



Full wwPDB EM Validation Report ⓘ

Nov 30, 2022 – 05:12 pm GMT

PDB ID : 8AP6
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 Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

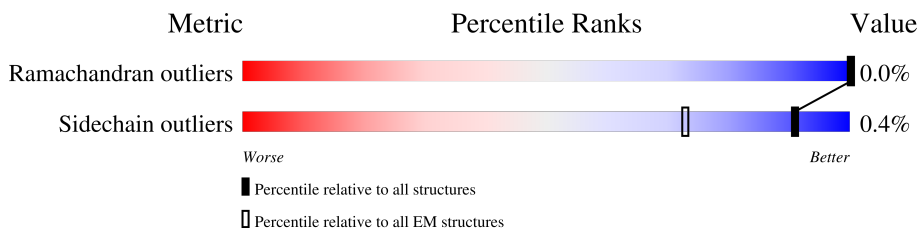
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	231	99% .
1	a	231	99% .
2	A1	584	9% 91% 9%
2	A2	584	9% 91% 9%
2	B1	584	8% 89% 10%
2	B2	584	8% 89% 10%
2	C1	584	5% 89% 10%
2	C2	584	5% 89% 10%
3	C	114	. 74% . 25%

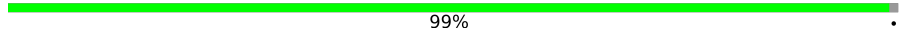
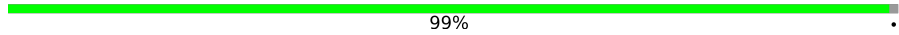
















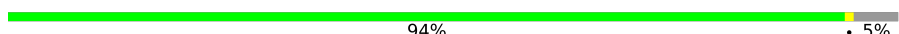
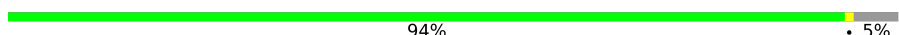





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Mol	Chain	Length	Quality of chain
3	c	114	74% 25%
4	D	370	89% 10%
4	d	370	89% 10%
5	D1	519	10% 94% 6%
5	D2	519	10% 94% 6%
5	E1	519	9% 93% 6%
5	E2	519	9% 93% 6%
5	F1	519	8% 94% 6%
5	F2	519	8% 94% 6%
6	E	396	96% ..
6	e	396	96% ..
7	F	145	92% 7%
7	f	145	92% 7%
8	G	269	10% 100%
8	g	269	10% 100%
9	G1	305	15% 98% ..
9	G2	305	14% 98% ..
10	H	157	6% 87% 13%
10	h	157	6% 87% 13%
11	H1	182	8% 88% 12%
11	H2	182	8% 88% 12%
12	I	104	99% .
12	i	104	99% .
13	I1	75	15% 87% 13%
13	I2	75	15% 87% 13%


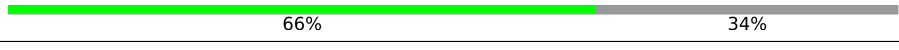
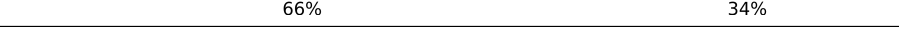




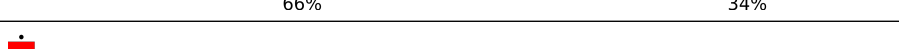



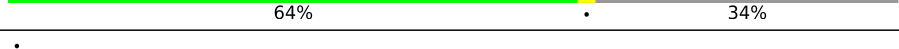
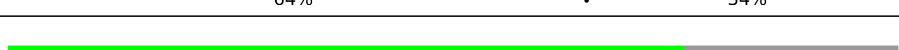
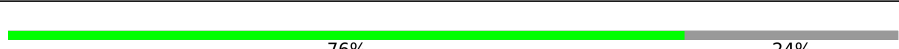


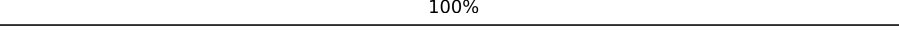
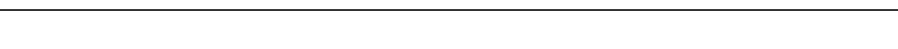
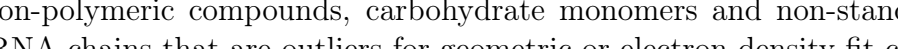

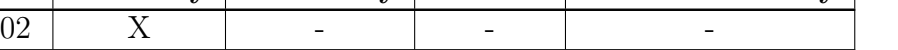
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Mol	Chain	Length	Quality of chain
14	J	169	 99%
14	j	169	 99%
15	J1	188	 32% 88% 12%
15	J2	188	 32% 88% 12%
15	K1	188	 11% 88% 12%
15	K2	188	 11% 88% 12%
15	L1	188	 21% 88% 12%
15	L2	188	 21% 88% 12%
16	K	124	 85% 15%
16	k	124	 85% 15%
17	L	92	 71% 29%
17	l	92	 71% 29%
18	M	144	 89% 10%
18	m	144	 89% 10%
19	M1	255	 12% 91% 8%
19	M2	255	 11% 91% 8%
20	N	156	 88% 11%
20	n	156	 88% 11%
21	O	101	 94% 5%
21	o	101	 94% 5%
22	O1	118	 66% 34%
22	O2	118	 66% 34%
22	P1	118	 66% 34%
22	P2	118	 66% 34%
22	Q1	118	 66% 34%

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Mol	Chain	Length	Quality of chain
22	Q2	118	 66% 34%
22	R1	118	 66% 34%
22	R2	118	 66% 34%
22	S1	118	 66% 34%
22	S2	118	 66% 34%
22	T1	118	 66% 34%
22	T2	118	 66% 34%
22	U1	118	 66% 34%
22	U2	118	 66% 34%
22	V1	118	 66% 34%
22	V2	118	 66% 34%
22	W1	118	 66% 34%
22	W2	118	 66% 34%
22	X1	118	 64% 34%
22	X2	118	 64% 34%
23	P	105	 76% 24%
23	p	105	 76% 24%
24	Q	98	 87% 13%
24	q	98	 87% 13%
25	R	62	 100%
25	r	62	 100%

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 ATP6B.

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	
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	
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	
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	
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	
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	
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

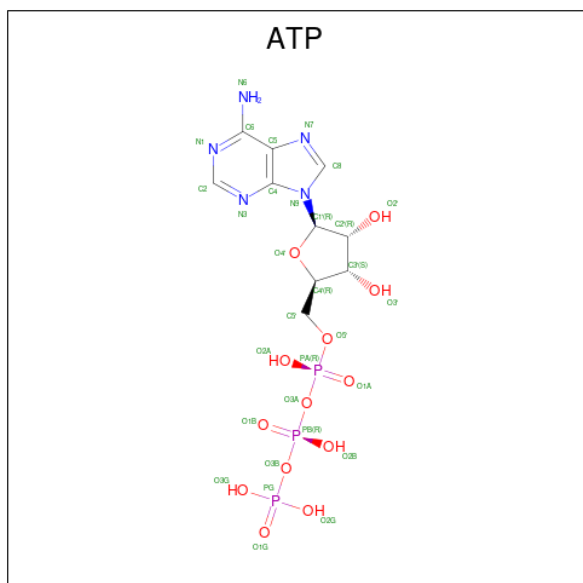
- Molecule 24 is a protein called ATPEG3.

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



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

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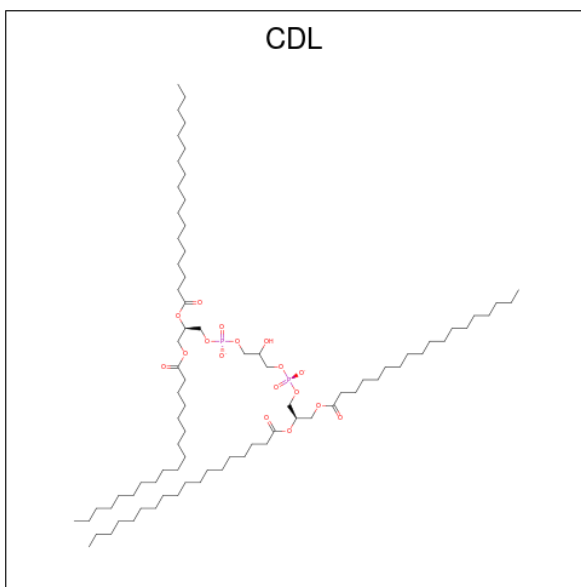
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Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
26	A2	1	43	10	12	5	13	3	0
26	B1	1	43	10	12	5	13	3	0
26	B2	1	43	10	12	5	13	3	0
26	C1	1	43	10	12	5	13	3	0
26	C2	1	43	10	12	5	13	3	0
26	F1	1	43	10	12	5	13	3	0
26	F2	1	43	10	12	5	13	3	0

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

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

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



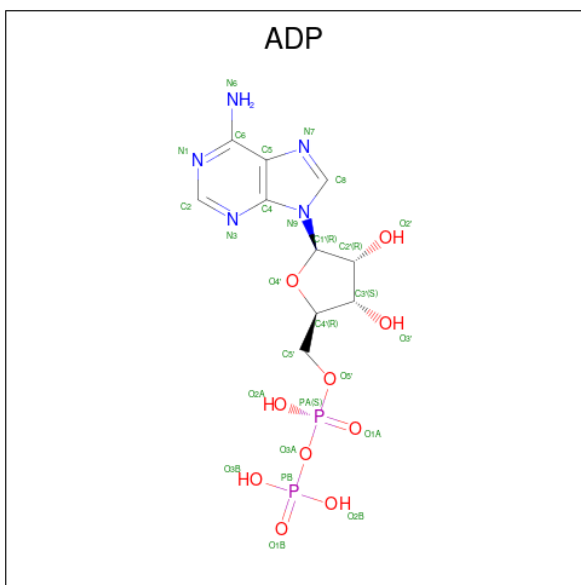
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
28	C	1	Total 256	C 81	H 156	O 17	P 2	0
28	E	1	Total 1280	C 405	H 780	O 85	P 10	0
28	E	1	Total 1280	C 405	H 780	O 85	P 10	0
28	E	1	Total 1280	C 405	H 780	O 85	P 10	0
28	E	1	Total 1280	C 405	H 780	O 85	P 10	0
28	E	1	Total 1280	C 405	H 780	O 85	P 10	0
28	E	1	Total 1280	C 405	H 780	O 85	P 10	0
28	F	1	Total 256	C 81	H 156	O 17	P 2	0
28	J	1	Total 512	C 162	H 312	O 34	P 4	0
28	J	1	Total 512	C 162	H 312	O 34	P 4	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
28	c	1	Total 256	C 81	H 156	O 17	P 2	0
28	e	1	Total 1280	C 405	H 780	O 85	P 10	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
28	e	1	Total	C	H	O	P	0
			1280	405	780	85	10	
28	e	1	Total	C	H	O	P	0
			1280	405	780	85	10	
28	e	1	Total	C	H	O	P	0
			1280	405	780	85	10	
28	e	1	Total	C	H	O	P	0
			1280	405	780	85	10	
28	f	1	Total	C	H	O	P	0
			256	81	156	17	2	
28	j	1	Total	C	H	O	P	0
			512	162	312	34	4	
28	j	1	Total	C	H	O	P	0
			512	162	312	34	4	
28	l	1	Total	C	H	O	P	0
			256	81	156	17	2	
28	m	1	Total	C	H	O	P	0
			256	81	156	17	2	
28	q	1	Total	C	H	O	P	0
			256	81	156	17	2	

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



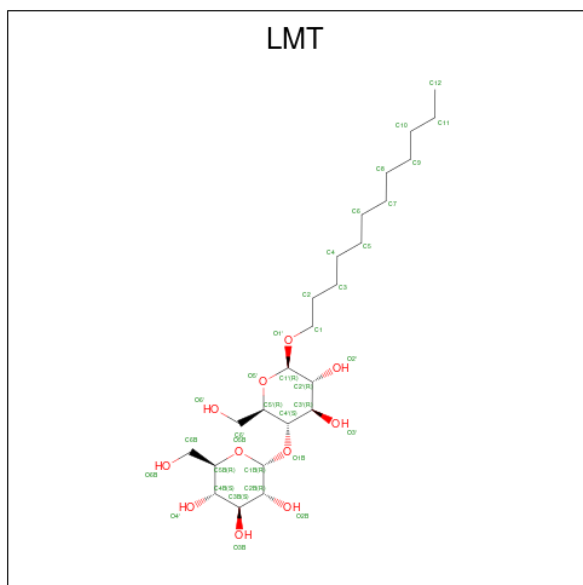
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
29	D1	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

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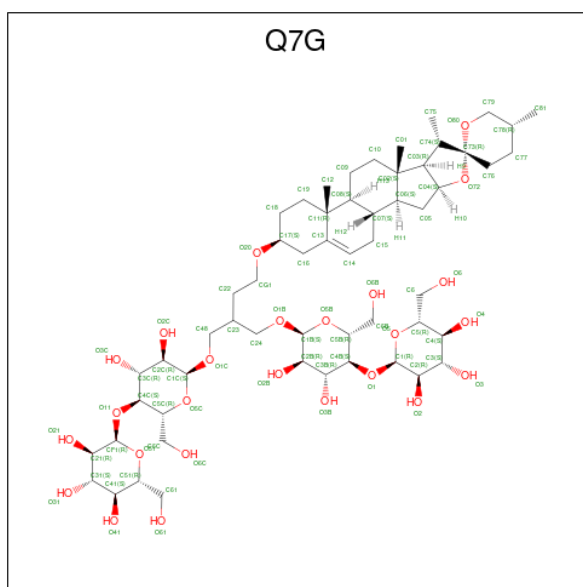
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
29	D2	1	39	10	12	5	10	2	0

- Molecule 30 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



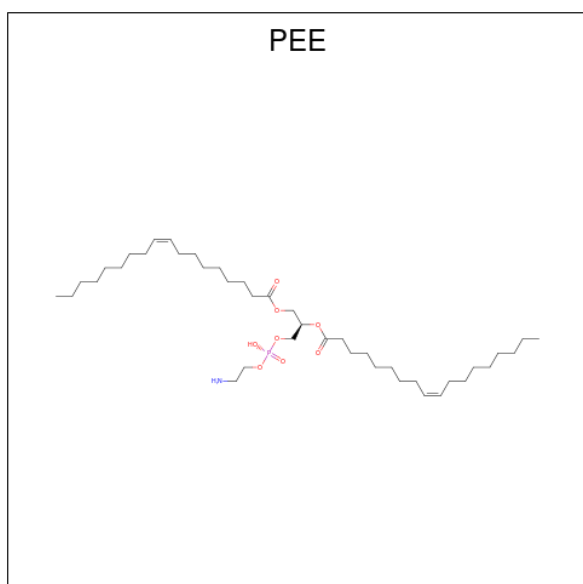
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
30	E	1	74	24	39	11	0
30	J	1	74	24	39	11	0
30	e	1	74	24	39	11	0
30	j	1	74	24	39	11	0

- 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 (three-letter code: Q7G) (formula: $C_{56}H_{92}O_{25}$).



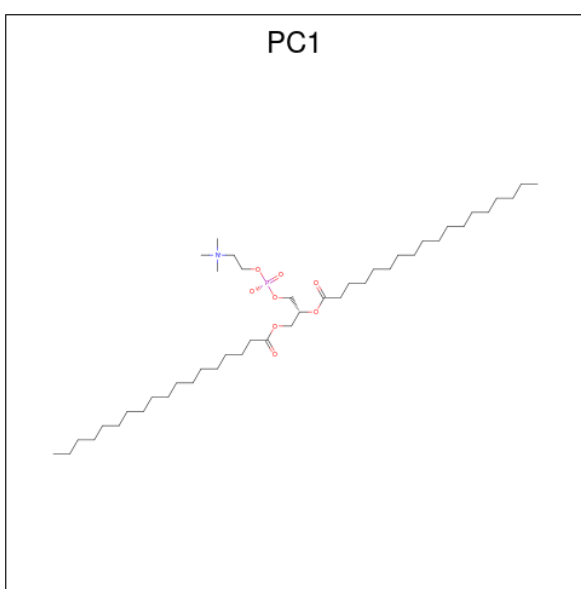
Mol	Chain	Residues	Atoms			AltConf	
			Total	C	H		O
31	E	1	108	38	60	10	0
31	N	1	129	44	70	15	0
31	e	1	108	38	60	10	0
31	n	1	129	44	70	15	0

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



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

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



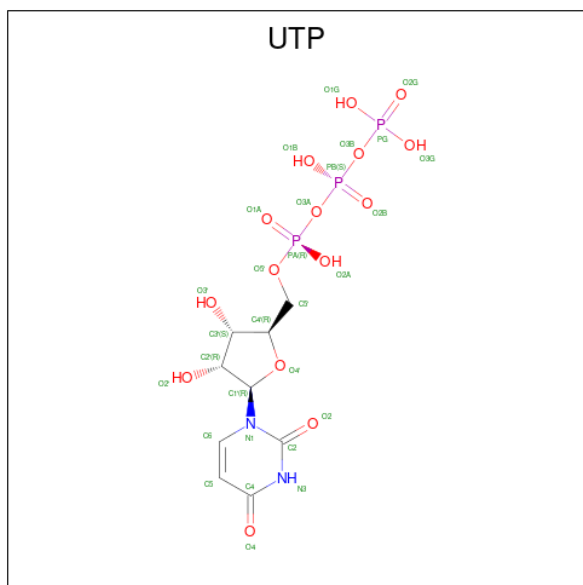
Mol	Chain	Residues	Atoms					AltConf	
33	F	1	Total	C	H	N	O	P	0
			284	88	176	2	16	2	
33	F	1	Total	C	H	N	O	P	0
			284	88	176	2	16	2	
33	I	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
33	J	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
33	f	1	Total	C	H	N	O	P	0
			284	88	176	2	16	2	
33	f	1	Total	C	H	N	O	P	0
			284	88	176	2	16	2	
33	i	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	

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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 (three-letter code: UTP) (formula: $C_9H_{15}N_2O_{15}P_3$) (labeled as "Ligand of Interest" by depositor).

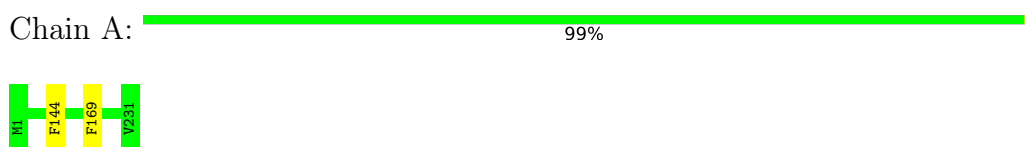


Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
34	H1	1	40	9	11	2	15	3	0
34	H2	1	40	9	11	2	15	3	0

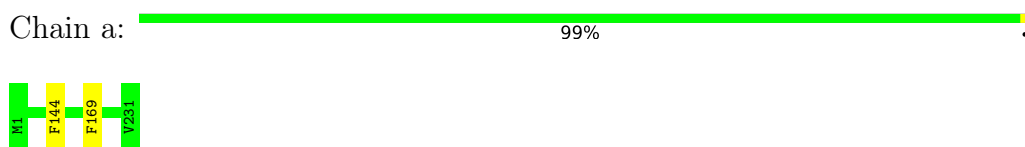
3 Residue-property plots [i](#)

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

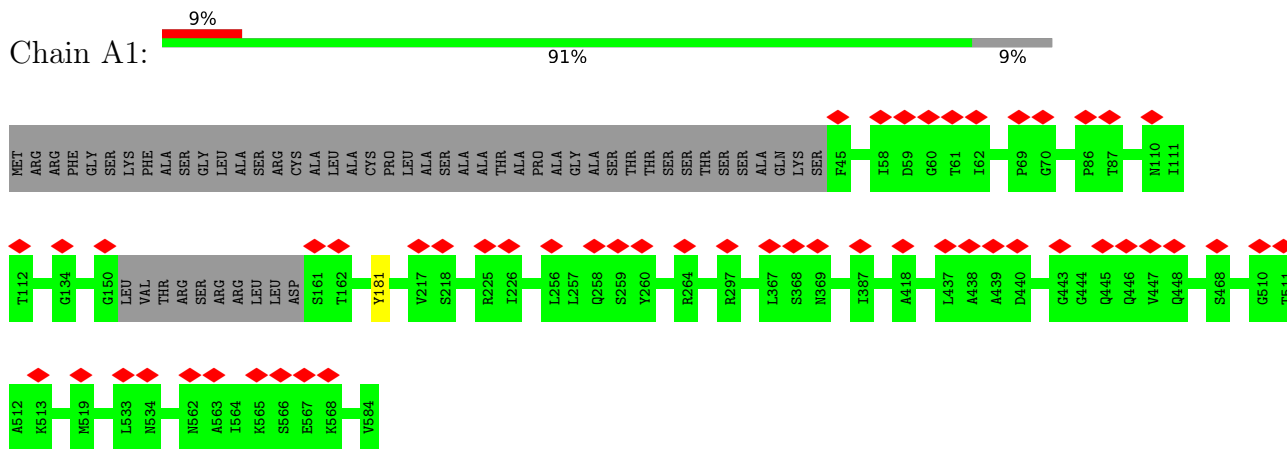
- Molecule 1: ATP synthase subunit a



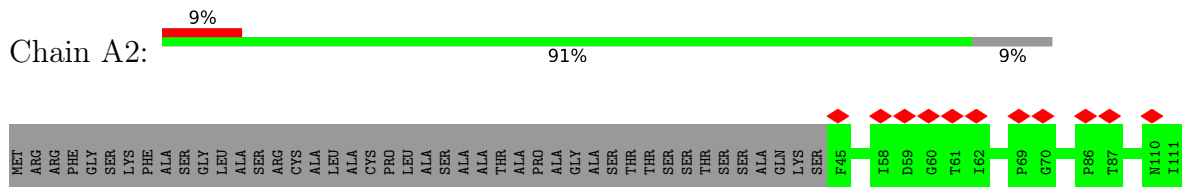
- Molecule 1: ATP synthase subunit a

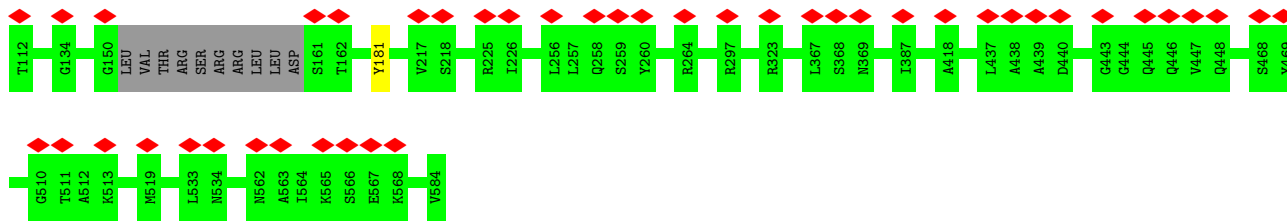


- Molecule 2: ATP synthase subunit alpha, mitochondrial

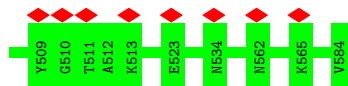
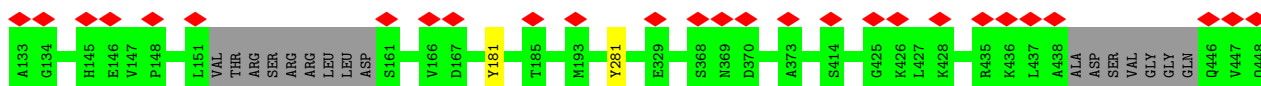
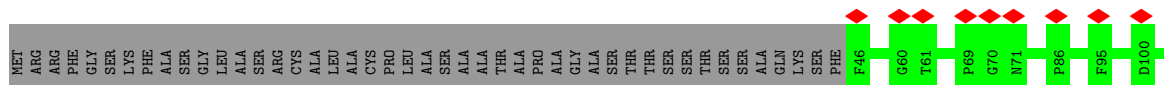
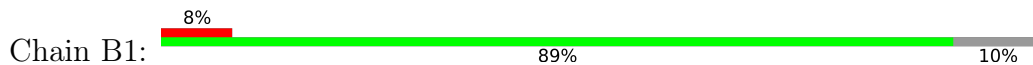


- Molecule 2: ATP synthase subunit alpha, mitochondrial

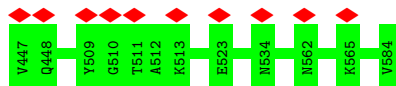
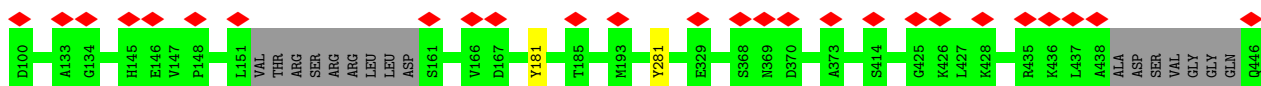
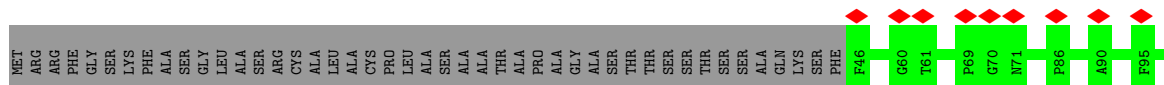
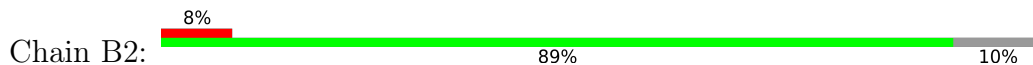




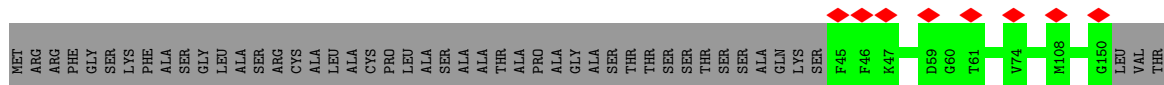
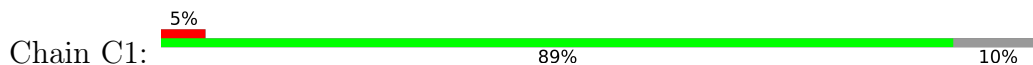
• Molecule 2: ATP synthase subunit alpha, mitochondrial



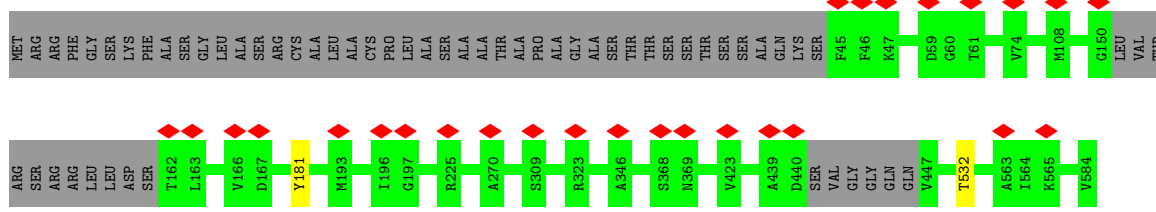
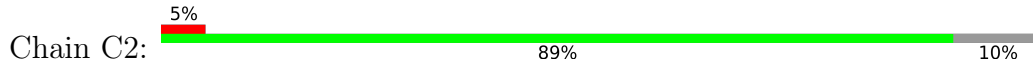
• Molecule 2: ATP synthase subunit alpha, mitochondrial



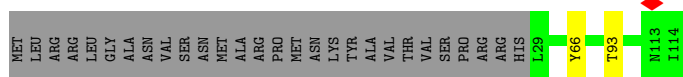
• Molecule 2: ATP synthase subunit alpha, mitochondrial



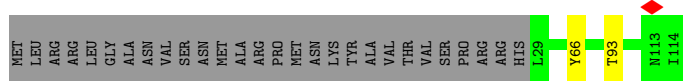
• Molecule 2: ATP synthase subunit alpha, mitochondrial



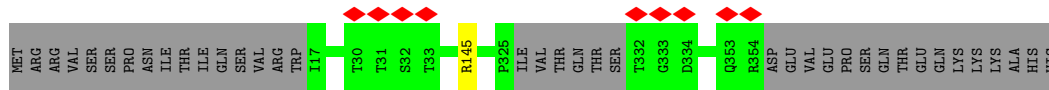
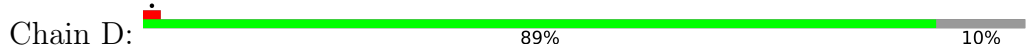
- Molecule 3: subunit-8



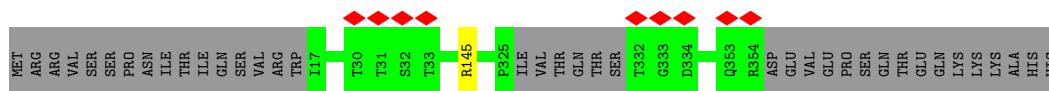
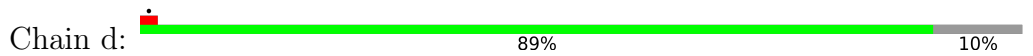
- Molecule 3: subunit-8



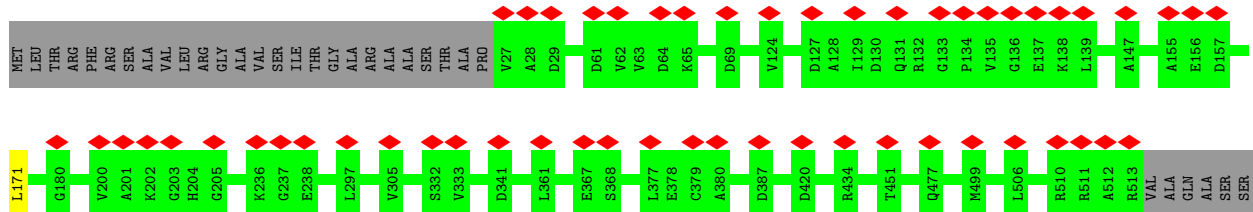
- Molecule 4: subunit-d



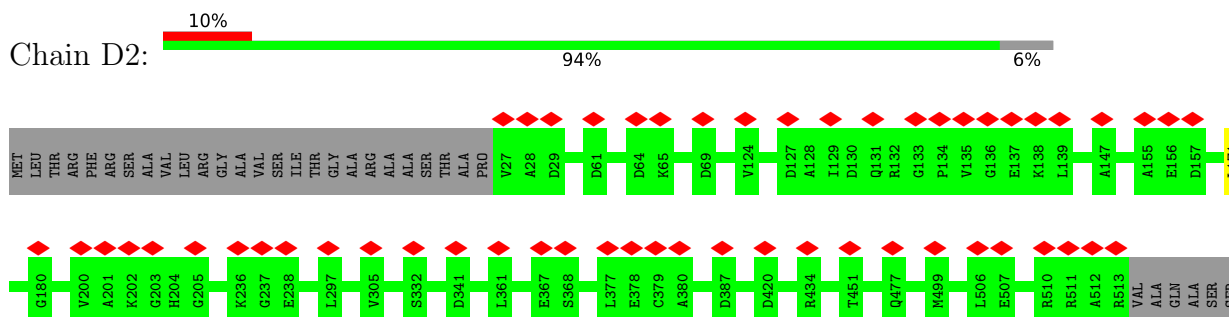
- Molecule 4: subunit-d



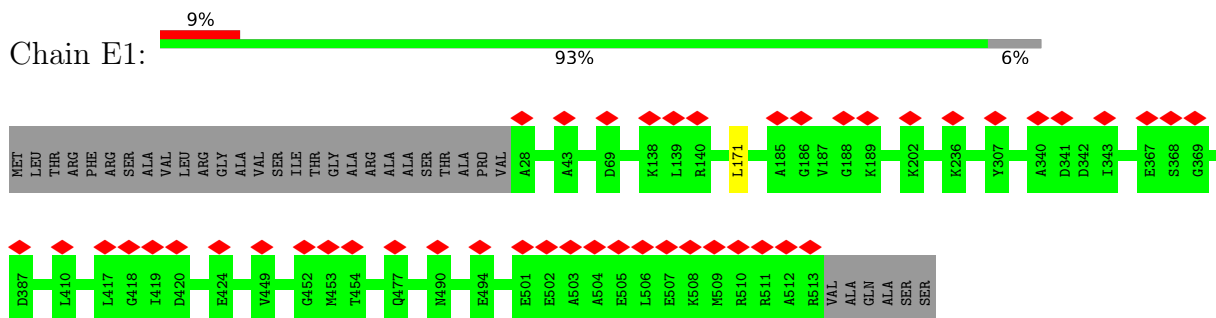
- Molecule 5: ATP synthase subunit beta, mitochondrial



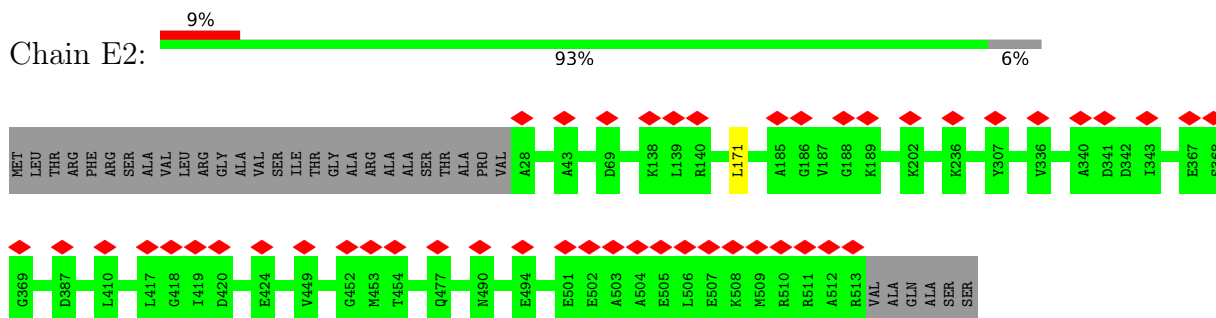
- Molecule 5: ATP synthase subunit beta, mitochondrial



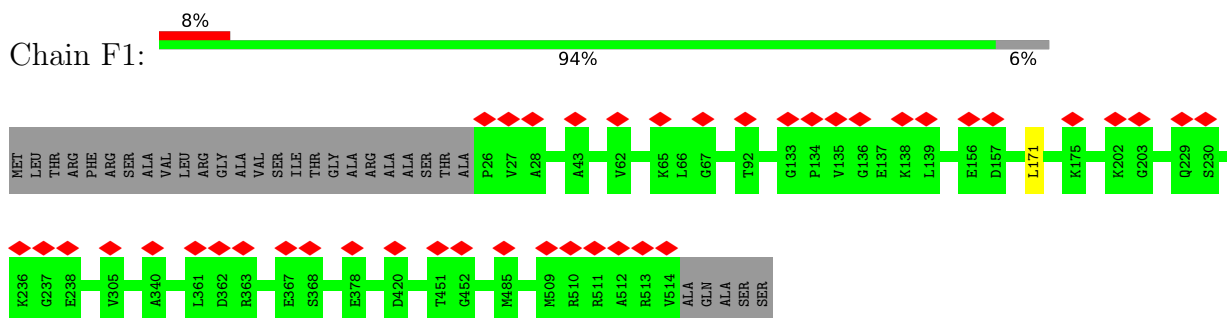
- Molecule 5: ATP synthase subunit beta, mitochondrial



