	U2	56/89 (63%)	56 (100%)	0	100	100
22	V1	56/89 (63%)	56 (100%)	0	100	100
22	V2	56/89 (63%)	56 (100%)	0	100	100
22	W1	56/89 (63%)	56 (100%)	0	100	100
22	W2	56/89 (63%)	56 (100%)	0	100	100
22	X1	56/89 (63%)	54 (96%)	2 (4%)	31	63
22	X2	56/89 (63%)	54 (96%)	2 (4%)	31	63
23	P	75/94 (80%)	75 (100%)	0	100	100
23	p	75/94 (80%)	75 (100%)	0	100	100
24	Q	80/92 (87%)	80 (100%)	0	100	100
24	q	80/92 (87%)	80 (100%)	0	100	100
25	R	56/56 (100%)	56 (100%)	0	100	100
25	r	56/56 (100%)	56 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	12866/14484 (89%)	12838 (100%)	28 (0%)	85 89

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	N	105	GLU
20	n	132	GLU
22	X1	107	PHE
7	f	42	ASN
22	X1	104	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
15	K2	82	GLN
7	f	34	GLN
19	M1	112	ASN
23	P	95	GLN
20	n	144	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	AME	e	1	6	9,10,11	0.29	0	9,11,13	0.43	0
6	AME	E	1	6	9,10,11	0.28	0	9,11,13	0.44	0

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
6	AME	e	1	6	-	3/9/10/12	-
6	AME	E	1	6	-	3/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	1	AME	N-CA-CB-CG
6	e	1	AME	N-CA-CB-CG
6	E	1	AME	C-CA-CB-CG
6	e	1	AME	C-CA-CB-CG
6	E	1	AME	CB-CA-N-CT1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 66 ligands modelled in this entry, 10 are monoatomic - leaving 56 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
28	CDL	E	403	-	99,99,99	0.29	0	105,111,111	0.26	0
28	CDL	M	201	-	99,99,99	0.30	0	105,111,111	0.29	0
32	PEE	r	101	-	50,50,50	0.75	2 (4%)	53,55,55	0.53	0
28	CDL	e	405	-	99,99,99	0.29	0	105,111,111	0.26	0
28	CDL	C	201	-	99,99,99	0.29	0	105,111,111	0.26	0
28	CDL	j	202	-	99,99,99	0.29	0	105,111,111	0.26	0
28	CDL	l	101	-	99,99,99	0.29	0	105,111,111	0.26	0
33	PC1	I	201	-	53,53,53	0.28	0	59,61,61	0.29	0
28	CDL	f	201	-	99,99,99	0.29	0	105,111,111	0.27	0
29	ADP	D1	601	27	28,29,29	0.40	0	43,45,45	0.48	0
28	CDL	e	401	-	99,99,99	0.29	0	105,111,111	0.26	0
30	LMT	E	401	-	36,36,36	0.15	0	47,47,47	0.47	1 (2%)
33	PC1	J	204	-	53,53,53	0.28	0	59,61,61	0.28	0
34	UTP	H2	201	-	29,30,30	0.29	0	43,47,47	0.32	0
28	CDL	Q	101	-	99,99,99	0.29	0	105,111,111	0.29	0
28	CDL	e	402	-	99,99,99	0.29	0	105,111,111	0.28	0
28	CDL	q	101	-	99,99,99	0.29	0	105,111,111	0.29	0
28	CDL	e	403	-	99,99,99	0.28	0	105,111,111	0.26	0
30	LMT	j	204	-	36,36,36	0.16	0	47,47,47	0.55	0
28	CDL	E	406	-	99,99,99	0.29	0	105,111,111	0.25	0
28	CDL	e	404	-	99,99,99	0.29	0	105,111,111	0.25	0
33	PC1	j	203	-	53,53,53	0.28	0	59,61,61	0.28	0
28	CDL	j	201	-	99,99,99	0.29	0	105,111,111	0.26	0
26	ATP	B2	601	27	32,33,33	0.27	0	48,52,52	0.28	0
32	PEE	f	202	-	50,50,50	0.78	2 (4%)	53,55,55	0.46	0
34	UTP	H1	201	-	29,30,30	0.29	0	43,47,47	0.32	0
31	Q7G	e	407	-	54,54,90	0.13	0	80,84,138	0.26	0
33	PC1	F	203	-	53,53,53	0.28	0	59,61,61	0.28	0
32	PEE	R	101	-	50,50,50	0.75	2 (4%)	53,55,55	0.52	0
28	CDL	J	203	-	99,99,99	0.29	0	105,111,111	0.26	0
33	PC1	i	201	-	53,53,53	0.28	0	59,61,61	0.29	0
32	PEE	F	202	-	50,50,50	0.78	2 (4%)	53,55,55	0.46	0
26	ATP	A1	601	27	32,33,33	0.27	0	48,52,52	0.28	0
28	CDL	F	201	-	99,99,99	0.29	0	105,111,111	0.27	0
33	PC1	f	203	-	53,53,53	0.28	0	59,61,61	0.28	0
28	CDL	m	201	-	99,99,99	0.30	0	105,111,111	0.29	0
28	CDL	E	404	-	99,99,99	0.29	0	105,111,111	0.28	0
28	CDL	E	407	-	99,99,99	0.29	0	105,111,111	0.26	0
28	CDL	L	101	-	99,99,99	0.29	0	105,111,111	0.25	0
30	LMT	e	406	-	36,36,36	0.14	0	47,47,47	0.47	1 (2%)
31	Q7G	E	402	-	54,54,90	0.13	0	80,84,138	0.26	0
30	LMT	J	201	-	36,36,36	0.16	0	47,47,47	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	Q7G	n	201	-	66,66,90	0.14	0	98,102,138	0.31	0
26	ATP	C2	601	27	32,33,33	0.27	0	48,52,52	0.28	0
33	PC1	F	204	-	53,53,53	0.27	0	59,61,61	0.28	0
26	ATP	F1	601	27	32,33,33	0.27	0	48,52,52	0.27	0
28	CDL	J	202	-	99,99,99	0.29	0	105,111,111	0.26	0
31	Q7G	N	201	-	66,66,90	0.13	0	98,102,138	0.31	0
26	ATP	C1	601	27	32,33,33	0.27	0	48,52,52	0.28	0
33	PC1	f	204	-	53,53,53	0.27	0	59,61,61	0.28	0
26	ATP	A2	601	27	32,33,33	0.27	0	48,52,52	0.28	0
26	ATP	B1	601	27	32,33,33	0.27	0	48,52,52	0.28	0
26	ATP	F2	601	27	32,33,33	0.28	0	48,52,52	0.27	0
28	CDL	E	405	-	99,99,99	0.29	0	105,111,111	0.27	0
28	CDL	c	201	-	99,99,99	0.29	0	105,111,111	0.26	0
29	ADP	D2	601	27	28,29,29	0.40	0	43,45,45	0.48	0

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
28	CDL	E	403	-	-	23/110/110/110	-
28	CDL	M	201	-	-	41/110/110/110	-
32	PEE	r	101	-	-	28/54/54/54	-
28	CDL	e	405	-	-	34/110/110/110	-
28	CDL	C	201	-	-	24/110/110/110	-
28	CDL	j	202	-	-	29/110/110/110	-
28	CDL	l	101	-	-	24/110/110/110	-
33	PC1	I	201	-	-	10/57/57/57	-
28	CDL	f	201	-	-	21/110/110/110	-
29	ADP	D1	601	27	-	1/16/32/32	0/3/3/3
28	CDL	e	401	-	-	23/110/110/110	-
30	LMT	E	401	-	-	1/21/61/61	0/2/2/2
33	PC1	J	204	-	-	12/57/57/57	-
34	UTP	H2	201	-	-	4/22/38/38	0/2/2/2
28	CDL	Q	101	-	-	26/110/110/110	-
28	CDL	e	402	-	-	30/110/110/110	-
28	CDL	q	101	-	-	26/110/110/110	-
28	CDL	e	403	-	-	29/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMT	j	204	-	-	5/21/61/61	0/2/2/2
28	CDL	E	406	-	-	19/110/110/110	-
28	CDL	e	404	-	-	19/110/110/110	-
33	PC1	j	203	-	-	12/57/57/57	-
28	CDL	j	201	-	-	24/110/110/110	-
26	ATP	B2	601	27	-	4/22/38/38	0/3/3/3
32	PEE	f	202	-	-	16/54/54/54	-
34	UTP	H1	201	-	-	4/22/38/38	0/2/2/2
31	Q7G	e	407	-	1/1/19/34	5/15/123/200	0/7/7/10
33	PC1	F	203	-	-	10/57/57/57	-
32	PEE	R	101	-	-	28/54/54/54	-
28	CDL	J	203	-	-	29/110/110/110	-
33	PC1	i	201	-	-	10/57/57/57	-
32	PEE	F	202	-	-	16/54/54/54	-
26	ATP	A1	601	27	-	6/22/38/38	0/3/3/3
28	CDL	F	201	-	-	21/110/110/110	-
33	PC1	f	203	-	-	10/57/57/57	-
28	CDL	m	201	-	-	41/110/110/110	-
31	Q7G	E	402	-	1/1/19/34	5/15/123/200	0/7/7/10
28	CDL	E	404	-	-	30/110/110/110	-
28	CDL	E	407	-	-	35/110/110/110	-
28	CDL	L	101	-	-	24/110/110/110	-
30	LMT	e	406	-	-	1/21/61/61	0/2/2/2
30	LMT	J	201	-	-	5/21/61/61	0/2/2/2
31	Q7G	n	201	-	2/2/24/34	6/20/148/200	0/8/8/10
26	ATP	C2	601	27	-	6/22/38/38	0/3/3/3
33	PC1	F	204	-	-	10/57/57/57	-
26	ATP	F1	601	27	-	5/22/38/38	0/3/3/3
31	Q7G	N	201	-	2/2/24/34	6/20/148/200	0/8/8/10
28	CDL	J	202	-	-	24/110/110/110	-
26	ATP	C1	601	27	-	6/22/38/38	0/3/3/3
33	PC1	f	204	-	-	10/57/57/57	-
26	ATP	A2	601	27	-	6/22/38/38	0/3/3/3
26	ATP	B1	601	27	-	4/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	ATP	F2	601	27	-	5/22/38/38	0/3/3/3
28	CDL	E	405	-	-	29/110/110/110	-
28	CDL	c	201	-	-	24/110/110/110	-
29	ADP	D2	601	27	-	1/16/32/32	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	f	202	PEE	C39-C38	3.66	1.52	1.31
32	F	202	PEE	C39-C38	3.64	1.52	1.31
32	f	202	PEE	C18-C19	3.60	1.52	1.31
32	F	202	PEE	C18-C19	3.60	1.52	1.31
32	r	101	PEE	C18-C19	3.55	1.51	1.31

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	e	406	LMT	C1'-O5'-C5'	-2.12	109.58	113.72
30	E	401	LMT	C1'-O5'-C5'	-2.10	109.61	113.72

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
31	E	402	Q7G	C1B
31	N	201	Q7G	C1B
31	N	201	Q7G	C1C
31	e	407	Q7G	C1B
31	n	201	Q7G	C1B

5 of 907 torsion outliers are listed below:

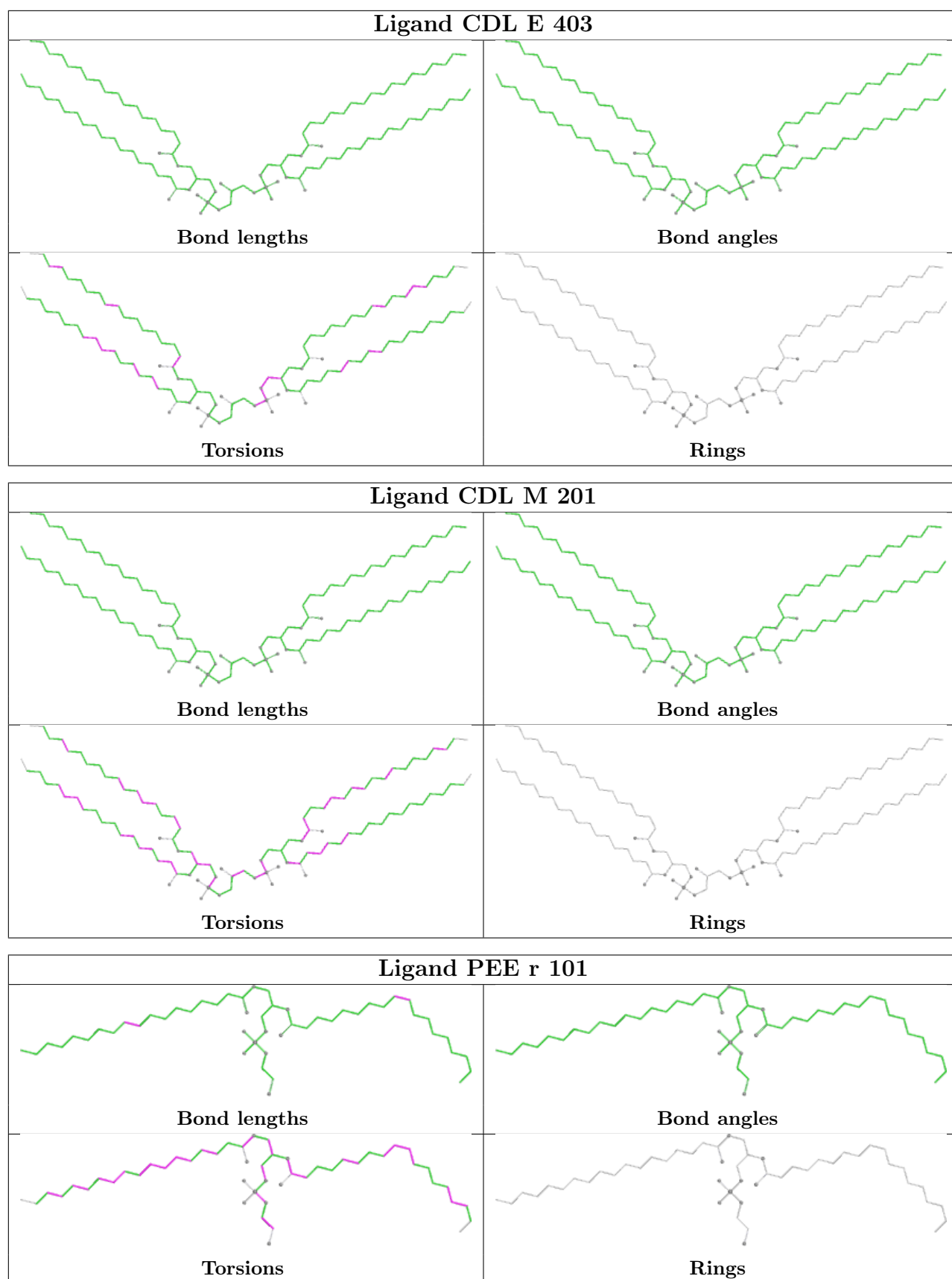
Mol	Chain	Res	Type	Atoms
26	A1	601	ATP	PB-O3B-PG-O2G
26	A2	601	ATP	PB-O3B-PG-O2G
26	B1	601	ATP	PB-O3B-PG-O3G
26	B2	601	ATP	PB-O3B-PG-O3G
26	C1	601	ATP	PB-O3B-PG-O2G