- Molecule 5: ATP synthase subunit beta, mitochondrial

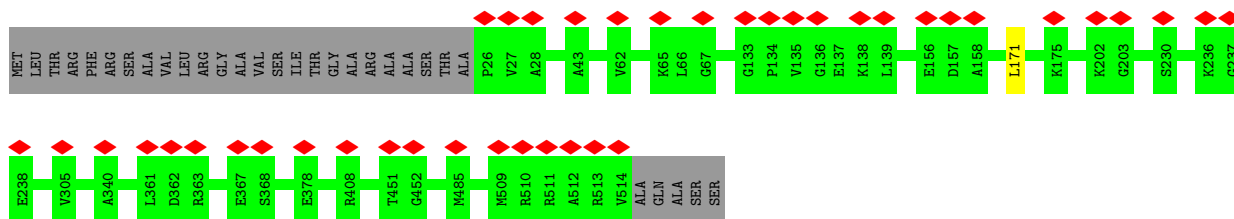


- Molecule 5: ATP synthase subunit beta, mitochondrial

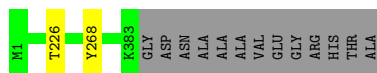


- Molecule 5: ATP synthase subunit beta, mitochondrial

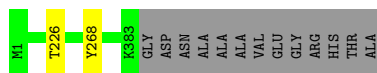




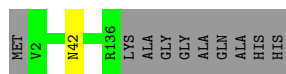
• Molecule 6: ATPTB1



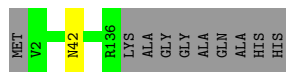
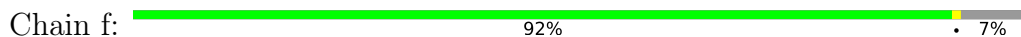
• Molecule 6: ATPTB1



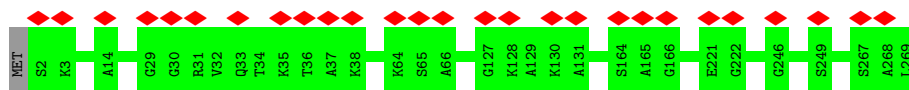
• Molecule 7: subunit-f



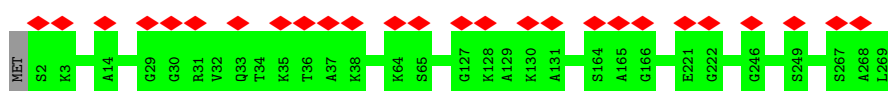
• Molecule 7: subunit-f



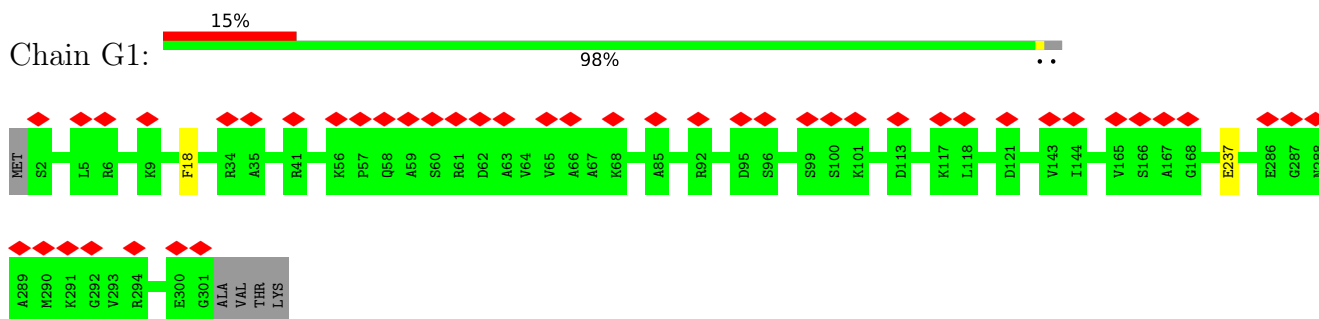
• Molecule 8: ATPTB3



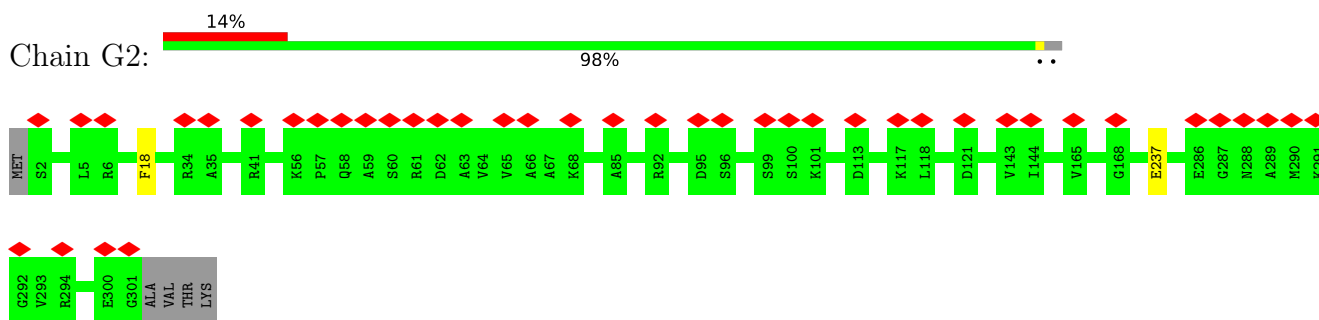
• Molecule 8: ATPTB3



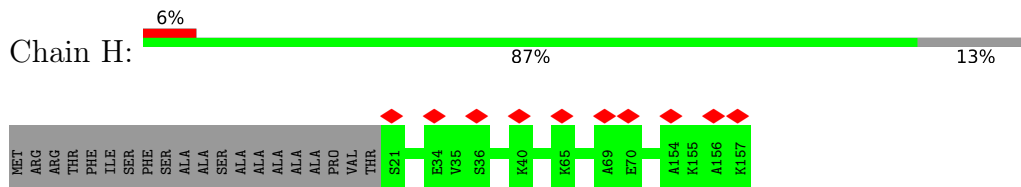
- Molecule 9: ATP synthase gamma subunit



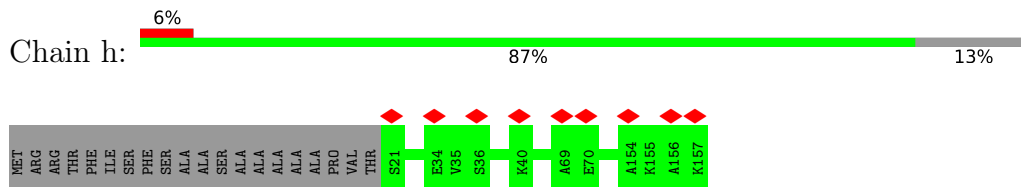
- Molecule 9: ATP synthase gamma subunit



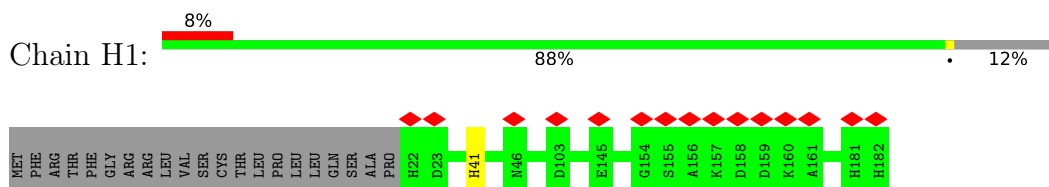
- Molecule 10: ATPTB4



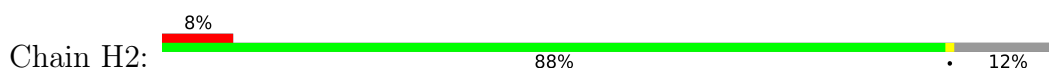
- Molecule 10: ATPTB4

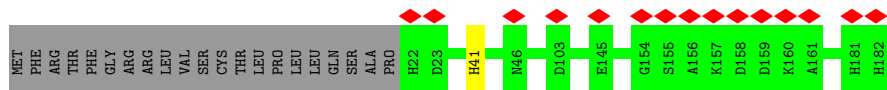


- Molecule 11: ATP synthase, epsilon chain, putative



- Molecule 11: ATP synthase, epsilon chain, putative





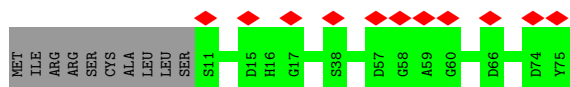
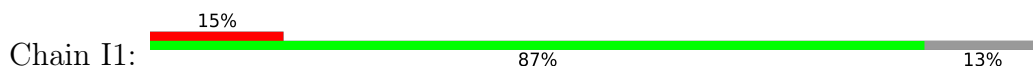
• Molecule 12: subunit-i/j



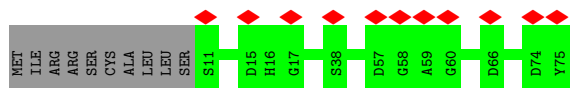
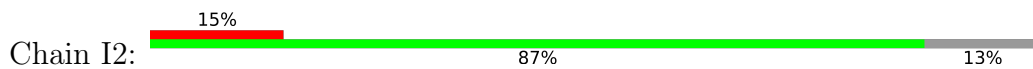
• Molecule 12: subunit-i/j



• Molecule 13: ATP synthase subunit epsilon, mitochondrial



• Molecule 13: ATP synthase subunit epsilon, mitochondrial



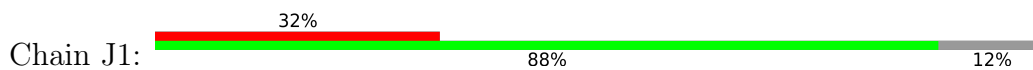
• Molecule 14: ATPTB6

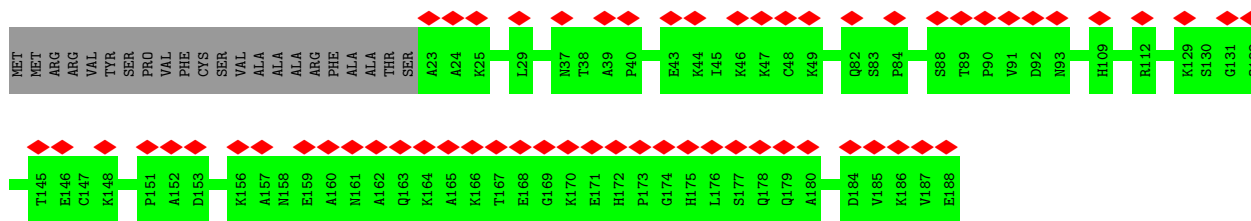


• Molecule 14: ATPTB6

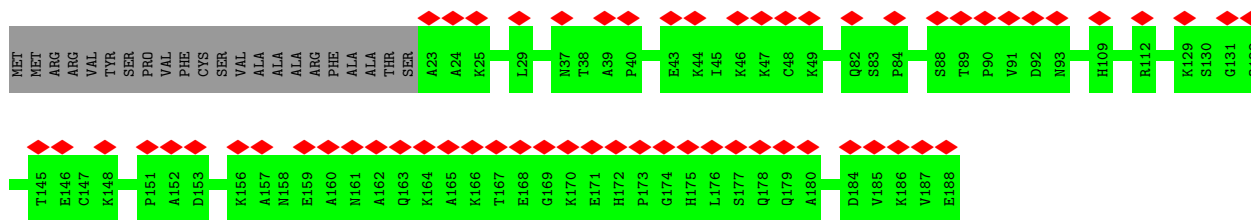
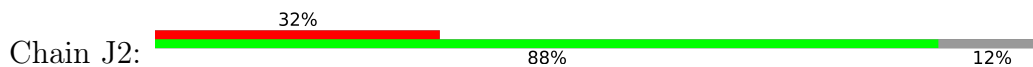


• Molecule 15: ATP synthase subunit p18, mitochondrial

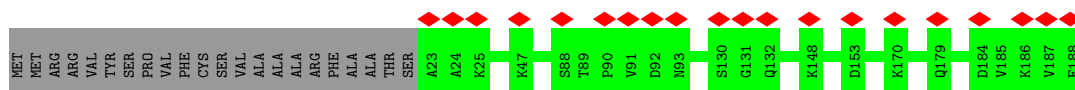
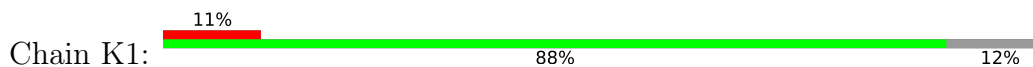




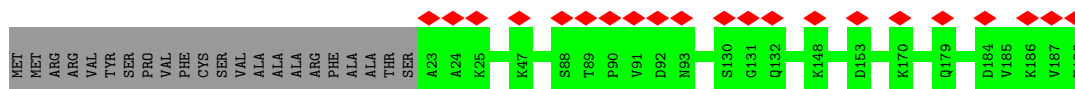
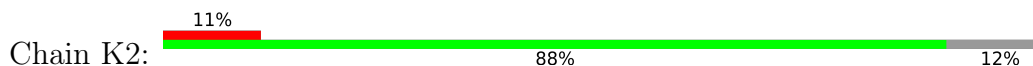
• Molecule 15: ATP synthase subunit p18, mitochondrial



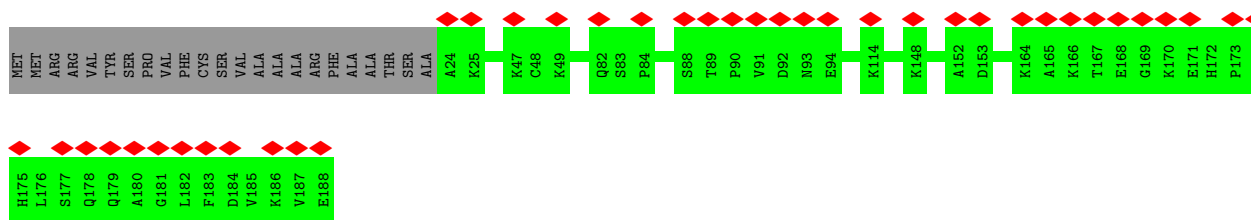
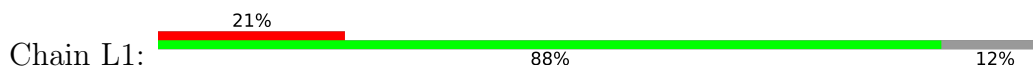
• Molecule 15: ATP synthase subunit p18, mitochondrial



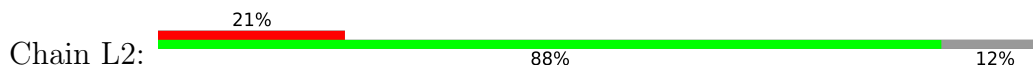
• Molecule 15: ATP synthase subunit p18, mitochondrial

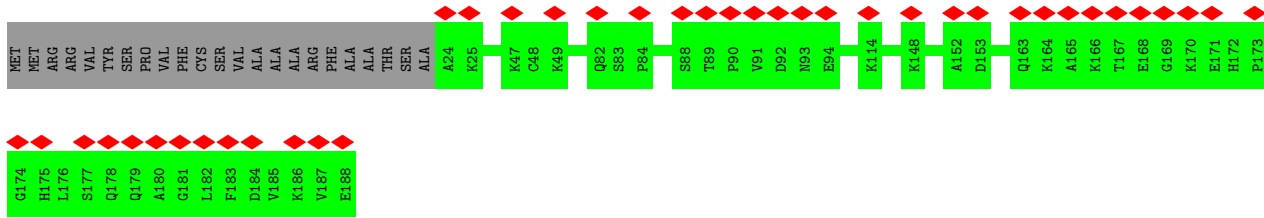


• Molecule 15: ATP synthase subunit p18, mitochondrial

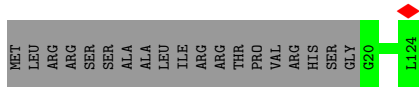
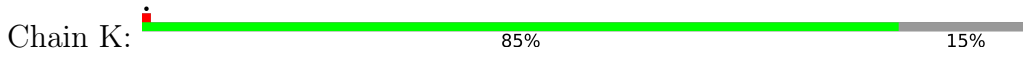


• Molecule 15: ATP synthase subunit p18, mitochondrial

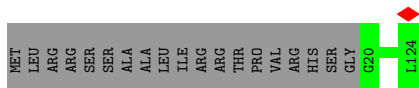
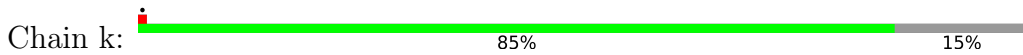




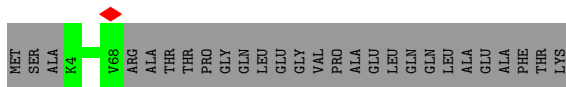
• Molecule 16: subunit-k



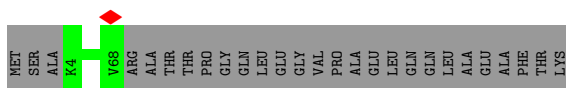
• Molecule 16: subunit-k



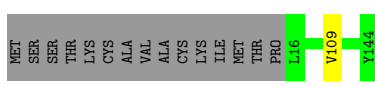
• Molecule 17: subunit-e



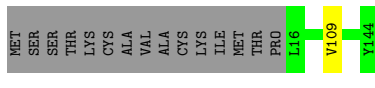
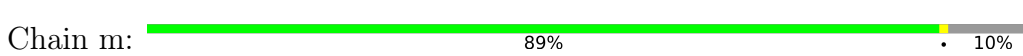
• Molecule 17: subunit-e



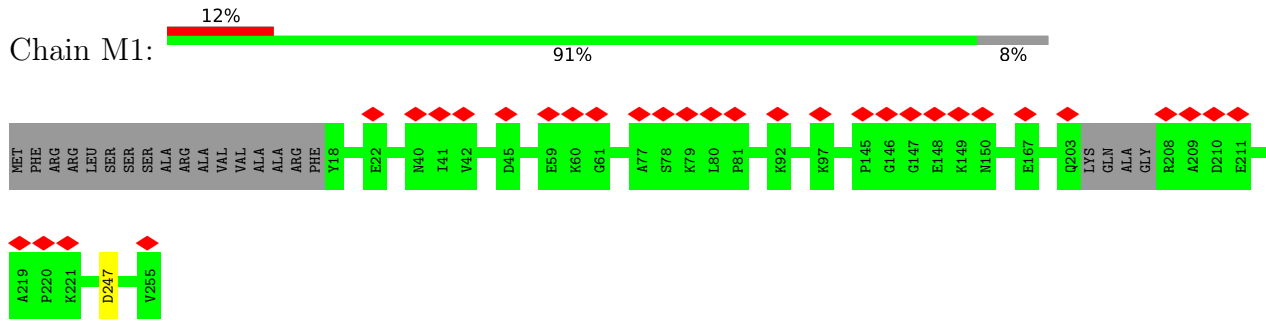
• Molecule 18: subunit-g



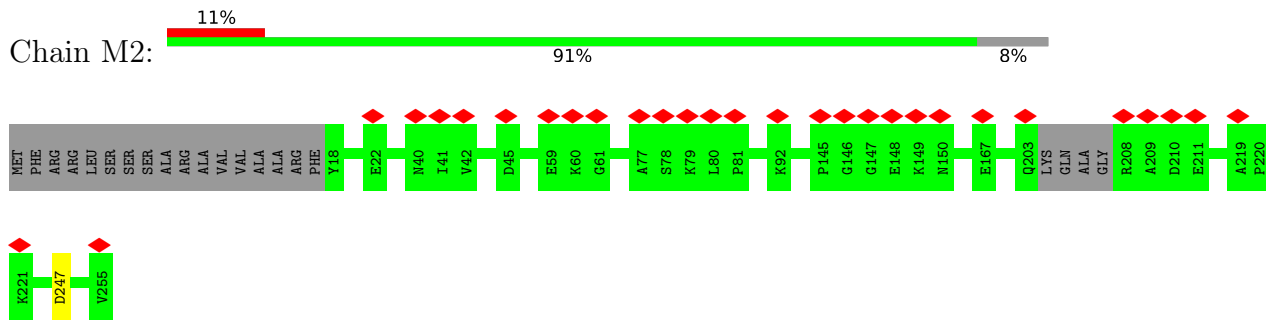
• Molecule 18: subunit-g



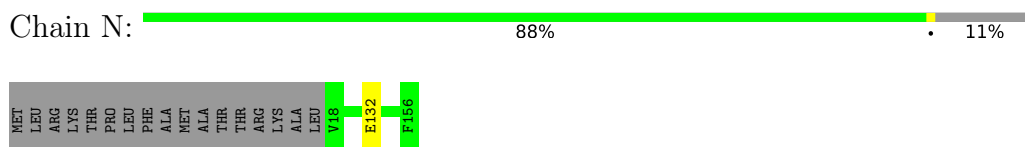
• Molecule 19: oligomycin sensitivity conferring protein



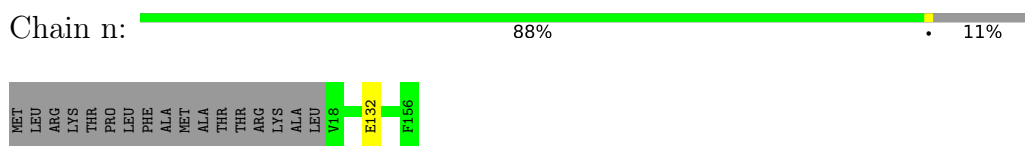
• Molecule 19: oligomycin sensitivity conferring protein



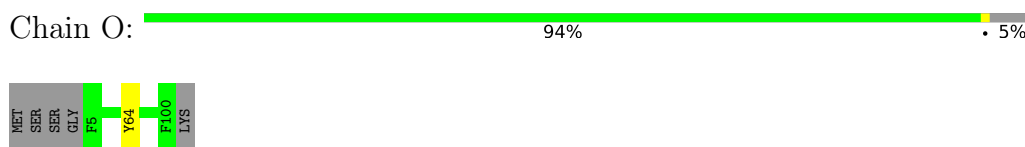
• Molecule 20: ATPTB11



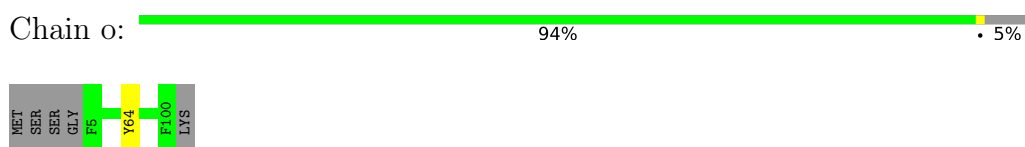
• Molecule 20: ATPTB11



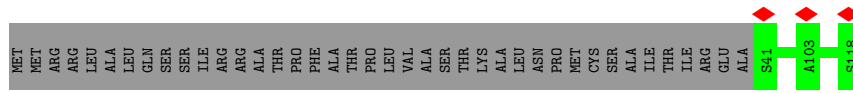
• Molecule 21: ATPTB12



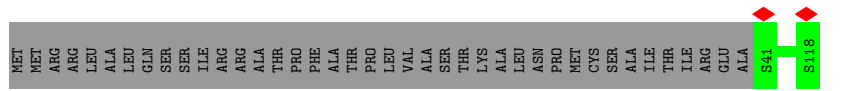
• Molecule 21: ATPTB12



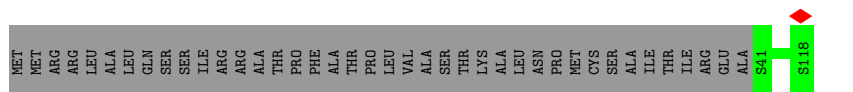
• Molecule 22: ATPase subunit 9, putative



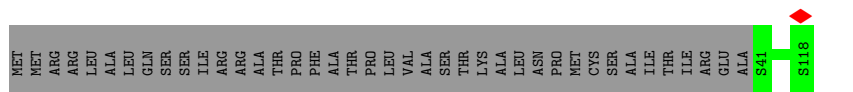
• Molecule 22: ATPase subunit 9, putative



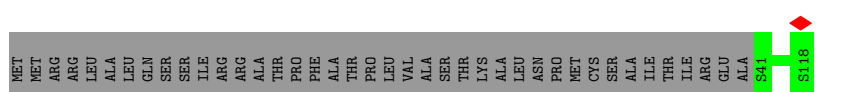
• Molecule 22: ATPase subunit 9, putative



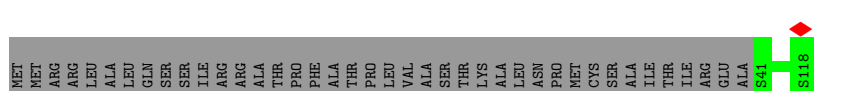
• Molecule 22: ATPase subunit 9, putative



• Molecule 22: ATPase subunit 9, putative

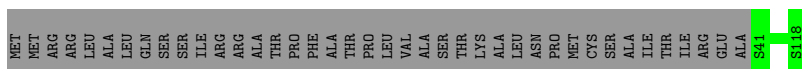


• Molecule 22: ATPase subunit 9, putative

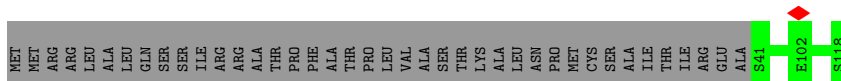


• Molecule 22: ATPase subunit 9, putative

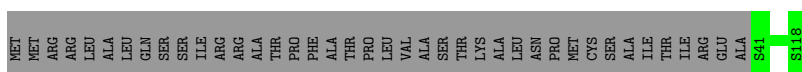




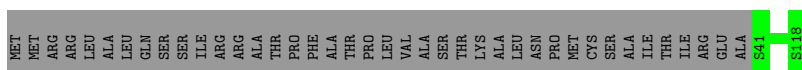
- Molecule 22: ATPase subunit 9, putative



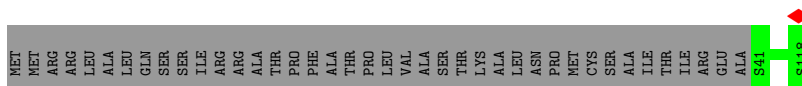
- Molecule 22: ATPase subunit 9, putative



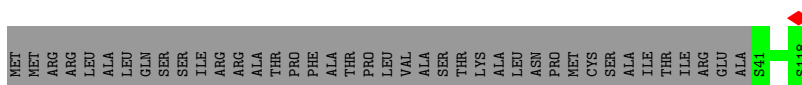
- Molecule 22: ATPase subunit 9, putative



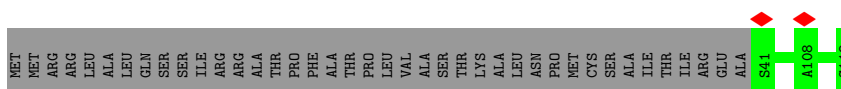
- Molecule 22: ATPase subunit 9, putative



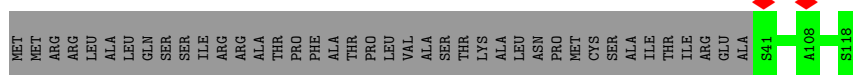
- Molecule 22: ATPase subunit 9, putative



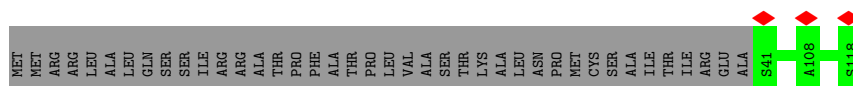
- Molecule 22: ATPase subunit 9, putative



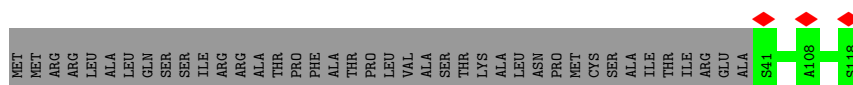
- Molecule 22: ATPase subunit 9, putative



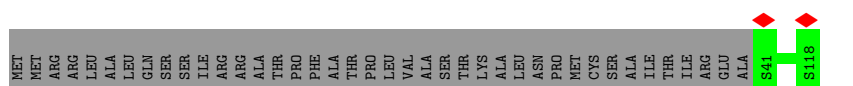
• Molecule 22: ATPase subunit 9, putative



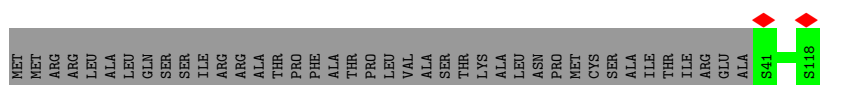
• Molecule 22: ATPase subunit 9, putative



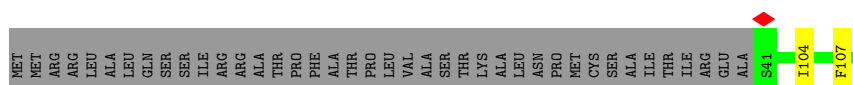
• Molecule 22: ATPase subunit 9, putative



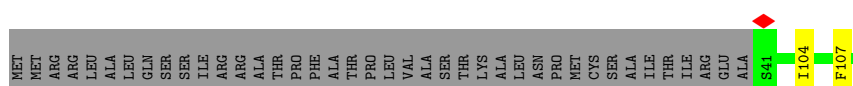
• Molecule 22: ATPase subunit 9, putative




• Molecule 22: ATPase subunit 9, putative

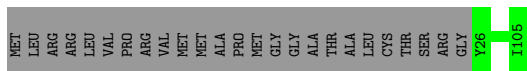


• Molecule 22: ATPase subunit 9, putative




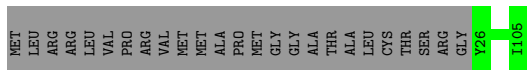
- Molecule 23: subunit-b

Chain P:  76% 24%




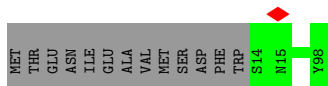
- Molecule 23: subunit-b

Chain p:  76% 24%




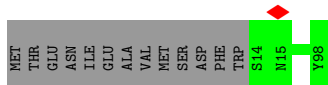
- Molecule 24: ATPEG3

Chain Q:  87% 13%



- Molecule 24: ATPEG3

Chain q:  87% 13%



- Molecule 25: ATPEG4

Chain R:  100%

There are no outlier residues recorded for this chain.

- Molecule 25: ATPEG4

Chain r:  100%

There are no outlier residues recorded for this chain.

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
Maximum map value	0.091	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	464.8, 464.8, 464.8	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.34	0/2111	0.41	0/2861
1	a	0.34	0/2111	0.41	0/2861
2	A1	0.24	0/4159	0.47	0/5632
2	A2	0.24	0/4159	0.47	0/5632
2	B1	0.24	0/4110	0.46	0/5566
2	B2	0.24	0/4110	0.46	0/5566
2	C1	0.24	0/4113	0.47	0/5569
2	C2	0.24	0/4113	0.47	0/5569
3	C	0.30	0/772	0.44	0/1054
3	c	0.30	0/772	0.45	0/1054
4	D	0.25	0/2786	0.50	0/3760
4	d	0.25	0/2786	0.50	0/3760
5	D1	0.24	0/3745	0.46	0/5077
5	D2	0.24	0/3745	0.47	0/5077
5	E1	0.24	0/3738	0.46	0/5067
5	E2	0.24	0/3738	0.46	0/5067
5	F1	0.24	0/3760	0.47	0/5098
5	F2	0.24	0/3760	0.47	0/5098
6	E	0.28	0/3305	0.45	0/4482
6	e	0.28	0/3305	0.45	0/4482
7	F	0.31	0/1183	0.50	0/1601
7	f	0.31	0/1183	0.50	0/1601
8	G	0.24	0/1953	0.45	0/2650
8	g	0.24	0/1953	0.45	0/2650
9	G1	0.24	0/2427	0.47	0/3268
9	G2	0.24	0/2427	0.47	0/3268
10	H	0.24	0/1088	0.39	0/1466
10	h	0.24	0/1088	0.39	0/1466
11	H1	0.25	0/1274	0.45	0/1728
11	H2	0.25	0/1274	0.45	0/1728
12	I	0.30	0/913	0.47	0/1240
12	i	0.30	0/913	0.47	0/1240

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
13	I1	0.23	0/547	0.48	0/738
13	I2	0.23	0/547	0.48	0/738
14	J	0.27	0/1462	0.48	0/1973
14	j	0.27	0/1462	0.48	0/1973
15	J1	0.23	0/1341	0.39	0/1810
15	J2	0.23	0/1341	0.39	0/1810
15	K1	0.23	0/1342	0.38	0/1810
15	K2	0.23	0/1342	0.38	0/1810
15	L1	0.23	0/1337	0.39	0/1803
15	L2	0.23	0/1337	0.38	0/1803
16	K	0.27	0/904	0.49	0/1228
16	k	0.27	0/904	0.49	0/1228
17	L	0.27	0/547	0.44	0/735
17	l	0.27	0/547	0.44	0/735
18	M	0.29	0/1049	0.44	0/1423
18	m	0.29	0/1049	0.44	0/1423
19	M1	0.24	0/1916	0.41	0/2591
19	M2	0.24	0/1916	0.41	0/2591
20	N	0.30	0/1166	0.45	0/1581
20	n	0.30	0/1166	0.45	0/1581
21	O	0.27	0/814	0.39	0/1100
21	o	0.27	0/814	0.39	0/1100
22	O1	0.25	0/574	0.40	0/777
22	O2	0.25	0/574	0.41	0/777
22	P1	0.26	0/574	0.41	0/777
22	P2	0.26	0/574	0.41	0/777
22	Q1	0.25	0/574	0.40	0/777
22	Q2	0.25	0/574	0.40	0/777
22	R1	0.25	0/574	0.40	0/777
22	R2	0.25	0/574	0.40	0/777
22	S1	0.25	0/574	0.39	0/777
22	S2	0.24	0/574	0.39	0/777
22	T1	0.25	0/574	0.39	0/777
22	T2	0.25	0/574	0.39	0/777
22	U1	0.24	0/574	0.38	0/777
22	U2	0.24	0/574	0.38	0/777
22	V1	0.24	0/574	0.38	0/777
22	V2	0.24	0/574	0.38	0/777
22	W1	0.25	0/574	0.39	0/777
22	W2	0.25	0/574	0.39	0/777
22	X1	0.25	0/574	0.38	0/777
22	X2	0.25	0/574	0.38	0/777
23	P	0.30	0/707	0.44	0/957

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
23	p	0.30	0/707	0.44	0/957
24	Q	0.29	0/799	0.50	0/1091
24	q	0.29	0/799	0.50	0/1091
25	R	0.32	0/567	0.45	0/767
25	r	0.32	0/567	0.45	0/767
All	All	0.26	0/123350	0.45	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](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	47	79
2	C2	517/584 (88%)	512 (99%)	4 (1%)	1 (0%)	47	79
3	C	84/114 (74%)	83 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	223 (99%)	2 (1%)	78	91
1	a	225/225 (100%)	223 (99%)	2 (1%)	78	91
2	A1	439/479 (92%)	438 (100%)	1 (0%)	93	98
2	A2	439/479 (92%)	438 (100%)	1 (0%)	93	98
2	B1	435/479 (91%)	433 (100%)	2 (0%)	88	95
2	B2	435/479 (91%)	433 (100%)	2 (0%)	88	95
2	C1	434/479 (91%)	433 (100%)	1 (0%)	93	98
2	C2	434/479 (91%)	433 (100%)	1 (0%)	93	98
3	C	80/104 (77%)	78 (98%)	2 (2%)	47	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	c	80/104 (77%)	78 (98%)	2 (2%)	47	77
4	D	297/334 (89%)	296 (100%)	1 (0%)	92	96
4	d	297/334 (89%)	296 (100%)	1 (0%)	92	96
5	D1	398/420 (95%)	397 (100%)	1 (0%)	92	96
5	D2	398/420 (95%)	397 (100%)	1 (0%)	92	96
5	E1	397/420 (94%)	396 (100%)	1 (0%)	92	96
5	E2	397/420 (94%)	396 (100%)	1 (0%)	92	96
5	F1	400/420 (95%)	399 (100%)	1 (0%)	92	96
5	F2	400/420 (95%)	399 (100%)	1 (0%)	92	96
6	E	334/341 (98%)	332 (99%)	2 (1%)	86	94
6	e	334/341 (98%)	332 (99%)	2 (1%)	86	94
7	F	119/124 (96%)	118 (99%)	1 (1%)	81	93
7	f	119/124 (96%)	118 (99%)	1 (1%)	81	93
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%)	251 (99%)	2 (1%)	81	93
9	G2	253/257 (98%)	251 (99%)	2 (1%)	81	93
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%)	84	94
11	H2	137/156 (88%)	136 (99%)	1 (1%)	84	94
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	78	91
18	m	111/124 (90%)	110 (99%)	1 (1%)	78	91
19	M1	200/215 (93%)	199 (100%)	1 (0%)	88	95
19	M2	200/215 (93%)	199 (100%)	1 (0%)	88	95
20	N	123/137 (90%)	122 (99%)	1 (1%)	81	93
20	n	123/137 (90%)	122 (99%)	1 (1%)	81	93
21	O	82/86 (95%)	81 (99%)	1 (1%)	71	88
21	o	82/86 (95%)	81 (99%)	1 (1%)	71	88
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	W2	56/89 (63%)	56 (100%)	0	100	100
22	X1	56/89 (63%)	54 (96%)	2 (4%)	35	69
22	X2	56/89 (63%)	54 (96%)	2 (4%)	35	69
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
All	All	12866/14484 (89%)	12818 (100%)	48 (0%)	91	95

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	PHE
1	A	169	PHE
2	A1	181	TYR
2	A2	181	TYR
2	B1	181	TYR
2	B1	281	TYR
2	B2	181	TYR
2	B2	281	TYR
3	C	66	TYR
3	C	93	THR
2	C1	181	TYR
2	C2	181	TYR
4	D	145	ARG
5	D1	171	LEU
5	D2	171	LEU
6	E	226	THR
6	E	268	TYR
5	E1	171	LEU
5	E2	171	LEU
7	F	42	ASN
5	F1	171	LEU
5	F2	171	LEU
9	G1	18	PHE
9	G1	237	GLU
9	G2	18	PHE

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Mol	Chain	Res	Type
9	G2	237	GLU
11	H1	41	HIS
11	H2	41	HIS
18	M	109	VAL
19	M1	247	ASP
19	M2	247	ASP
20	N	132	GLU
21	O	64	TYR
22	X1	104	ILE
22	X1	107	PHE
22	X2	104	ILE
22	X2	107	PHE
1	a	144	PHE
1	a	169	PHE
3	c	66	TYR
3	c	93	THR
4	d	145	ARG
6	e	226	THR
6	e	268	TYR
7	f	42	ASN
18	m	109	VAL
20	n	132	GLU
21	o	64	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
2	A1	339	HIS
2	A2	339	HIS
3	C	101	GLN
9	G1	162	ASN
9	G1	233	ASN
9	G2	162	ASN
9	G2	233	ASN
15	J1	93	ASN
15	J2	93	ASN
15	K1	82	GLN
22	V1	75	ASN
22	V2	75	ASN
1	a	150	ASN

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	0.24	0	9,11,13	0.49	0
6	AME	e	1	6	9,10,11	0.25	0	9,11,13	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
6	AME	E	1	6	-	2/9/10/12	-
6	AME	e	1	6	-	2/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) 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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	j	202	-	99,99,99	0.29	0	105,111,111	0.26	0
28	CDL	E	406	-	99,99,99	0.29	0	105,111,111	0.25	0
26	ATP	A1	601	27	26,33,33	0.60	0	31,52,52	0.60	1 (3%)
26	ATP	B2	601	27	26,33,33	0.61	0	31,52,52	0.61	1 (3%)
28	CDL	Q	101	-	99,99,99	0.29	0	105,111,111	0.29	0
31	Q7G	E	402	-	54,54,90	0.13	0	82,84,138	0.32	0
33	PC1	J	204	-	53,53,53	0.28	0	59,61,61	0.27	0
32	PEE	r	101	-	50,50,50	0.74	2 (4%)	53,55,55	0.51	0
26	ATP	F2	601	27	26,33,33	0.62	0	31,52,52	0.60	1 (3%)
34	UTP	H2	201	-	22,30,30	0.91	1 (4%)	27,47,47	0.85	1 (3%)
26	ATP	F1	601	27	26,33,33	0.62	0	31,52,52	0.60	1 (3%)
28	CDL	J	203	-	99,99,99	0.29	0	105,111,111	0.26	0
31	Q7G	e	407	-	54,54,90	0.13	0	82,84,138	0.31	0
33	PC1	j	203	-	53,53,53	0.29	0	59,61,61	0.27	0
30	LMT	j	204	-	36,36,36	0.17	0	47,47,47	0.54	0
29	ADP	D1	601	27	24,29,29	0.70	0	29,45,45	0.79	1 (3%)
33	PC1	I	201	-	53,53,53	0.28	0	59,61,61	0.27	0
33	PC1	f	204	-	53,53,53	0.27	0	59,61,61	0.27	0
28	CDL	q	101	-	99,99,99	0.29	0	105,111,111	0.29	0
26	ATP	A2	601	27	26,33,33	0.61	0	31,52,52	0.61	1 (3%)
30	LMT	E	401	-	36,36,36	0.15	0	47,47,47	0.46	1 (2%)
26	ATP	C1	601	27	26,33,33	0.61	0	31,52,52	0.61	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	UTP	H1	201	-	22,30,30	0.91	1 (4%)	27,47,47	0.85	1 (3%)
28	CDL	e	401	-	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	0.28	0
29	ADP	D2	601	27	24,29,29	0.69	0	29,45,45	0.79	1 (3%)
30	LMT	e	406	-	36,36,36	0.15	0	47,47,47	0.47	1 (2%)
28	CDL	e	402	-	99,99,99	0.30	0	105,111,111	0.28	0
28	CDL	e	404	-	99,99,99	0.29	0	105,111,111	0.25	0
33	PC1	i	201	-	53,53,53	0.29	0	59,61,61	0.27	0
28	CDL	e	405	-	99,99,99	0.29	0	105,111,111	0.26	0
31	Q7G	N	201	-	66,66,90	0.13	0	100,102,138	0.31	0
28	CDL	E	403	-	99,99,99	0.29	0	105,111,111	0.26	0
28	CDL	j	201	-	99,99,99	0.29	0	105,111,111	0.25	0
28	CDL	C	201	-	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	F	201	-	99,99,99	0.29	0	105,111,111	0.26	0
28	CDL	E	404	-	99,99,99	0.30	0	105,111,111	0.28	0
26	ATP	B1	601	27	26,33,33	0.61	0	31,52,52	0.61	1 (3%)
28	CDL	M	201	-	99,99,99	0.30	0	105,111,111	0.28	0
26	ATP	C2	601	27	26,33,33	0.61	0	31,52,52	0.61	1 (3%)
28	CDL	l	101	-	99,99,99	0.30	0	105,111,111	0.26	0
32	PEE	f	202	-	50,50,50	0.76	2 (4%)	53,55,55	0.45	0
33	PC1	F	203	-	53,53,53	0.28	0	59,61,61	0.27	0
33	PC1	f	203	-	53,53,53	0.28	0	59,61,61	0.28	0
32	PEE	F	202	-	50,50,50	0.76	2 (4%)	53,55,55	0.45	0
28	CDL	e	403	-	99,99,99	0.29	0	105,111,111	0.26	0
32	PEE	R	101	-	50,50,50	0.73	2 (4%)	53,55,55	0.51	0
28	CDL	L	101	-	99,99,99	0.29	0	105,111,111	0.25	0
33	PC1	F	204	-	53,53,53	0.27	0	59,61,61	0.27	0
28	CDL	f	201	-	99,99,99	0.29	0	105,111,111	0.26	0
30	LMT	J	201	-	36,36,36	0.16	0	47,47,47	0.54	0
31	Q7G	n	201	-	66,66,90	0.14	0	100,102,138	0.31	0
28	CDL	E	407	-	99,99,99	0.29	0	105,111,111	0.26	0
28	CDL	E	405	-	99,99,99	0.29	0	105,111,111	0.27	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	j	202	-	-	29/110/110/110	-
28	CDL	E	406	-	-	19/110/110/110	-
26	ATP	A1	601	27	-	5/18/38/38	0/3/3/3
31	Q7G	E	402	-	1/1/19/34	5/15/123/200	0/7/7/10
26	ATP	B2	601	27	-	4/18/38/38	0/3/3/3
28	CDL	Q	101	-	-	28/110/110/110	-
33	PC1	J	204	-	-	14/57/57/57	-
32	PEE	r	101	-	-	29/54/54/54	-
26	ATP	F2	601	27	-	4/18/38/38	0/3/3/3
34	UTP	H2	201	-	-	5/20/38/38	0/2/2/2
26	ATP	F1	601	27	-	4/18/38/38	0/3/3/3
28	CDL	J	203	-	-	29/110/110/110	-
31	Q7G	e	407	-	1/1/19/34	5/15/123/200	0/7/7/10
33	PC1	j	203	-	-	14/57/57/57	-
30	LMT	j	204	-	-	5/21/61/61	0/2/2/2
29	ADP	D1	601	27	-	1/12/32/32	0/3/3/3
33	PC1	I	201	-	-	10/57/57/57	-
33	PC1	f	204	-	-	10/57/57/57	-
28	CDL	q	101	-	-	28/110/110/110	-
26	ATP	A2	601	27	-	5/18/38/38	0/3/3/3
30	LMT	E	401	-	-	1/21/61/61	0/2/2/2
26	ATP	C1	601	27	-	6/18/38/38	0/3/3/3
34	UTP	H1	201	-	-	4/20/38/38	0/2/2/2
28	CDL	e	401	-	-	23/110/110/110	-
28	CDL	m	201	-	-	41/110/110/110	-
29	ADP	D2	601	27	-	1/12/32/32	0/3/3/3
30	LMT	e	406	-	-	1/21/61/61	0/2/2/2
28	CDL	e	402	-	-	30/110/110/110	-
28	CDL	e	404	-	-	19/110/110/110	-
33	PC1	i	201	-	-	10/57/57/57	-
31	Q7G	N	201	-	2/2/24/34	6/20/148/200	0/8/8/10
28	CDL	e	405	-	-	34/110/110/110	-
28	CDL	E	403	-	-	23/110/110/110	-
28	CDL	j	201	-	-	25/110/110/110	-
28	CDL	C	201	-	-	24/110/110/110	-
28	CDL	c	201	-	-	24/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CDL	J	202	-	-	25/110/110/110	-
28	CDL	F	201	-	-	22/110/110/110	-
28	CDL	E	404	-	-	30/110/110/110	-
26	ATP	B1	601	27	-	4/18/38/38	0/3/3/3
28	CDL	M	201	-	-	42/110/110/110	-
26	ATP	C2	601	27	-	6/18/38/38	0/3/3/3
28	CDL	l	101	-	-	23/110/110/110	-
32	PEE	f	202	-	-	17/54/54/54	-
33	PC1	F	203	-	-	10/57/57/57	-
33	PC1	f	203	-	-	10/57/57/57	-
32	PEE	F	202	-	-	17/54/54/54	-
28	CDL	e	403	-	-	30/110/110/110	-
32	PEE	R	101	-	-	29/54/54/54	-
28	CDL	L	101	-	-	23/110/110/110	-
33	PC1	F	204	-	-	10/57/57/57	-
28	CDL	f	201	-	-	22/110/110/110	-
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
28	CDL	E	407	-	-	35/110/110/110	-
28	CDL	E	405	-	-	30/110/110/110	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	f	202	PEE	C39-C38	3.57	1.52	1.31
32	F	202	PEE	C39-C38	3.56	1.52	1.31
32	f	202	PEE	C18-C19	3.51	1.52	1.31
32	F	202	PEE	C18-C19	3.51	1.52	1.31
32	r	101	PEE	C18-C19	3.46	1.51	1.31
32	R	101	PEE	C18-C19	3.45	1.51	1.31
32	r	101	PEE	C39-C38	3.35	1.51	1.31
32	R	101	PEE	C39-C38	3.35	1.51	1.31
34	H2	201	UTP	C4-N3	3.08	1.38	1.33
34	H1	201	UTP	C4-N3	3.05	1.38	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	H2	201	UTP	C5-C4-N3	-3.87	114.79	123.31
34	H1	201	UTP	C5-C4-N3	-3.86	114.82	123.31
26	C2	601	ATP	C5-C6-N6	2.35	123.92	120.35
26	B2	601	ATP	C5-C6-N6	2.35	123.92	120.35
29	D1	601	ADP	C5-C6-N6	2.34	123.90	120.35
29	D2	601	ADP	C5-C6-N6	2.34	123.90	120.35
26	C1	601	ATP	C5-C6-N6	2.33	123.90	120.35
26	F1	601	ATP	C5-C6-N6	2.33	123.89	120.35
26	A2	601	ATP	C5-C6-N6	2.33	123.89	120.35
26	F2	601	ATP	C5-C6-N6	2.31	123.87	120.35
26	B1	601	ATP	C5-C6-N6	2.31	123.86	120.35
26	A1	601	ATP	C5-C6-N6	2.31	123.86	120.35
30	e	406	LMT	C1'-O5'-C5'	-2.09	109.58	113.69
30	E	401	LMT	C1'-O5'-C5'	-2.08	109.61	113.69

All (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
31	n	201	Q7G	C1C

All (921) 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
26	C2	601	ATP	PB-O3B-PG-O2G
26	F1	601	ATP	PB-O3B-PG-O2G
26	F2	601	ATP	PB-O3B-PG-O2G
28	C	201	CDL	CB3-OB5-PB2-OB4
28	E	403	CDL	CB2-OB2-PB2-OB3
28	E	403	CDL	CB2-OB2-PB2-OB4
28	E	403	CDL	CB2-OB2-PB2-OB5
28	E	403	CDL	CB3-OB5-PB2-OB3
28	E	404	CDL	CA3-OA5-PA1-OA2
28	E	404	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
28	E	404	CDL	CA3-OA5-PA1-OA4
28	E	406	CDL	CA3-OA5-PA1-OA4
28	E	406	CDL	CB3-OB5-PB2-OB3
28	E	406	CDL	CB3-OB5-PB2-OB4
28	E	407	CDL	CA3-OA5-PA1-OA2
28	E	407	CDL	CA3-OA5-PA1-OA3
28	E	407	CDL	CA3-OA5-PA1-OA4
28	E	407	CDL	CB3-OB5-PB2-OB4
28	E	407	CDL	OB5-CB3-CB4-OB6
28	J	202	CDL	CB2-C1-CA2-OA2
28	J	202	CDL	CA2-OA2-PA1-OA3
28	J	202	CDL	CA3-OA5-PA1-OA2
28	J	202	CDL	CA3-OA5-PA1-OA3
28	J	202	CDL	CA3-OA5-PA1-OA4
28	J	203	CDL	CA2-OA2-PA1-OA4
28	J	203	CDL	CB3-OB5-PB2-OB4
28	L	101	CDL	CA2-OA2-PA1-OA3
28	L	101	CDL	CA2-OA2-PA1-OA4
28	L	101	CDL	CB2-OB2-PB2-OB5
28	M	201	CDL	CA3-OA5-PA1-OA3
28	M	201	CDL	CA3-OA5-PA1-OA4
28	M	201	CDL	OA6-CA4-CA6-OA8
28	M	201	CDL	CB2-OB2-PB2-OB3
28	M	201	CDL	CB2-OB2-PB2-OB4
28	M	201	CDL	CB2-OB2-PB2-OB5
28	M	201	CDL	CB3-OB5-PB2-OB3
28	Q	101	CDL	OA5-CA3-CA4-OA6
28	Q	101	CDL	CB2-OB2-PB2-OB3
28	Q	101	CDL	CB2-OB2-PB2-OB4
28	Q	101	CDL	CB3-OB5-PB2-OB3
28	c	201	CDL	CB3-OB5-PB2-OB4
28	e	401	CDL	CB2-OB2-PB2-OB3
28	e	401	CDL	CB2-OB2-PB2-OB4
28	e	401	CDL	CB2-OB2-PB2-OB5
28	e	401	CDL	CB3-OB5-PB2-OB3
28	e	402	CDL	CA3-OA5-PA1-OA2
28	e	402	CDL	CA3-OA5-PA1-OA3
28	e	402	CDL	CA3-OA5-PA1-OA4
28	e	404	CDL	CA3-OA5-PA1-OA4
28	e	404	CDL	CB3-OB5-PB2-OB3
28	e	404	CDL	CB3-OB5-PB2-OB4
28	e	405	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
28	e	405	CDL	CA3-OA5-PA1-OA3
28	e	405	CDL	CA3-OA5-PA1-OA4
28	e	405	CDL	CB3-OB5-PB2-OB4
28	e	405	CDL	OB5-CB3-CB4-OB6
28	j	201	CDL	CB2-C1-CA2-OA2
28	j	201	CDL	CA2-OA2-PA1-OA3
28	j	201	CDL	CA3-OA5-PA1-OA2
28	j	201	CDL	CA3-OA5-PA1-OA3
28	j	201	CDL	CA3-OA5-PA1-OA4
28	j	202	CDL	CA2-OA2-PA1-OA4
28	j	202	CDL	CB3-OB5-PB2-OB4
28	l	101	CDL	CA2-OA2-PA1-OA3
28	l	101	CDL	CA2-OA2-PA1-OA4
28	l	101	CDL	CB2-OB2-PB2-OB5
28	m	201	CDL	CA3-OA5-PA1-OA3
28	m	201	CDL	CA3-OA5-PA1-OA4
28	m	201	CDL	OA6-CA4-CA6-OA8
28	m	201	CDL	CB2-OB2-PB2-OB3
28	m	201	CDL	CB2-OB2-PB2-OB4
28	m	201	CDL	CB2-OB2-PB2-OB5
28	m	201	CDL	CB3-OB5-PB2-OB3
28	q	101	CDL	OA5-CA3-CA4-OA6
28	q	101	CDL	CB2-OB2-PB2-OB3
28	q	101	CDL	CB2-OB2-PB2-OB4
28	q	101	CDL	CB3-OB5-PB2-OB3
30	J	201	LMT	O5'-C1'-O1'-C1
30	J	201	LMT	C2-C1-O1'-C1'
30	j	204	LMT	O5'-C1'-O1'-C1
30	j	204	LMT	C2-C1-O1'-C1'
31	E	402	Q7G	C2B-C1B-O1B-C24
31	E	402	Q7G	O5B-C1B-O1B-C24
31	E	402	Q7G	CG1-C22-C23-C48
31	N	201	Q7G	C2B-C1B-O1B-C24
31	N	201	Q7G	O5B-C1B-O1B-C24
31	e	407	Q7G	C2B-C1B-O1B-C24
31	e	407	Q7G	O5B-C1B-O1B-C24
31	e	407	Q7G	CG1-C22-C23-C48
31	n	201	Q7G	C2B-C1B-O1B-C24
31	n	201	Q7G	O5B-C1B-O1B-C24
32	F	202	PEE	C1-O3P-P-O2P
32	F	202	PEE	C1-O3P-P-O1P
32	R	101	PEE	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
32	R	101	PEE	C4-O4P-P-O2P
32	R	101	PEE	C4-O4P-P-O1P
32	R	101	PEE	O4P-C4-C5-N
32	f	202	PEE	C1-O3P-P-O2P
32	f	202	PEE	C1-O3P-P-O1P
32	r	101	PEE	C4-O4P-P-O3P
32	r	101	PEE	C4-O4P-P-O2P
32	r	101	PEE	C4-O4P-P-O1P
32	r	101	PEE	O4P-C4-C5-N
33	F	203	PC1	C11-O13-P-O12
33	F	203	PC1	C1-O11-P-O14
33	F	204	PC1	O13-C11-C12-N
33	I	201	PC1	C11-O13-P-O12
33	I	201	PC1	C11-O13-P-O14
33	I	201	PC1	C11-O13-P-O11
33	I	201	PC1	O13-C11-C12-N
33	J	204	PC1	C11-O13-P-O14
33	J	204	PC1	C1-O11-P-O12
33	J	204	PC1	C1-O11-P-O14
33	J	204	PC1	C1-O11-P-O13
33	f	203	PC1	C11-O13-P-O12
33	f	203	PC1	C1-O11-P-O14
33	f	204	PC1	O13-C11-C12-N
33	i	201	PC1	C11-O13-P-O12
33	i	201	PC1	C11-O13-P-O14
33	i	201	PC1	C11-O13-P-O11
33	i	201	PC1	O13-C11-C12-N
33	j	203	PC1	C11-O13-P-O14
33	j	203	PC1	C1-O11-P-O12
33	j	203	PC1	C1-O11-P-O14
33	j	203	PC1	C1-O11-P-O13
34	H1	201	UTP	C5'-O5'-PA-O2A
34	H1	201	UTP	C5'-O5'-PA-O3A
34	H2	201	UTP	C5'-O5'-PA-O2A
34	H2	201	UTP	C5'-O5'-PA-O3A
28	C	201	CDL	O1-C1-CA2-OA2
28	J	202	CDL	O1-C1-CA2-OA2
28	M	201	CDL	O1-C1-CB2-OB2
28	c	201	CDL	O1-C1-CA2-OA2
28	j	201	CDL	O1-C1-CA2-OA2
28	m	201	CDL	O1-C1-CB2-OB2
28	E	405	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
28	e	403	CDL	C11-CA5-OA6-CA4
28	E	403	CDL	C77-C78-C79-C80
28	e	401	CDL	C77-C78-C79-C80
28	E	405	CDL	OA7-CA5-OA6-CA4
28	e	403	CDL	OA7-CA5-OA6-CA4
28	M	201	CDL	CA2-C1-CB2-OB2
28	Q	101	CDL	CA2-C1-CB2-OB2
28	m	201	CDL	CA2-C1-CB2-OB2
28	q	101	CDL	CA2-C1-CB2-OB2
28	M	201	CDL	C34-C35-C36-C37
28	m	201	CDL	C34-C35-C36-C37
32	R	101	PEE	C31-C32-C33-C34
32	r	101	PEE	C31-C32-C33-C34
28	L	101	CDL	O1-C1-CA2-OA2
28	l	101	CDL	O1-C1-CA2-OA2
30	J	201	LMT	C2'-C1'-O1'-C1
30	j	204	LMT	C2'-C1'-O1'-C1
28	E	404	CDL	C31-CA7-OA8-CA6
28	e	402	CDL	C31-CA7-OA8-CA6
28	E	407	CDL	CA7-C31-C32-C33
28	M	201	CDL	CB5-C51-C52-C53
28	e	405	CDL	CA7-C31-C32-C33
28	m	201	CDL	CB5-C51-C52-C53
28	M	201	CDL	CA5-C11-C12-C13
28	m	201	CDL	CA5-C11-C12-C13
28	E	406	CDL	O1-C1-CA2-OA2
28	Q	101	CDL	O1-C1-CB2-OB2
28	e	404	CDL	O1-C1-CA2-OA2
28	q	101	CDL	O1-C1-CB2-OB2
28	E	407	CDL	C11-CA5-OA6-CA4
28	M	201	CDL	C51-CB5-OB6-CB4
28	e	405	CDL	C11-CA5-OA6-CA4
28	m	201	CDL	C51-CB5-OB6-CB4
28	C	201	CDL	CB3-OB5-PB2-OB2
28	E	403	CDL	CB3-OB5-PB2-OB2
28	E	406	CDL	CA3-OA5-PA1-OA2
28	E	406	CDL	CB3-OB5-PB2-OB2
28	E	407	CDL	CB3-OB5-PB2-OB2
28	F	201	CDL	CA2-OA2-PA1-OA5
28	F	201	CDL	CB3-OB5-PB2-OB2
28	J	203	CDL	CB3-OB5-PB2-OB2
28	L	101	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
28	L	101	CDL	CA3-OA5-PA1-OA2
28	M	201	CDL	CA3-OA5-PA1-OA2
28	M	201	CDL	CB3-OB5-PB2-OB2
28	Q	101	CDL	CA2-OA2-PA1-OA5
28	Q	101	CDL	CB2-OB2-PB2-OB5
28	c	201	CDL	CB3-OB5-PB2-OB2
28	e	401	CDL	CB3-OB5-PB2-OB2
28	e	404	CDL	CA3-OA5-PA1-OA2
28	e	404	CDL	CB3-OB5-PB2-OB2
28	e	405	CDL	CB3-OB5-PB2-OB2
28	f	201	CDL	CA2-OA2-PA1-OA5
28	f	201	CDL	CB3-OB5-PB2-OB2
28	j	202	CDL	CB3-OB5-PB2-OB2
28	l	101	CDL	CA2-OA2-PA1-OA5
28	l	101	CDL	CA3-OA5-PA1-OA2
28	m	201	CDL	CA3-OA5-PA1-OA2
28	m	201	CDL	CB3-OB5-PB2-OB2
28	q	101	CDL	CA2-OA2-PA1-OA5
28	q	101	CDL	CB2-OB2-PB2-OB5
32	F	202	PEE	C1-O3P-P-O4P
32	F	202	PEE	C4-O4P-P-O3P
32	f	202	PEE	C1-O3P-P-O4P
32	f	202	PEE	C4-O4P-P-O3P
33	F	203	PC1	C11-O13-P-O11
33	F	203	PC1	C1-O11-P-O13
33	F	204	PC1	C11-O13-P-O11
33	J	204	PC1	C11-O13-P-O11
33	f	203	PC1	C11-O13-P-O11
33	f	203	PC1	C1-O11-P-O13
33	f	204	PC1	C11-O13-P-O11
33	j	203	PC1	C11-O13-P-O11
28	E	404	CDL	OA9-CA7-OA8-CA6
28	e	402	CDL	OA9-CA7-OA8-CA6
28	E	404	CDL	C74-C75-C76-C77
28	e	402	CDL	C74-C75-C76-C77
28	C	201	CDL	CB2-C1-CA2-OA2
28	J	203	CDL	CA2-C1-CB2-OB2
28	c	201	CDL	CB2-C1-CA2-OA2
28	j	202	CDL	CA2-C1-CB2-OB2
28	E	407	CDL	OA7-CA5-OA6-CA4
28	e	405	CDL	OA7-CA5-OA6-CA4
28	M	201	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
28	m	201	CDL	OB7-CB5-OB6-CB4
28	J	202	CDL	CA7-C31-C32-C33
28	j	201	CDL	CA7-C31-C32-C33
28	M	201	CDL	OA5-CA3-CA4-OA6
28	m	201	CDL	OA5-CA3-CA4-OA6
28	E	406	CDL	O1-C1-CB2-OB2
28	J	203	CDL	O1-C1-CB2-OB2
28	e	404	CDL	O1-C1-CB2-OB2
28	j	202	CDL	O1-C1-CB2-OB2
28	J	203	CDL	C74-C75-C76-C77
28	j	202	CDL	C74-C75-C76-C77
28	J	202	CDL	C13-C14-C15-C16
28	j	201	CDL	C13-C14-C15-C16
28	Q	101	CDL	OA7-CA5-OA6-CA4
28	q	101	CDL	OA7-CA5-OA6-CA4
28	Q	101	CDL	C11-CA5-OA6-CA4
28	q	101	CDL	C11-CA5-OA6-CA4
28	J	203	CDL	C78-C79-C80-C81
28	j	202	CDL	C78-C79-C80-C81
28	E	405	CDL	C71-C72-C73-C74
28	e	403	CDL	C71-C72-C73-C74
30	E	401	LMT	C2-C1-O1'-C1'
30	e	406	LMT	C2-C1-O1'-C1'
28	M	201	CDL	CA7-C31-C32-C33
28	m	201	CDL	CA7-C31-C32-C33
28	C	201	CDL	C55-C56-C57-C58
28	c	201	CDL	C55-C56-C57-C58
28	J	203	CDL	C11-CA5-OA6-CA4
28	j	202	CDL	C11-CA5-OA6-CA4
31	E	402	Q7G	CG1-C22-C23-C24
31	e	407	Q7G	CG1-C22-C23-C24
28	E	406	CDL	CA2-C1-CB2-OB2
28	e	404	CDL	CA2-C1-CB2-OB2
28	E	405	CDL	C14-C15-C16-C17
28	e	403	CDL	C14-C15-C16-C17
28	J	203	CDL	OA7-CA5-OA6-CA4
28	j	202	CDL	OA7-CA5-OA6-CA4
28	E	406	CDL	C17-C18-C19-C20
28	M	201	CDL	C36-C37-C38-C39
28	e	404	CDL	C17-C18-C19-C20
28	m	201	CDL	C36-C37-C38-C39
28	J	203	CDL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
28	j	202	CDL	C15-C16-C17-C18
28	q	101	CDL	CB7-C71-C72-C73
28	E	405	CDL	C78-C79-C80-C81
28	e	403	CDL	C78-C79-C80-C81
28	Q	101	CDL	CB7-C71-C72-C73
28	E	407	CDL	C40-C41-C42-C43
28	e	405	CDL	C40-C41-C42-C43
28	J	202	CDL	C81-C82-C83-C84
28	j	201	CDL	C81-C82-C83-C84
28	Q	101	CDL	CA5-C11-C12-C13
28	q	101	CDL	CA5-C11-C12-C13
28	E	406	CDL	C11-CA5-OA6-CA4
28	J	203	CDL	C51-CB5-OB6-CB4
28	e	404	CDL	C11-CA5-OA6-CA4
28	j	202	CDL	C51-CB5-OB6-CB4
32	F	202	PEE	C11-C10-O2-C2
32	f	202	PEE	C11-C10-O2-C2
28	E	405	CDL	O1-C1-CA2-OA2
28	e	403	CDL	O1-C1-CA2-OA2
28	E	406	CDL	OA7-CA5-OA6-CA4
28	J	203	CDL	OB7-CB5-OB6-CB4
28	e	404	CDL	OA7-CA5-OA6-CA4
28	j	202	CDL	OB7-CB5-OB6-CB4
28	C	201	CDL	C34-C35-C36-C37
28	E	407	CDL	C57-C58-C59-C60
28	c	201	CDL	C34-C35-C36-C37
28	e	405	CDL	C57-C58-C59-C60
28	E	407	CDL	C56-C57-C58-C59
28	J	202	CDL	C34-C35-C36-C37
28	e	405	CDL	C56-C57-C58-C59
28	j	201	CDL	C34-C35-C36-C37
28	E	407	CDL	C71-C72-C73-C74
28	e	405	CDL	C71-C72-C73-C74
28	m	201	CDL	C12-C13-C14-C15
32	F	202	PEE	C42-C43-C44-C45
32	f	202	PEE	C42-C43-C44-C45
31	N	201	Q7G	O5C-C5C-C6C-O6C
31	n	201	Q7G	O5C-C5C-C6C-O6C
28	M	201	CDL	C12-C13-C14-C15
28	E	405	CDL	C51-CB5-OB6-CB4
28	e	403	CDL	C51-CB5-OB6-CB4
28	J	203	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
28	j	202	CDL	CA2-OA2-PA1-OA5
28	C	201	CDL	OA5-CA3-CA4-CA6
28	J	203	CDL	OA5-CA3-CA4-CA6
28	M	201	CDL	OA5-CA3-CA4-CA6
28	Q	101	CDL	OA5-CA3-CA4-CA6
28	c	201	CDL	OA5-CA3-CA4-CA6
28	j	202	CDL	OA5-CA3-CA4-CA6
28	m	201	CDL	OA5-CA3-CA4-CA6
28	q	101	CDL	OA5-CA3-CA4-CA6
28	J	202	CDL	C62-C63-C64-C65
28	j	201	CDL	C62-C63-C64-C65
28	F	201	CDL	C77-C78-C79-C80
28	M	201	CDL	C33-C34-C35-C36
28	f	201	CDL	C77-C78-C79-C80
28	m	201	CDL	C33-C34-C35-C36
32	R	101	PEE	C22-C23-C24-C25
28	M	201	CDL	C73-C74-C75-C76
32	r	101	PEE	C22-C23-C24-C25
28	m	201	CDL	C73-C74-C75-C76
33	F	203	PC1	C1-C2-C3-O31
33	f	203	PC1	C1-C2-C3-O31
28	C	201	CDL	C51-C52-C53-C54
28	c	201	CDL	C51-C52-C53-C54
28	e	401	CDL	C18-C19-C20-C21
28	E	403	CDL	C18-C19-C20-C21
28	E	405	CDL	C17-C18-C19-C20
28	e	403	CDL	C17-C18-C19-C20
28	E	404	CDL	C11-C12-C13-C14
28	e	402	CDL	C11-C12-C13-C14
30	J	201	LMT	O5B-C5B-C6B-O6B
30	j	204	LMT	O5B-C5B-C6B-O6B
28	E	407	CDL	C76-C77-C78-C79
28	e	401	CDL	C81-C82-C83-C84
28	e	405	CDL	C76-C77-C78-C79
28	E	403	CDL	C81-C82-C83-C84
28	E	407	CDL	C53-C54-C55-C56
28	e	405	CDL	C53-C54-C55-C56
28	L	101	CDL	C14-C15-C16-C17
28	l	101	CDL	C14-C15-C16-C17
28	E	407	CDL	C11-C12-C13-C14
28	e	405	CDL	C11-C12-C13-C14
28	C	201	CDL	CA4-CA6-OA8-CA7

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Mol	Chain	Res	Type	Atoms
28	c	201	CDL	CA4-CA6-OA8-CA7
28	E	406	CDL	OB6-CB4-CB6-OB8
28	F	201	CDL	OB6-CB4-CB6-OB8
28	L	101	CDL	OA6-CA4-CA6-OA8
28	e	404	CDL	OB6-CB4-CB6-OB8
28	f	201	CDL	OB6-CB4-CB6-OB8
28	l	101	CDL	OA6-CA4-CA6-OA8
28	C	201	CDL	C39-C40-C41-C42
28	c	201	CDL	C39-C40-C41-C42
32	r	101	PEE	C23-C24-C25-C26
33	F	204	PC1	C37-C38-C39-C3A
33	f	204	PC1	C37-C38-C39-C3A
32	F	202	PEE	O4-C10-O2-C2
32	f	202	PEE	O4-C10-O2-C2
28	J	203	CDL	C76-C77-C78-C79
32	R	101	PEE	C23-C24-C25-C26
28	j	202	CDL	C76-C77-C78-C79
32	R	101	PEE	C31-C30-O3-C3
32	r	101	PEE	C31-C30-O3-C3
26	F1	601	ATP	PG-O3B-PB-O1B
26	F2	601	ATP	PG-O3B-PB-O1B
28	F	201	CDL	C11-CA5-OA6-CA4
28	f	201	CDL	C11-CA5-OA6-CA4
33	I	201	PC1	C32-C31-O31-C3
33	i	201	PC1	C32-C31-O31-C3
28	E	404	CDL	C78-C79-C80-C81
28	L	101	CDL	C31-C32-C33-C34
28	M	201	CDL	C83-C84-C85-C86
28	l	101	CDL	C31-C32-C33-C34
28	m	201	CDL	C83-C84-C85-C86
32	R	101	PEE	C17-C18-C19-C20
32	r	101	PEE	C17-C18-C19-C20
28	E	407	CDL	CB7-C71-C72-C73
28	e	405	CDL	CB7-C71-C72-C73
28	e	402	CDL	C78-C79-C80-C81
32	r	101	PEE	C43-C44-C45-C46
32	R	101	PEE	C43-C44-C45-C46
28	J	203	CDL	C79-C80-C81-C82
28	j	202	CDL	C79-C80-C81-C82
28	E	405	CDL	CB5-C51-C52-C53
28	e	403	CDL	CB5-C51-C52-C53
28	C	201	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
28	J	202	CDL	CA4-CA3-OA5-PA1
28	c	201	CDL	CA4-CA3-OA5-PA1
28	j	201	CDL	CA4-CA3-OA5-PA1
28	E	405	CDL	C12-C13-C14-C15
28	L	101	CDL	C64-C65-C66-C67
28	e	403	CDL	C12-C13-C14-C15
28	l	101	CDL	C64-C65-C66-C67
28	E	407	CDL	CB3-CB4-CB6-OB8
28	e	405	CDL	CB3-CB4-CB6-OB8
32	F	202	PEE	C1-C2-C3-O3
32	R	101	PEE	C1-C2-C3-O3
32	f	202	PEE	C1-C2-C3-O3
32	r	101	PEE	C1-C2-C3-O3
28	e	403	CDL	C83-C84-C85-C86
28	E	405	CDL	C83-C84-C85-C86
28	F	201	CDL	C12-C13-C14-C15
28	f	201	CDL	C12-C13-C14-C15
28	J	202	CDL	CA2-OA2-PA1-OA5
28	j	201	CDL	CA2-OA2-PA1-OA5
28	C	201	CDL	OA5-CA3-CA4-OA6
28	E	403	CDL	OB5-CB3-CB4-OB6
28	F	201	CDL	OA5-CA3-CA4-OA6
28	c	201	CDL	OA5-CA3-CA4-OA6
28	e	401	CDL	OB5-CB3-CB4-OB6
28	f	201	CDL	OA5-CA3-CA4-OA6
28	E	407	CDL	C59-C60-C61-C62
28	e	405	CDL	C59-C60-C61-C62
28	f	201	CDL	C13-C14-C15-C16
32	R	101	PEE	O5-C30-O3-C3
32	r	101	PEE	O5-C30-O3-C3
28	F	201	CDL	C13-C14-C15-C16
28	e	401	CDL	C43-C44-C45-C46
28	E	403	CDL	C43-C44-C45-C46
33	i	201	PC1	C2C-C2D-C2E-C2F
33	F	203	PC1	O21-C2-C3-O31
33	f	203	PC1	O21-C2-C3-O31
28	J	203	CDL	C72-C73-C74-C75
28	j	202	CDL	C72-C73-C74-C75
33	I	201	PC1	C2C-C2D-C2E-C2F
28	Q	101	CDL	CB2-C1-CA2-OA2
28	q	101	CDL	CB2-C1-CA2-OA2
31	N	201	Q7G	C24-C23-C48-O1C