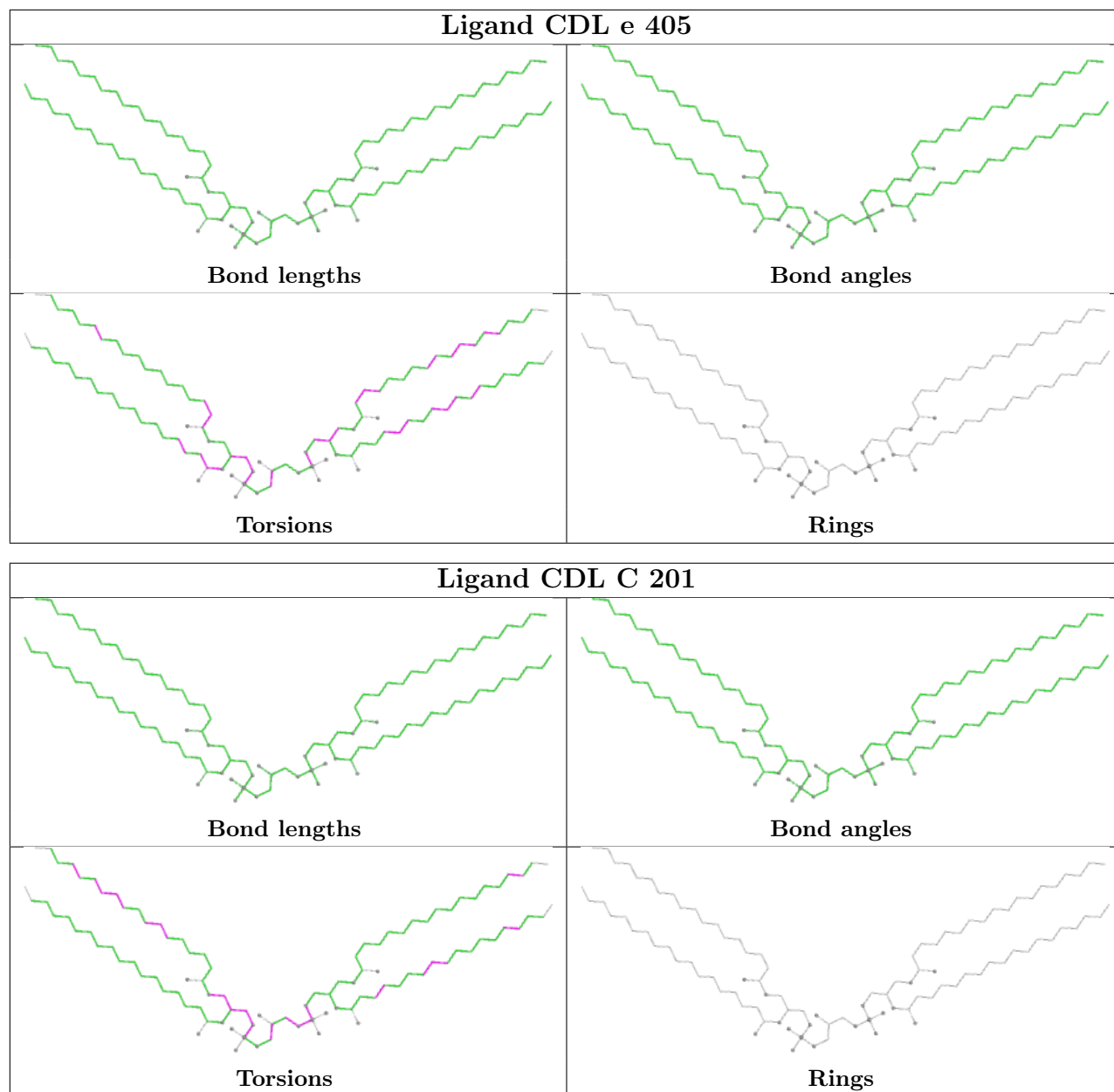
There are no ring outliers.

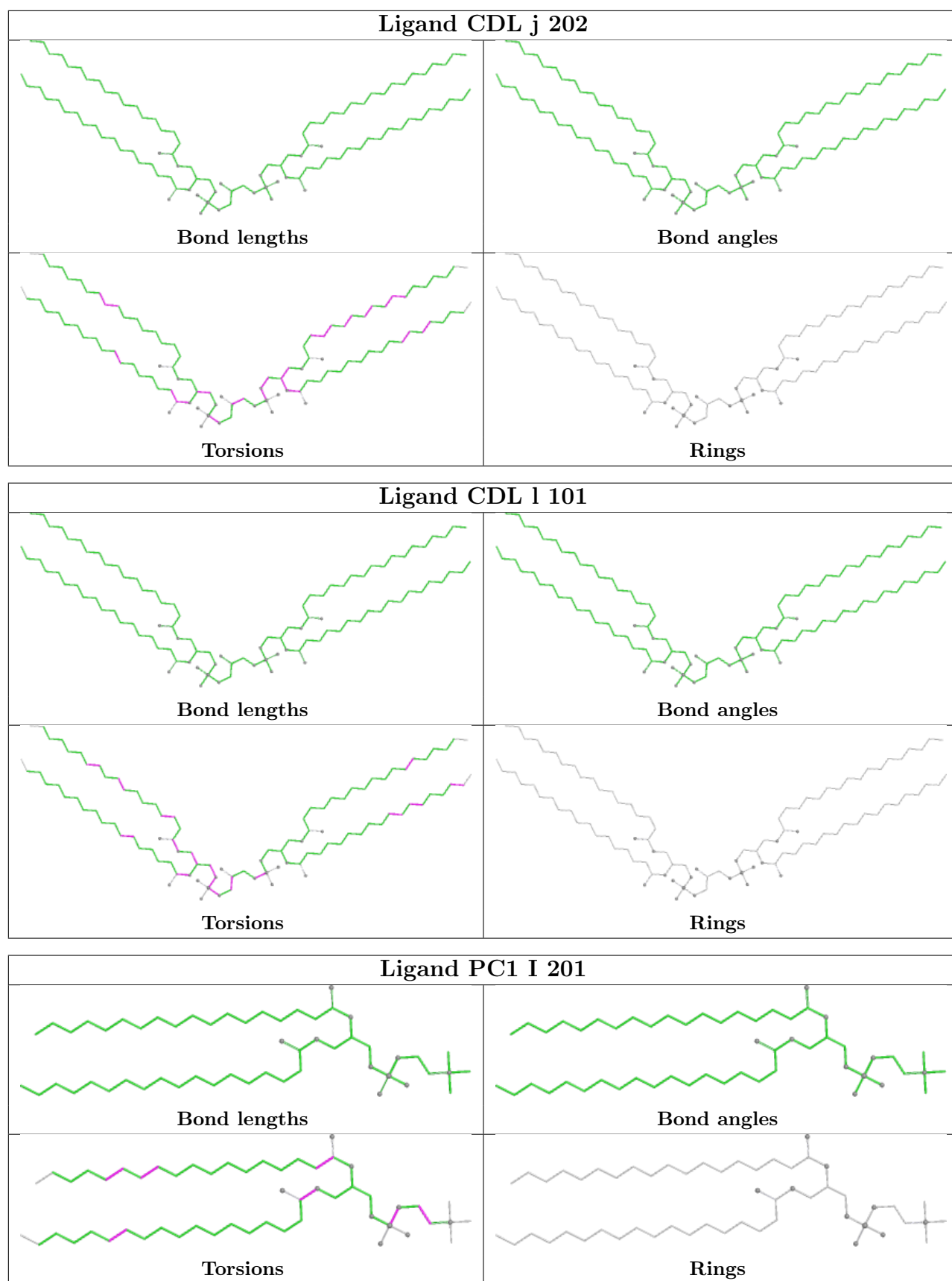
16 monomers are involved in 19 short contacts:

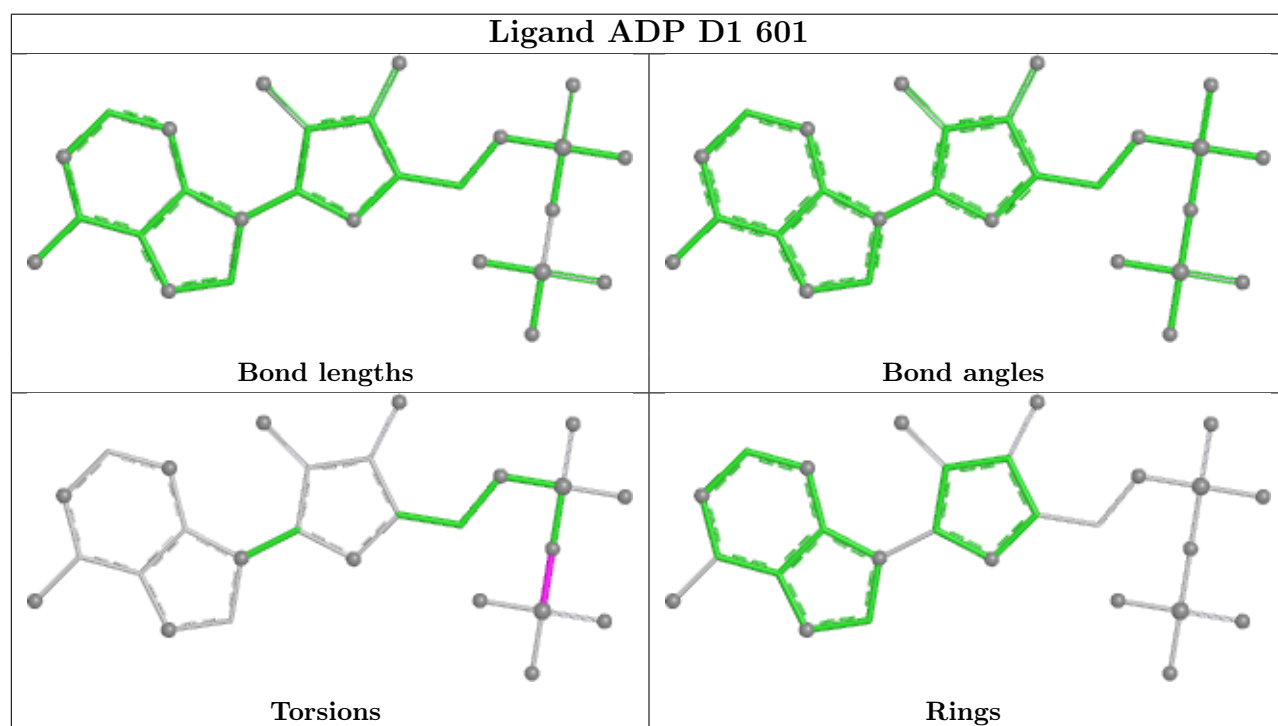
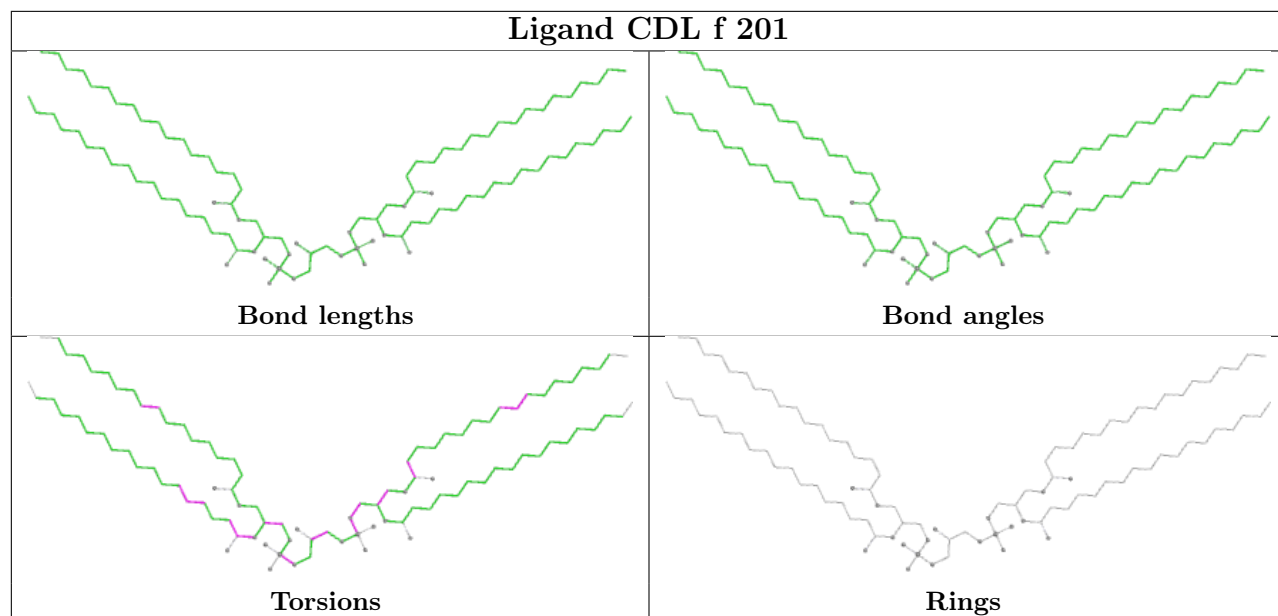
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	M	201	CDL	1	0
32	r	101	PEE	1	0
28	C	201	CDL	1	0
28	j	202	CDL	1	0
34	H2	201	UTP	2	0
28	Q	101	CDL	1	0
28	e	402	CDL	3	0
28	e	403	CDL	2	0
26	B2	601	ATP	1	0
34	H1	201	UTP	2	0
28	J	203	CDL	1	0
28	E	404	CDL	3	0
33	F	204	PC1	1	0
33	f	204	PC1	1	0
28	E	405	CDL	2	0
28	c	201	CDL	1	0

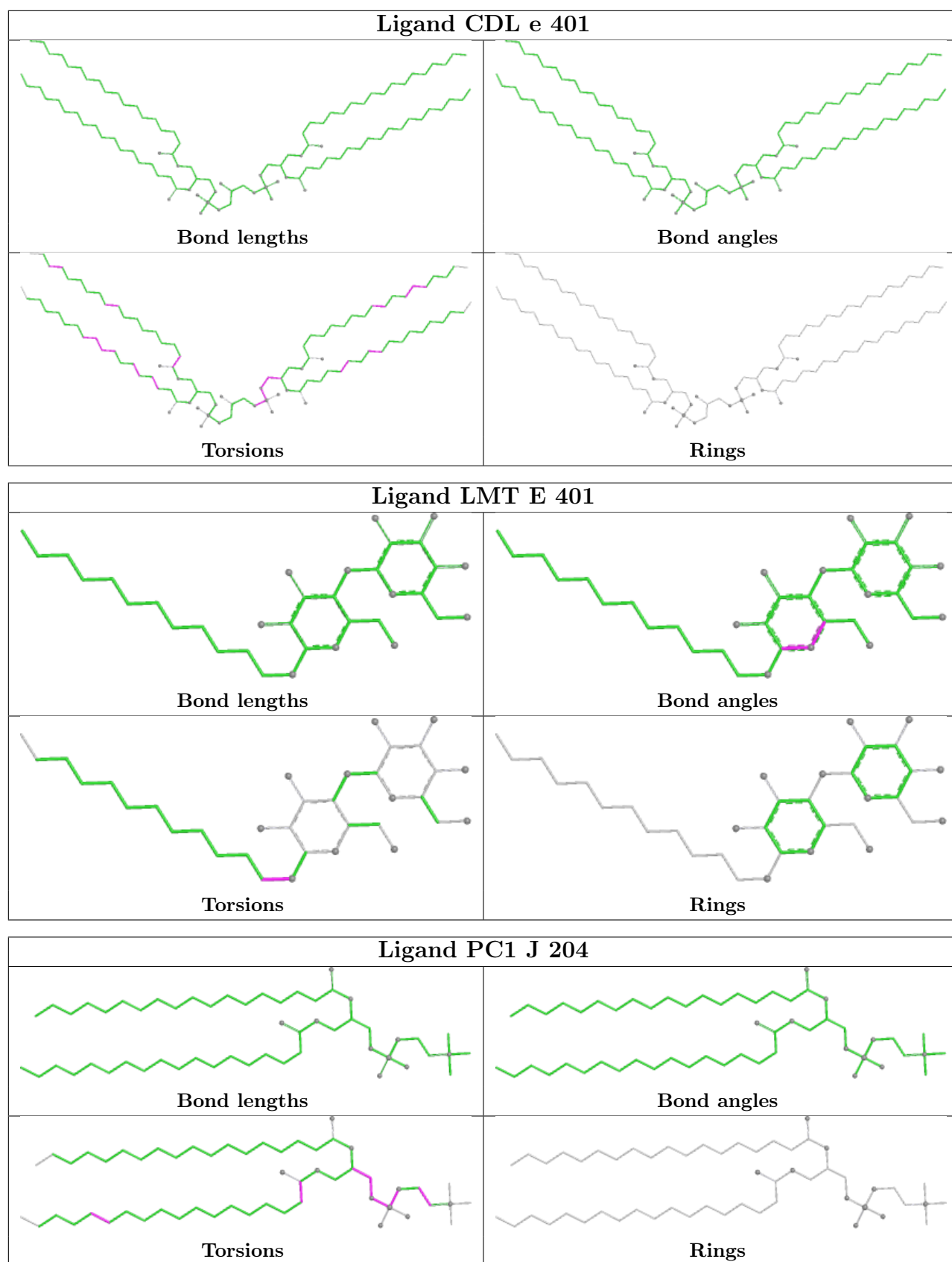
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