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Mol	Chain	Res	Type	Atoms
31	n	201	Q7G	C24-C23-C48-O1C
28	E	405	CDL	OB7-CB5-OB6-CB4
28	F	201	CDL	OA7-CA5-OA6-CA4
28	e	403	CDL	OB7-CB5-OB6-CB4
28	f	201	CDL	OA7-CA5-OA6-CA4
28	J	202	CDL	C55-C56-C57-C58
28	j	201	CDL	C55-C56-C57-C58
28	E	403	CDL	CB4-CB3-OB5-PB2
28	E	404	CDL	CA4-CA3-OA5-PA1
28	L	101	CDL	CA4-CA3-OA5-PA1
28	e	401	CDL	CB4-CB3-OB5-PB2
28	e	402	CDL	CA4-CA3-OA5-PA1
28	l	101	CDL	CA4-CA3-OA5-PA1
33	J	204	PC1	C2-C1-O11-P
33	j	203	PC1	C2-C1-O11-P
32	R	101	PEE	C39-C40-C41-C42
32	r	101	PEE	C39-C40-C41-C42
28	E	407	CDL	C52-C53-C54-C55
28	E	407	CDL	C78-C79-C80-C81
28	e	405	CDL	C52-C53-C54-C55
28	e	405	CDL	C78-C79-C80-C81
28	m	201	CDL	C78-C79-C80-C81
28	M	201	CDL	C78-C79-C80-C81
28	e	401	CDL	C56-C57-C58-C59
28	E	403	CDL	C56-C57-C58-C59
33	I	201	PC1	O32-C31-O31-C3
33	i	201	PC1	O32-C31-O31-C3
28	E	403	CDL	OB5-CB3-CB4-CB6
28	E	407	CDL	OB5-CB3-CB4-CB6
28	J	202	CDL	OB5-CB3-CB4-CB6
28	e	401	CDL	OB5-CB3-CB4-CB6
28	e	405	CDL	OB5-CB3-CB4-CB6
28	j	201	CDL	OB5-CB3-CB4-CB6
28	E	404	CDL	C34-C35-C36-C37
28	e	402	CDL	C34-C35-C36-C37
28	j	201	CDL	C77-C78-C79-C80
28	E	404	CDL	CA6-CA4-OA6-CA5
28	Q	101	CDL	CB3-CB4-OB6-CB5
28	e	402	CDL	CA6-CA4-OA6-CA5
28	q	101	CDL	CB3-CB4-OB6-CB5
28	C	201	CDL	C83-C84-C85-C86
28	J	202	CDL	C77-C78-C79-C80

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Mol	Chain	Res	Type	Atoms
28	c	201	CDL	C83-C84-C85-C86
28	E	403	CDL	C13-C14-C15-C16
28	e	401	CDL	C13-C14-C15-C16
28	J	203	CDL	C61-C62-C63-C64
28	C	201	CDL	CA3-CA4-CA6-OA8
28	E	404	CDL	C1-CB2-OB2-PB2
28	E	406	CDL	CB3-CB4-CB6-OB8
28	F	201	CDL	CB4-CB3-OB5-PB2
28	J	202	CDL	C1-CB2-OB2-PB2
28	J	203	CDL	CB4-CB3-OB5-PB2
28	c	201	CDL	CA3-CA4-CA6-OA8
28	e	402	CDL	C1-CB2-OB2-PB2
28	e	404	CDL	CB3-CB4-CB6-OB8
28	f	201	CDL	CB4-CB3-OB5-PB2
28	j	201	CDL	C1-CB2-OB2-PB2
28	j	202	CDL	CB4-CB3-OB5-PB2
32	R	101	PEE	C2-C1-O3P-P
32	r	101	PEE	C2-C1-O3P-P
28	E	404	CDL	OB5-CB3-CB4-OB6
28	E	407	CDL	OA5-CA3-CA4-OA6
28	e	402	CDL	OB5-CB3-CB4-OB6
28	e	405	CDL	OA5-CA3-CA4-OA6
28	j	202	CDL	C61-C62-C63-C64
28	M	201	CDL	C42-C43-C44-C45
28	m	201	CDL	C42-C43-C44-C45
28	E	406	CDL	CB2-C1-CA2-OA2
28	e	404	CDL	CB2-C1-CA2-OA2
32	R	101	PEE	O4-C10-O2-C2
32	r	101	PEE	O4-C10-O2-C2
26	B1	601	ATP	PB-O3B-PG-O2G
26	B2	601	ATP	PB-O3B-PG-O2G
30	J	201	LMT	C2-C3-C4-C5
30	j	204	LMT	C2-C3-C4-C5
28	E	404	CDL	C81-C82-C83-C84
28	e	402	CDL	C81-C82-C83-C84
28	E	405	CDL	OA6-CA4-CA6-OA8
28	e	403	CDL	OA6-CA4-CA6-OA8
32	R	101	PEE	O2-C2-C3-O3
32	r	101	PEE	O2-C2-C3-O3
28	L	101	CDL	C31-CA7-OA8-CA6
28	l	101	CDL	C31-CA7-OA8-CA6
26	B2	601	ATP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
26	C1	601	ATP	PA-O3A-PB-O2B
26	C2	601	ATP	PA-O3A-PB-O2B
31	N	201	Q7G	C16-C17-O20-CG1
31	N	201	Q7G	C18-C17-O20-CG1
31	n	201	Q7G	C16-C17-O20-CG1
31	n	201	Q7G	C18-C17-O20-CG1
28	e	402	CDL	C75-C76-C77-C78
28	E	404	CDL	C75-C76-C77-C78
33	J	204	PC1	C3C-C3D-C3E-C3F
33	j	203	PC1	C3C-C3D-C3E-C3F
28	E	407	CDL	CA4-CA3-OA5-PA1
28	e	405	CDL	CA4-CA3-OA5-PA1
28	E	403	CDL	CB3-OB5-PB2-OB4
28	E	407	CDL	CB3-OB5-PB2-OB3
28	F	201	CDL	CA2-OA2-PA1-OA4
28	F	201	CDL	CB3-OB5-PB2-OB3
28	J	202	CDL	CA2-OA2-PA1-OA4
28	J	203	CDL	CA2-OA2-PA1-OA3
28	L	101	CDL	CA3-OA5-PA1-OA3
28	L	101	CDL	CB2-OB2-PB2-OB4
28	Q	101	CDL	CA2-OA2-PA1-OA3
28	e	401	CDL	CB3-OB5-PB2-OB4
28	e	405	CDL	CB3-OB5-PB2-OB3
28	f	201	CDL	CA2-OA2-PA1-OA4
28	f	201	CDL	CB3-OB5-PB2-OB3
28	j	201	CDL	CA2-OA2-PA1-OA4
28	j	202	CDL	CA2-OA2-PA1-OA3
28	l	101	CDL	CA3-OA5-PA1-OA3
28	l	101	CDL	CB2-OB2-PB2-OB4
28	q	101	CDL	CA2-OA2-PA1-OA3
32	F	202	PEE	C4-O4P-P-O2P
32	F	202	PEE	C4-O4P-P-O1P
32	f	202	PEE	C4-O4P-P-O2P
32	f	202	PEE	C4-O4P-P-O1P
33	F	203	PC1	C1-O11-P-O12
33	F	204	PC1	C11-O13-P-O12
33	f	203	PC1	C1-O11-P-O12
33	f	204	PC1	C11-O13-P-O12
28	E	406	CDL	OA5-CA3-CA4-CA6
28	e	404	CDL	OA5-CA3-CA4-CA6
32	r	101	PEE	C13-C14-C15-C16
32	R	101	PEE	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
28	M	201	CDL	C20-C21-C22-C23
28	m	201	CDL	C20-C21-C22-C23
28	C	201	CDL	C62-C63-C64-C65
28	c	201	CDL	C62-C63-C64-C65
33	F	204	PC1	C21-C22-C23-C24
33	f	204	PC1	C21-C22-C23-C24
28	E	406	CDL	OA5-CA3-CA4-OA6
28	J	202	CDL	OB5-CB3-CB4-OB6
28	J	203	CDL	OA5-CA3-CA4-OA6
28	e	404	CDL	OA5-CA3-CA4-OA6
28	j	201	CDL	OB5-CB3-CB4-OB6
28	j	202	CDL	OA5-CA3-CA4-OA6
31	E	402	Q7G	C23-C24-O1B-C1B
31	e	407	Q7G	C23-C24-O1B-C1B
28	E	404	CDL	C17-C18-C19-C20
28	e	402	CDL	C17-C18-C19-C20
28	L	101	CDL	OA9-CA7-OA8-CA6
28	l	101	CDL	OA9-CA7-OA8-CA6
28	J	202	CDL	C72-C73-C74-C75
28	j	201	CDL	C72-C73-C74-C75
28	E	404	CDL	C53-C54-C55-C56
28	M	201	CDL	CA3-CA4-CA6-OA8
28	m	201	CDL	CA3-CA4-CA6-OA8
28	q	101	CDL	C77-C78-C79-C80
33	F	203	PC1	O13-C11-C12-N
33	J	204	PC1	O13-C11-C12-N
33	f	203	PC1	O13-C11-C12-N
33	j	203	PC1	O13-C11-C12-N
28	E	407	CDL	OB6-CB4-CB6-OB8
28	e	405	CDL	OB6-CB4-CB6-OB8
32	F	202	PEE	O2-C2-C3-O3
32	f	202	PEE	O2-C2-C3-O3
28	e	402	CDL	C53-C54-C55-C56
28	Q	101	CDL	C77-C78-C79-C80
28	e	402	CDL	C79-C80-C81-C82
28	e	403	CDL	C62-C63-C64-C65
28	E	404	CDL	C79-C80-C81-C82
28	E	405	CDL	C62-C63-C64-C65
32	R	101	PEE	C34-C35-C36-C37
28	E	403	CDL	C53-C54-C55-C56
32	r	101	PEE	C34-C35-C36-C37
28	e	401	CDL	C53-C54-C55-C56

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Mol	Chain	Res	Type	Atoms
29	D1	601	ADP	PA-O3A-PB-O1B
29	D2	601	ADP	PA-O3A-PB-O1B
28	E	406	CDL	CA6-CA4-OA6-CA5
28	J	203	CDL	CB3-CB4-OB6-CB5
28	e	404	CDL	CA6-CA4-OA6-CA5
28	j	202	CDL	CB3-CB4-OB6-CB5
28	E	404	CDL	OB5-CB3-CB4-CB6
28	E	407	CDL	OA5-CA3-CA4-CA6
28	e	402	CDL	OB5-CB3-CB4-CB6
28	e	405	CDL	OA5-CA3-CA4-CA6
28	E	405	CDL	C51-C52-C53-C54
28	e	403	CDL	C51-C52-C53-C54
33	i	201	PC1	C2A-C2B-C2C-C2D
28	e	402	CDL	C55-C56-C57-C58
33	I	201	PC1	C2A-C2B-C2C-C2D
28	E	404	CDL	C55-C56-C57-C58
32	R	101	PEE	C11-C10-O2-C2
32	r	101	PEE	C11-C10-O2-C2
32	R	101	PEE	C38-C39-C40-C41
32	r	101	PEE	C38-C39-C40-C41
28	C	201	CDL	OA6-CA4-CA6-OA8
28	E	405	CDL	OB6-CB4-CB6-OB8
28	c	201	CDL	OA6-CA4-CA6-OA8
28	e	403	CDL	OB6-CB4-CB6-OB8
28	C	201	CDL	C35-C36-C37-C38
28	C	201	CDL	CA3-OA5-PA1-OA2
28	E	405	CDL	CB2-OB2-PB2-OB5
28	Q	101	CDL	CA3-OA5-PA1-OA2
28	Q	101	CDL	CB3-OB5-PB2-OB2
28	c	201	CDL	CA3-OA5-PA1-OA2
28	e	403	CDL	CB2-OB2-PB2-OB5
28	q	101	CDL	CA3-OA5-PA1-OA2
28	q	101	CDL	CB3-OB5-PB2-OB2
32	R	101	PEE	C1-O3P-P-O4P
32	r	101	PEE	C1-O3P-P-O4P
28	M	201	CDL	C72-C73-C74-C75
28	m	201	CDL	C72-C73-C74-C75
28	c	201	CDL	C35-C36-C37-C38
28	E	405	CDL	CA3-CA4-CA6-OA8
28	E	405	CDL	CB3-CB4-CB6-OB8
28	F	201	CDL	CB3-CB4-CB6-OB8
28	L	101	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
28	e	403	CDL	CA3-CA4-CA6-OA8
28	e	403	CDL	CB3-CB4-CB6-OB8
28	f	201	CDL	CB3-CB4-CB6-OB8
28	j	202	CDL	CB3-CB4-CB6-OB8
28	l	101	CDL	CA3-CA4-CA6-OA8
26	A1	601	ATP	PG-O3B-PB-O2B
26	A2	601	ATP	PG-O3B-PB-O2B
26	B1	601	ATP	PA-O3A-PB-O1B
26	B1	601	ATP	PA-O3A-PB-O2B
26	B2	601	ATP	PA-O3A-PB-O2B
26	C1	601	ATP	PG-O3B-PB-O2B
26	C2	601	ATP	PG-O3B-PB-O2B
26	F1	601	ATP	PG-O3B-PB-O2B
26	F2	601	ATP	PG-O3B-PB-O2B
28	E	405	CDL	C1-CA2-OA2-PA1
28	Q	101	CDL	C1-CB2-OB2-PB2
28	e	403	CDL	C1-CA2-OA2-PA1
28	q	101	CDL	C1-CB2-OB2-PB2
32	r	101	PEE	C36-C37-C38-C39
33	F	204	PC1	O31-C31-C32-C33
33	f	204	PC1	O31-C31-C32-C33
33	J	204	PC1	O11-C1-C2-O21
33	j	203	PC1	O11-C1-C2-O21
28	E	403	CDL	C80-C81-C82-C83
28	F	201	CDL	C78-C79-C80-C81
28	f	201	CDL	C78-C79-C80-C81
28	L	101	CDL	C36-C37-C38-C39
28	e	401	CDL	C80-C81-C82-C83
28	l	101	CDL	C36-C37-C38-C39
32	R	101	PEE	C36-C37-C38-C39
28	F	201	CDL	O1-C1-CB2-OB2
28	f	201	CDL	O1-C1-CB2-OB2
28	C	201	CDL	C1-CB2-OB2-PB2
28	c	201	CDL	C1-CB2-OB2-PB2
32	F	202	PEE	C16-C17-C18-C19
32	f	202	PEE	C16-C17-C18-C19
28	e	402	CDL	C54-C55-C56-C57
32	R	101	PEE	C33-C34-C35-C36
32	r	101	PEE	C33-C34-C35-C36
28	c	201	CDL	C40-C41-C42-C43
28	E	404	CDL	C54-C55-C56-C57
28	C	201	CDL	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
28	C	201	CDL	C42-C43-C44-C45
28	c	201	CDL	C42-C43-C44-C45
28	M	201	CDL	C75-C76-C77-C78
28	m	201	CDL	C75-C76-C77-C78
28	J	203	CDL	CB3-CB4-CB6-OB8
28	E	404	CDL	OA7-CA5-OA6-CA4
28	e	402	CDL	OA7-CA5-OA6-CA4
28	e	401	CDL	C16-C17-C18-C19
28	E	403	CDL	C16-C17-C18-C19
28	M	201	CDL	C21-C22-C23-C24
28	m	201	CDL	C21-C22-C23-C24
28	E	406	CDL	C78-C79-C80-C81
28	J	202	CDL	CA3-CA4-OA6-CA5
28	j	201	CDL	CA3-CA4-OA6-CA5
28	L	101	CDL	C39-C40-C41-C42
28	e	404	CDL	C78-C79-C80-C81
28	l	101	CDL	C39-C40-C41-C42
28	q	101	CDL	C75-C76-C77-C78
28	Q	101	CDL	C75-C76-C77-C78
33	f	204	PC1	O22-C21-O21-C2
33	J	204	PC1	O11-C1-C2-C3
33	j	203	PC1	O11-C1-C2-C3
28	E	403	CDL	C11-C12-C13-C14
33	F	204	PC1	O22-C21-O21-C2
28	e	401	CDL	C11-C12-C13-C14
28	j	201	CDL	C71-C72-C73-C74
28	J	202	CDL	C71-C72-C73-C74
28	L	101	CDL	CB2-C1-CA2-OA2
28	l	101	CDL	CB2-C1-CA2-OA2
28	C	201	CDL	C38-C39-C40-C41
28	E	404	CDL	C77-C78-C79-C80
28	e	402	CDL	C77-C78-C79-C80
28	j	202	CDL	C37-C38-C39-C40
28	C	201	CDL	C56-C57-C58-C59
28	c	201	CDL	C38-C39-C40-C41
28	c	201	CDL	C56-C57-C58-C59
28	J	203	CDL	C37-C38-C39-C40
28	e	403	CDL	C18-C19-C20-C21
28	E	403	CDL	C37-C38-C39-C40
28	E	405	CDL	C18-C19-C20-C21
33	f	204	PC1	C24-C25-C26-C27
28	e	401	CDL	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
33	F	204	PC1	C24-C25-C26-C27
28	e	403	CDL	C23-C24-C25-C26
28	E	405	CDL	C23-C24-C25-C26
28	E	403	CDL	C17-C18-C19-C20
28	E	407	CDL	O1-C1-CA2-OA2
28	e	405	CDL	O1-C1-CA2-OA2
28	E	405	CDL	C71-CB7-OB8-CB6
28	e	403	CDL	C71-CB7-OB8-CB6
28	e	401	CDL	C17-C18-C19-C20
32	F	202	PEE	O2-C10-C11-C12
28	F	201	CDL	C37-C38-C39-C40
32	f	202	PEE	O2-C10-C11-C12
28	f	201	CDL	C37-C38-C39-C40
28	m	201	CDL	C19-C20-C21-C22
33	F	204	PC1	C22-C21-O21-C2
33	f	204	PC1	C22-C21-O21-C2
28	M	201	CDL	C19-C20-C21-C22
32	R	101	PEE	C18-C19-C20-C21
32	r	101	PEE	C18-C19-C20-C21
33	F	203	PC1	O22-C21-O21-C2
33	f	203	PC1	O22-C21-O21-C2
28	E	405	CDL	OB9-CB7-OB8-CB6
26	C1	601	ATP	PB-O3B-PG-O1G
26	C2	601	ATP	PB-O3B-PG-O1G
26	F1	601	ATP	PB-O3B-PG-O1G
26	F2	601	ATP	PB-O3B-PG-O1G
28	F	201	CDL	C12-C11-CA5-OA6
28	f	201	CDL	C12-C11-CA5-OA6
28	E	407	CDL	C79-C80-C81-C82
28	e	403	CDL	OB9-CB7-OB8-CB6
28	E	403	CDL	C32-C31-CA7-OA8
28	e	401	CDL	C32-C31-CA7-OA8
28	e	405	CDL	C79-C80-C81-C82
28	L	101	CDL	OA7-CA5-OA6-CA4
28	l	101	CDL	OA7-CA5-OA6-CA4
28	M	201	CDL	C12-C11-CA5-OA6
28	m	201	CDL	C12-C11-CA5-OA6
28	L	101	CDL	C60-C61-C62-C63
28	J	203	CDL	C12-C11-CA5-OA6
28	j	202	CDL	C12-C11-CA5-OA6
32	F	202	PEE	C36-C37-C38-C39
32	f	202	PEE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
28	l	101	CDL	C60-C61-C62-C63
33	I	201	PC1	C3B-C3C-C3D-C3E
28	Q	101	CDL	OB5-CB3-CB4-OB6
28	q	101	CDL	OB5-CB3-CB4-OB6
28	M	201	CDL	C72-C71-CB7-OB8
33	i	201	PC1	C3B-C3C-C3D-C3E
28	m	201	CDL	C72-C71-CB7-OB8
28	E	406	CDL	C18-C19-C20-C21
28	e	404	CDL	C18-C19-C20-C21
26	A1	601	ATP	PB-O3B-PG-O3G
26	A2	601	ATP	PB-O3B-PG-O3G
28	F	201	CDL	C72-C71-CB7-OB8
28	f	201	CDL	C72-C71-CB7-OB8
33	F	203	PC1	C22-C21-O21-C2
33	f	203	PC1	C22-C21-O21-C2
28	E	407	CDL	C12-C11-CA5-OA6
28	J	202	CDL	C52-C51-CB5-OB6
28	e	405	CDL	C12-C11-CA5-OA6
28	j	201	CDL	C52-C51-CB5-OB6
33	J	204	PC1	O31-C31-C32-C33
33	j	203	PC1	O31-C31-C32-C33
32	F	202	PEE	C18-C19-C20-C21
32	R	101	PEE	C16-C17-C18-C19
32	f	202	PEE	C18-C19-C20-C21
32	r	101	PEE	C16-C17-C18-C19
28	Q	101	CDL	C72-C71-CB7-OB8
28	q	101	CDL	C72-C71-CB7-OB8
32	R	101	PEE	O2-C10-C11-C12
32	r	101	PEE	O2-C10-C11-C12
32	F	202	PEE	O4-C10-C11-C12
32	f	202	PEE	O4-C10-C11-C12
28	e	402	CDL	O1-C1-CA2-OA2
34	H1	201	UTP	O4'-C4'-C5'-O5'
34	H2	201	UTP	O4'-C4'-C5'-O5'
28	E	404	CDL	C52-C51-CB5-OB6
28	e	402	CDL	C52-C51-CB5-OB6
26	A1	601	ATP	PA-O3A-PB-O2B
26	A2	601	ATP	PA-O3A-PB-O2B
26	C1	601	ATP	PA-O3A-PB-O1B
26	C2	601	ATP	PA-O3A-PB-O1B
34	H1	201	UTP	PG-O3B-PB-O2B
34	H2	201	UTP	PG-O3B-PB-O1B

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Mol	Chain	Res	Type	Atoms
34	H2	201	UTP	PG-O3B-PB-O2B
28	E	404	CDL	C11-CA5-OA6-CA4
28	e	402	CDL	C11-CA5-OA6-CA4
32	R	101	PEE	C35-C36-C37-C38
32	r	101	PEE	C35-C36-C37-C38
28	j	202	CDL	C38-C39-C40-C41
28	J	203	CDL	C38-C39-C40-C41
28	M	201	CDL	C72-C71-CB7-OB9
28	e	405	CDL	C12-C11-CA5-OA7
28	e	402	CDL	C24-C25-C26-C27
28	E	407	CDL	C12-C11-CA5-OA7
28	J	203	CDL	C12-C11-CA5-OA7
28	m	201	CDL	C72-C71-CB7-OB9
28	e	405	CDL	C81-C82-C83-C84
28	E	404	CDL	C24-C25-C26-C27
28	E	407	CDL	C81-C82-C83-C84
28	m	201	CDL	C53-C54-C55-C56
28	m	201	CDL	C71-CB7-OB8-CB6
28	F	201	CDL	C12-C11-CA5-OA7
28	f	201	CDL	C12-C11-CA5-OA7
28	j	202	CDL	C12-C11-CA5-OA7
28	M	201	CDL	C53-C54-C55-C56
33	F	204	PC1	C2B-C2C-C2D-C2E
33	f	204	PC1	C2B-C2C-C2D-C2E
28	E	404	CDL	O1-C1-CA2-OA2
28	F	201	CDL	C72-C71-CB7-OB9
28	f	201	CDL	C72-C71-CB7-OB9
28	E	405	CDL	C32-C31-CA7-OA8
28	E	404	CDL	CB4-CB3-OB5-PB2
28	e	402	CDL	CB4-CB3-OB5-PB2
28	l	101	CDL	C58-C59-C60-C61
28	E	403	CDL	C32-C31-CA7-OA9
28	e	401	CDL	C32-C31-CA7-OA9
28	m	201	CDL	C12-C11-CA5-OA7
28	L	101	CDL	C58-C59-C60-C61
26	A1	601	ATP	C5'-O5'-PA-O1A
26	A2	601	ATP	C5'-O5'-PA-O1A
26	C1	601	ATP	C5'-O5'-PA-O1A
26	C2	601	ATP	C5'-O5'-PA-O1A
28	C	201	CDL	CB2-OB2-PB2-OB3
28	E	405	CDL	CB2-OB2-PB2-OB3
28	M	201	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
28	Q	101	CDL	CA3-OA5-PA1-OA3
28	c	201	CDL	CB2-OB2-PB2-OB3
28	e	403	CDL	CB2-OB2-PB2-OB3
28	m	201	CDL	CB3-OB5-PB2-OB4
28	q	101	CDL	CA3-OA5-PA1-OA3
33	J	204	PC1	C11-O13-P-O12
33	j	203	PC1	C11-O13-P-O12
28	M	201	CDL	C12-C11-CA5-OA7
32	R	101	PEE	O4-C10-C11-C12
28	E	405	CDL	C52-C51-CB5-OB6
28	e	403	CDL	C32-C31-CA7-OA8
28	e	403	CDL	C52-C51-CB5-OB6
28	F	201	CDL	OA5-CA3-CA4-CA6
28	Q	101	CDL	OB5-CB3-CB4-CB6
28	f	201	CDL	OA5-CA3-CA4-CA6
28	q	101	CDL	OB5-CB3-CB4-CB6
32	r	101	PEE	O4-C10-C11-C12
28	E	407	CDL	C32-C31-CA7-OA8
28	e	405	CDL	C32-C31-CA7-OA8
28	m	201	CDL	C51-C52-C53-C54
28	M	201	CDL	C71-CB7-OB8-CB6
28	M	201	CDL	C51-C52-C53-C54
28	q	101	CDL	C72-C71-CB7-OB9
28	E	407	CDL	CA3-CA4-OA6-CA5
28	J	202	CDL	CA6-CA4-OA6-CA5
28	j	201	CDL	CA6-CA4-OA6-CA5
33	J	204	PC1	C12-C11-O13-P
33	j	203	PC1	C12-C11-O13-P
28	M	201	CDL	OB9-CB7-OB8-CB6
28	m	201	CDL	OB9-CB7-OB8-CB6
28	Q	101	CDL	C72-C71-CB7-OB9
33	j	203	PC1	O32-C31-C32-C33
28	L	101	CDL	C80-C81-C82-C83
28	l	101	CDL	C80-C81-C82-C83
28	E	404	CDL	C32-C31-CA7-OA8
28	e	402	CDL	C32-C31-CA7-OA8
33	J	204	PC1	O32-C31-C32-C33
28	Q	101	CDL	C73-C74-C75-C76
28	j	202	CDL	C71-C72-C73-C74
28	J	203	CDL	C71-C72-C73-C74
28	e	403	CDL	C32-C33-C34-C35
28	E	405	CDL	C32-C33-C34-C35

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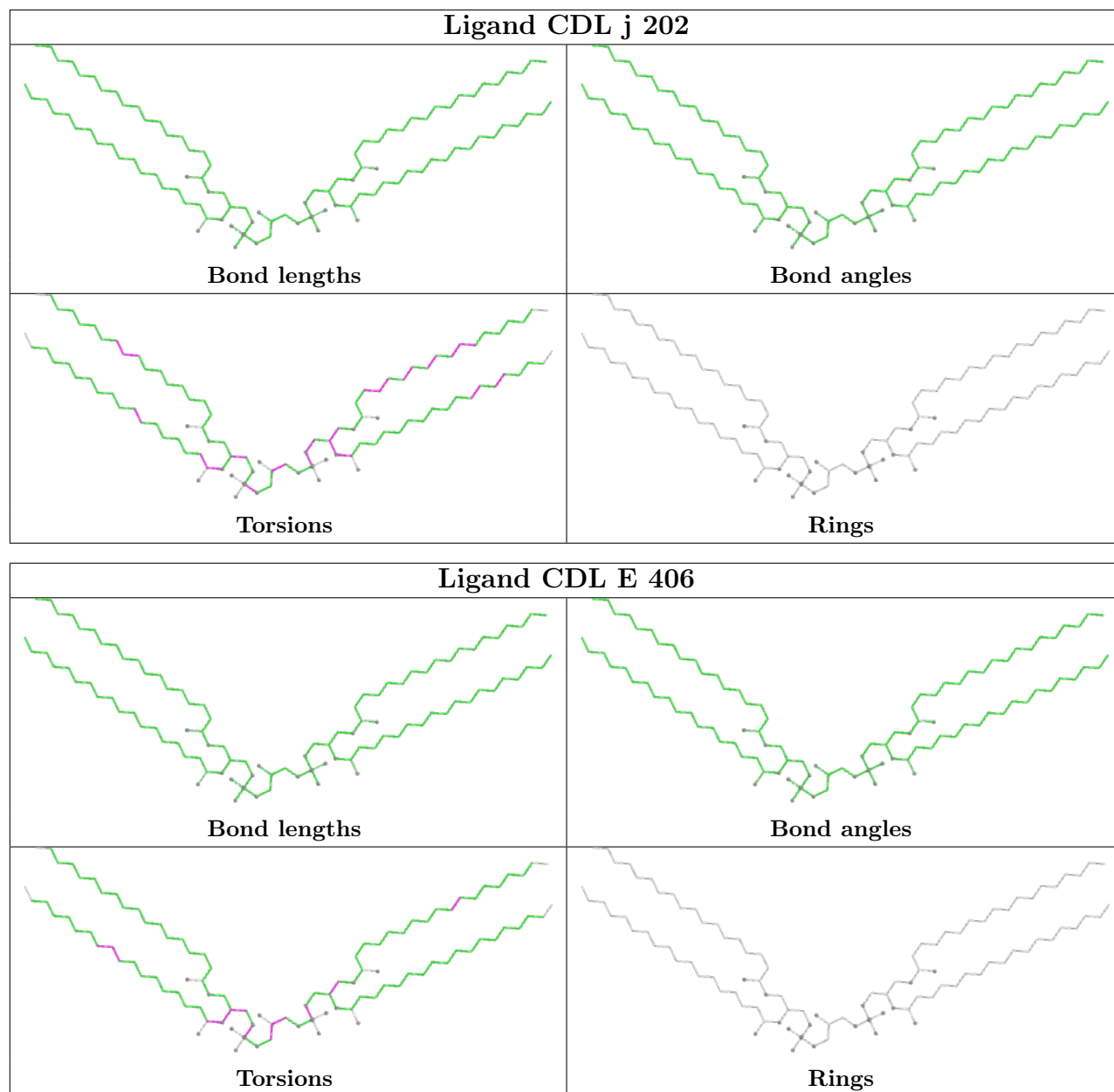
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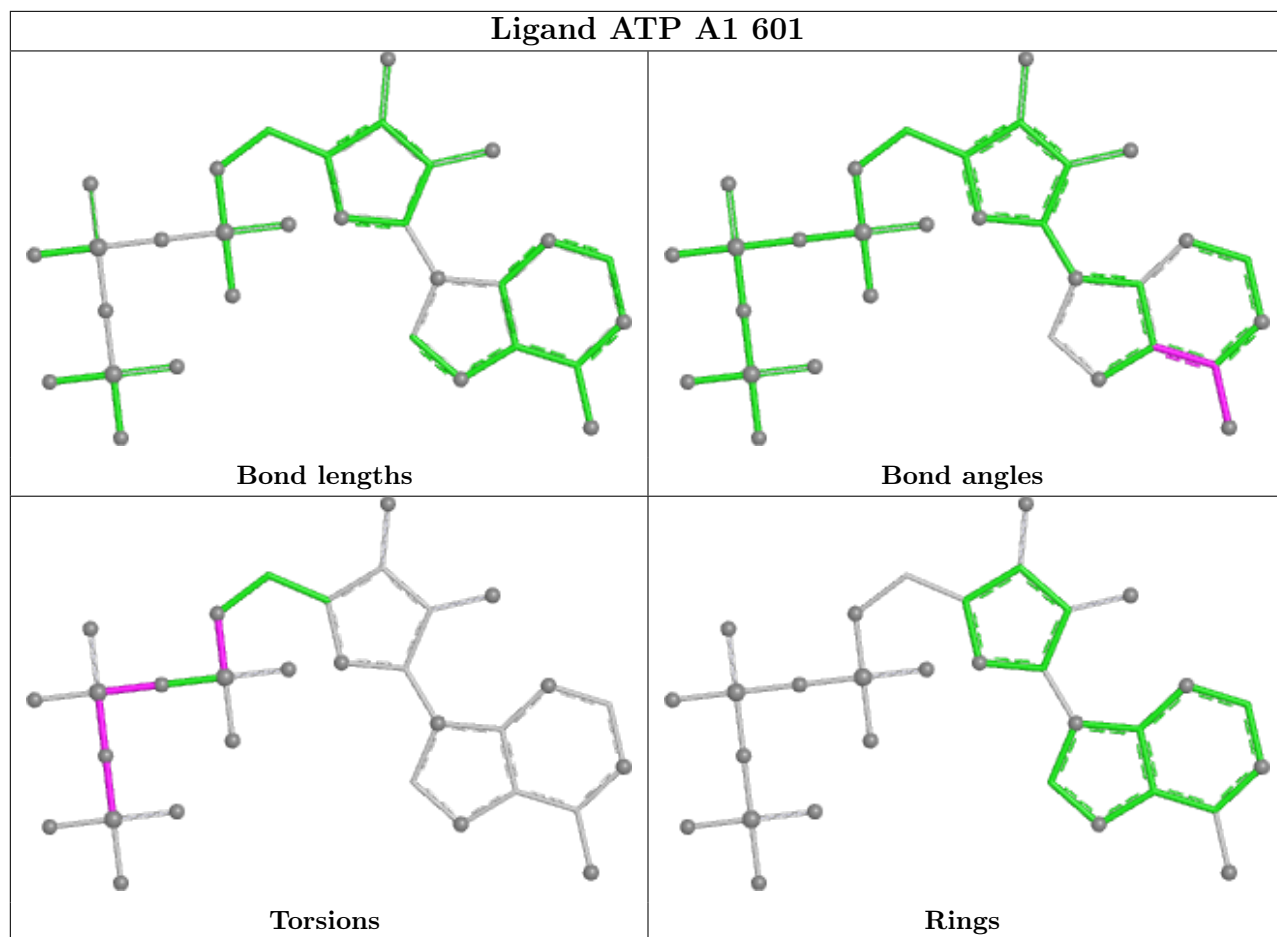
Mol	Chain	Res	Type	Atoms
28	q	101	CDL	C73-C74-C75-C76
32	R	101	PEE	C41-C42-C43-C44
28	J	203	CDL	C59-C60-C61-C62
28	j	202	CDL	C59-C60-C61-C62
28	E	404	CDL	C32-C31-CA7-OA9
32	r	101	PEE	C41-C42-C43-C44
32	F	202	PEE	O3-C30-C31-C32
32	f	202	PEE	O3-C30-C31-C32
28	E	405	CDL	C32-C31-CA7-OA9
28	e	402	CDL	C32-C31-CA7-OA9
28	e	403	CDL	C52-C51-CB5-OB7
33	i	201	PC1	O21-C21-C22-C23
28	E	405	CDL	C52-C51-CB5-OB7
28	e	403	CDL	C32-C31-CA7-OA9
28	e	405	CDL	C32-C31-CA7-OA9
28	Q	101	CDL	O1-C1-CA2-OA2
28	q	101	CDL	O1-C1-CA2-OA2
33	I	201	PC1	O21-C21-C22-C23
28	E	407	CDL	C32-C31-CA7-OA9
28	J	202	CDL	C52-C51-CB5-OB7
28	j	201	CDL	C52-C51-CB5-OB7
28	M	201	CDL	C14-C15-C16-C17
28	F	201	CDL	C52-C51-CB5-OB6
28	f	201	CDL	C52-C51-CB5-OB6

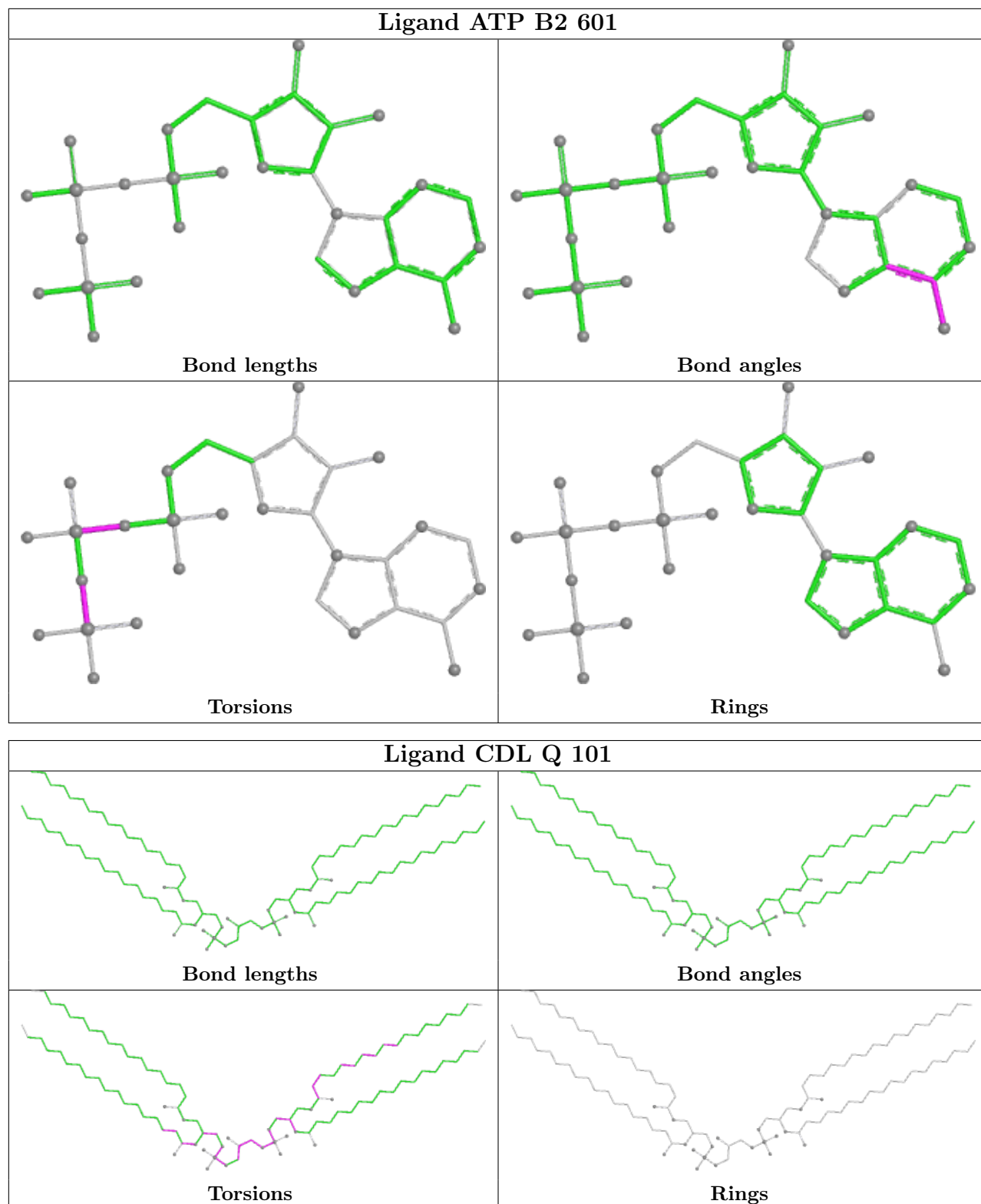
There are no ring outliers.

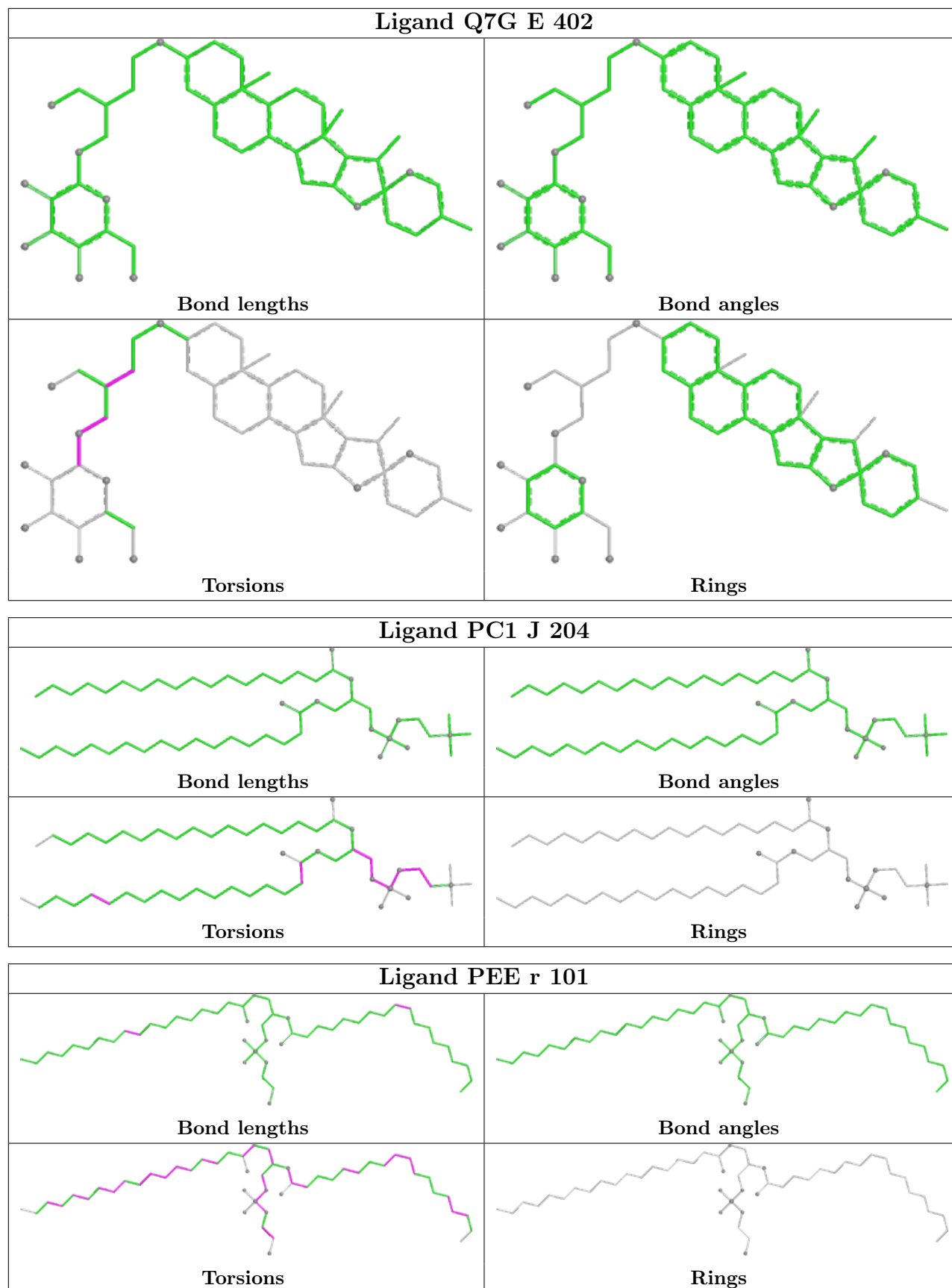
No monomer is involved in short contacts.

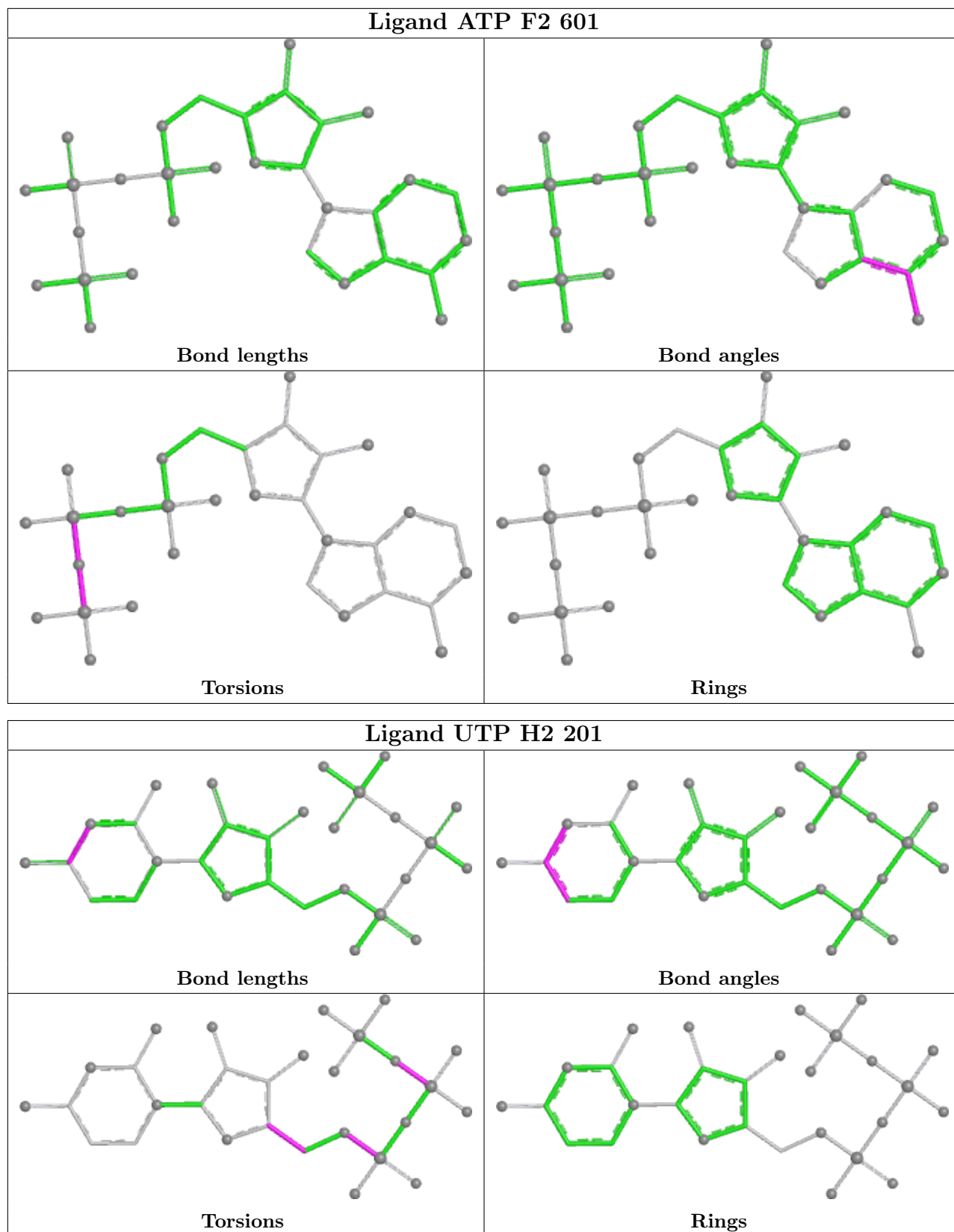
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

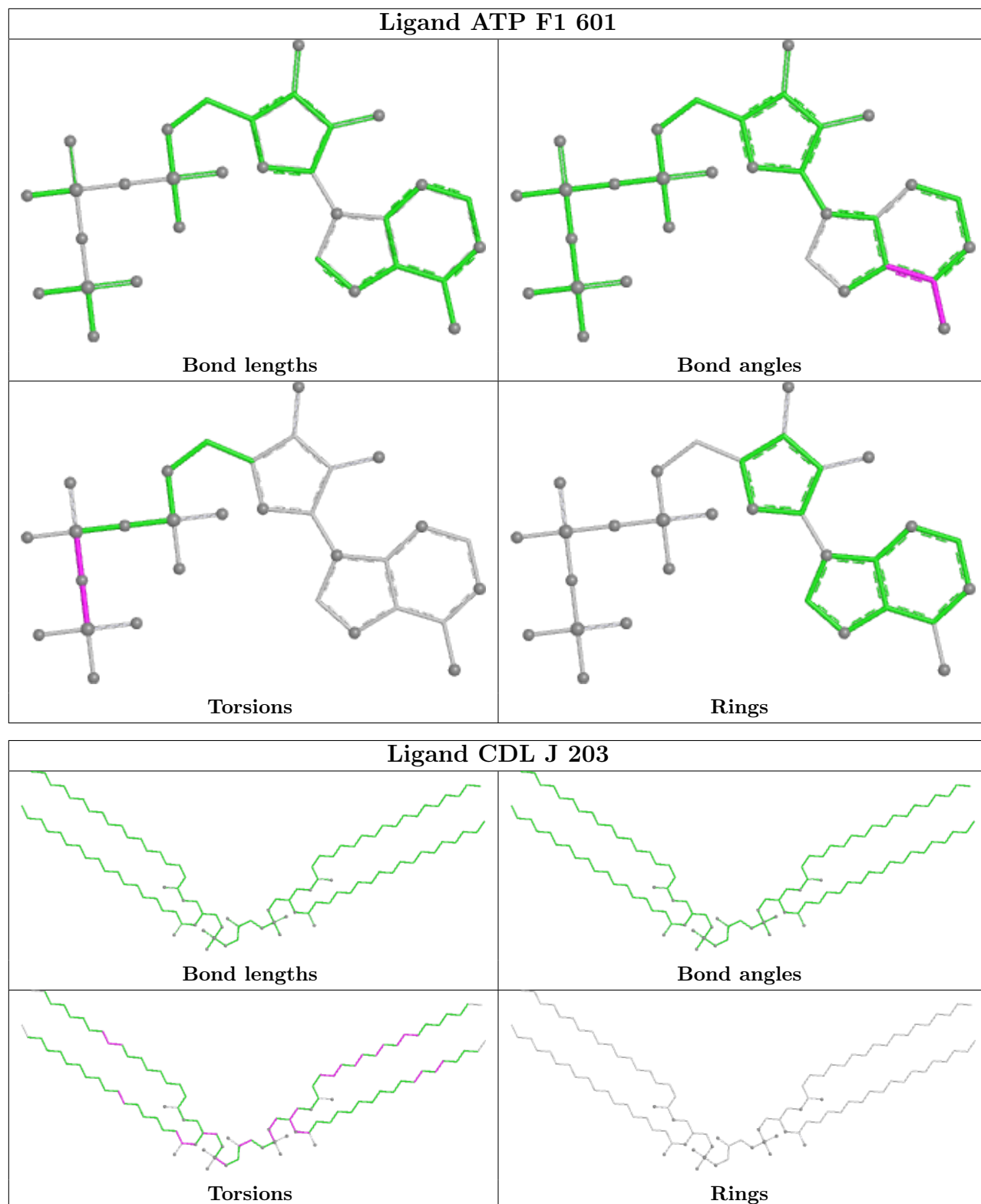


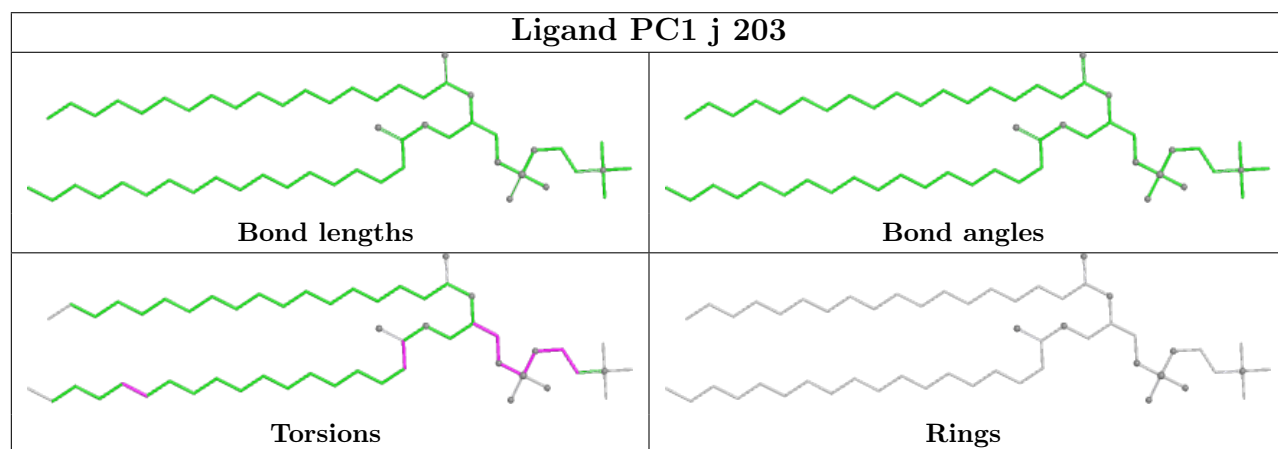
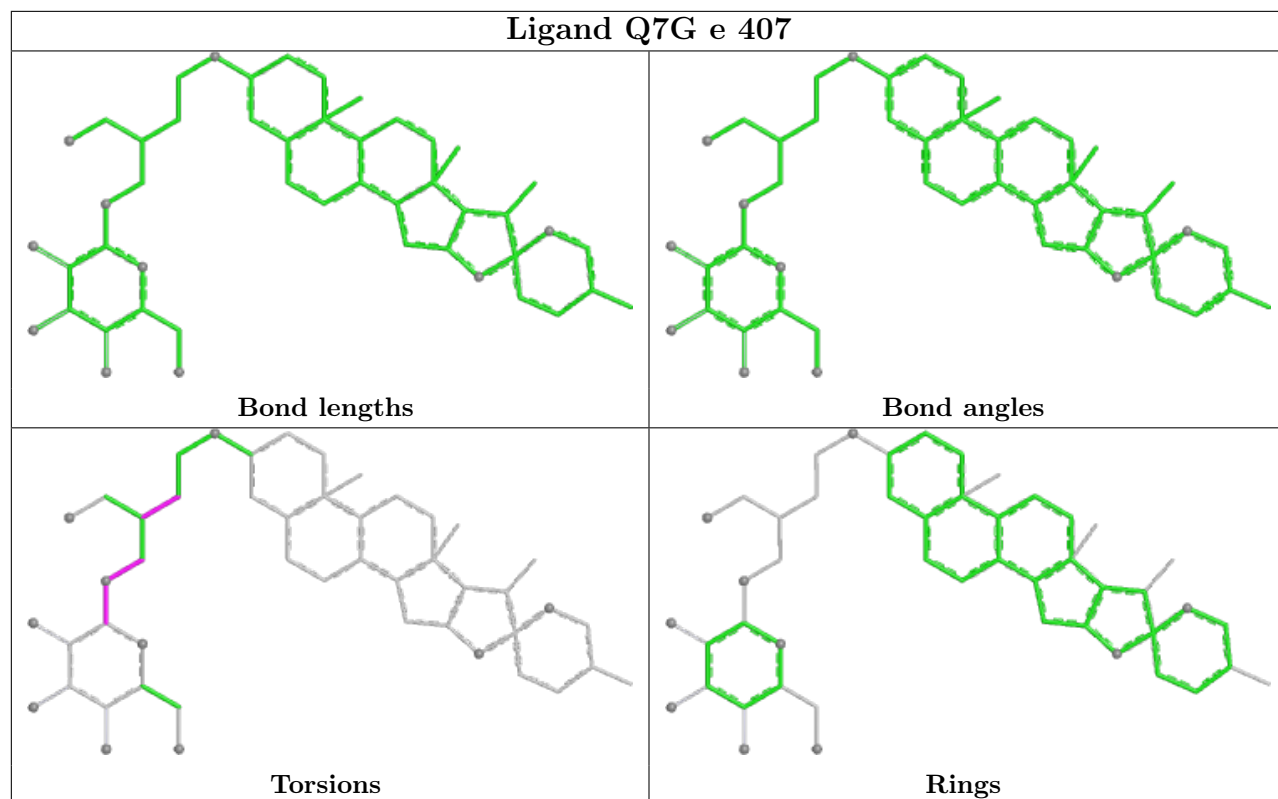