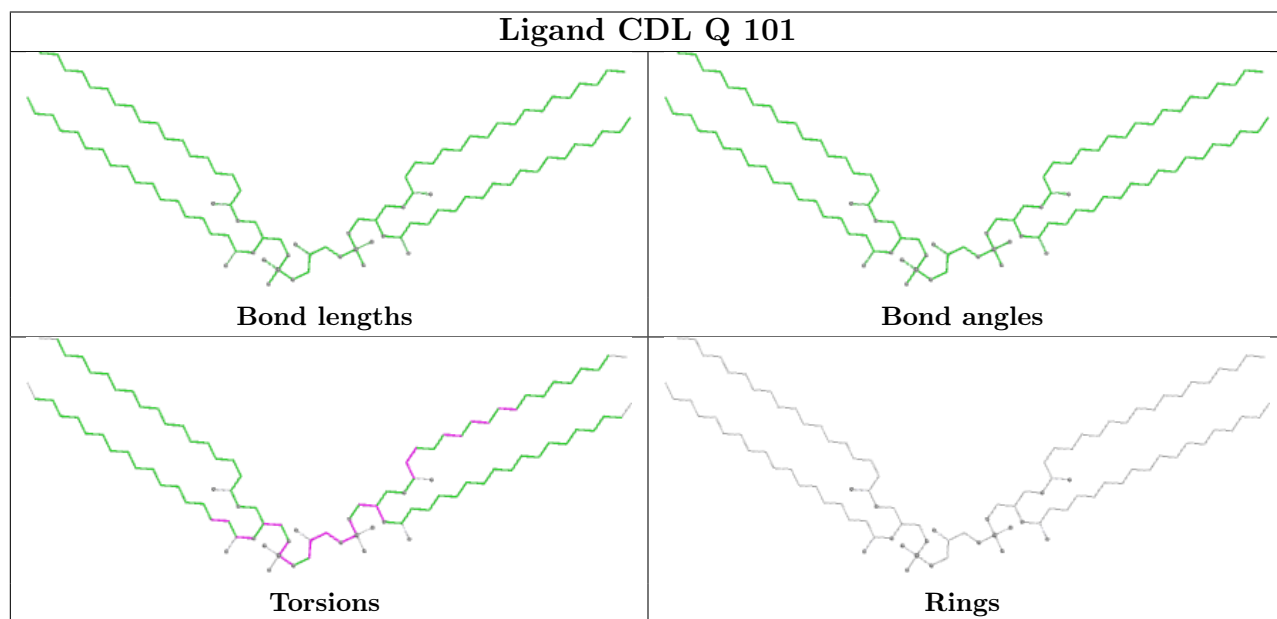
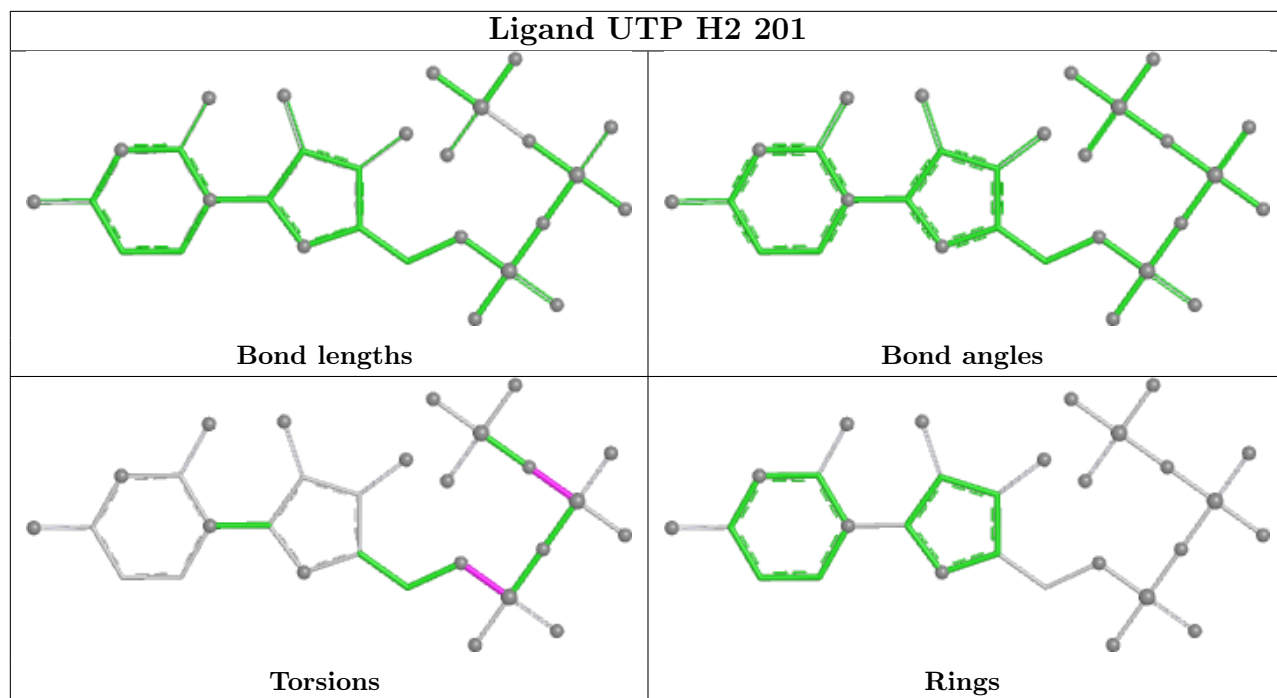


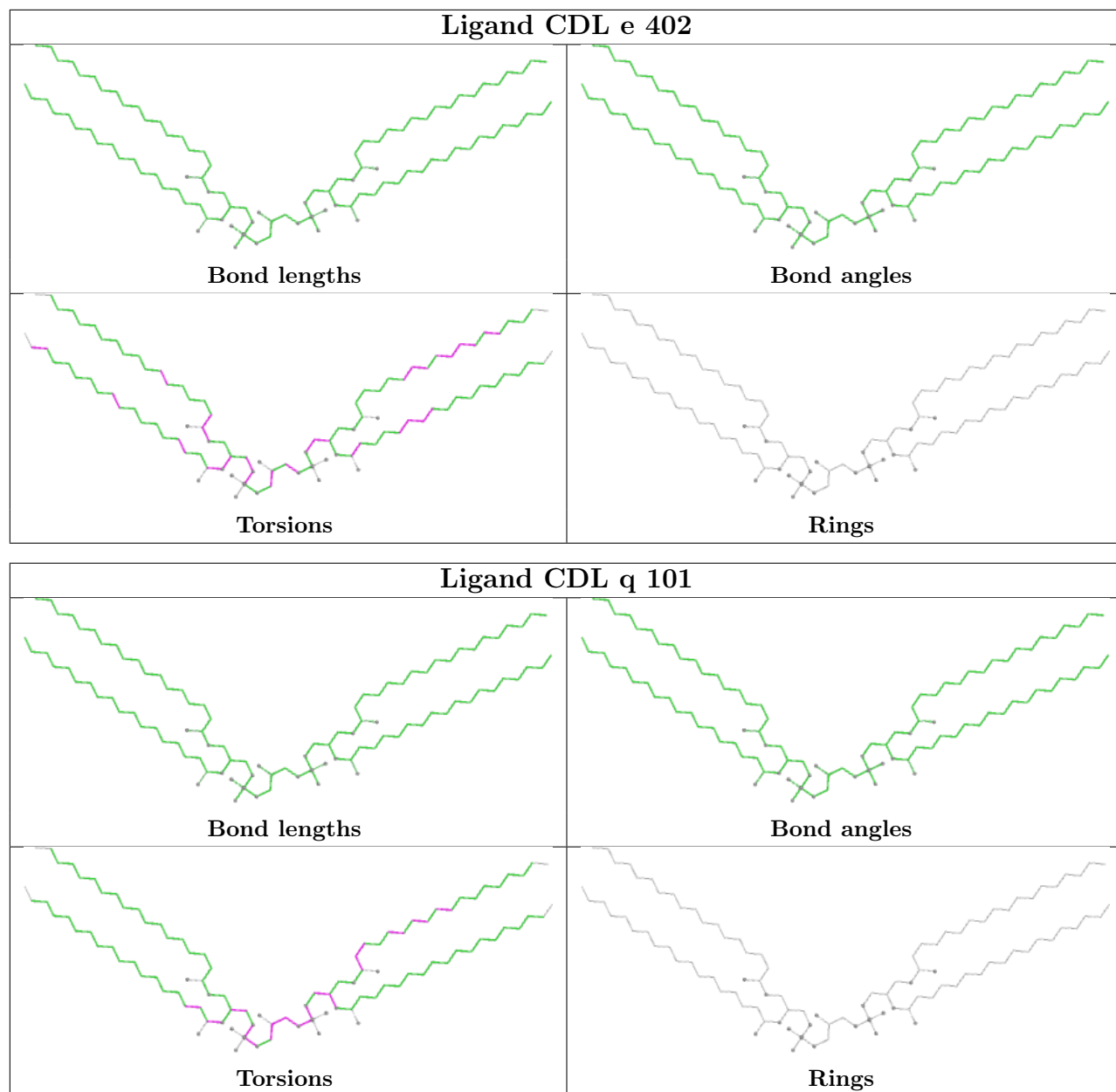


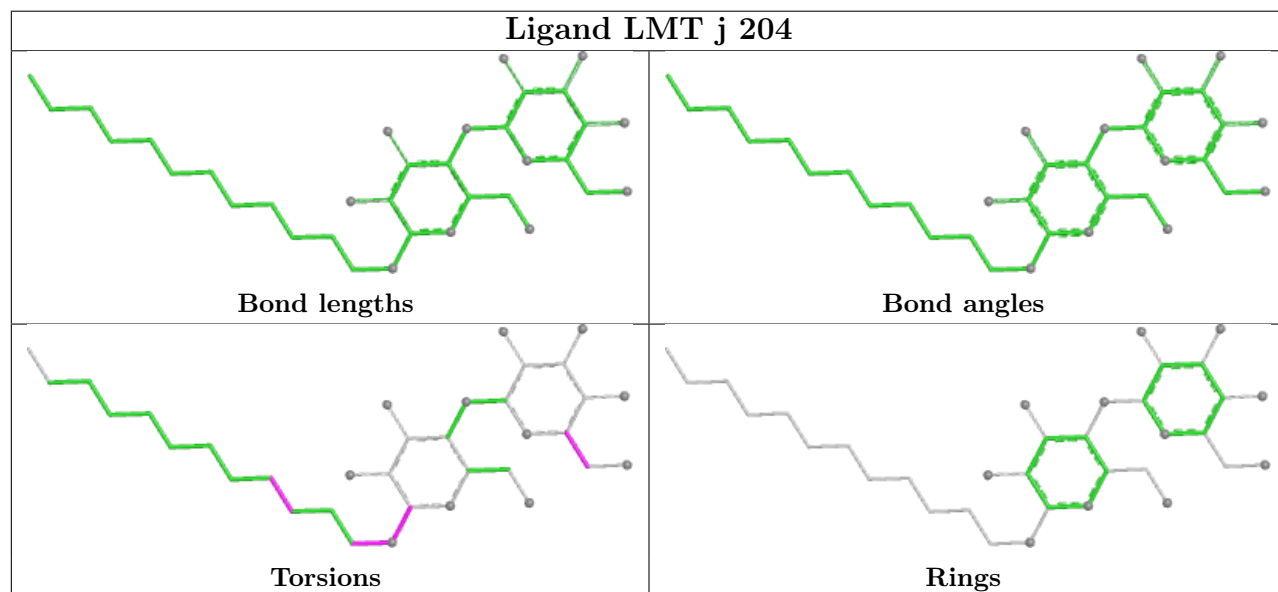
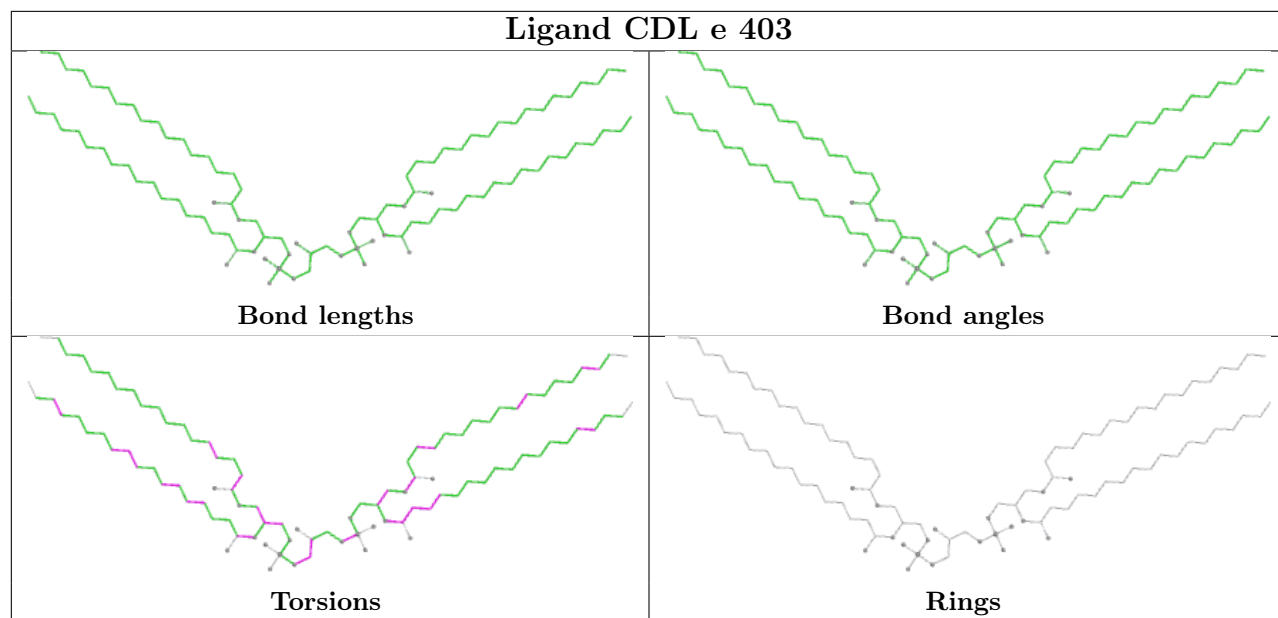


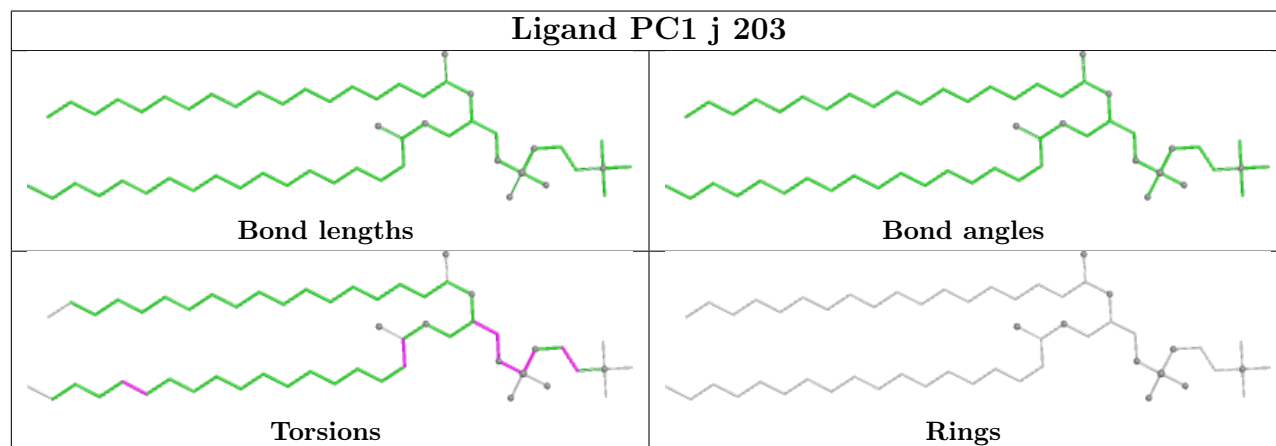
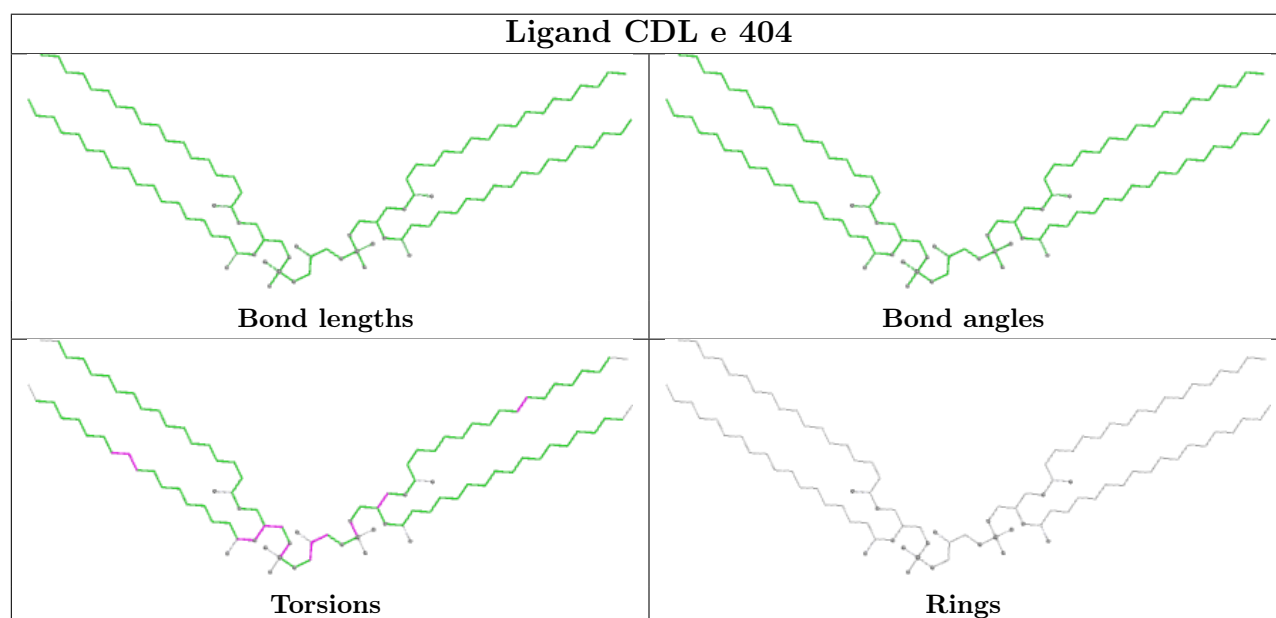
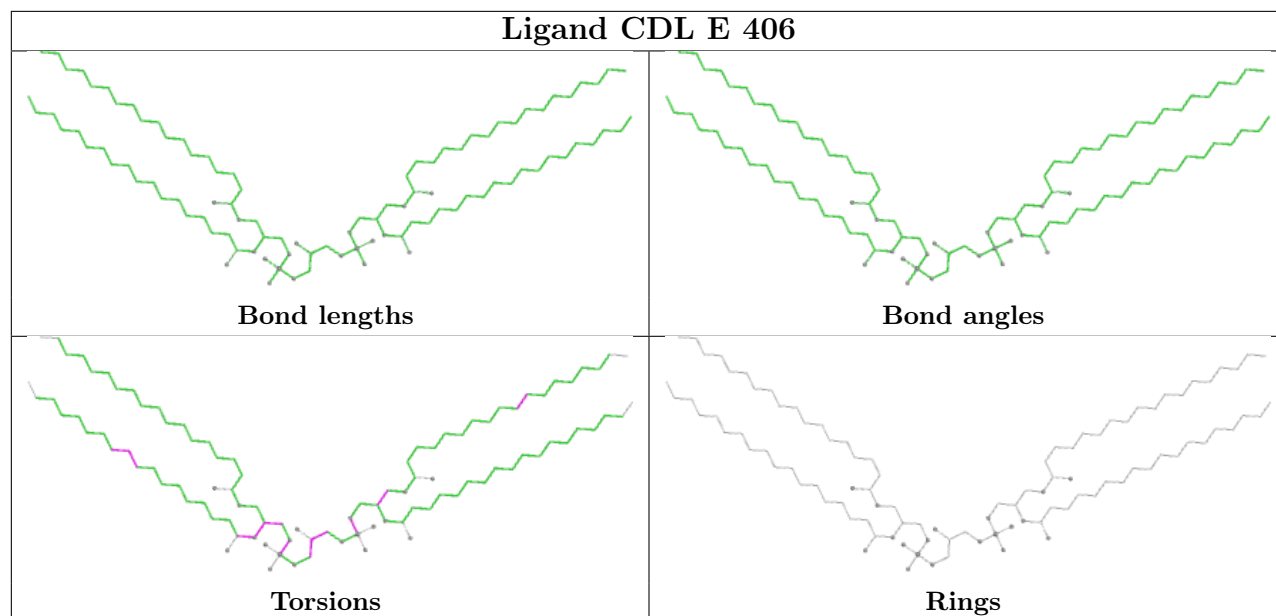


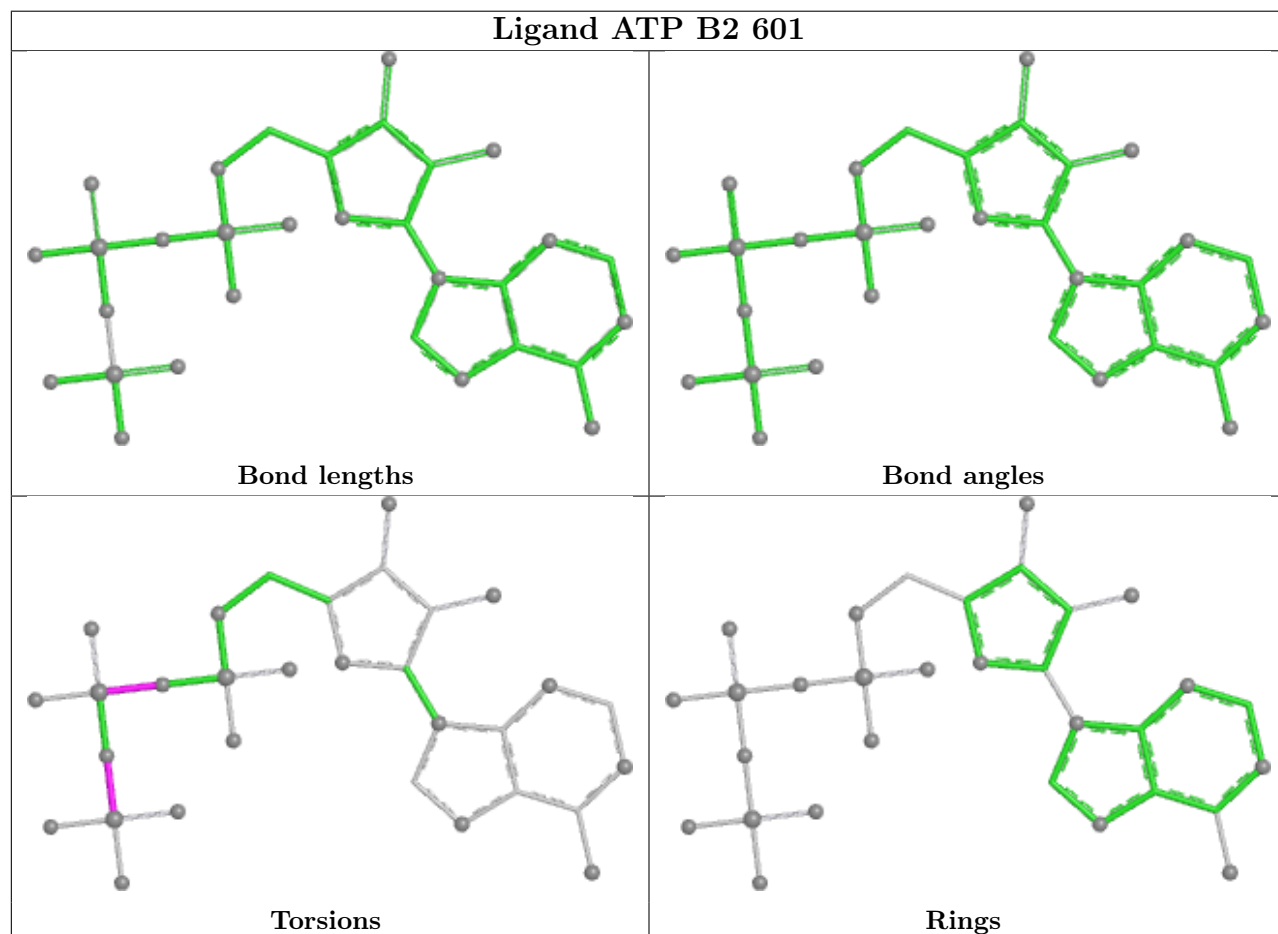
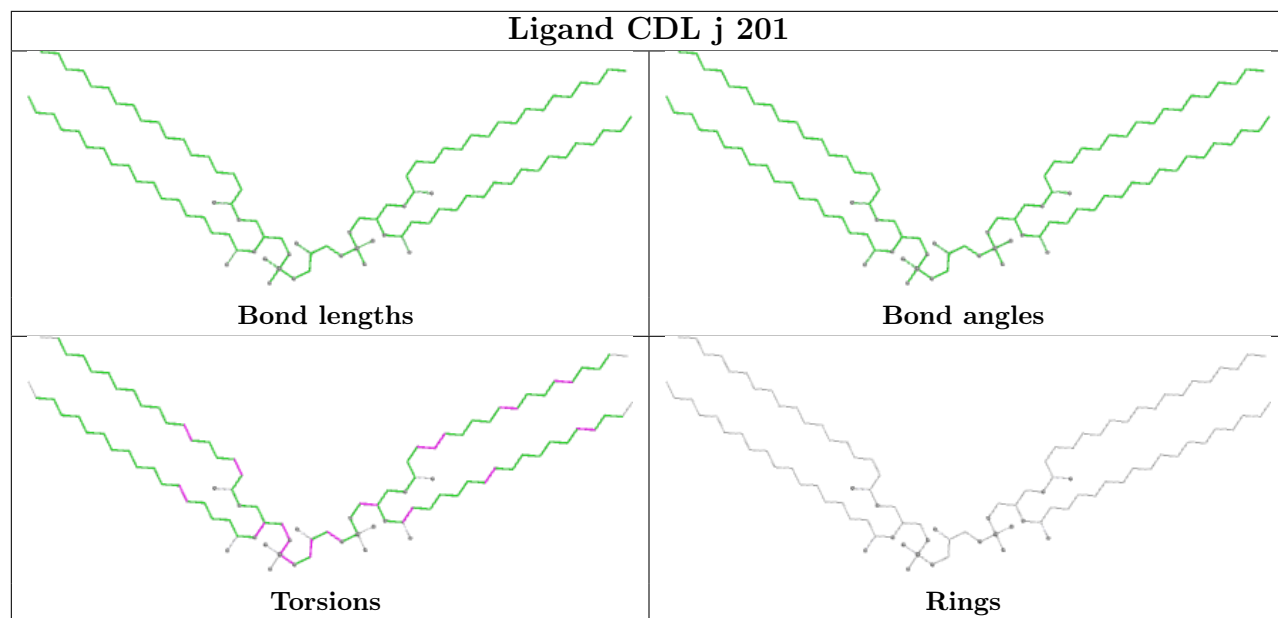


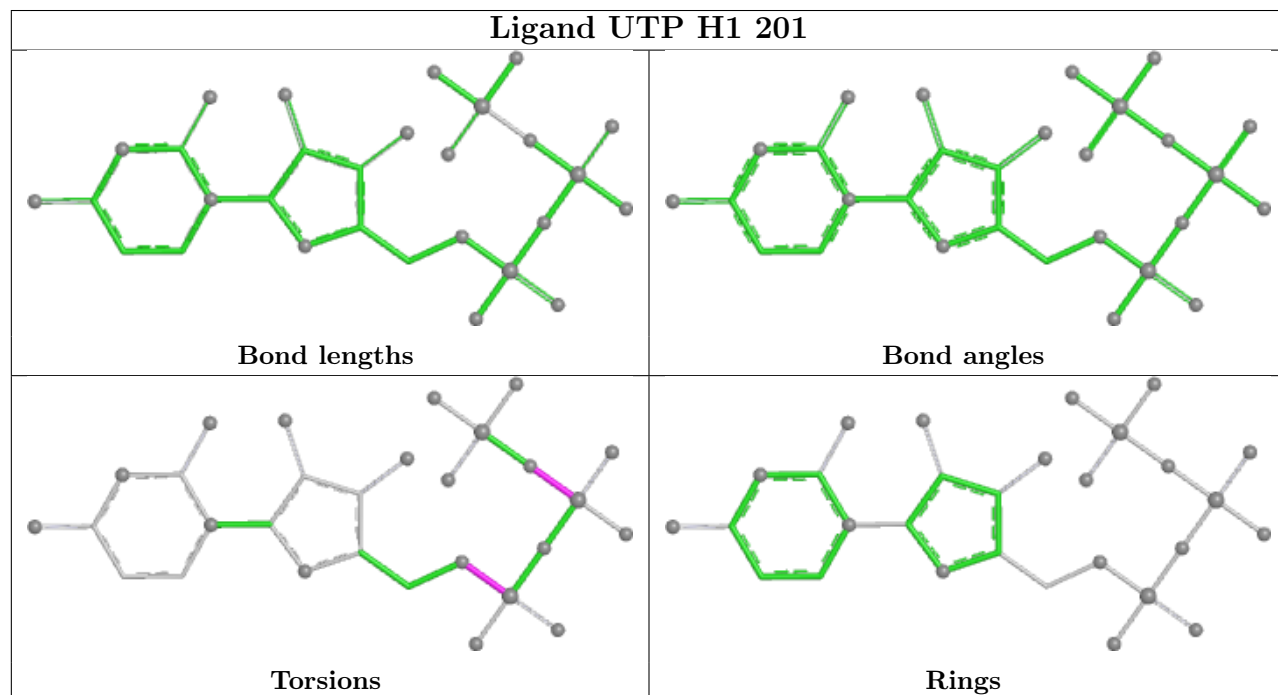
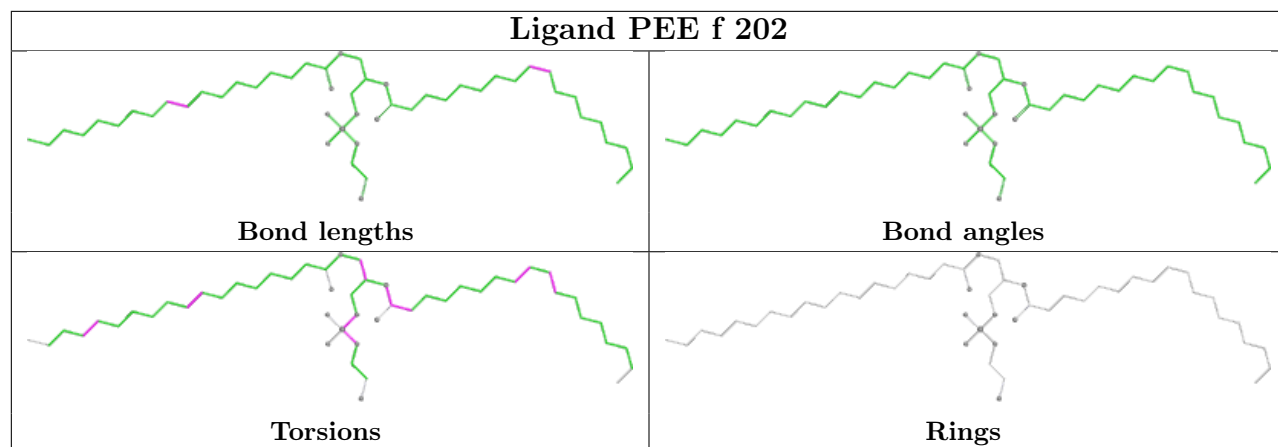