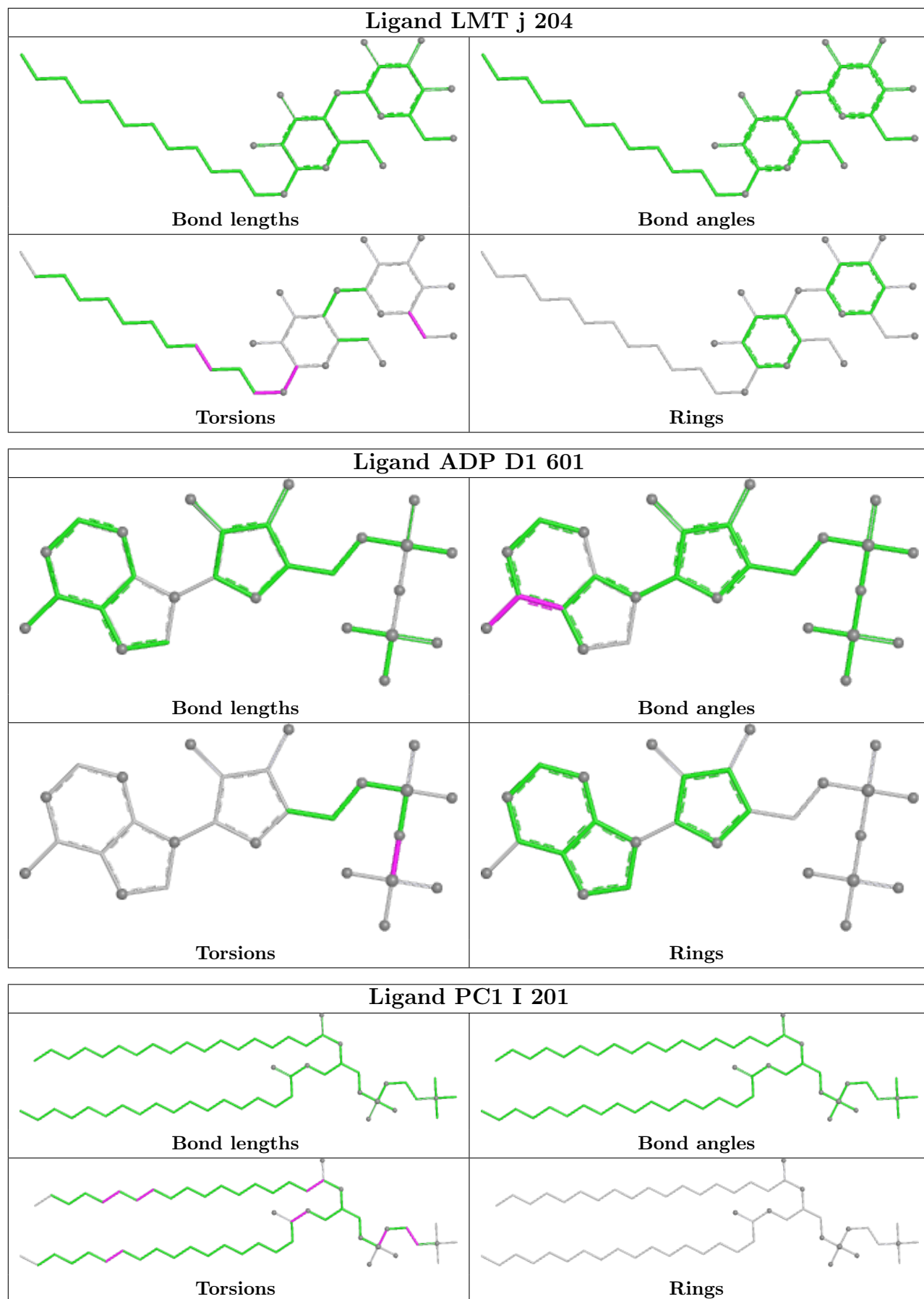


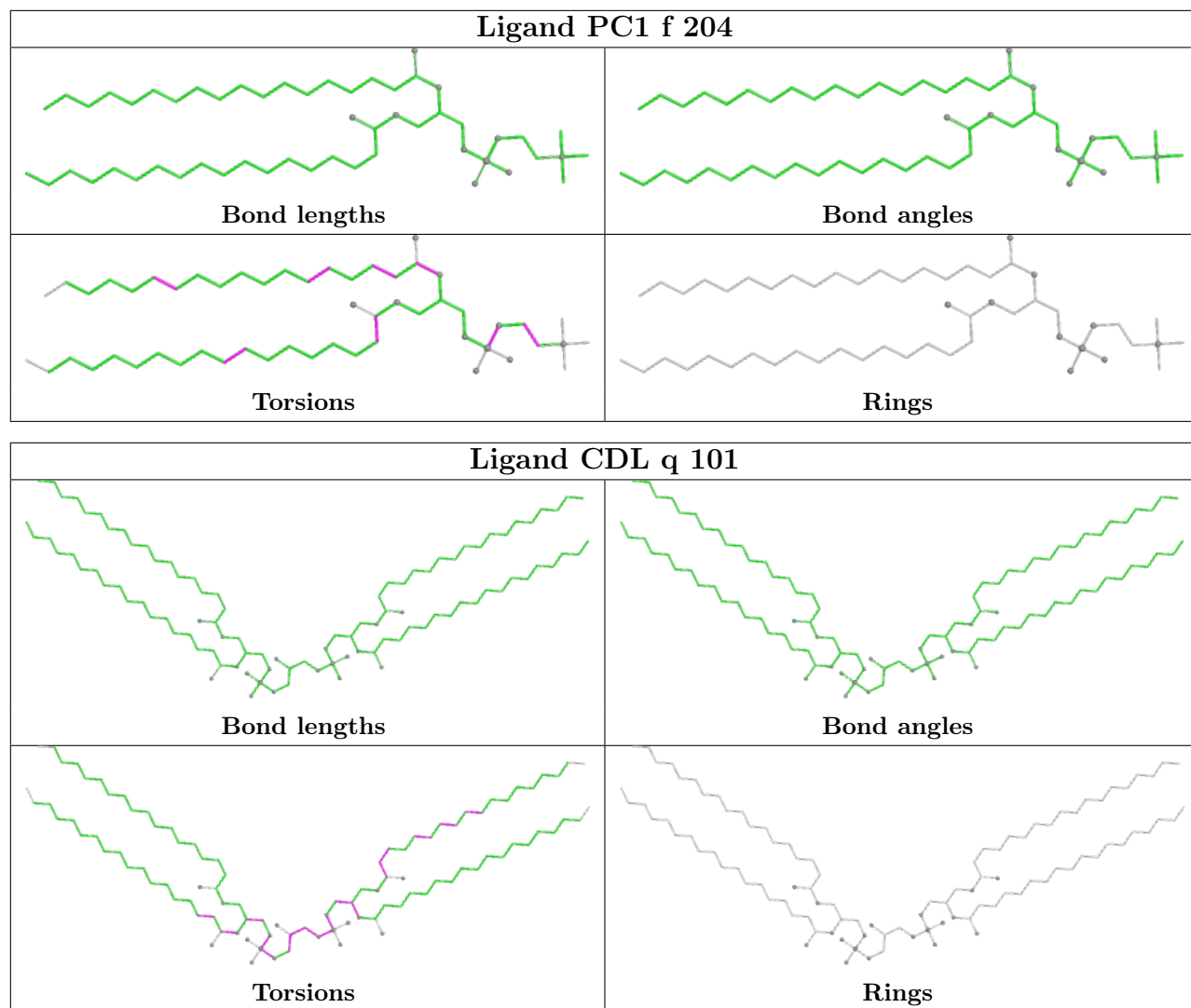


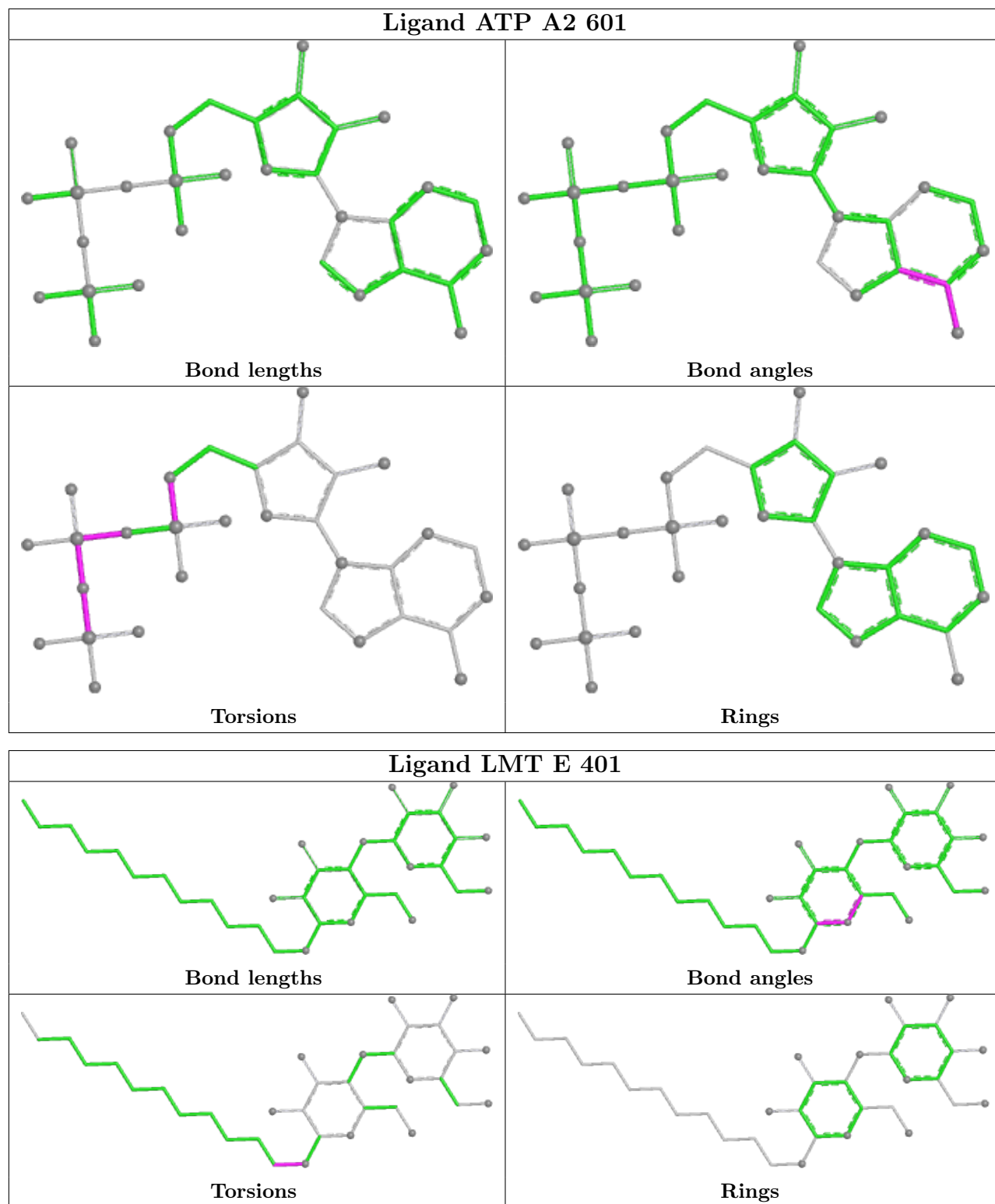


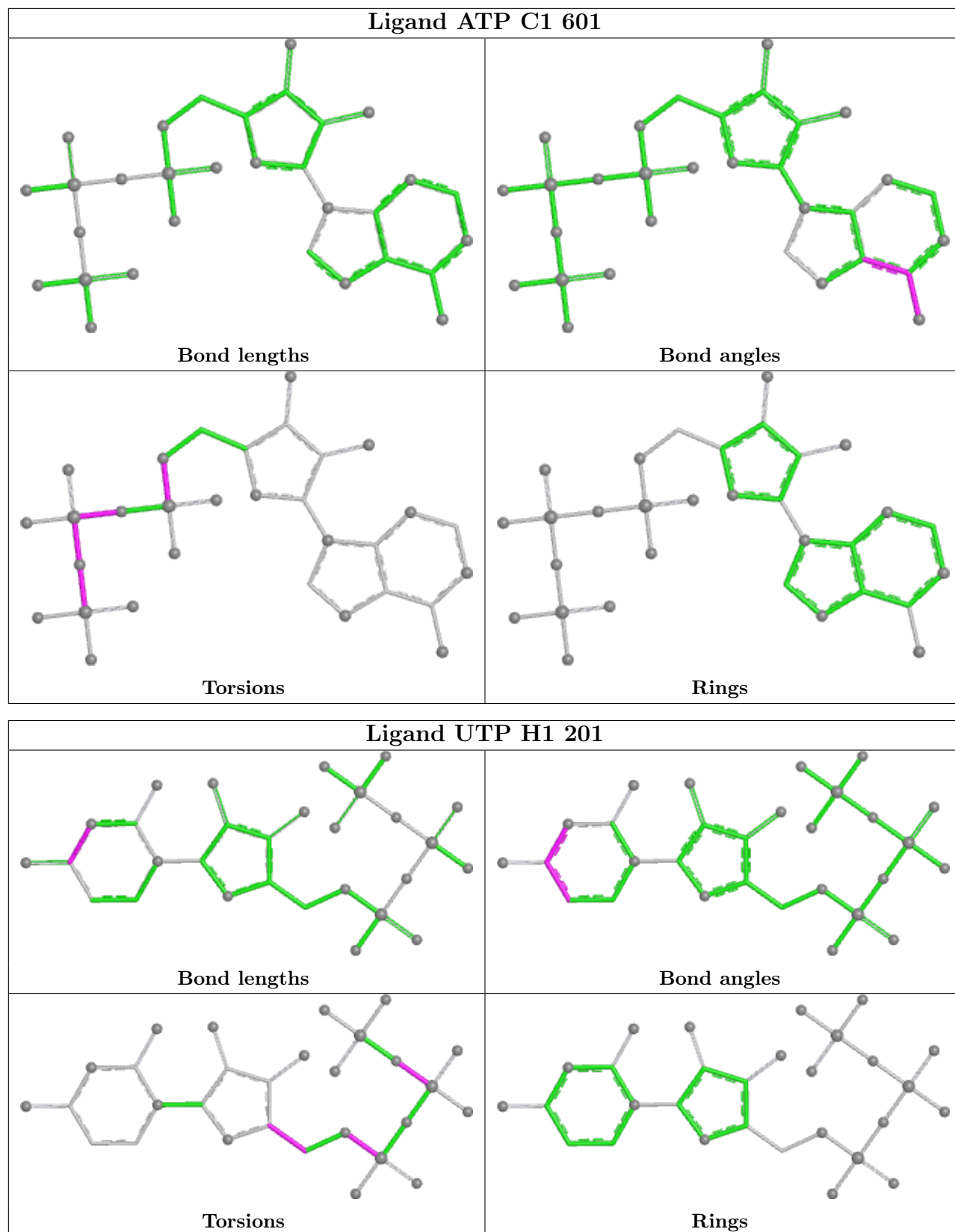


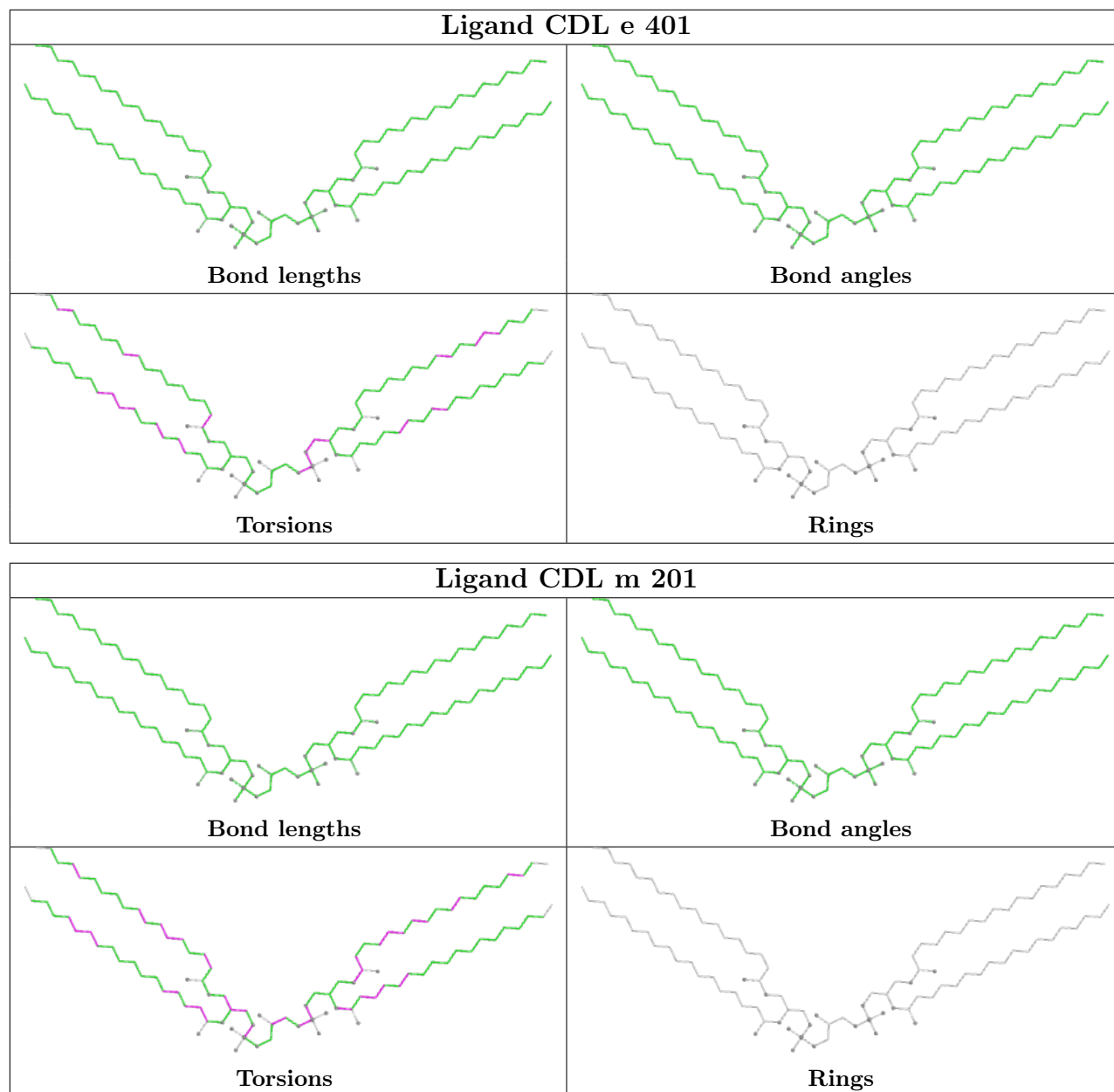


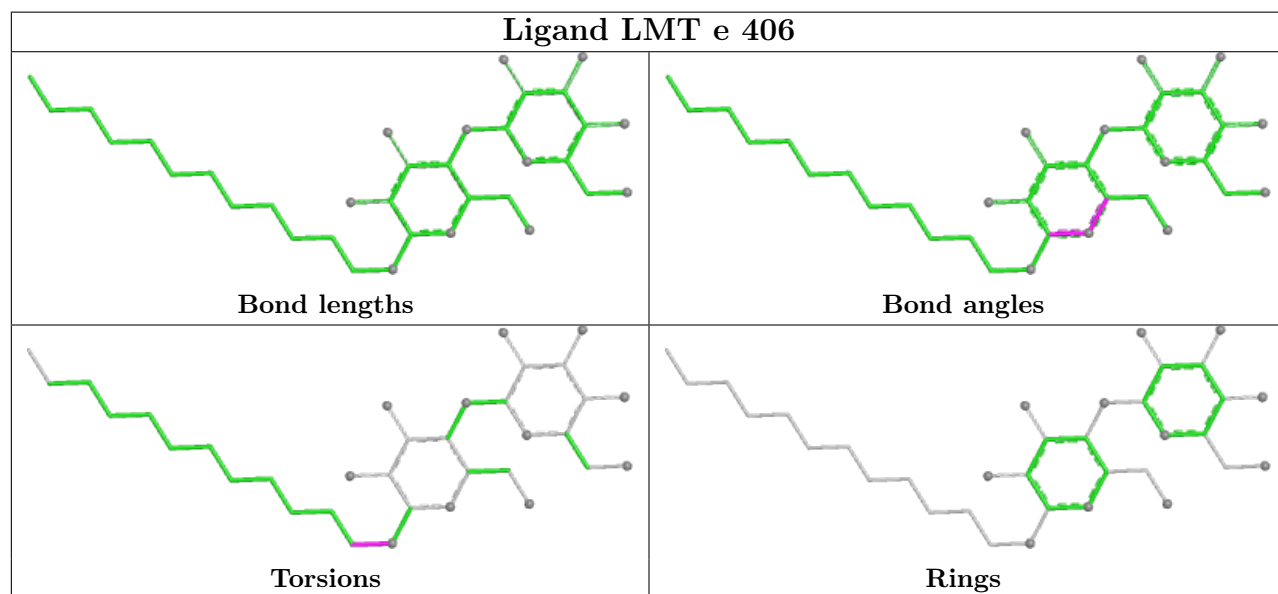
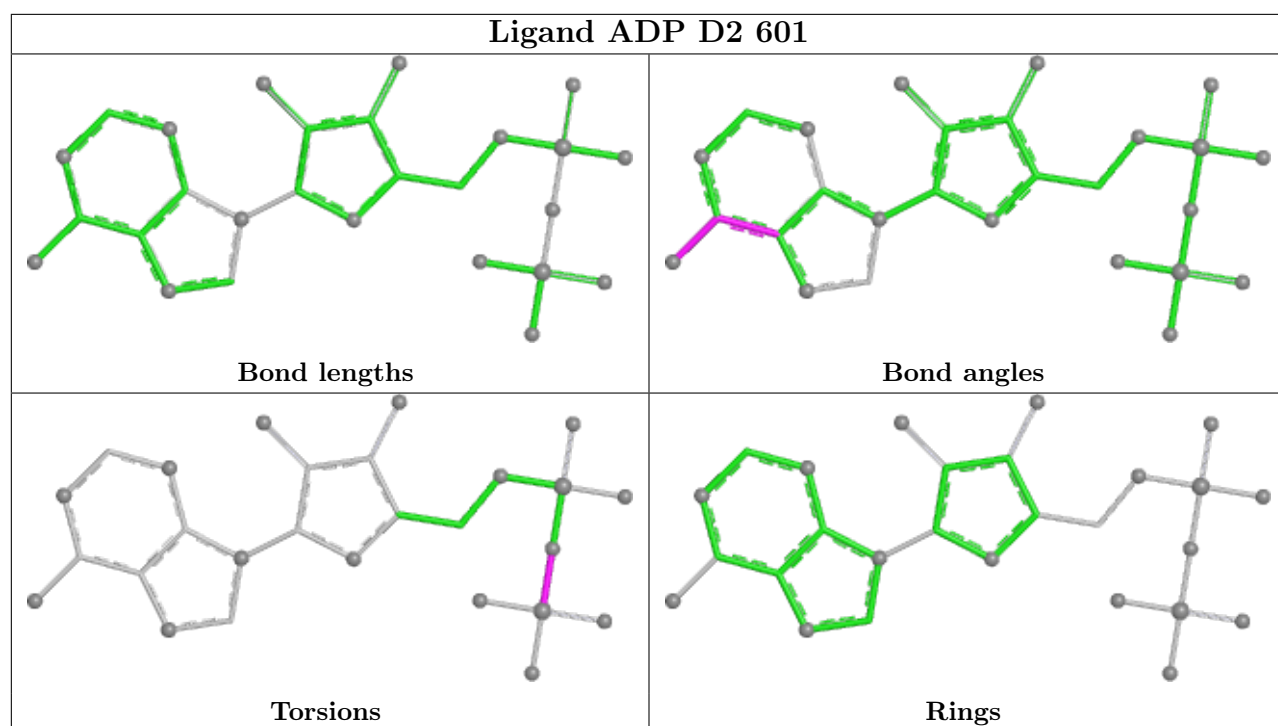


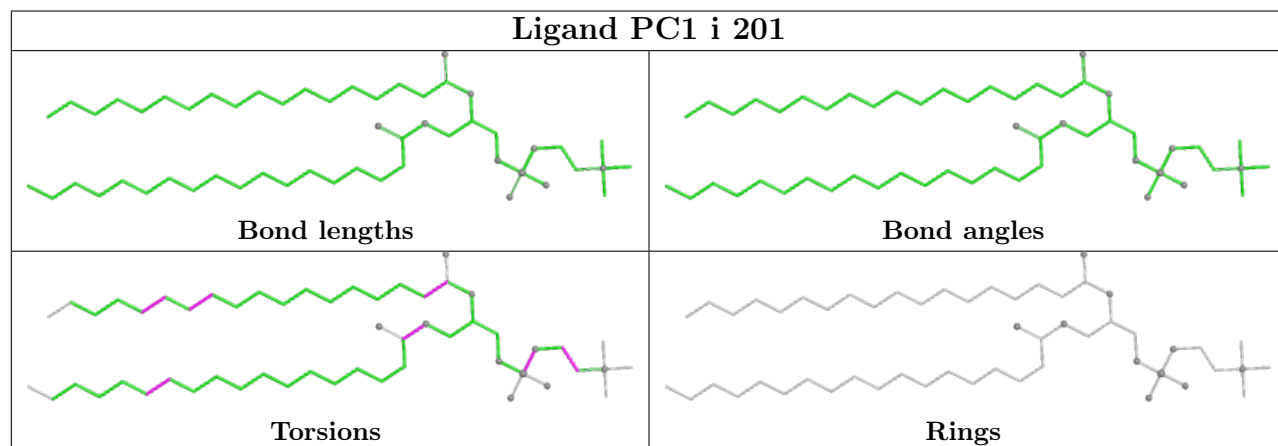
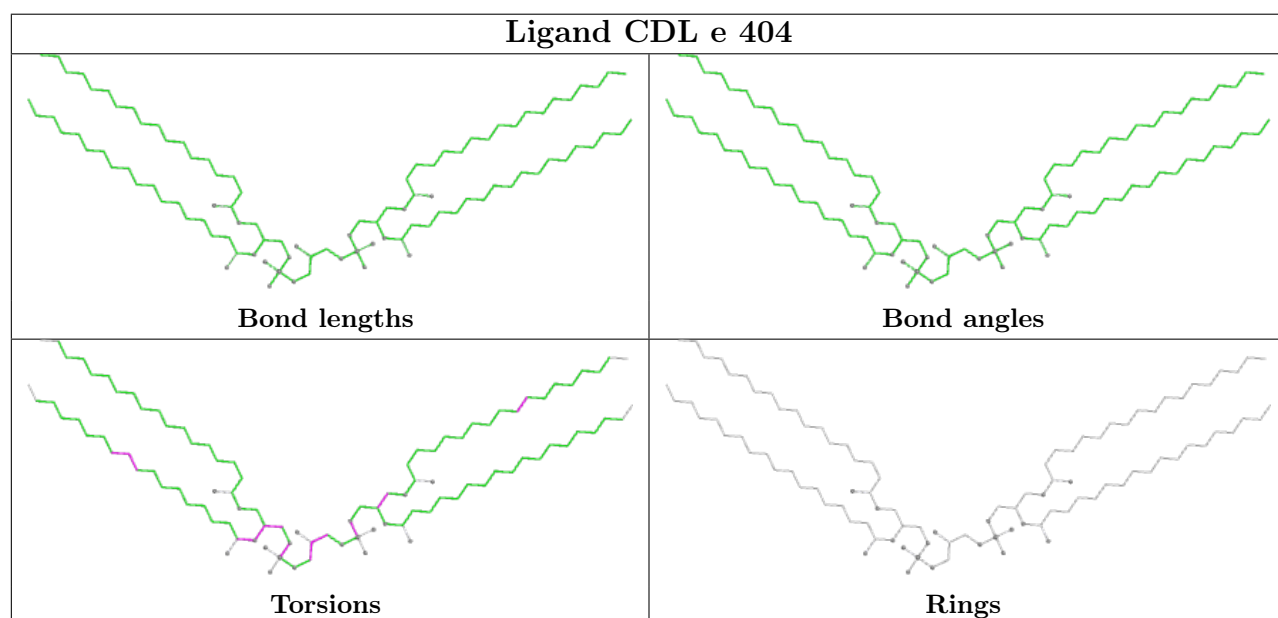
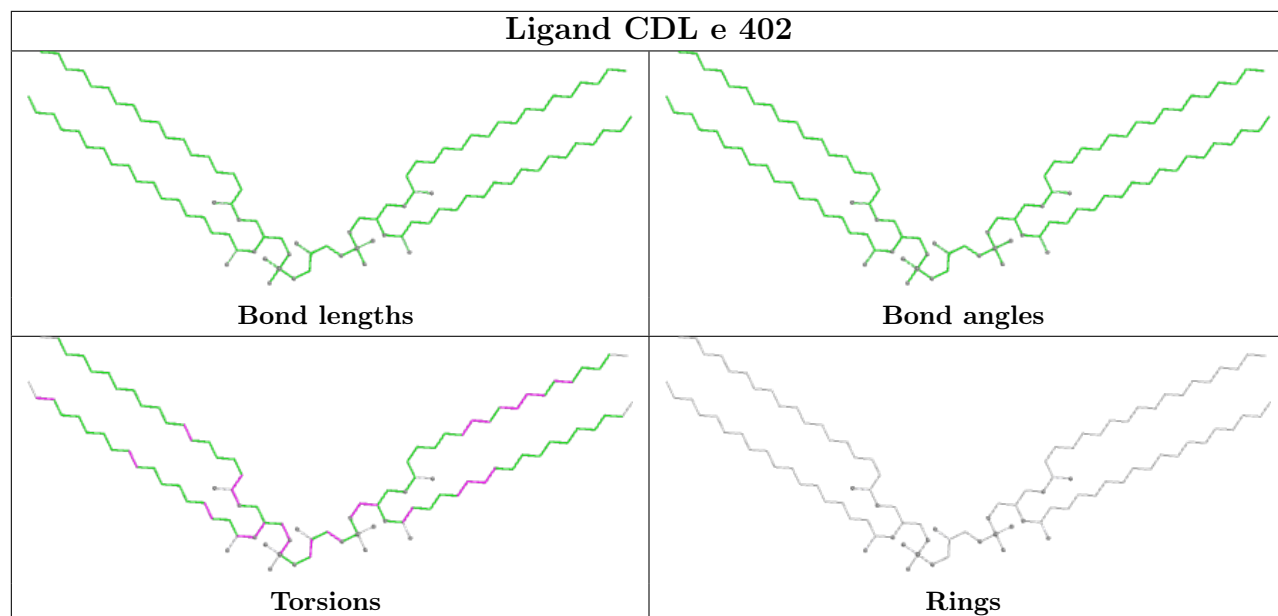


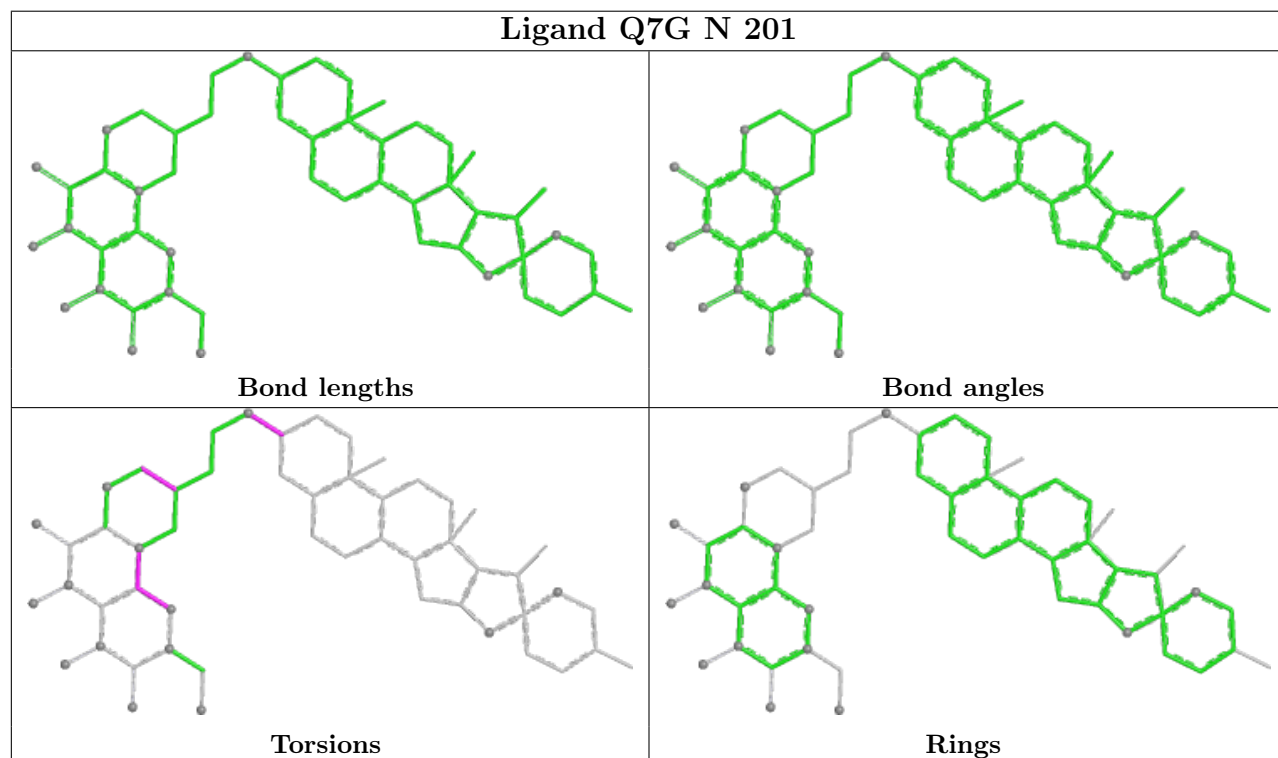
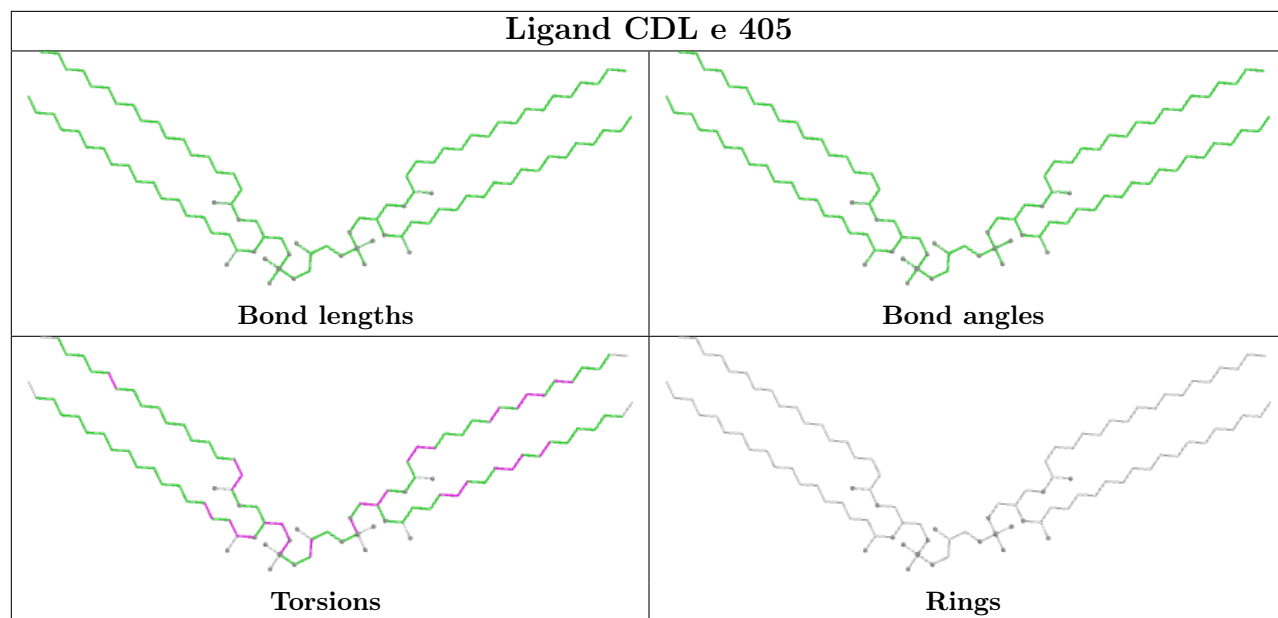


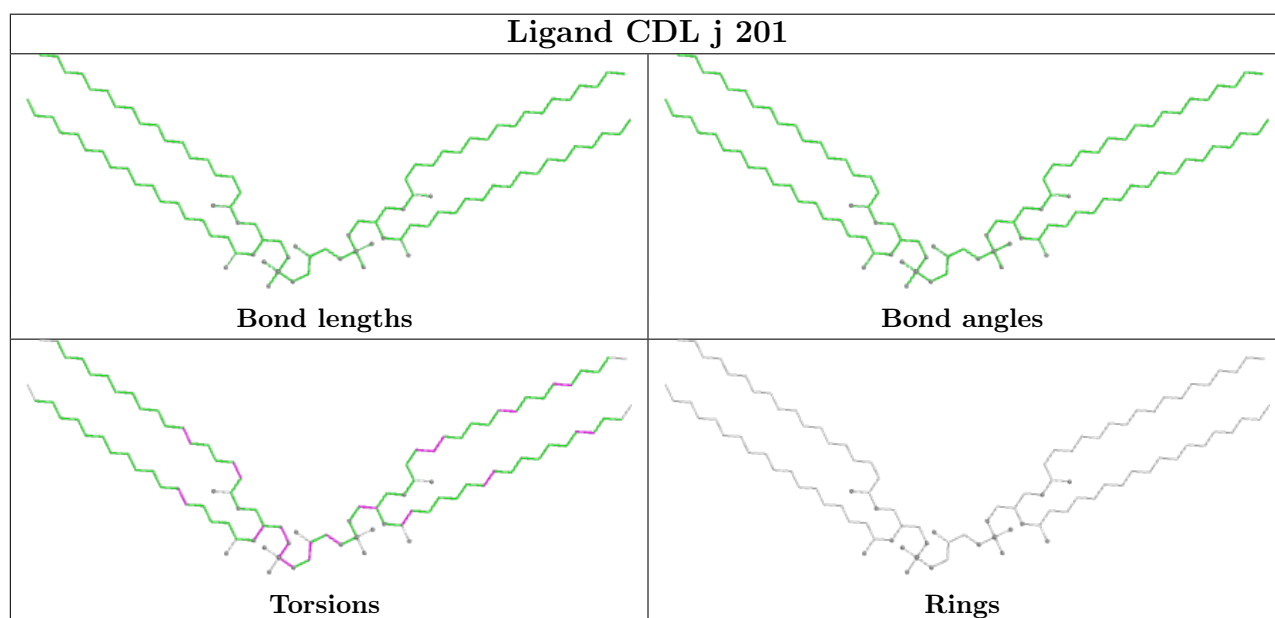
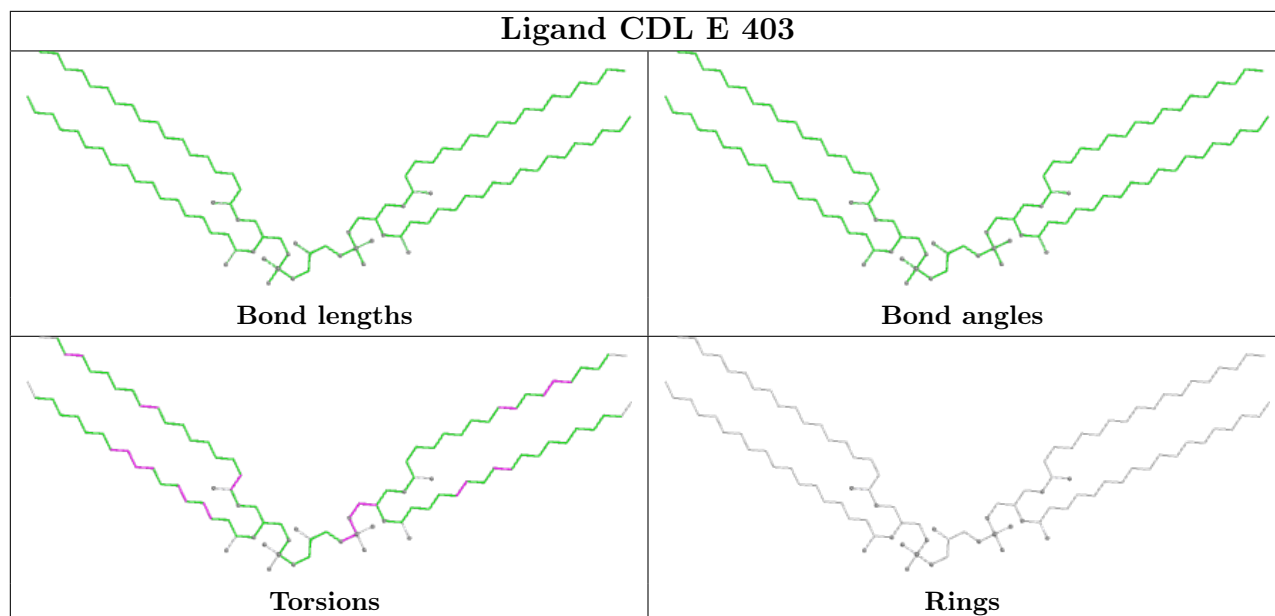


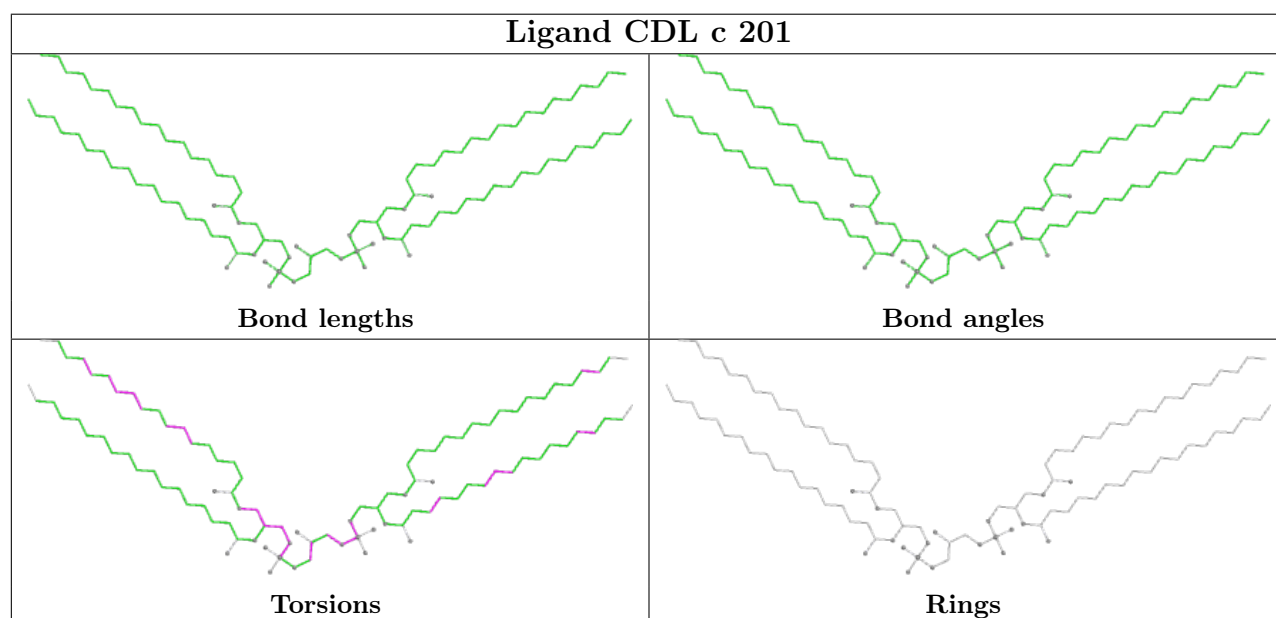
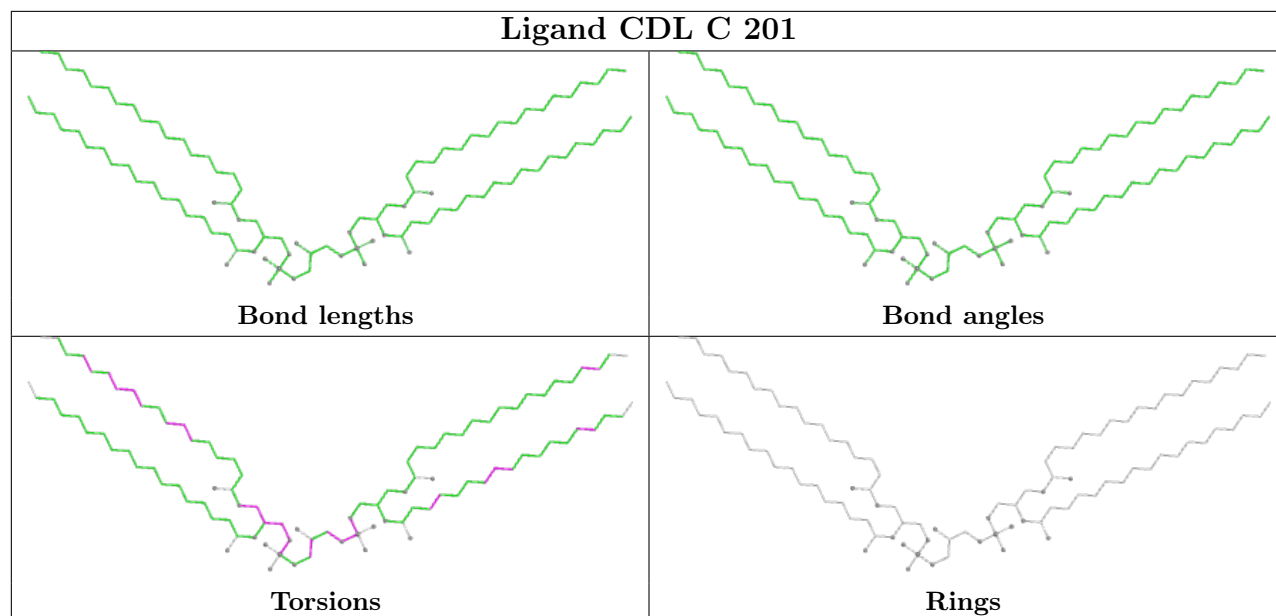