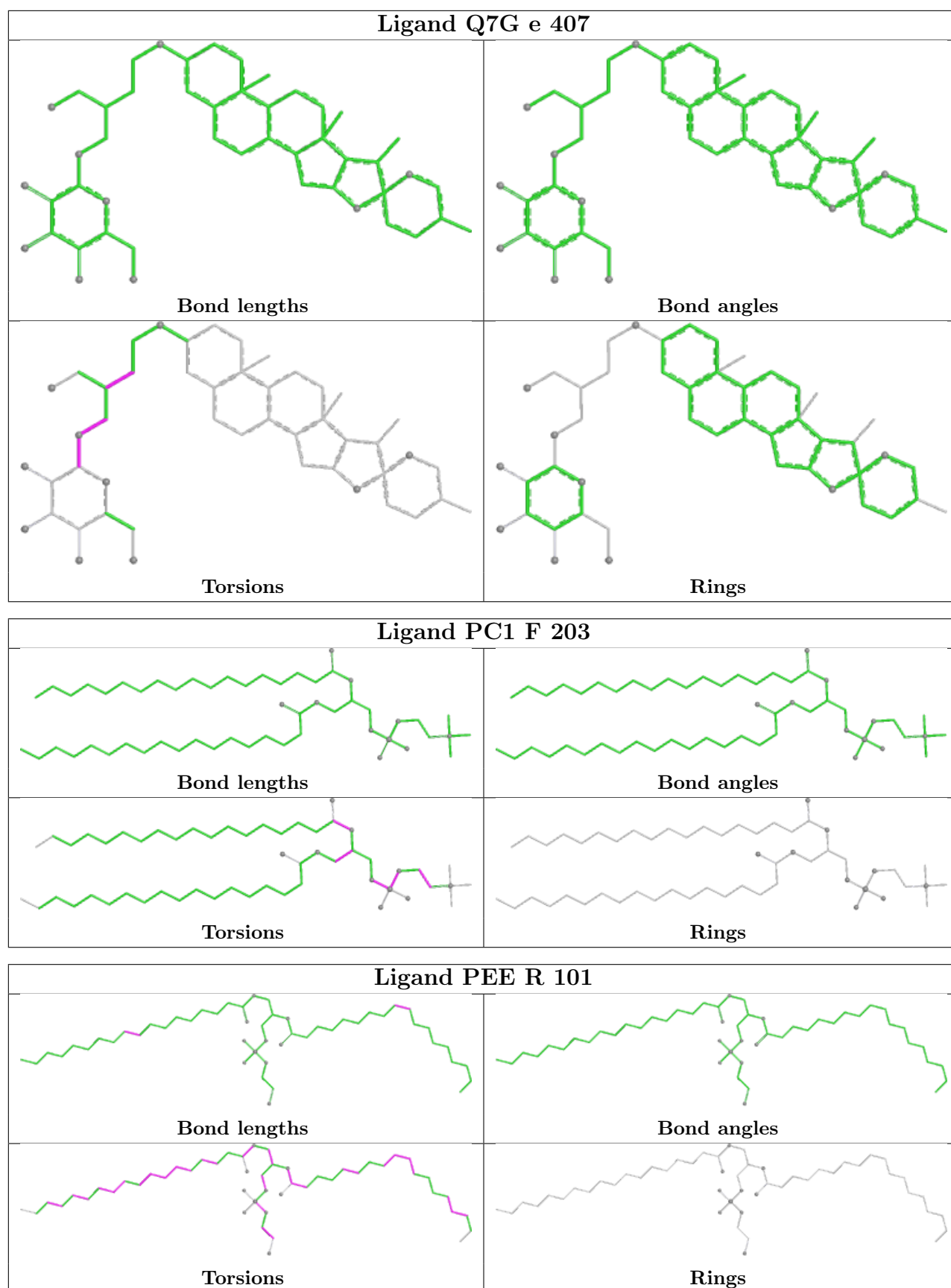


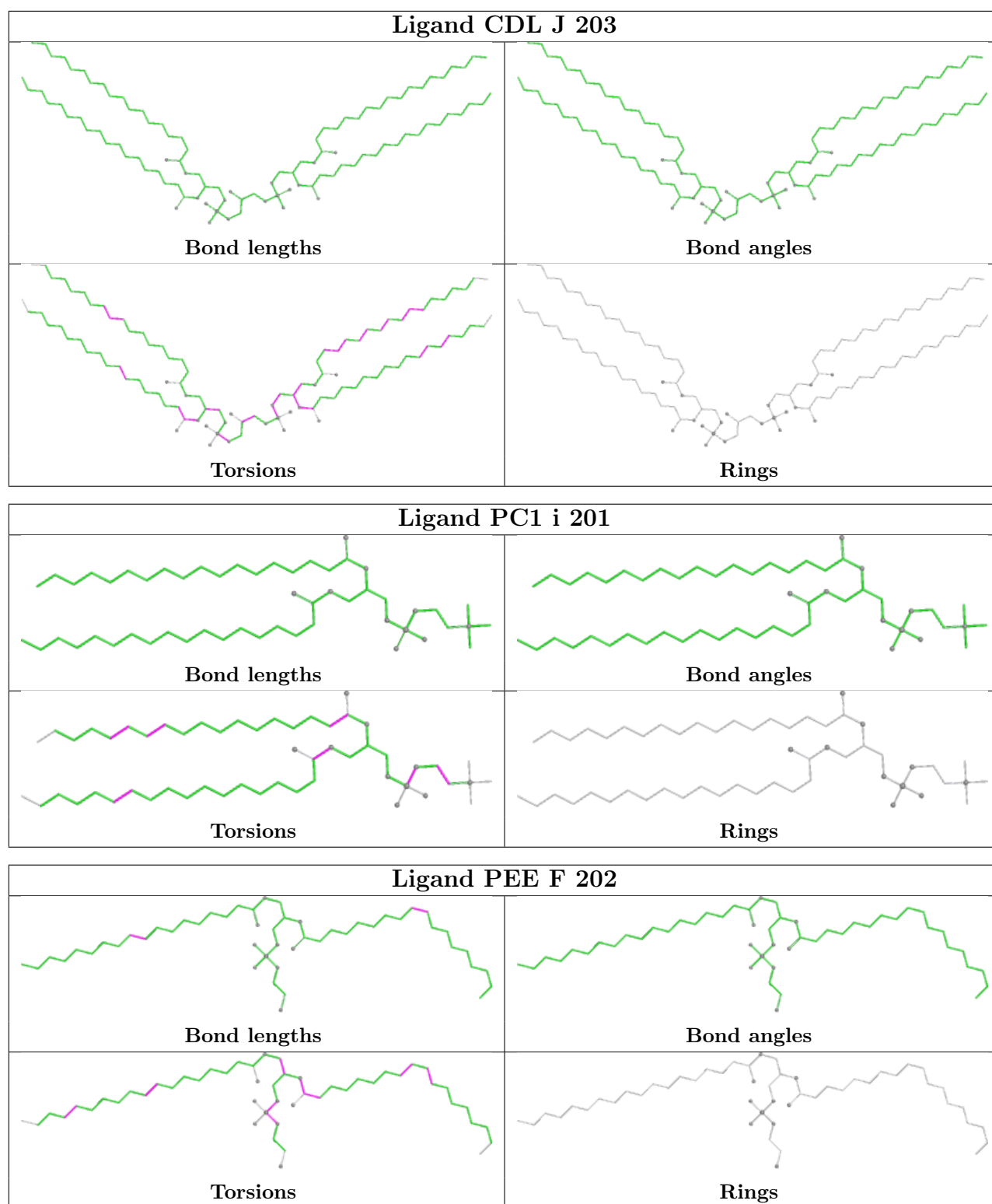


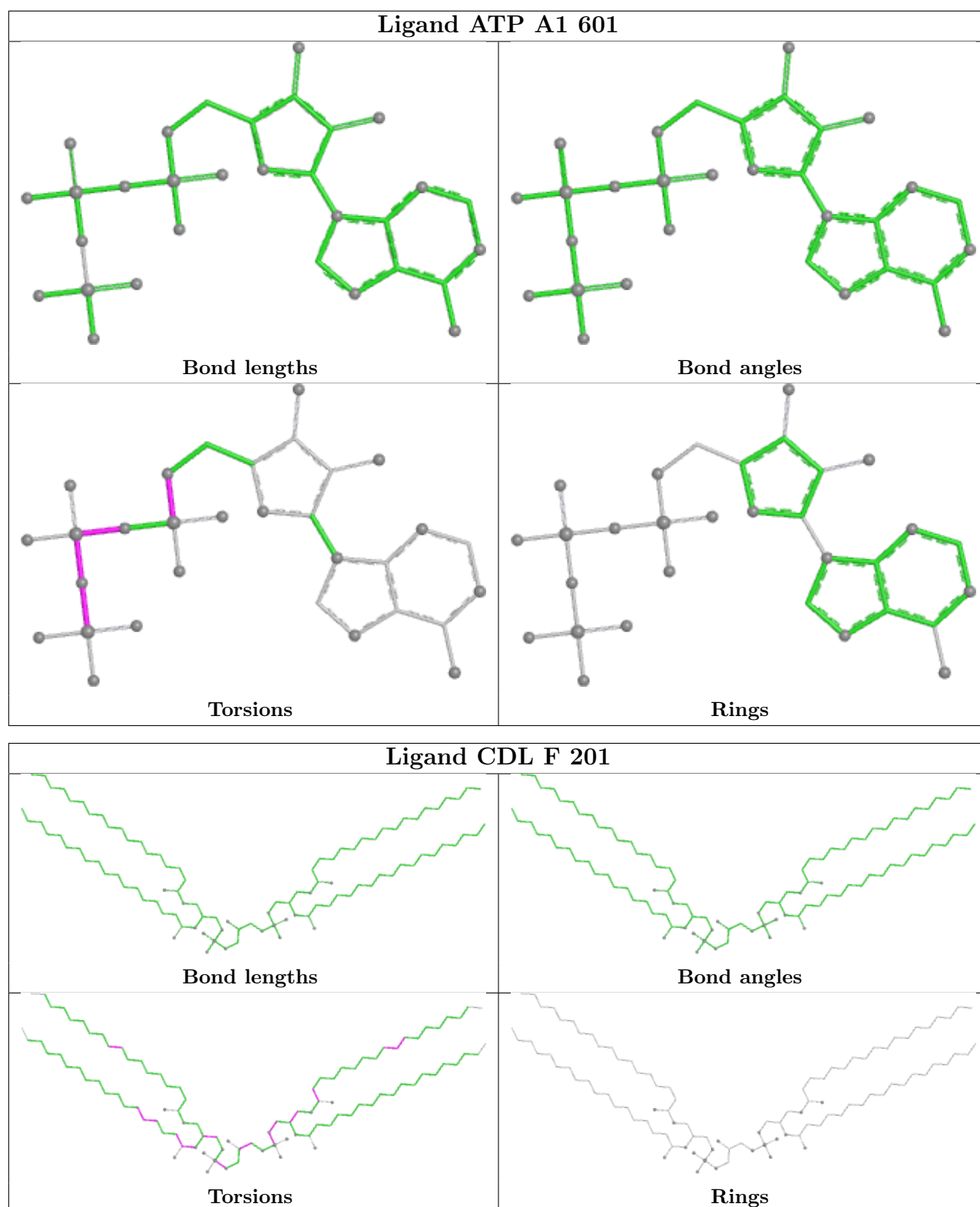


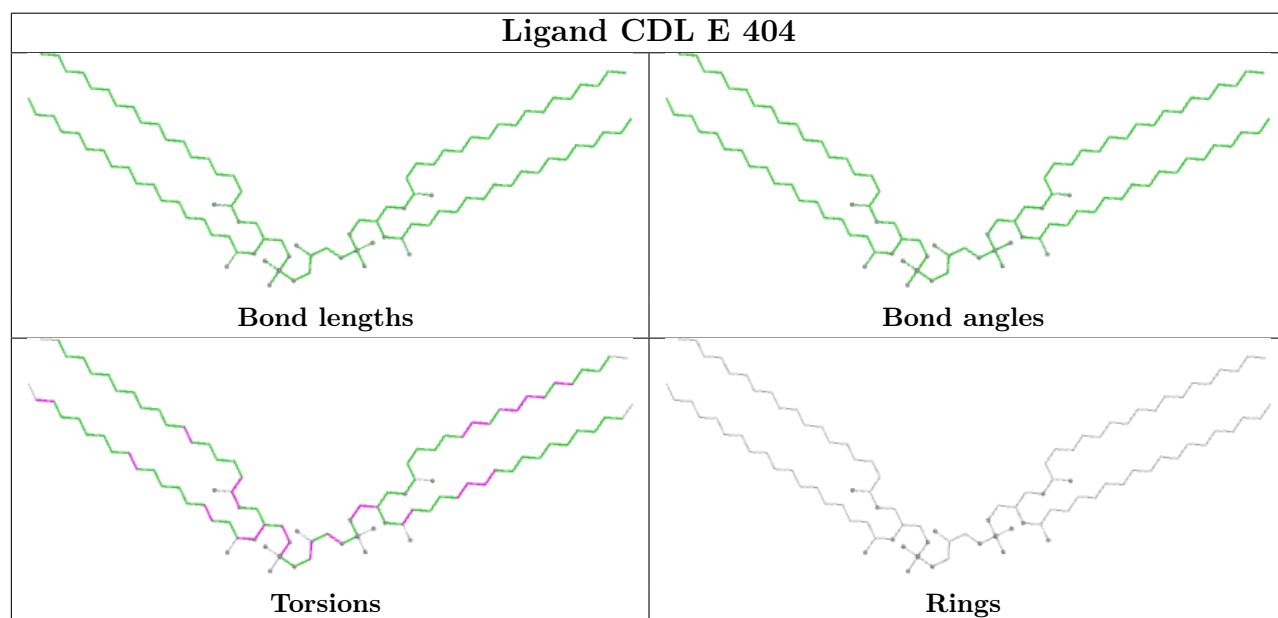
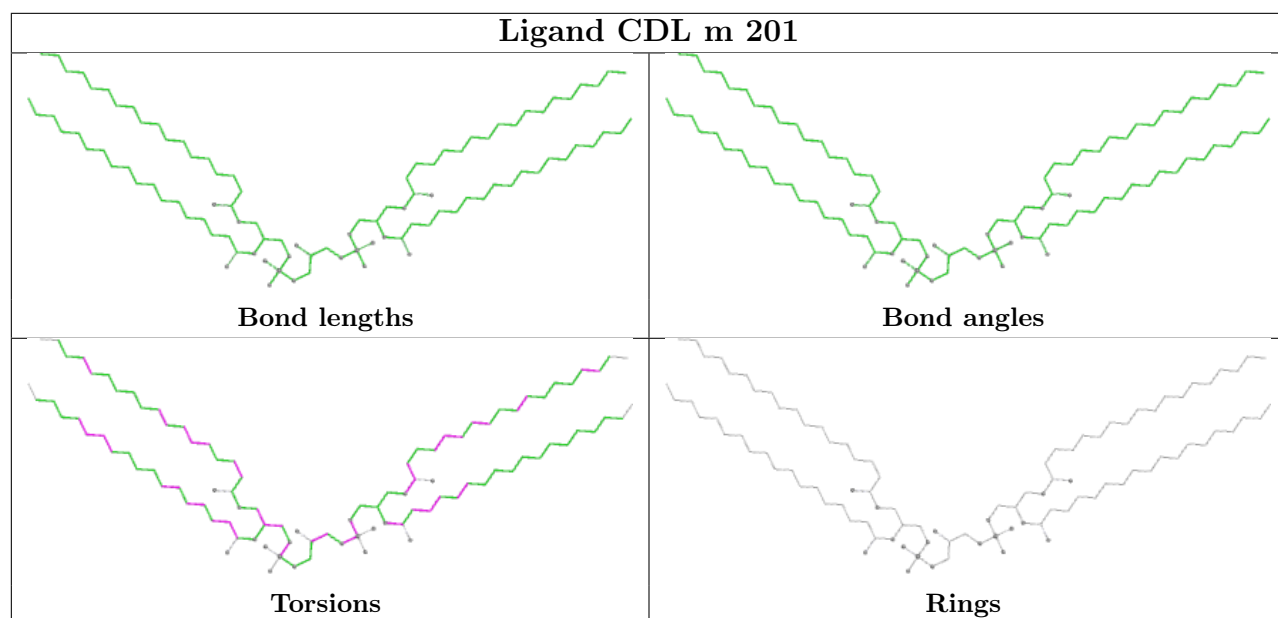
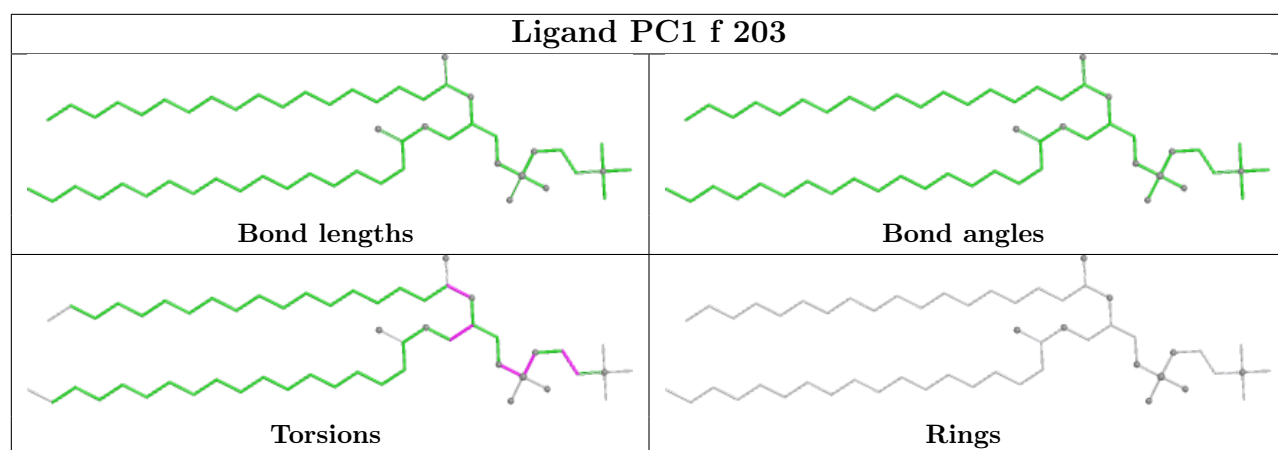


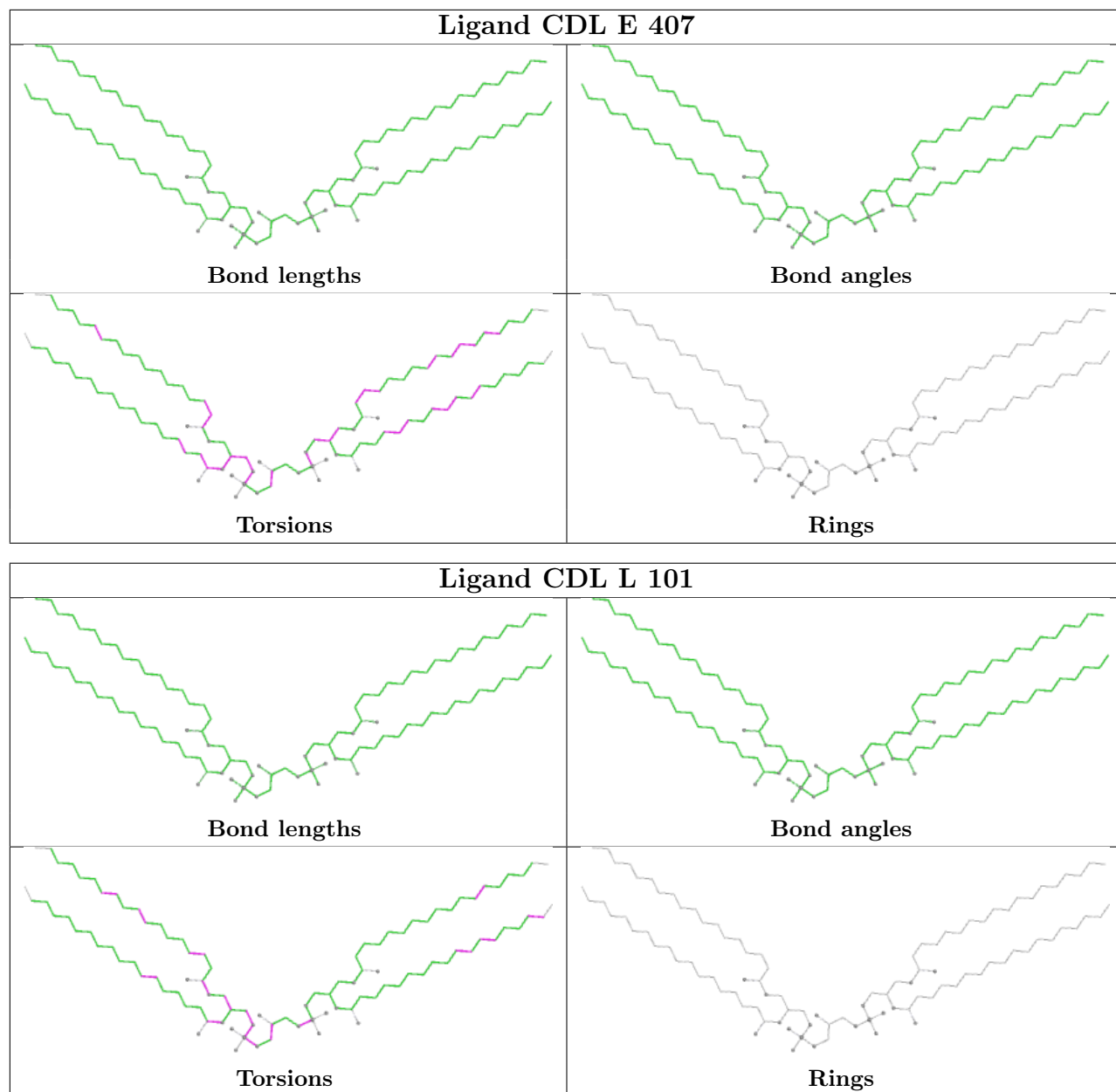


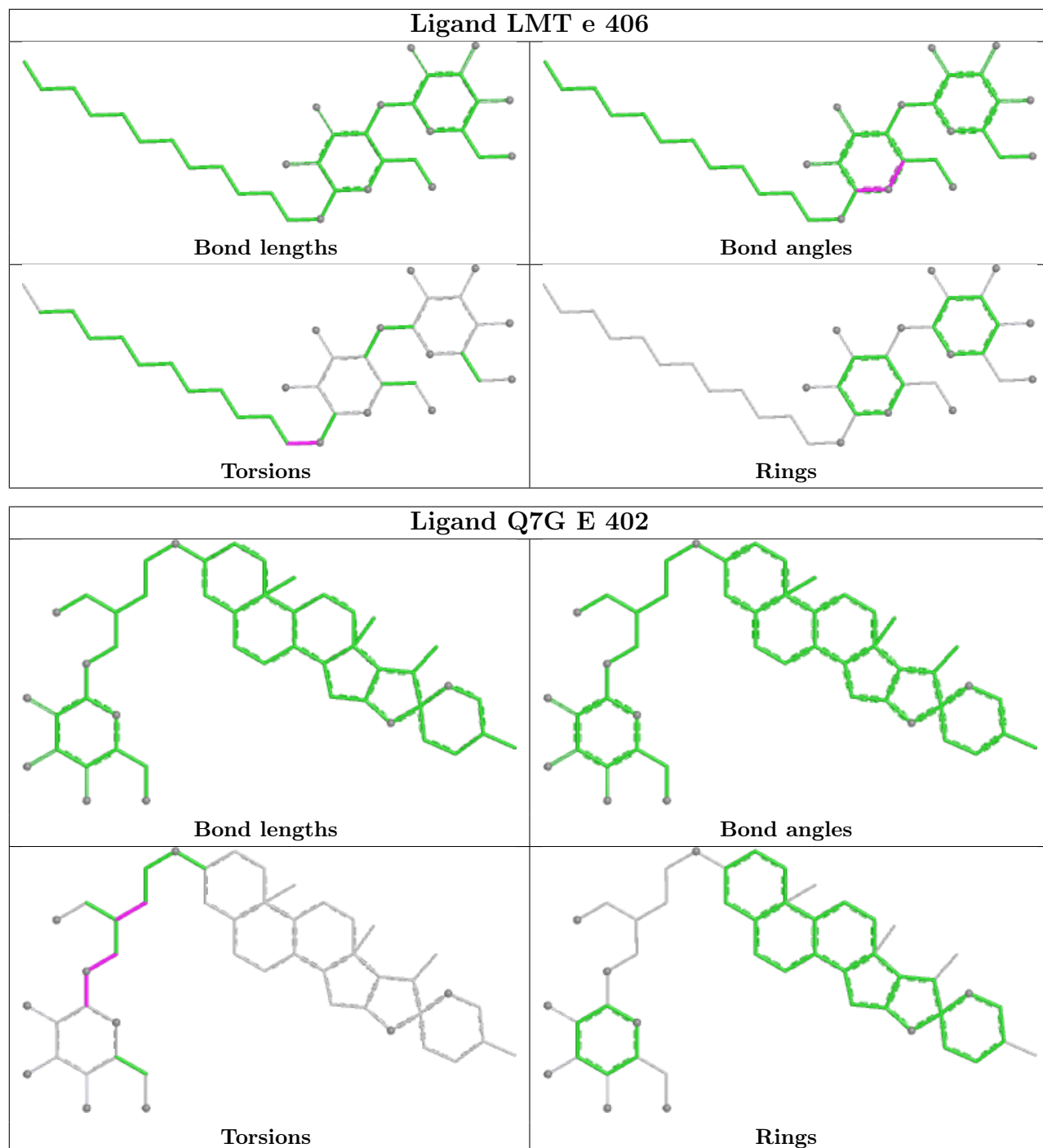


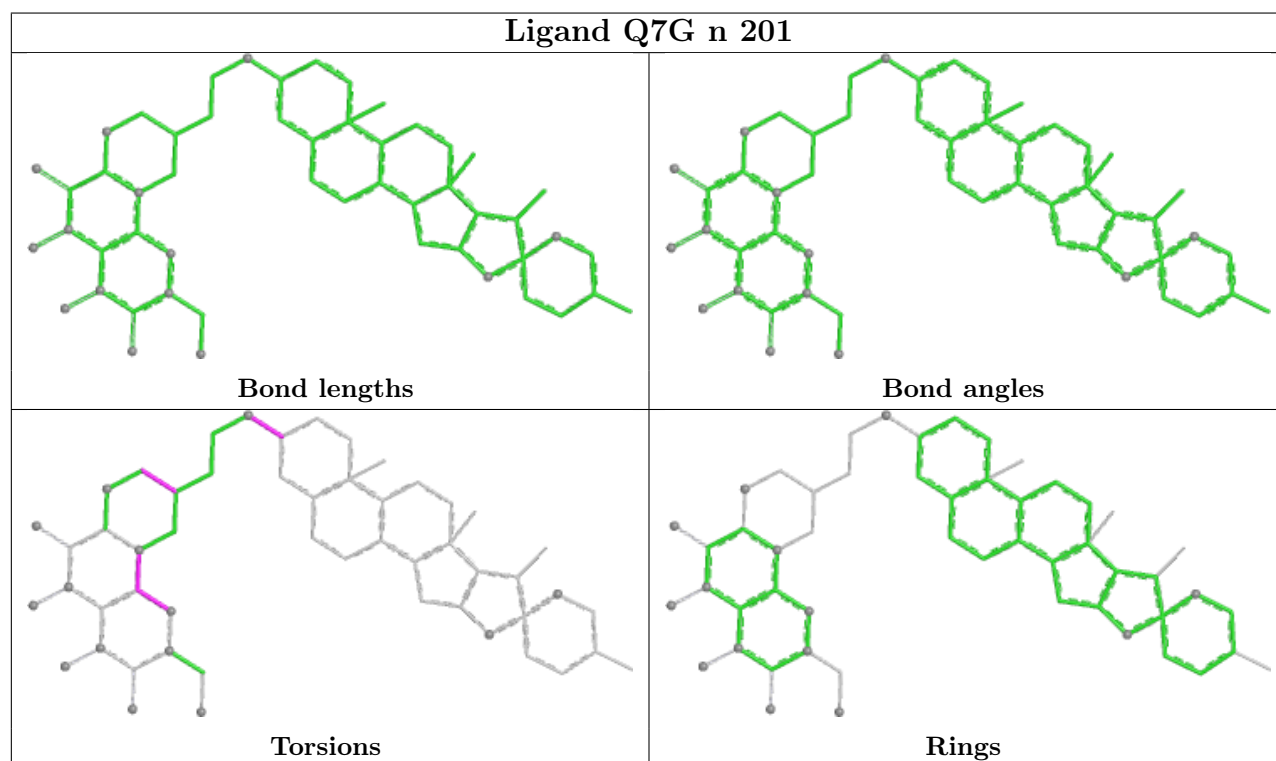
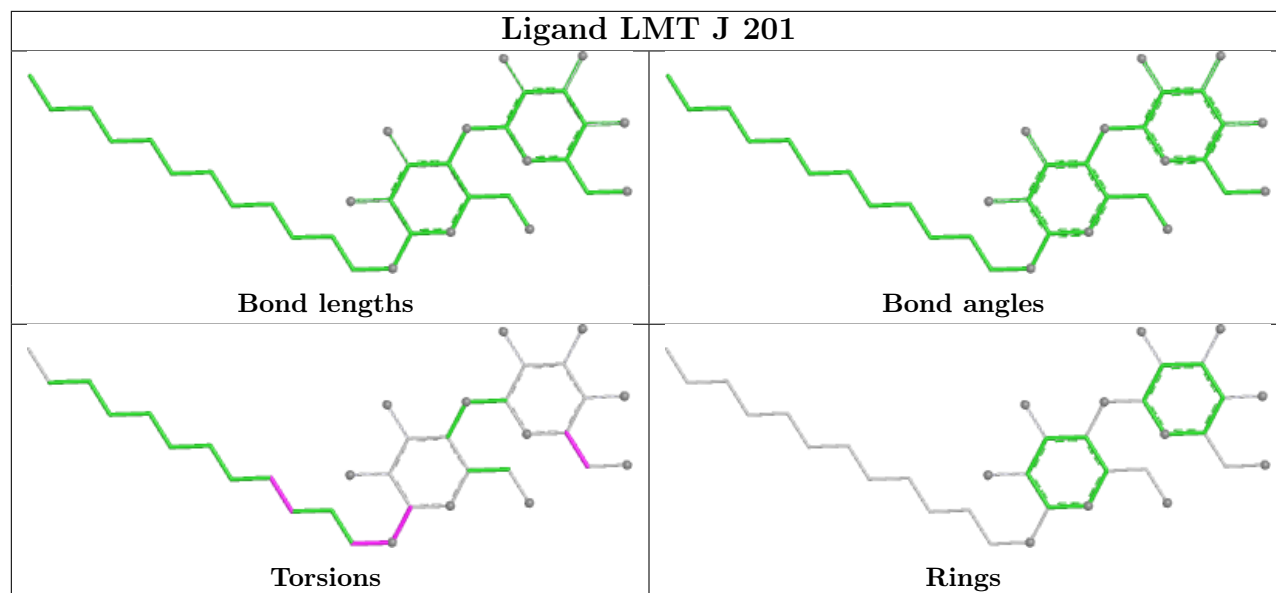