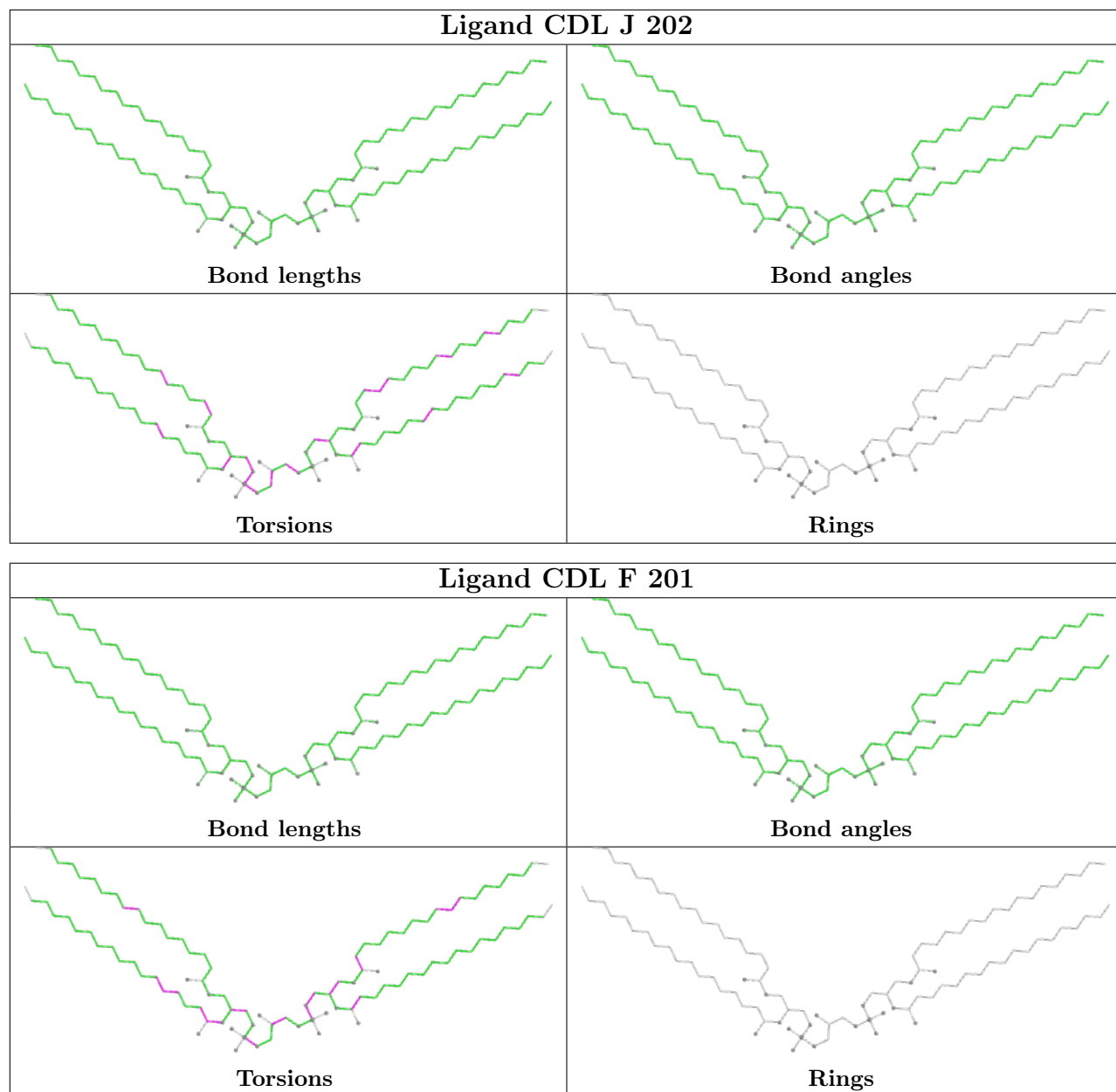


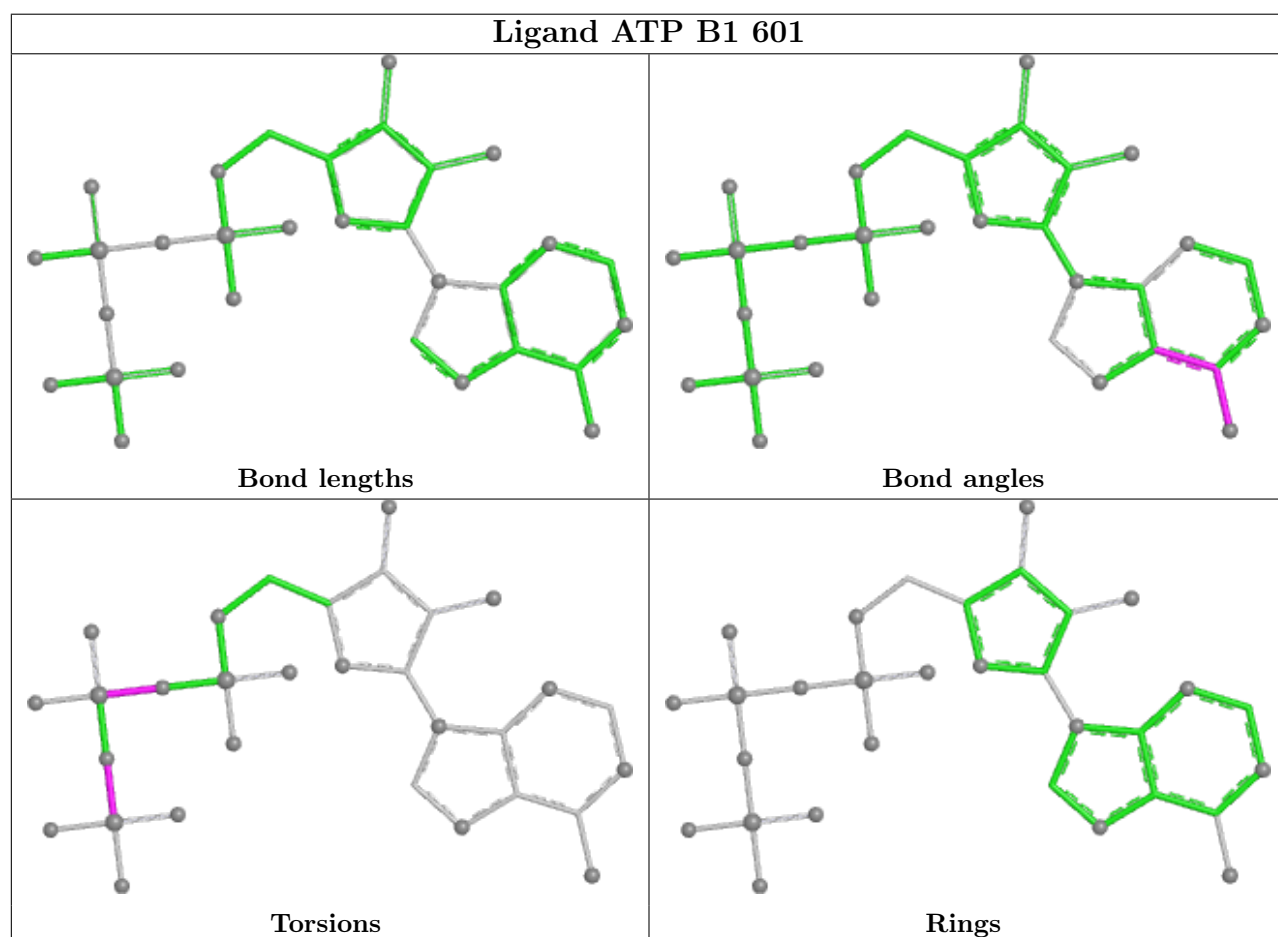
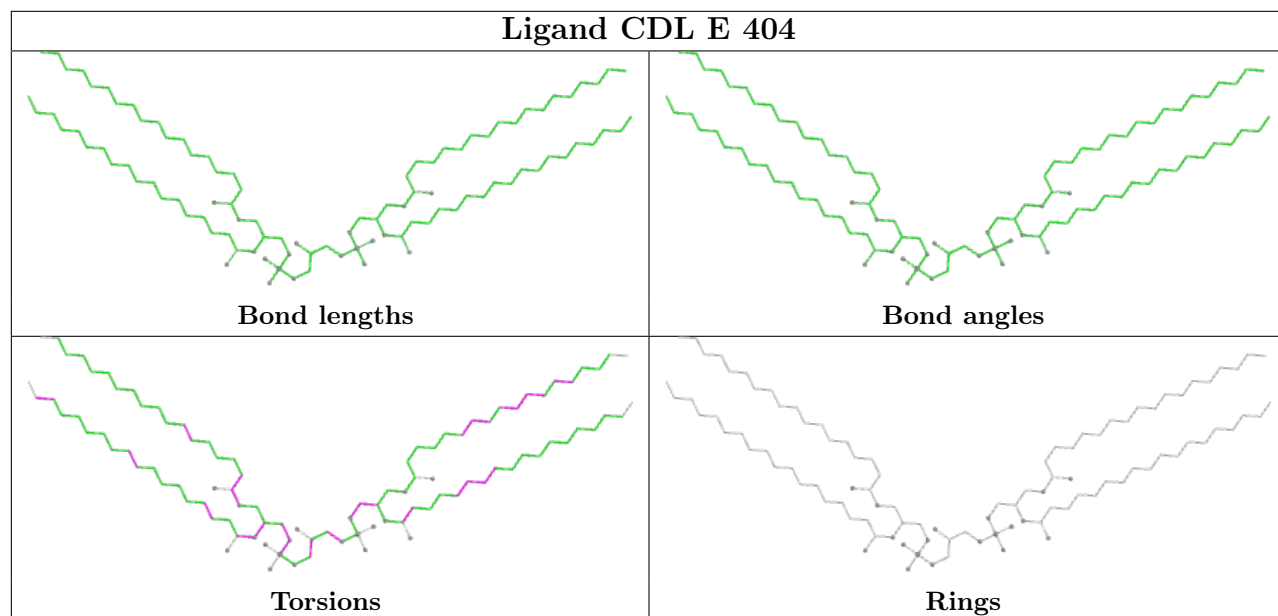


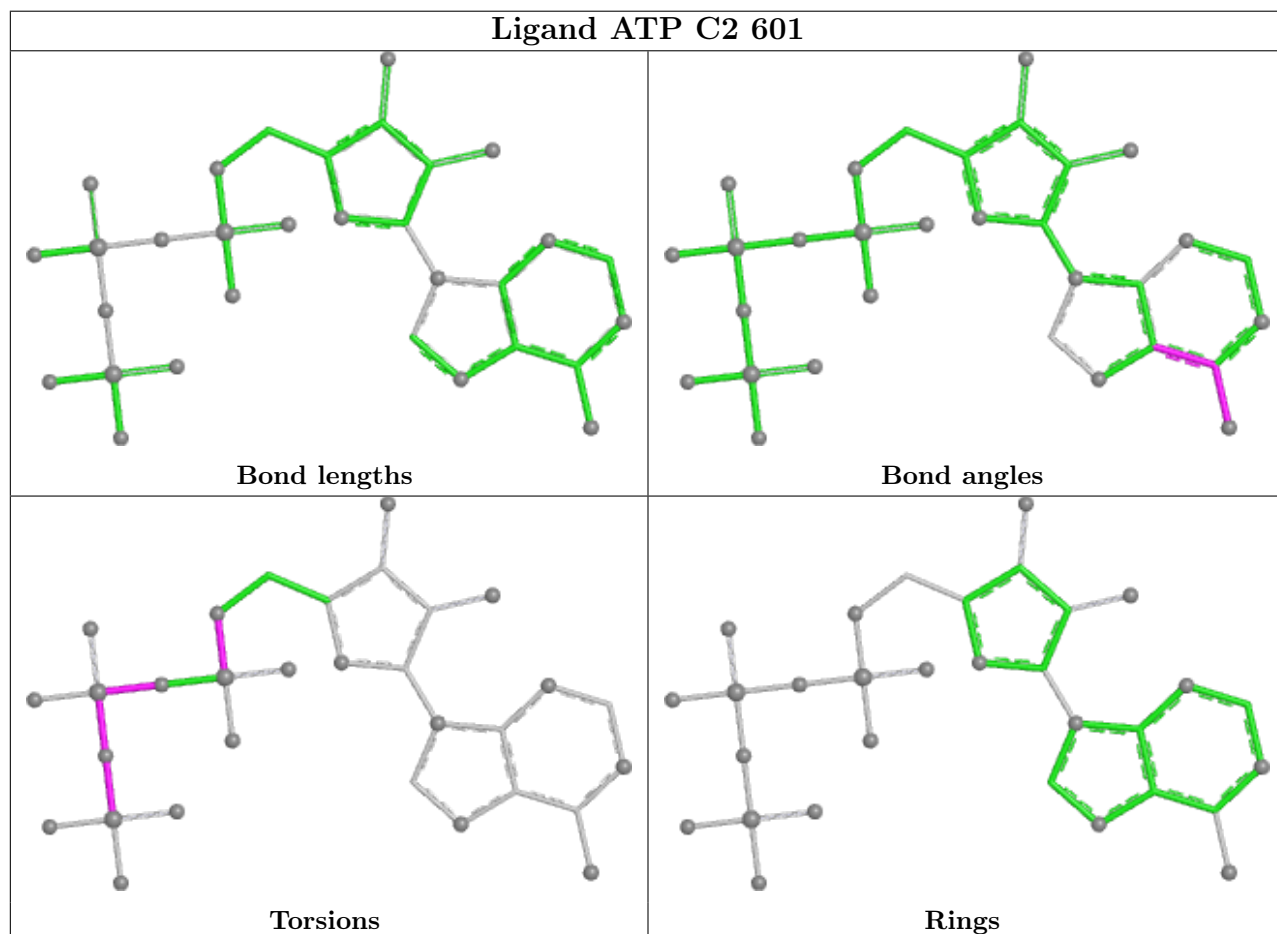
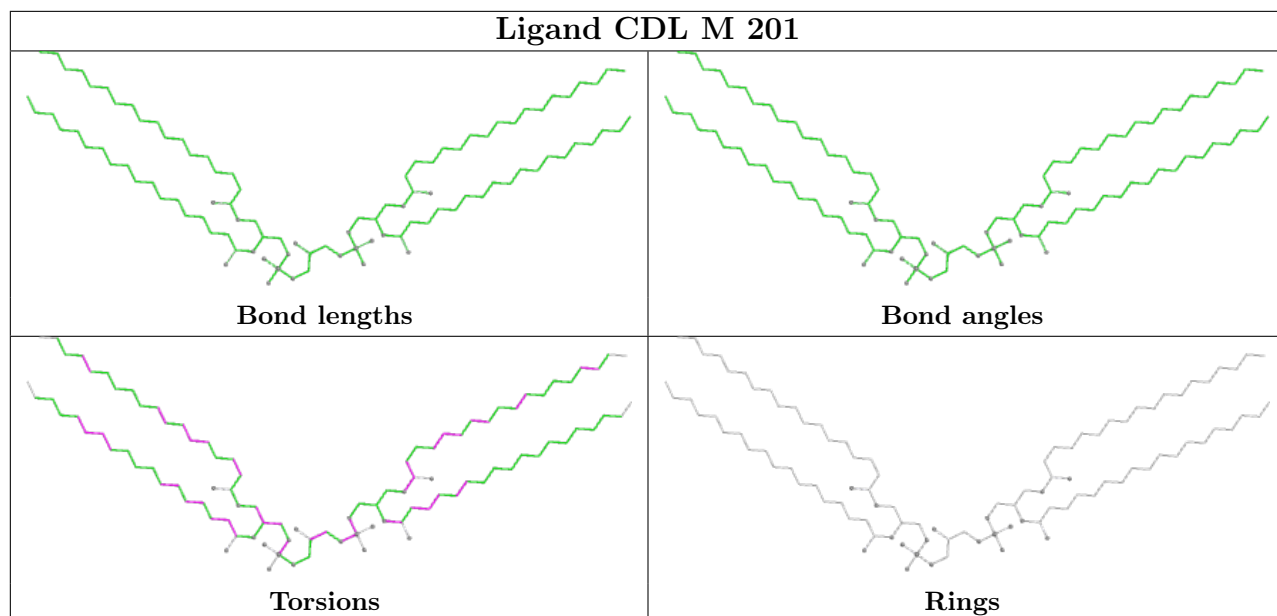


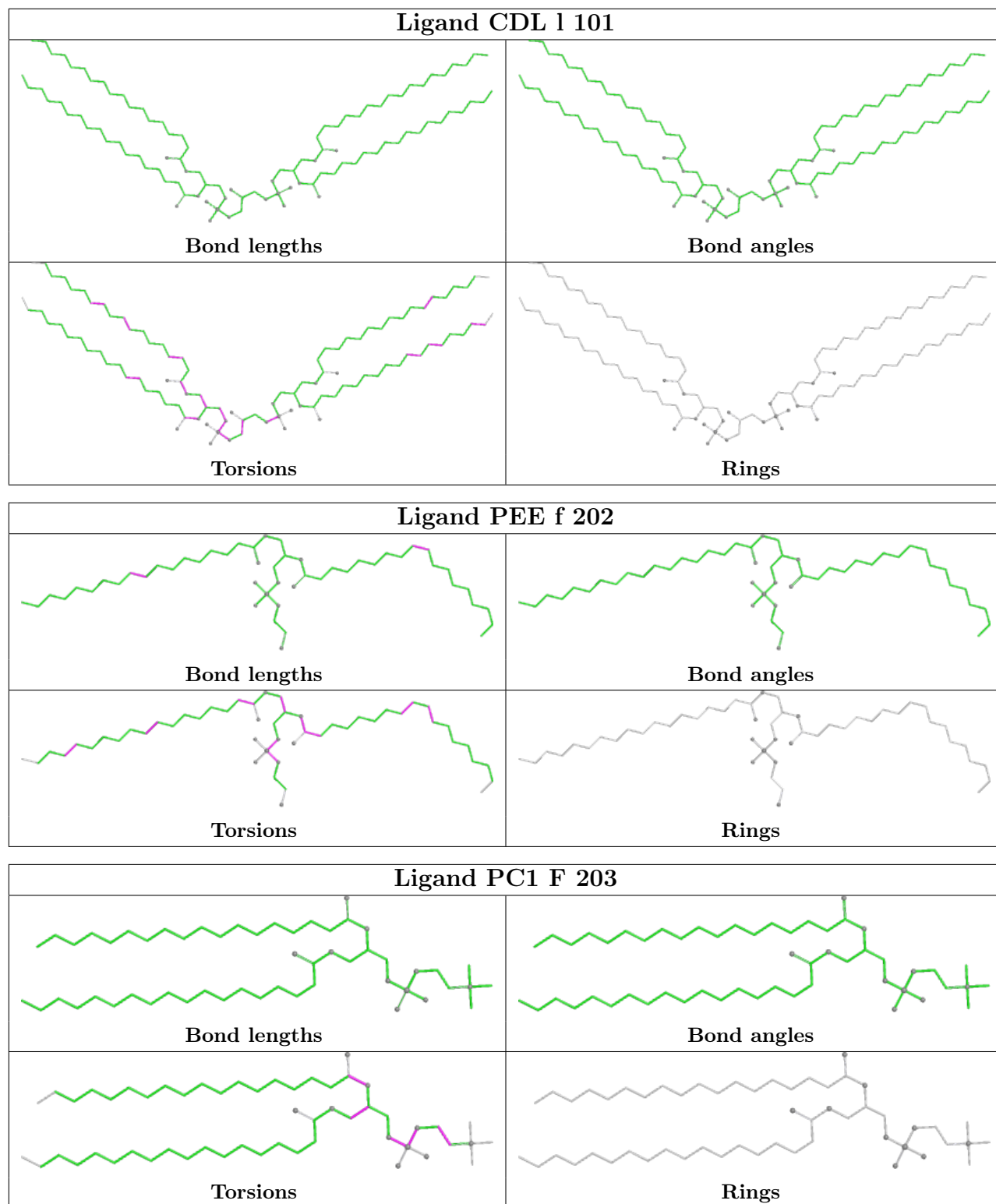


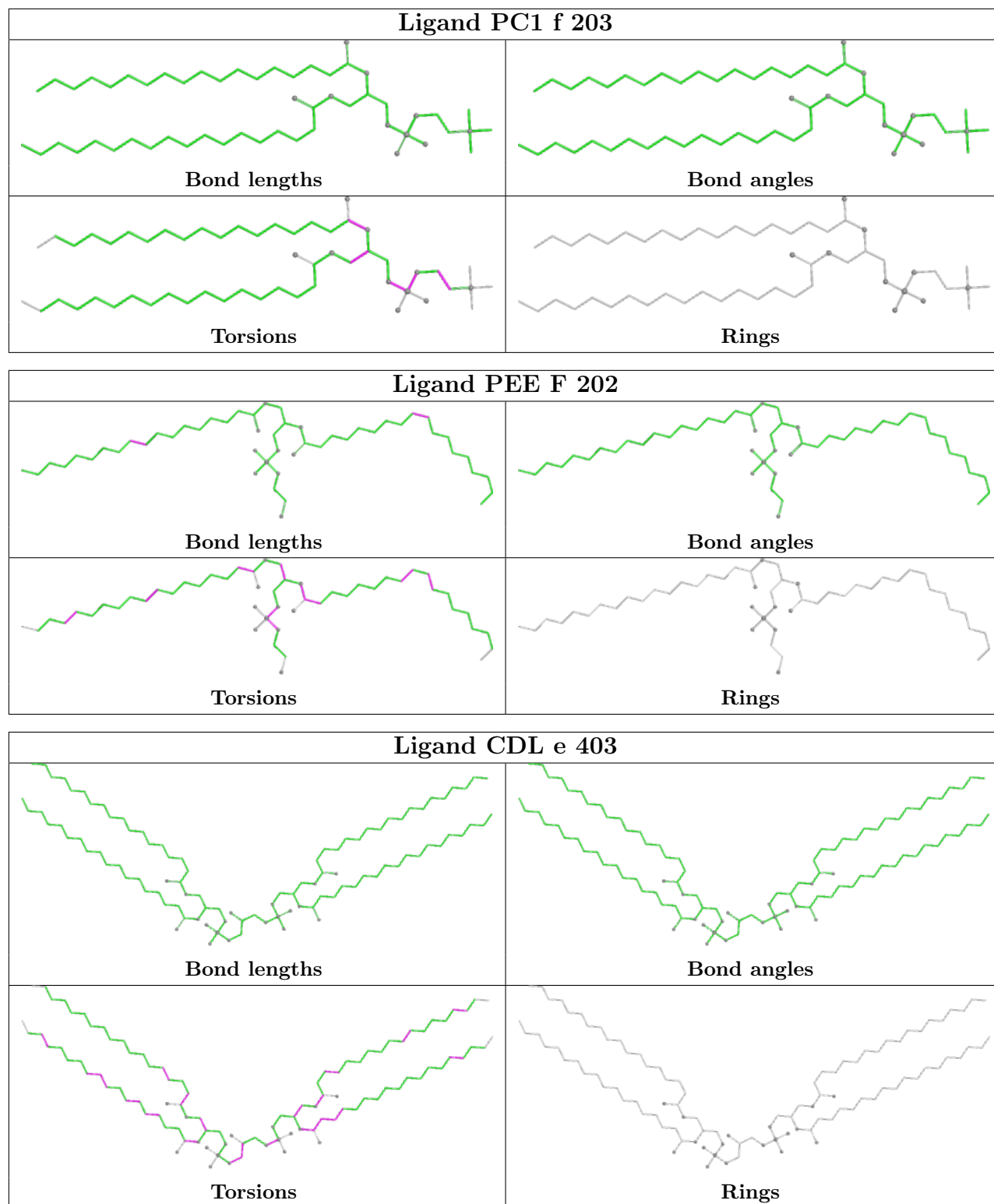


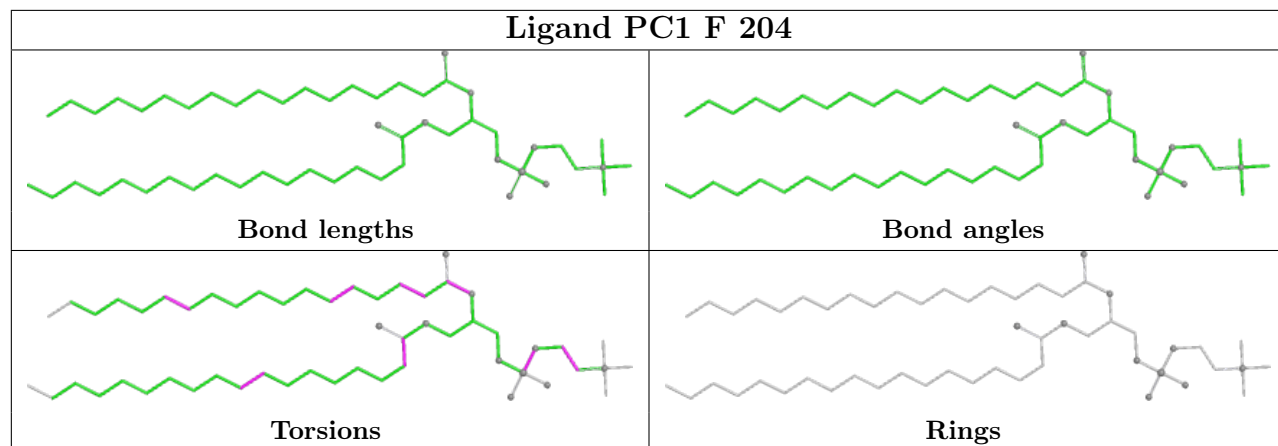
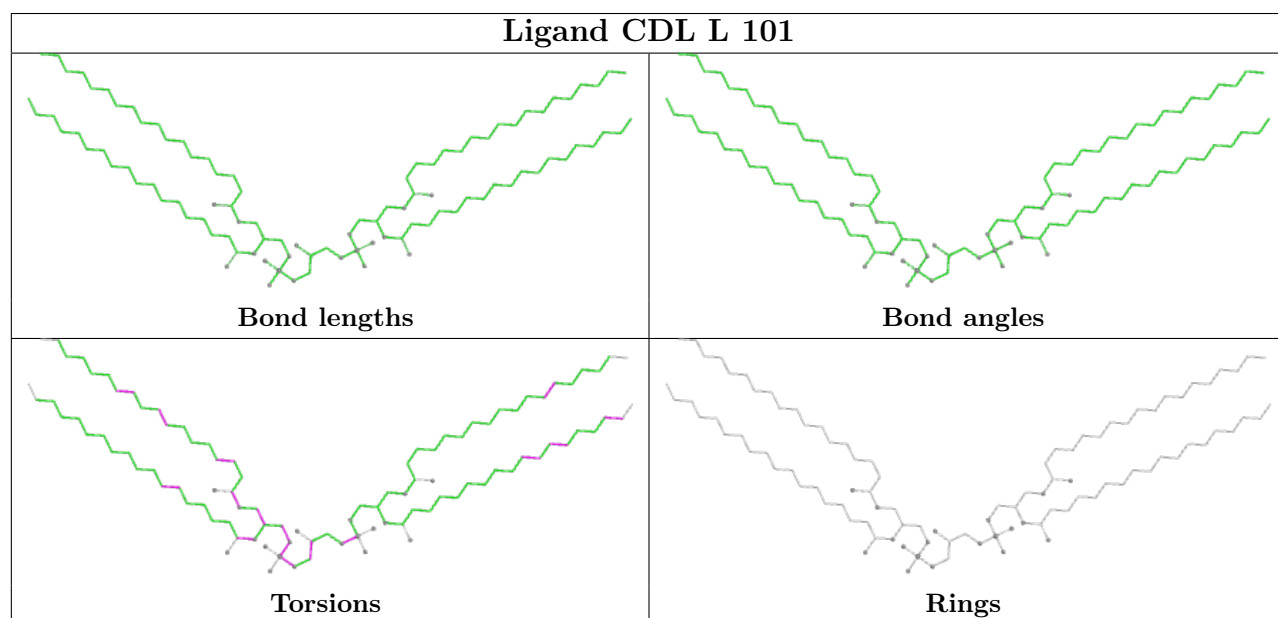
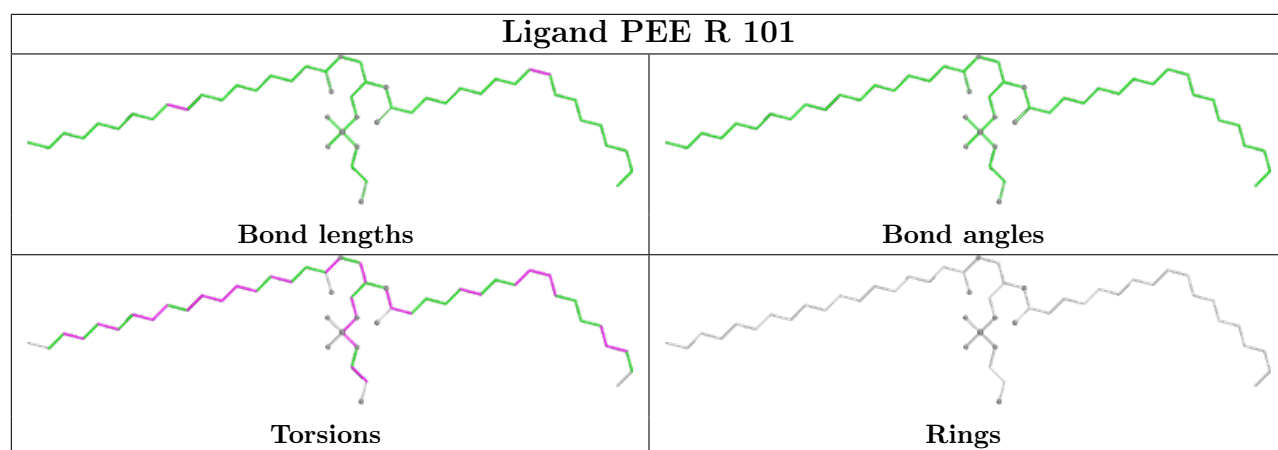


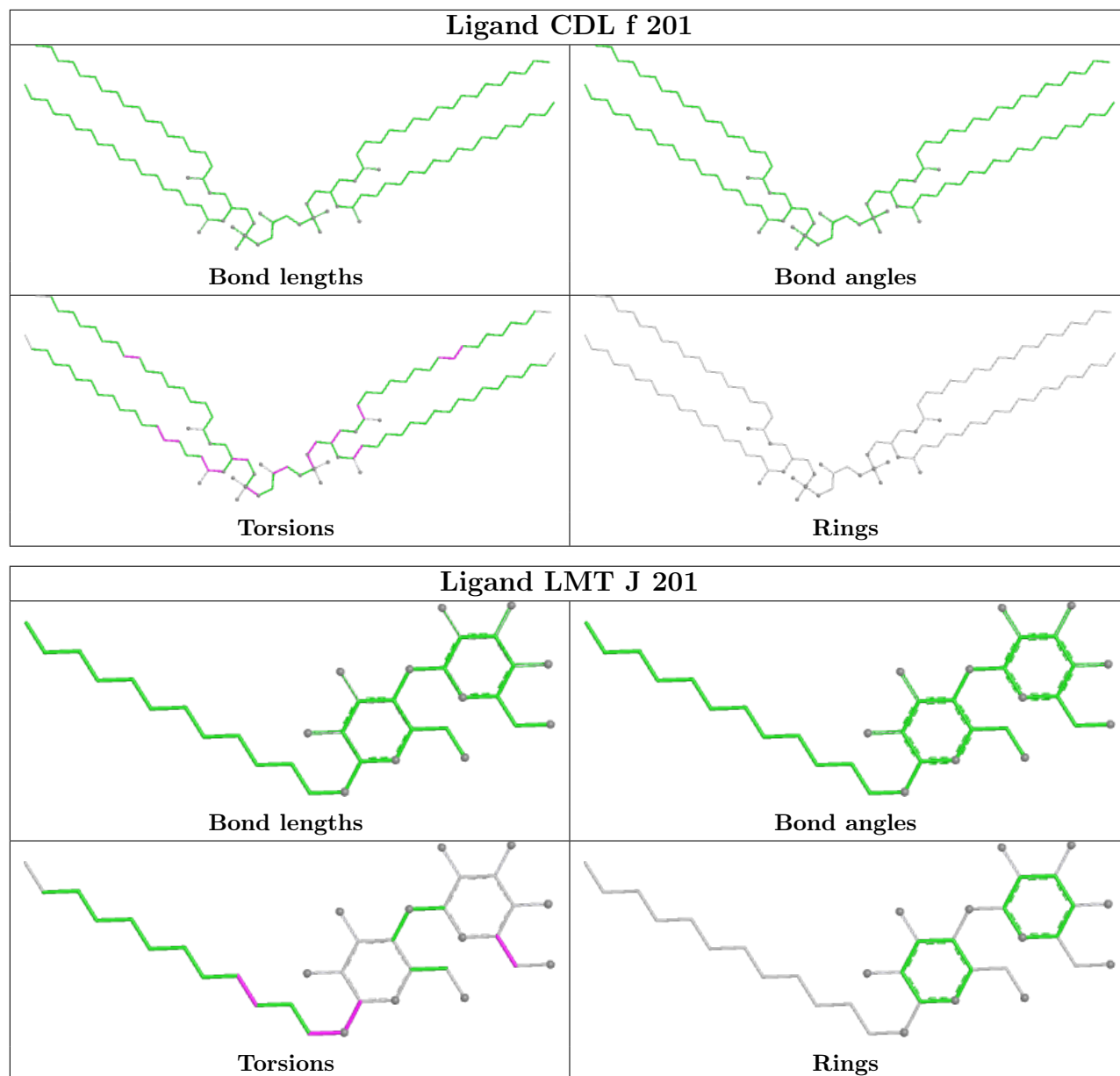


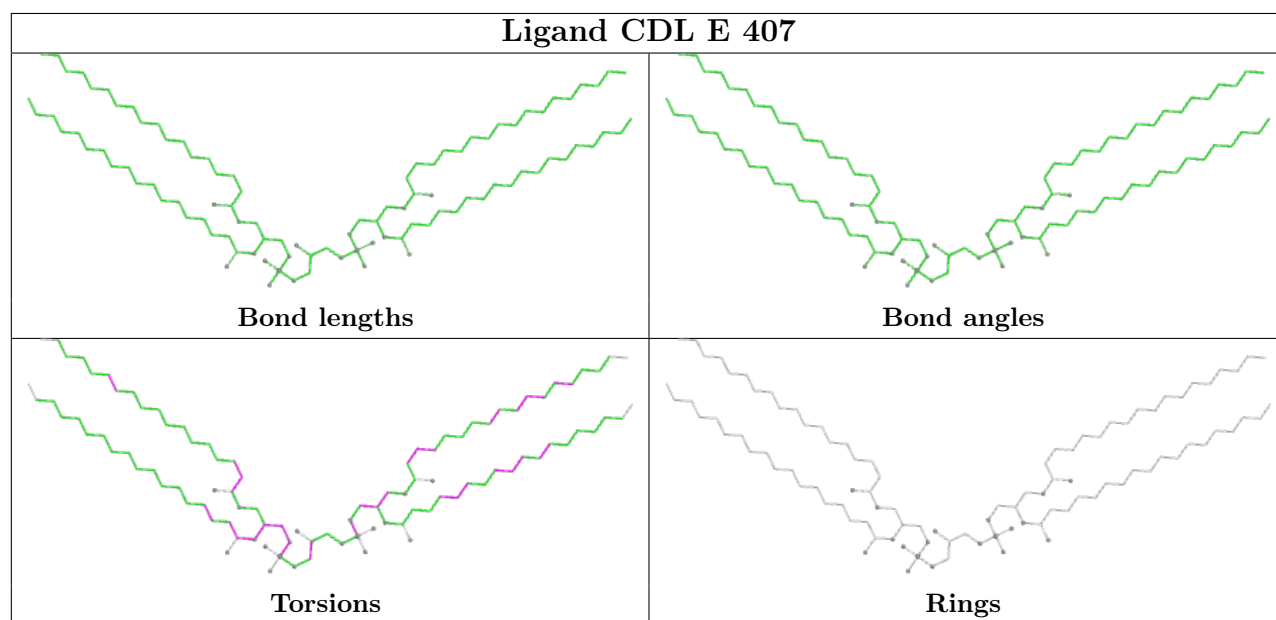
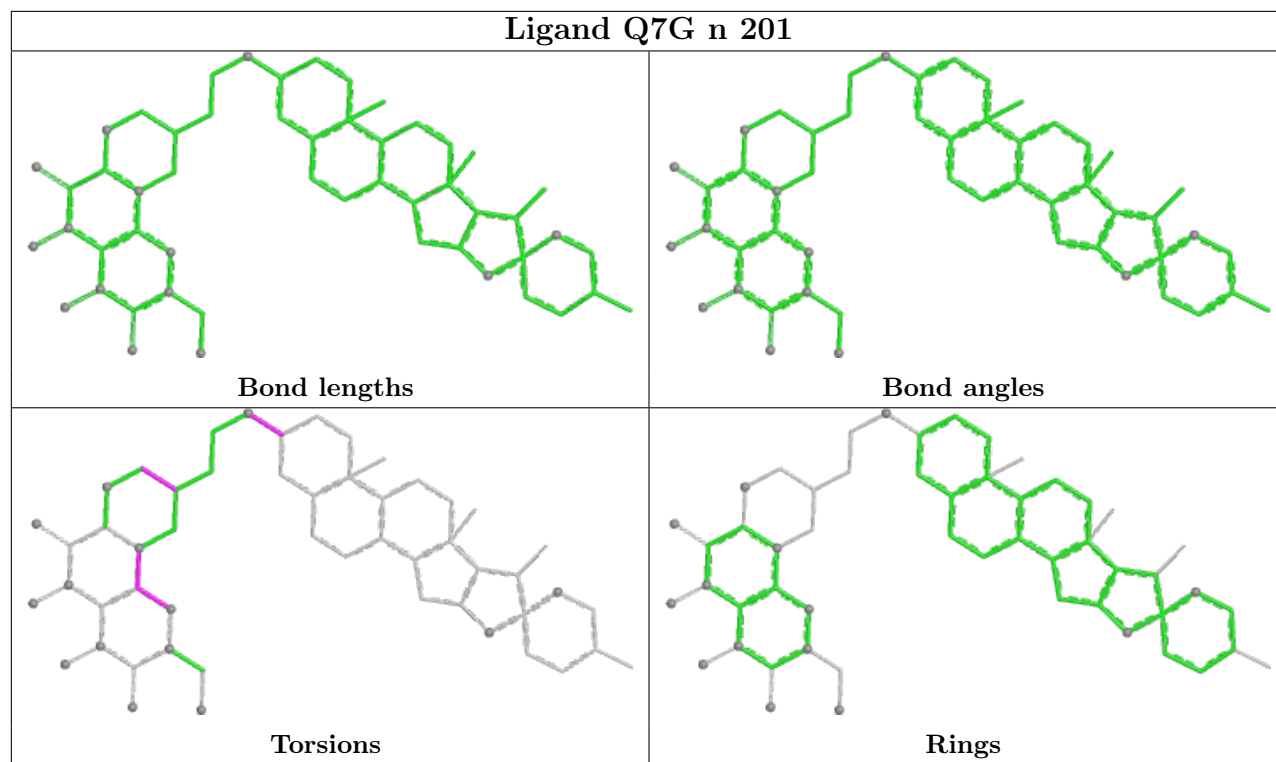


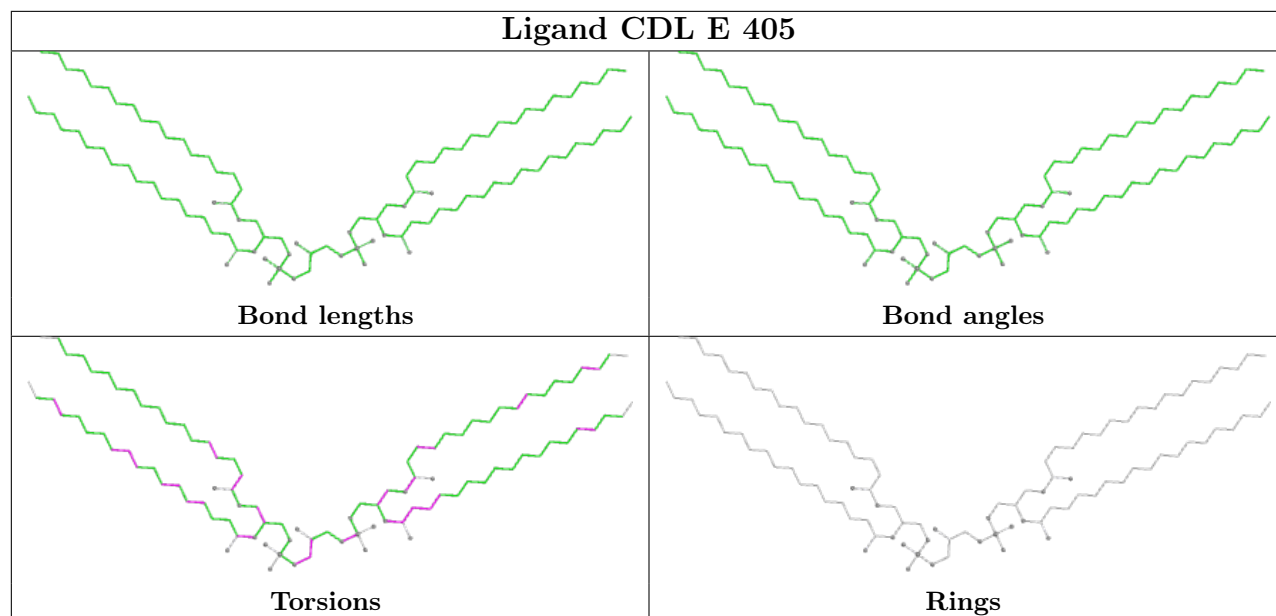












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

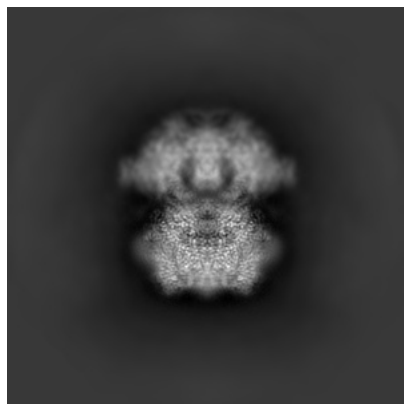
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15559. These allow visual inspection of the internal detail of the map and identification of artifacts.