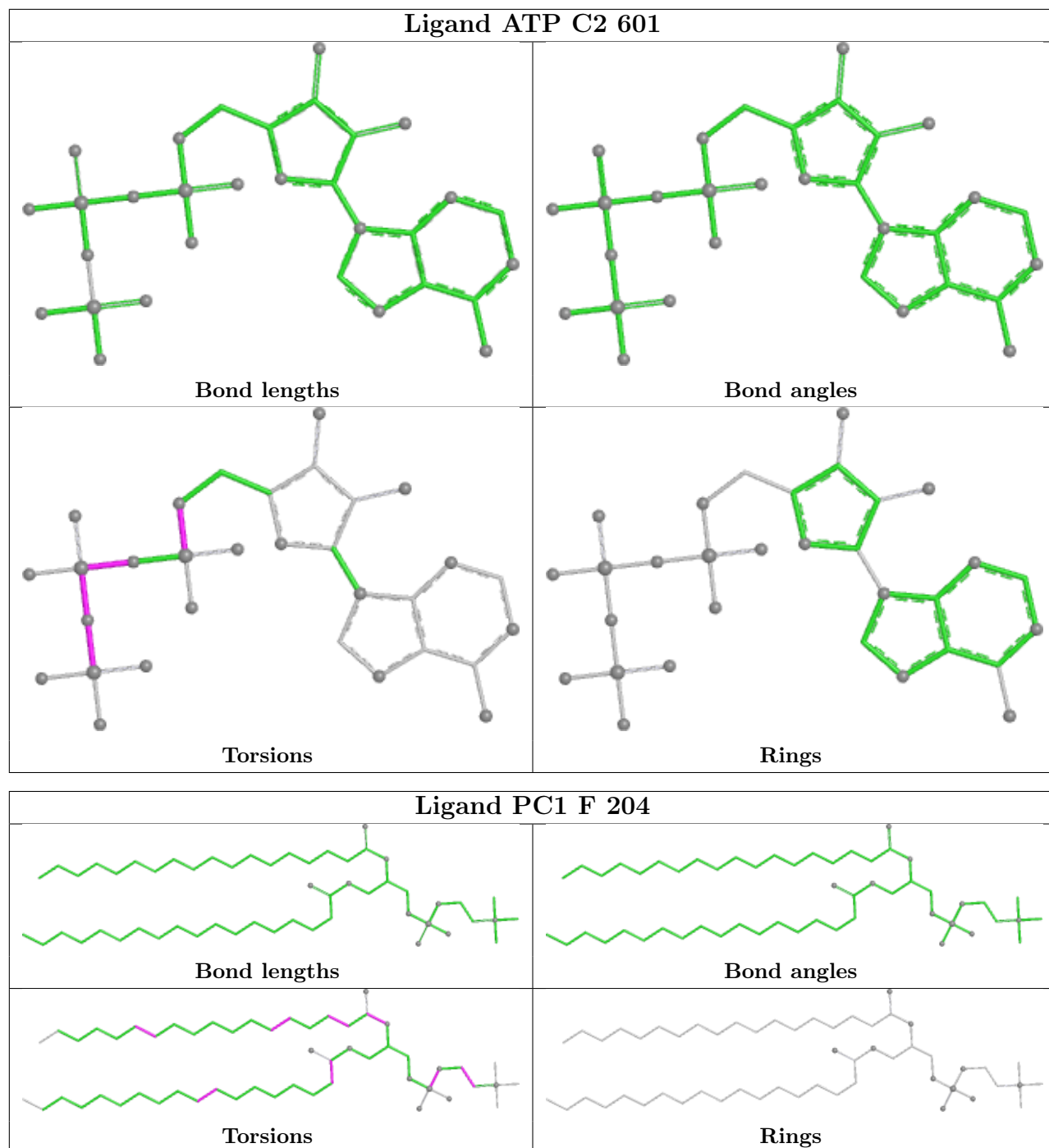


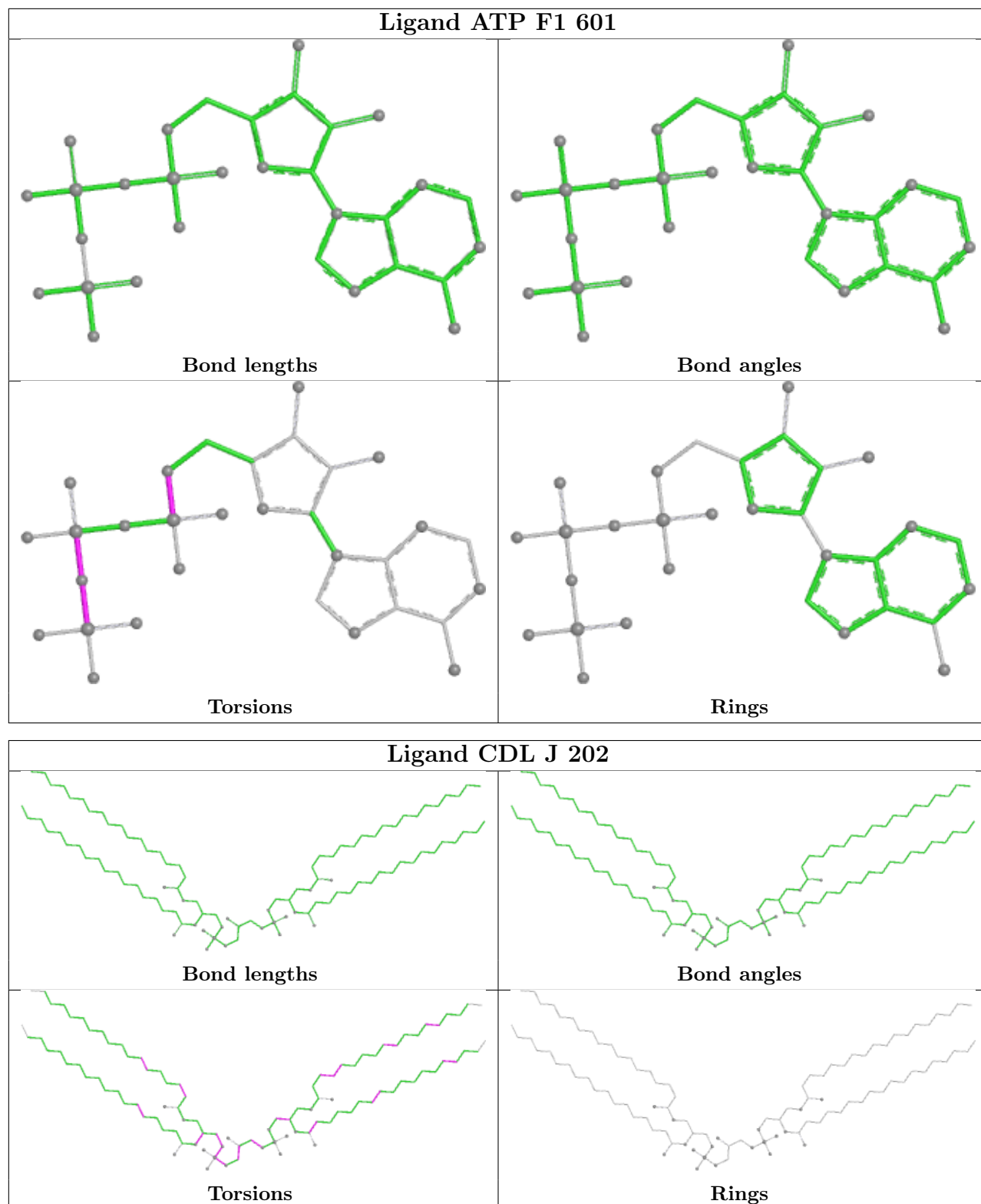


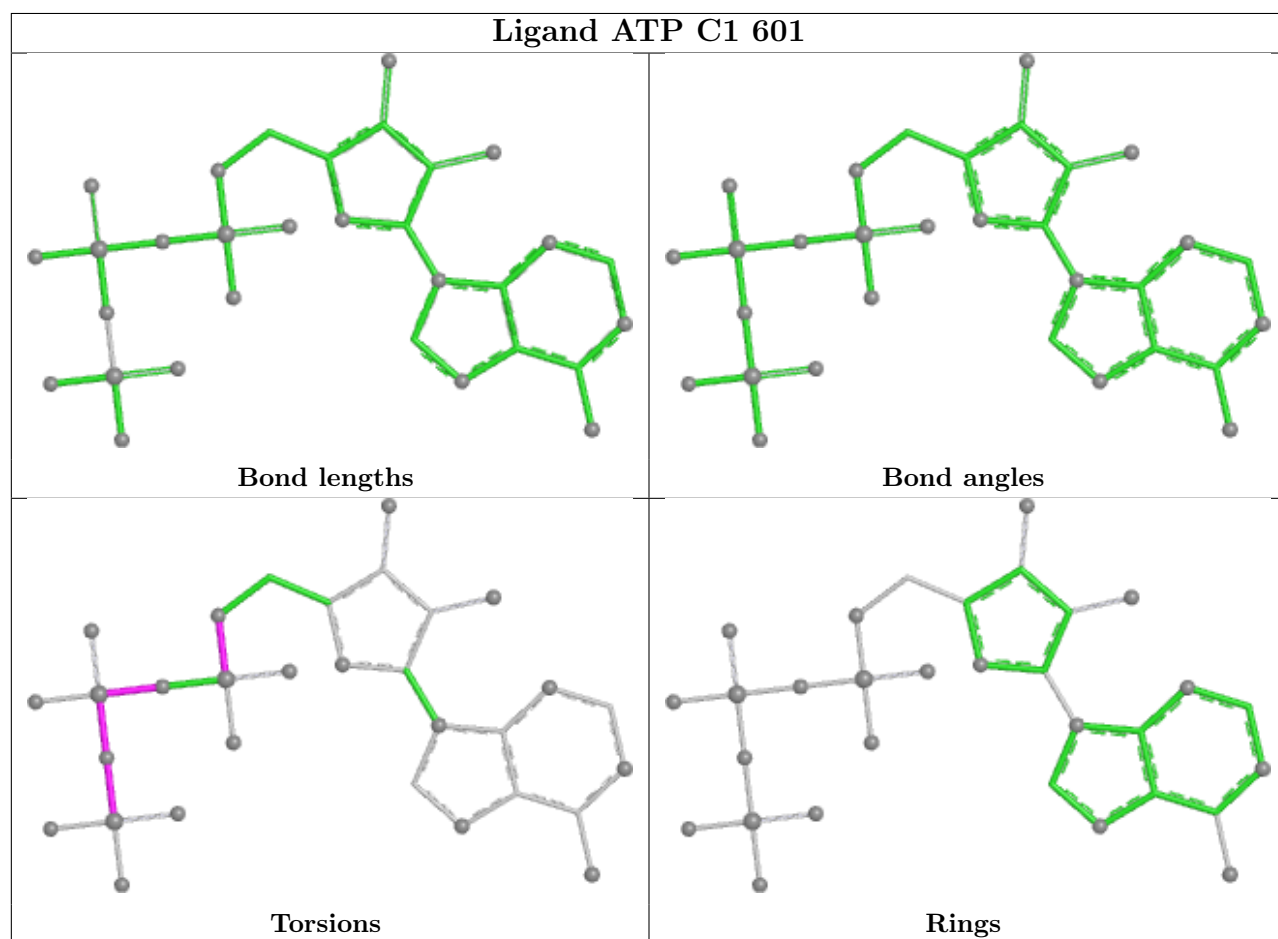
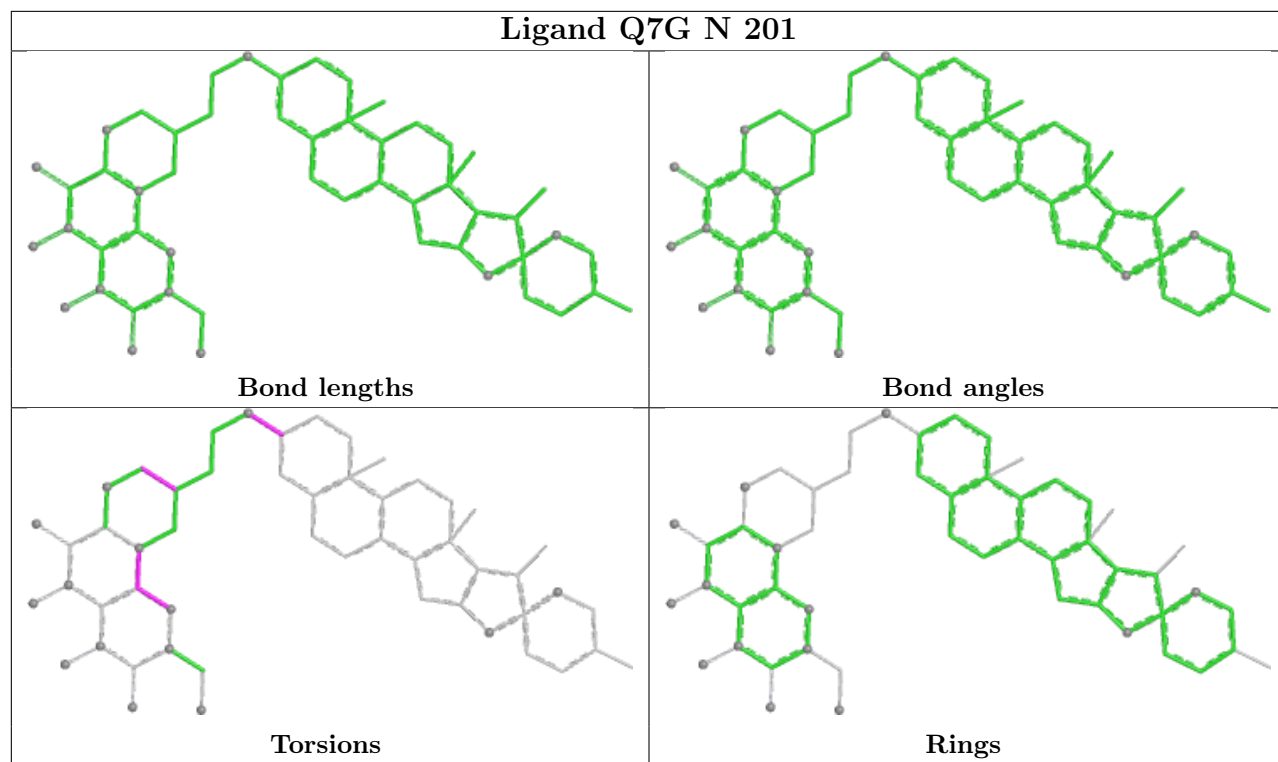


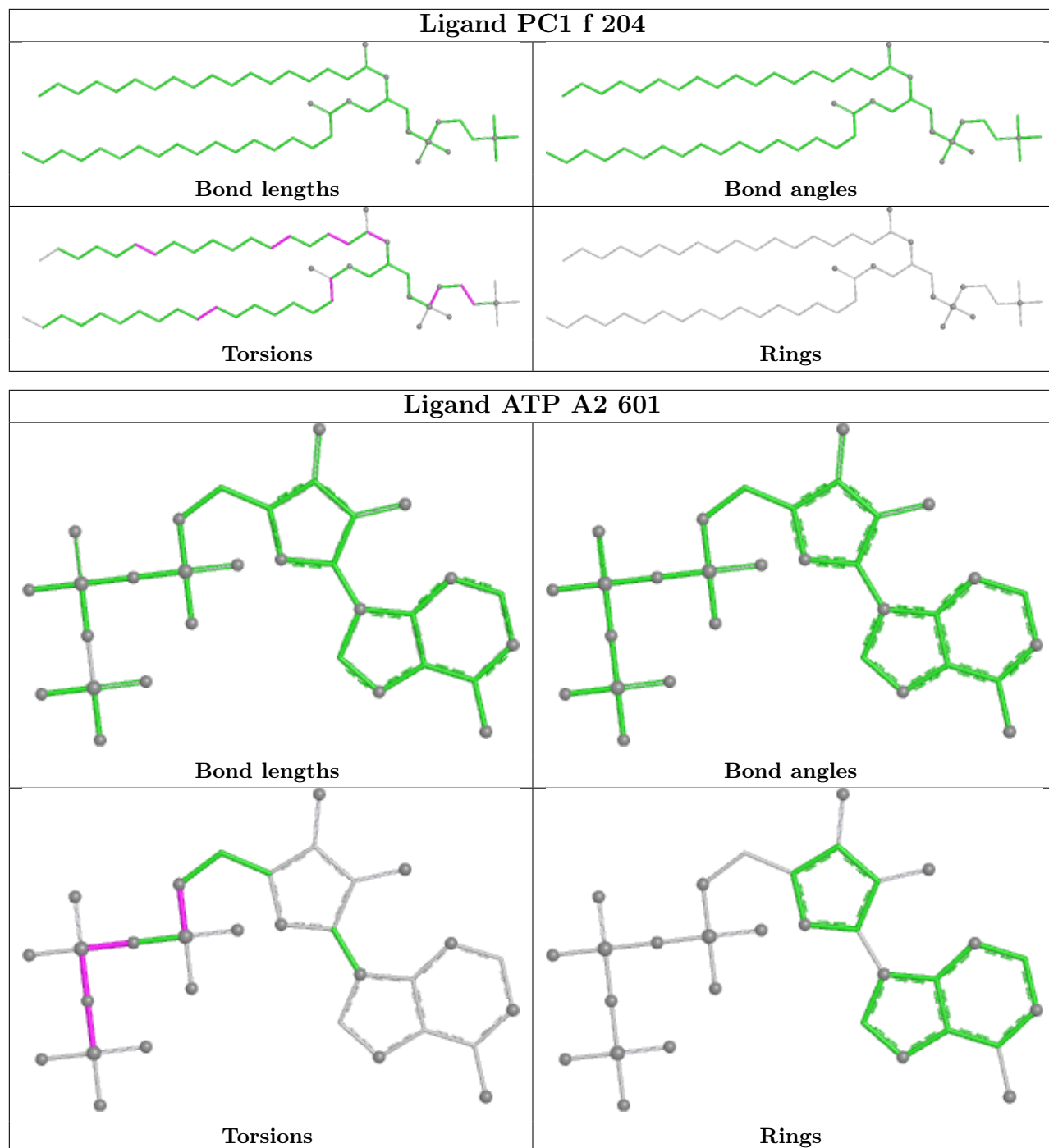


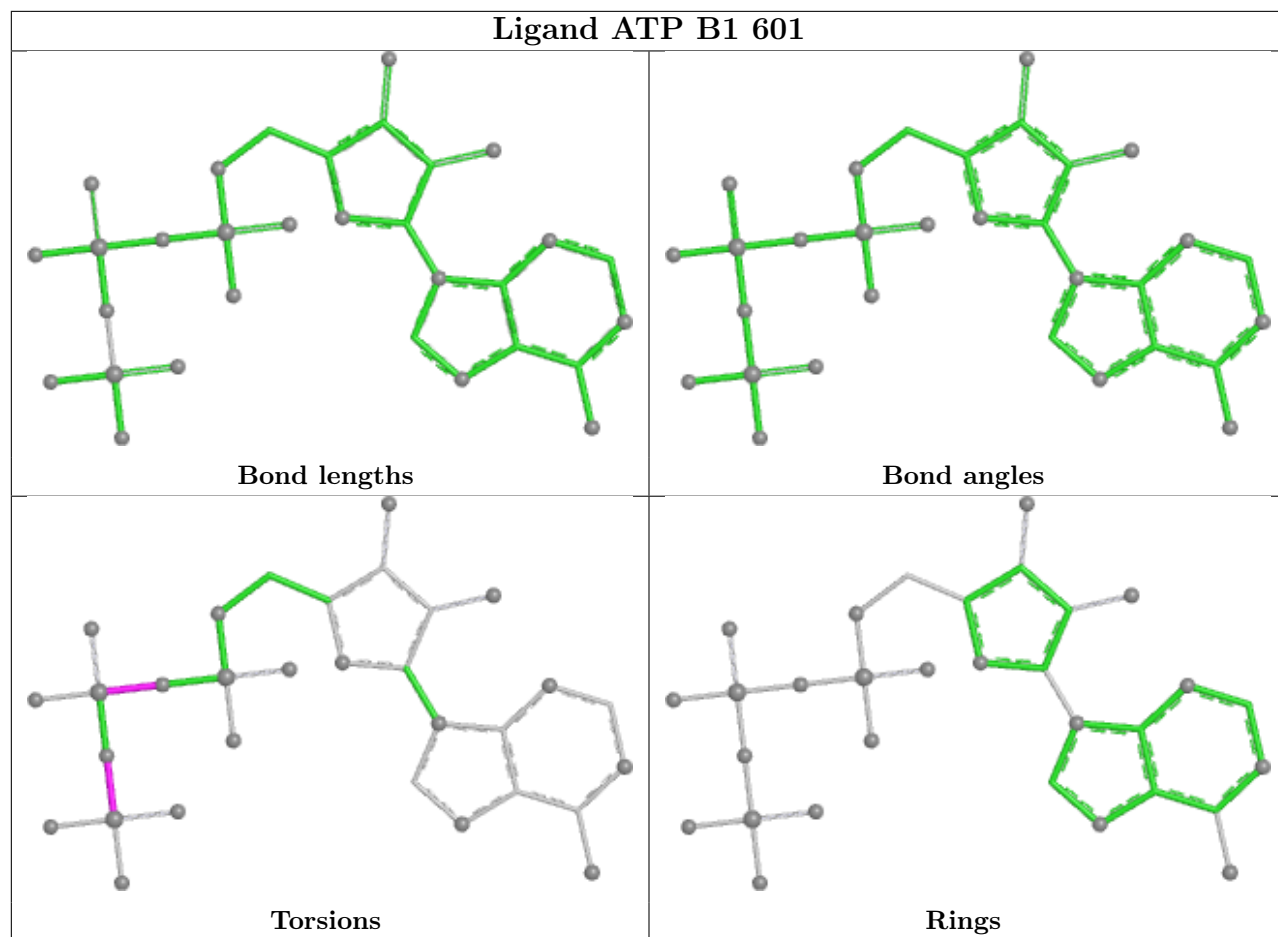


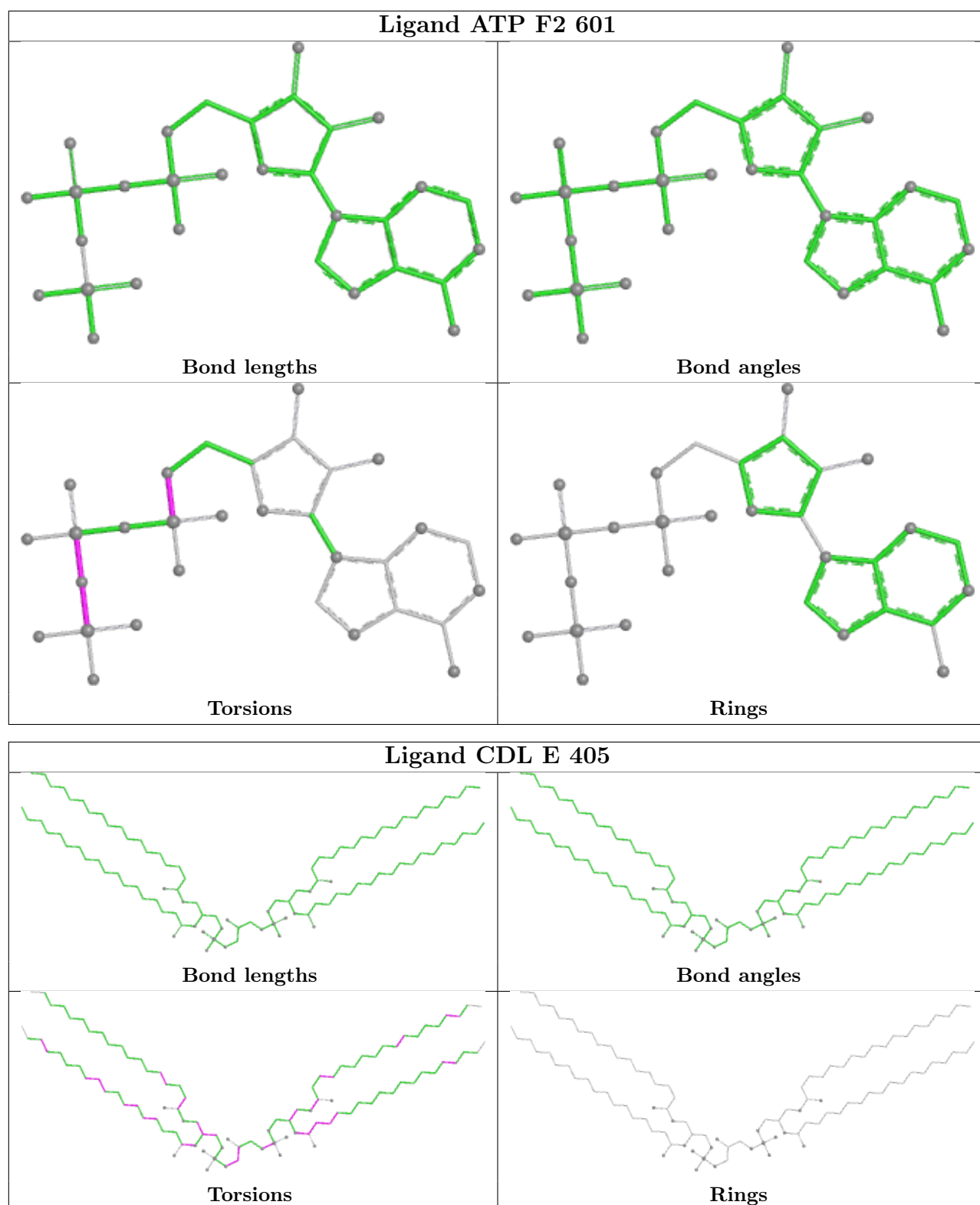


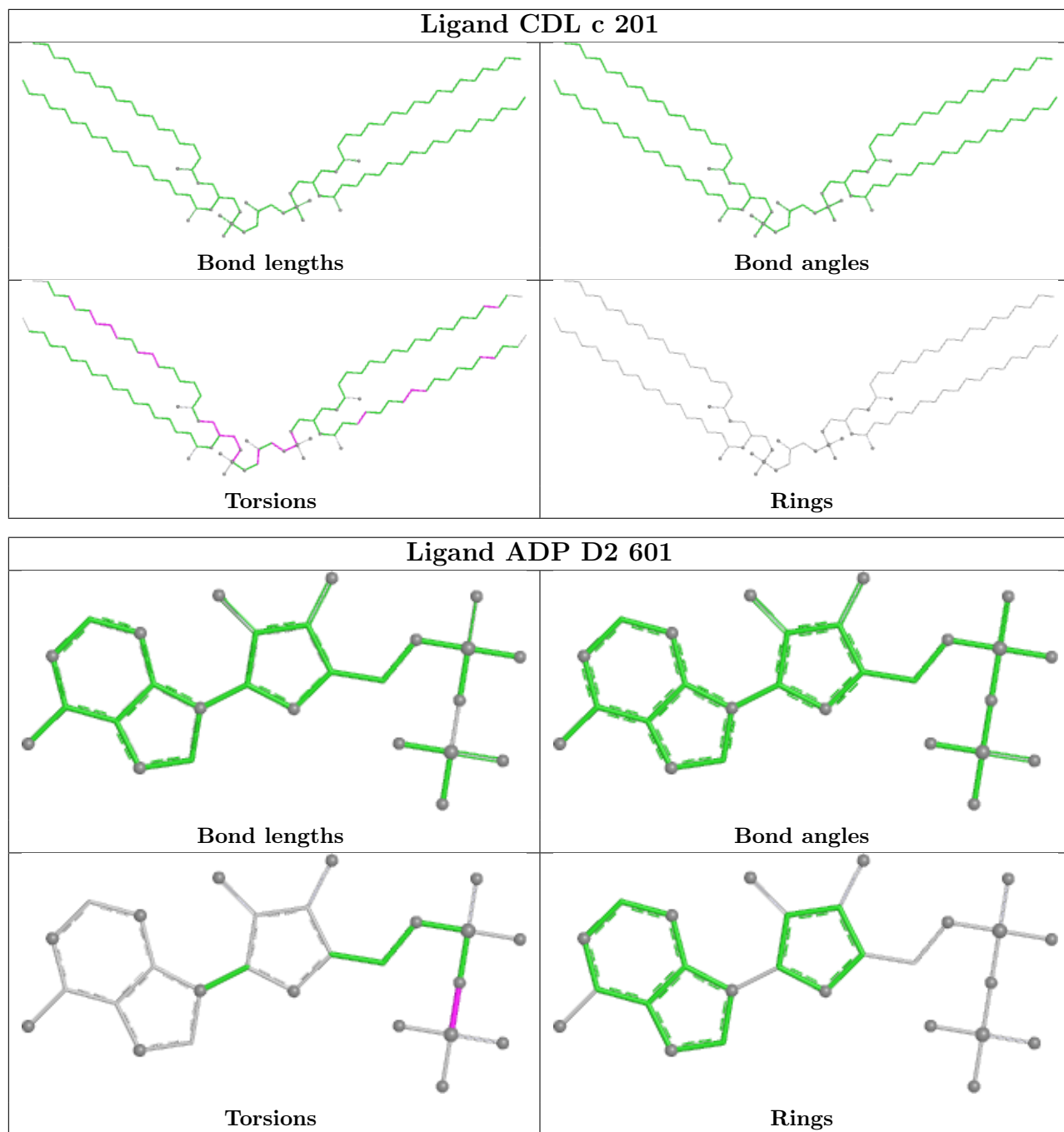












5.7 Other polymers [i](#)

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

This section contains visualisations of the EMDB entry EMD-15559. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis

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

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.