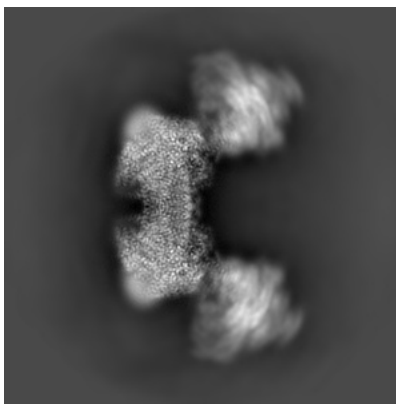
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

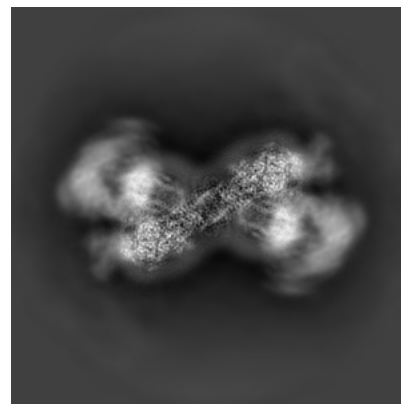
6.1.1 Primary map



X

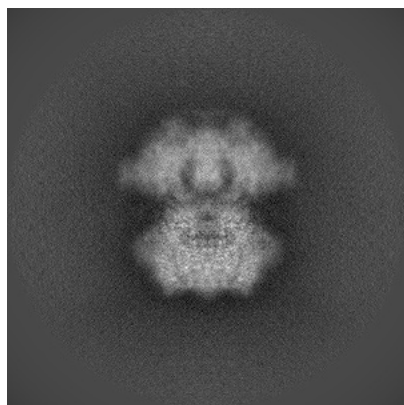


Y

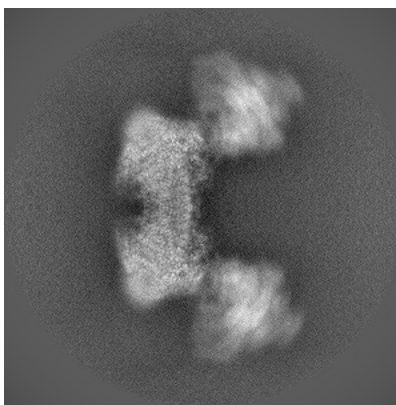


Z

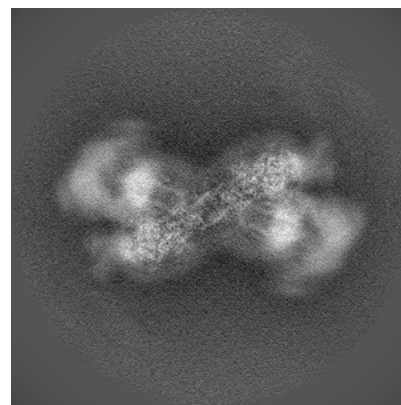
6.1.2 Raw map



X



Y

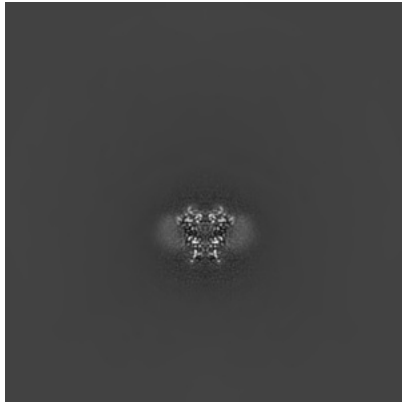


Z

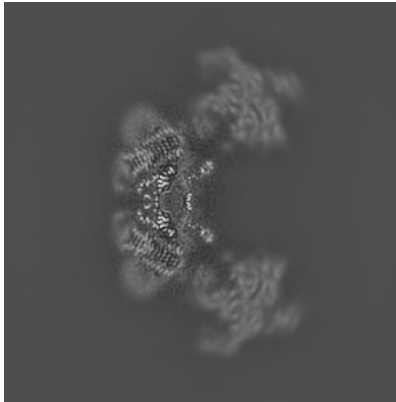
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

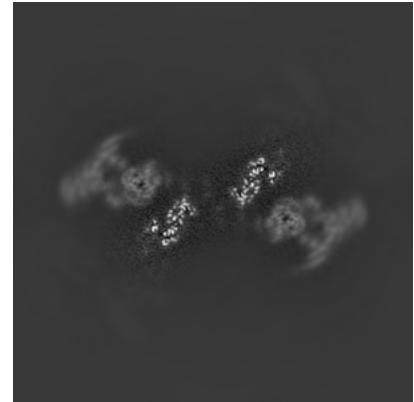
6.2.1 Primary map



X Index: 280

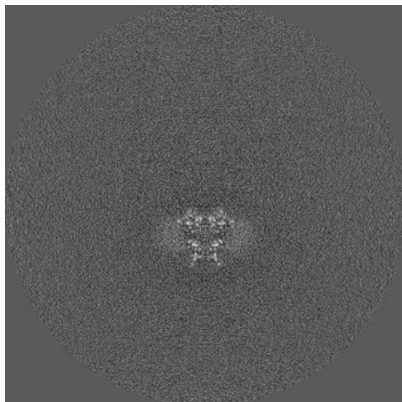


Y Index: 280

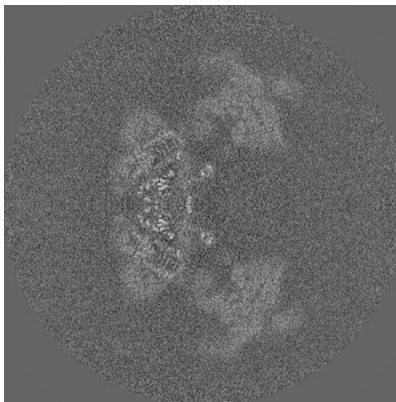


Z Index: 280

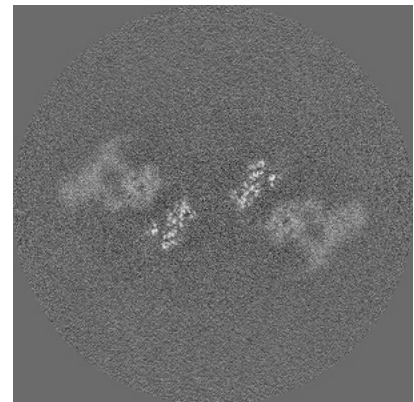
6.2.2 Raw map



X Index: 280



Y Index: 280

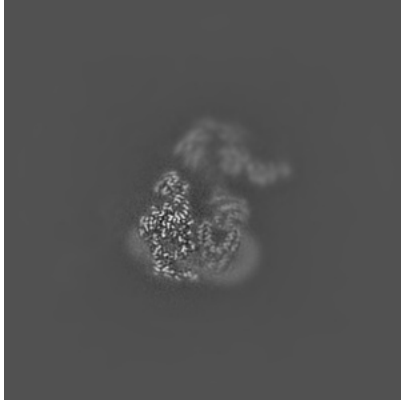


Z Index: 280

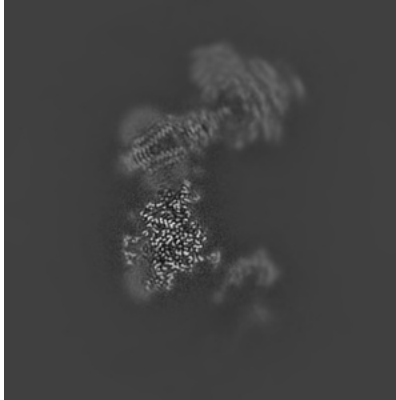
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

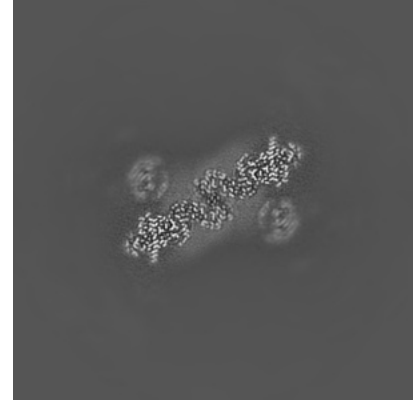
6.3.1 Primary map



X Index: 195

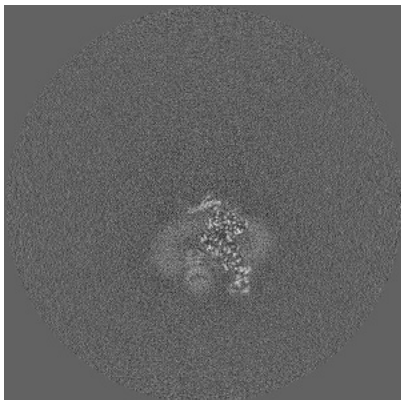


Y Index: 256

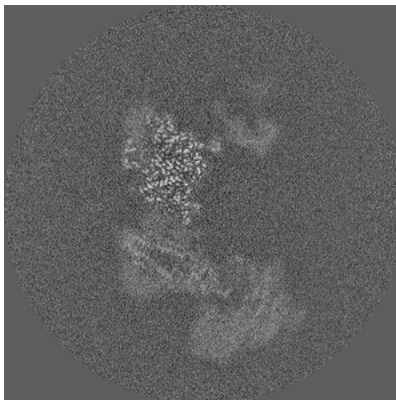


Z Index: 254

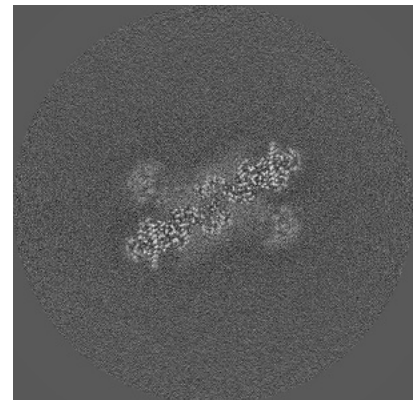
6.3.2 Raw map



X Index: 322



Y Index: 304

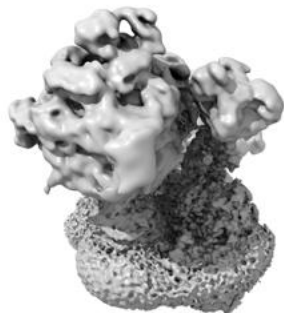


Z Index: 255

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



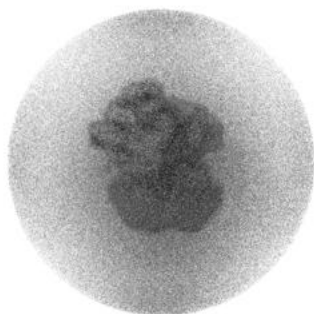
Y



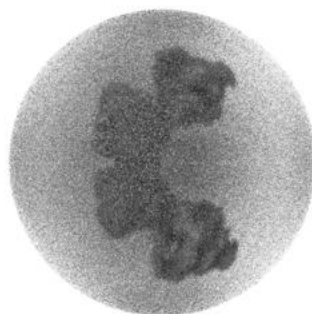
Z

The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

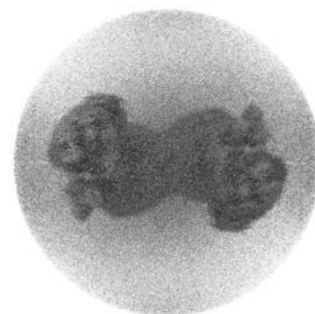
6.4.2 Raw map



X



Y



Z

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

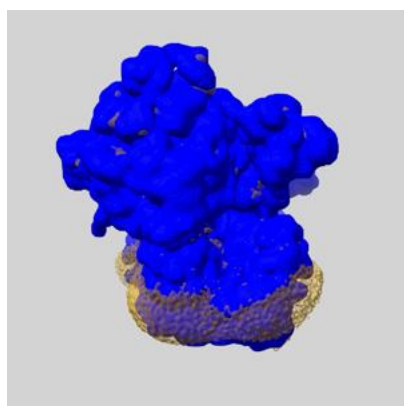
6.5 Mask visualisation [i](#)

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

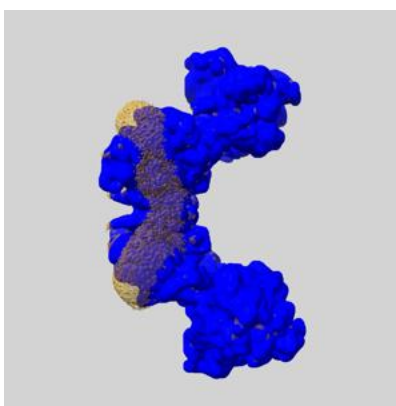
A mask typically either:

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

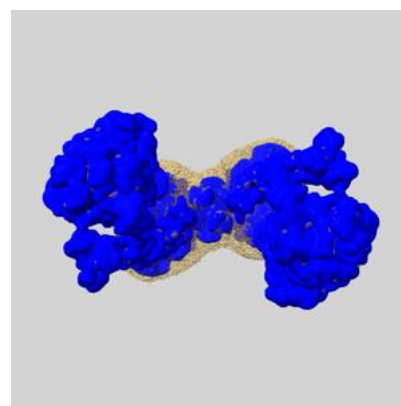
6.5.1 emd_15559_msk_1.map [i](#)



X



Y

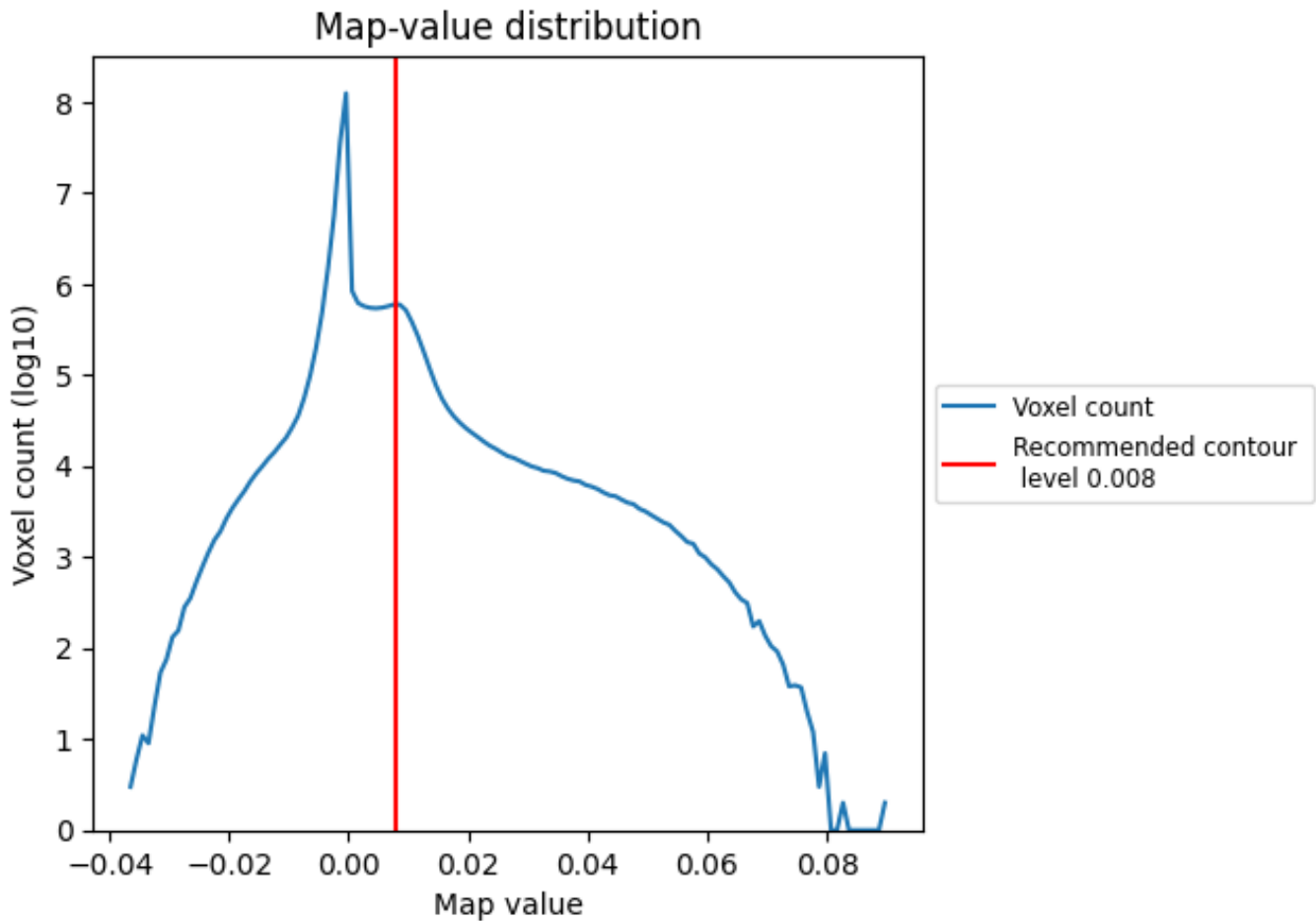


Z

7 Map analysis [i](#)

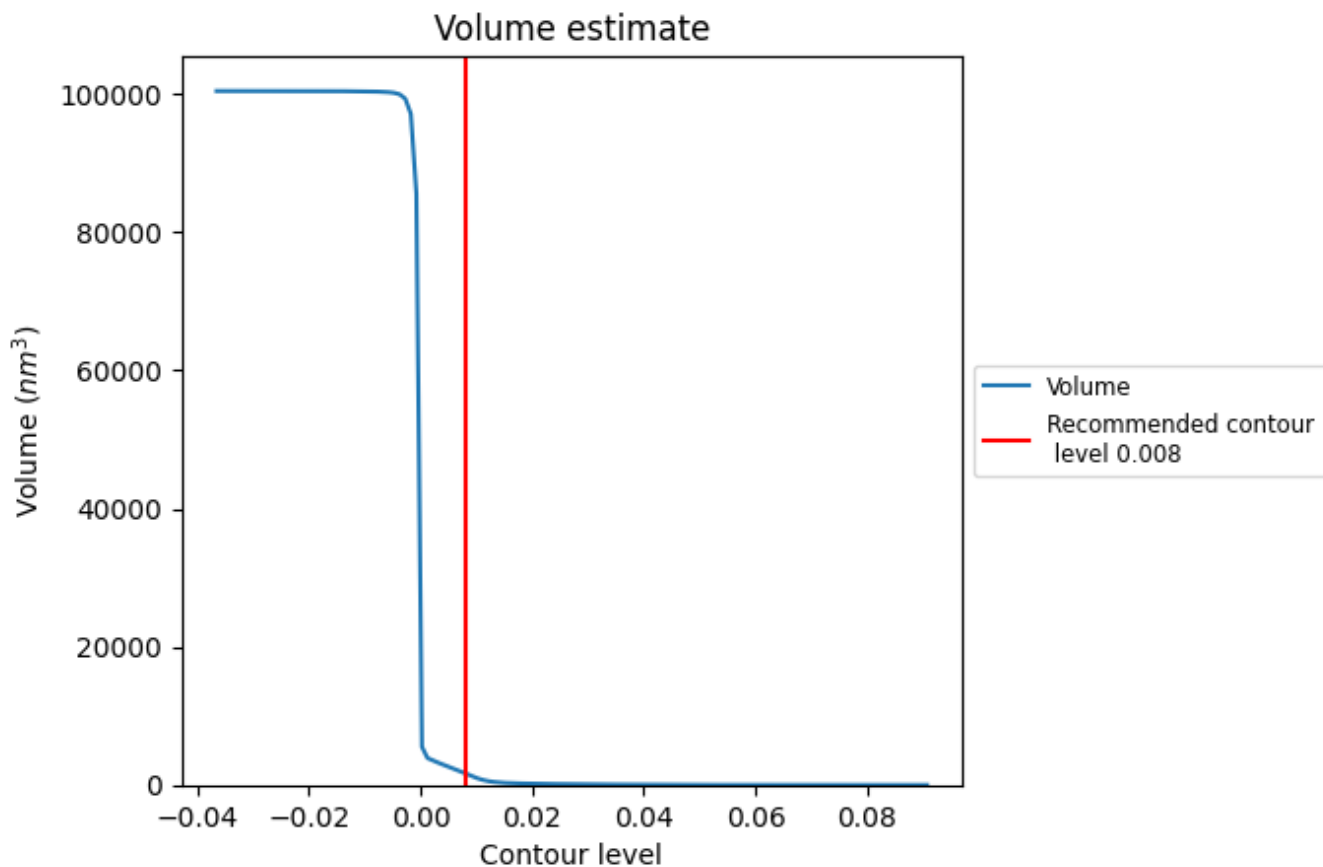
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

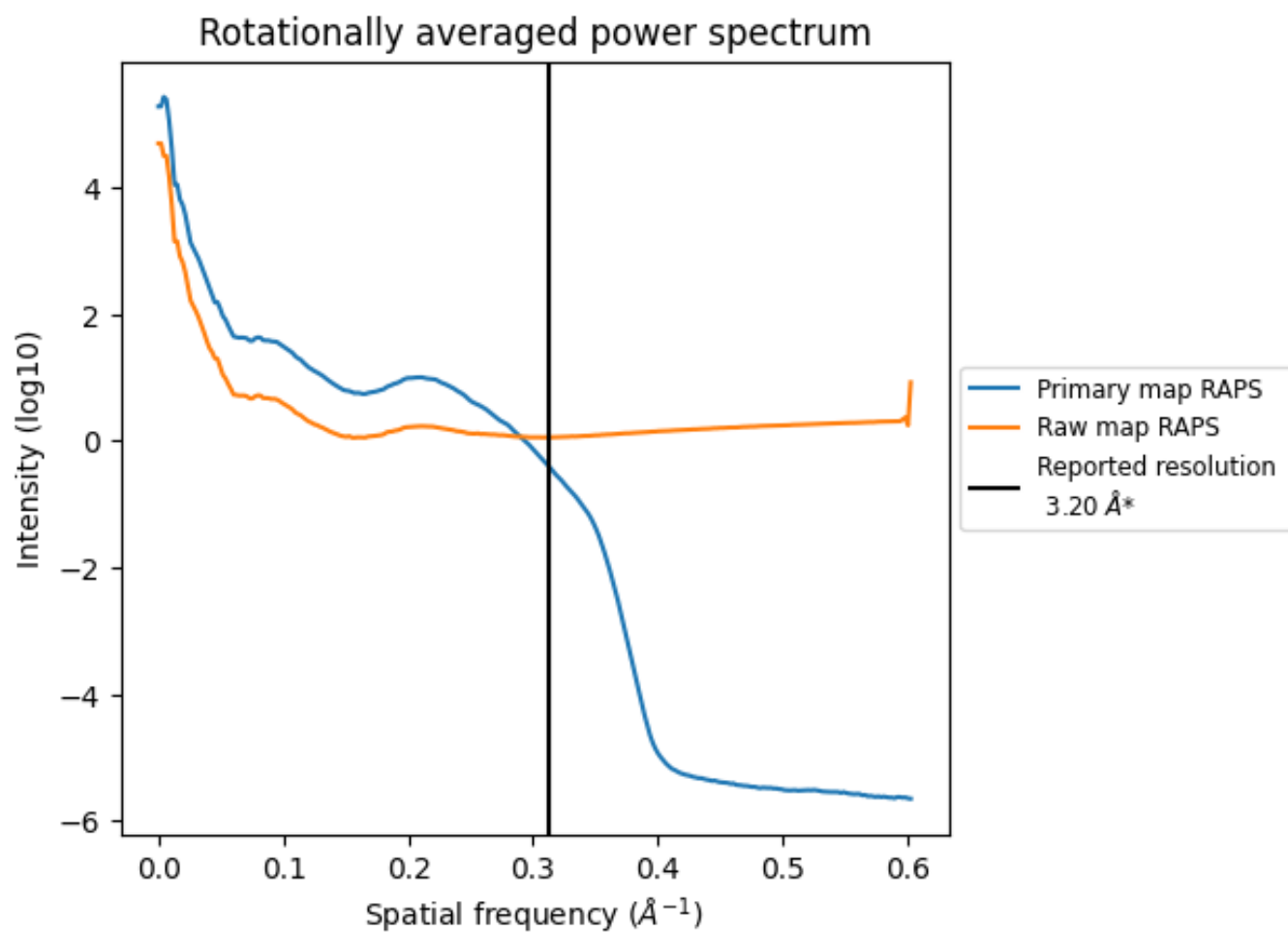
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1696 nm^3 ; this corresponds to an approximate mass of 1532 kDa.

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

7.3 Rotationally averaged power spectrum i

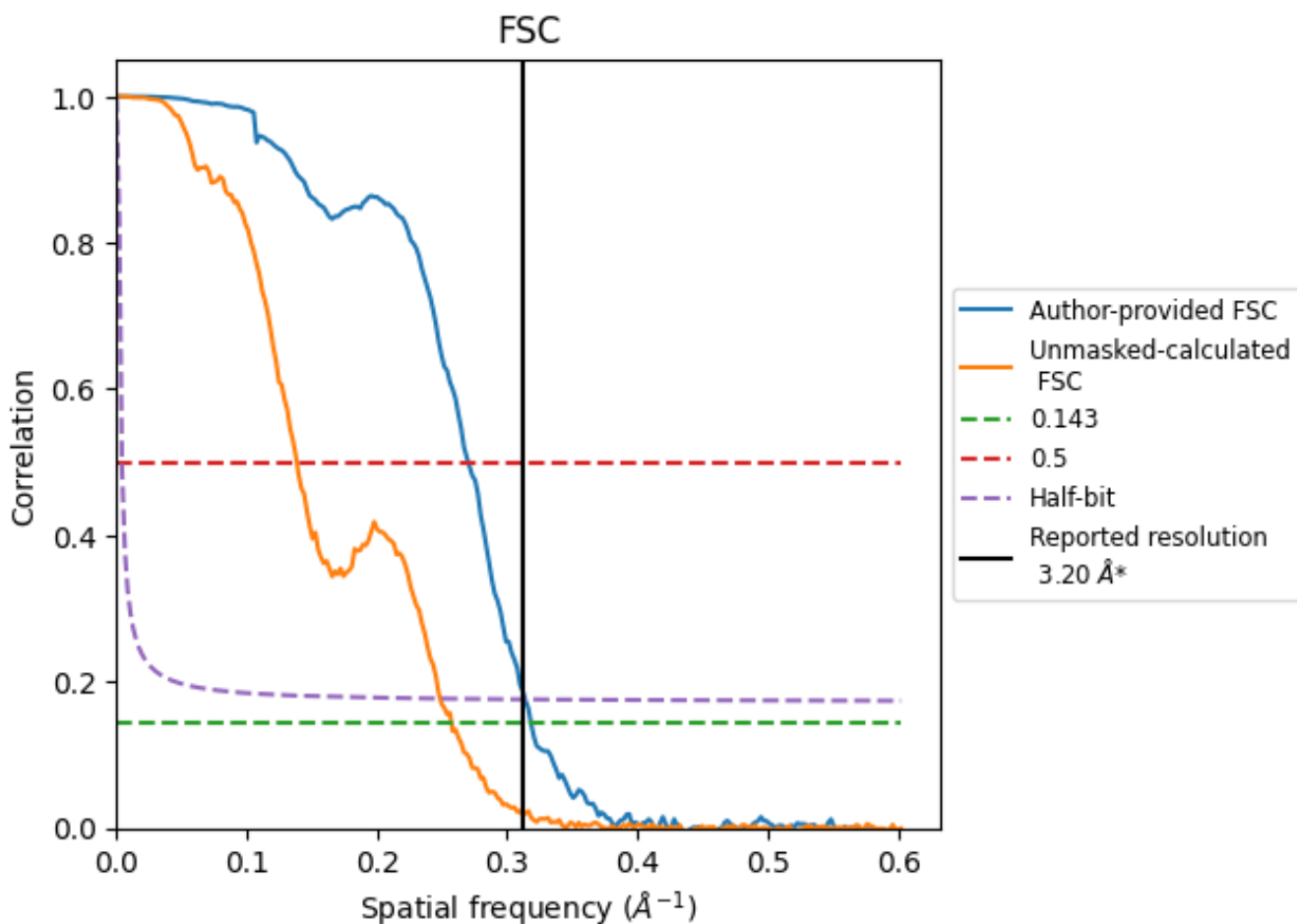


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

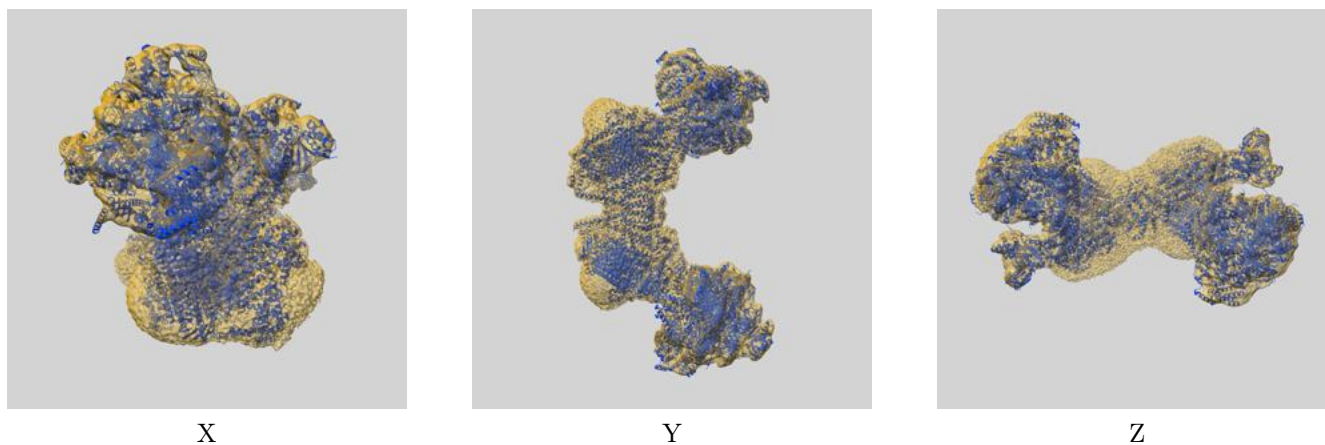
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.14	3.70	3.19
Unmasked-calculated*	3.89	7.22	4.02

*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 3.89 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15559 and PDB model 8AP6. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)

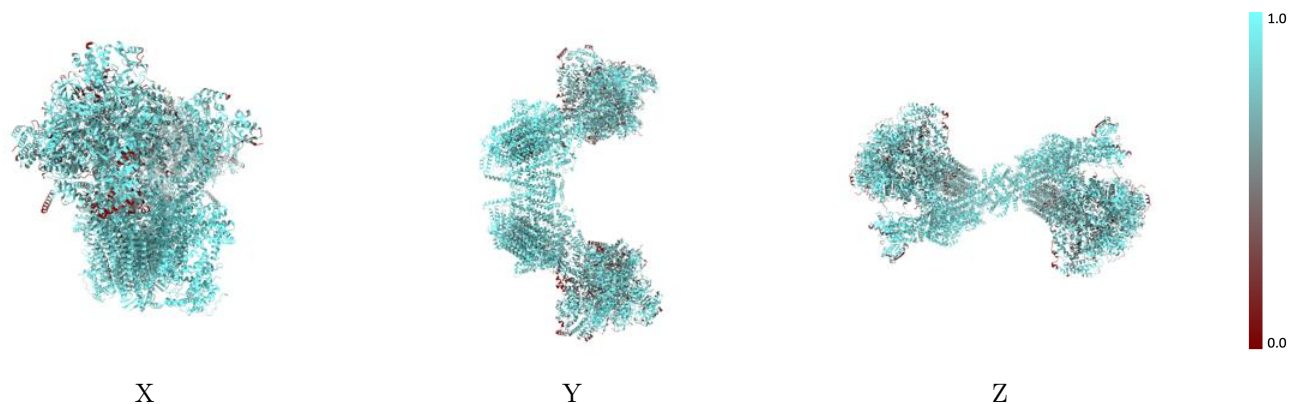


The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

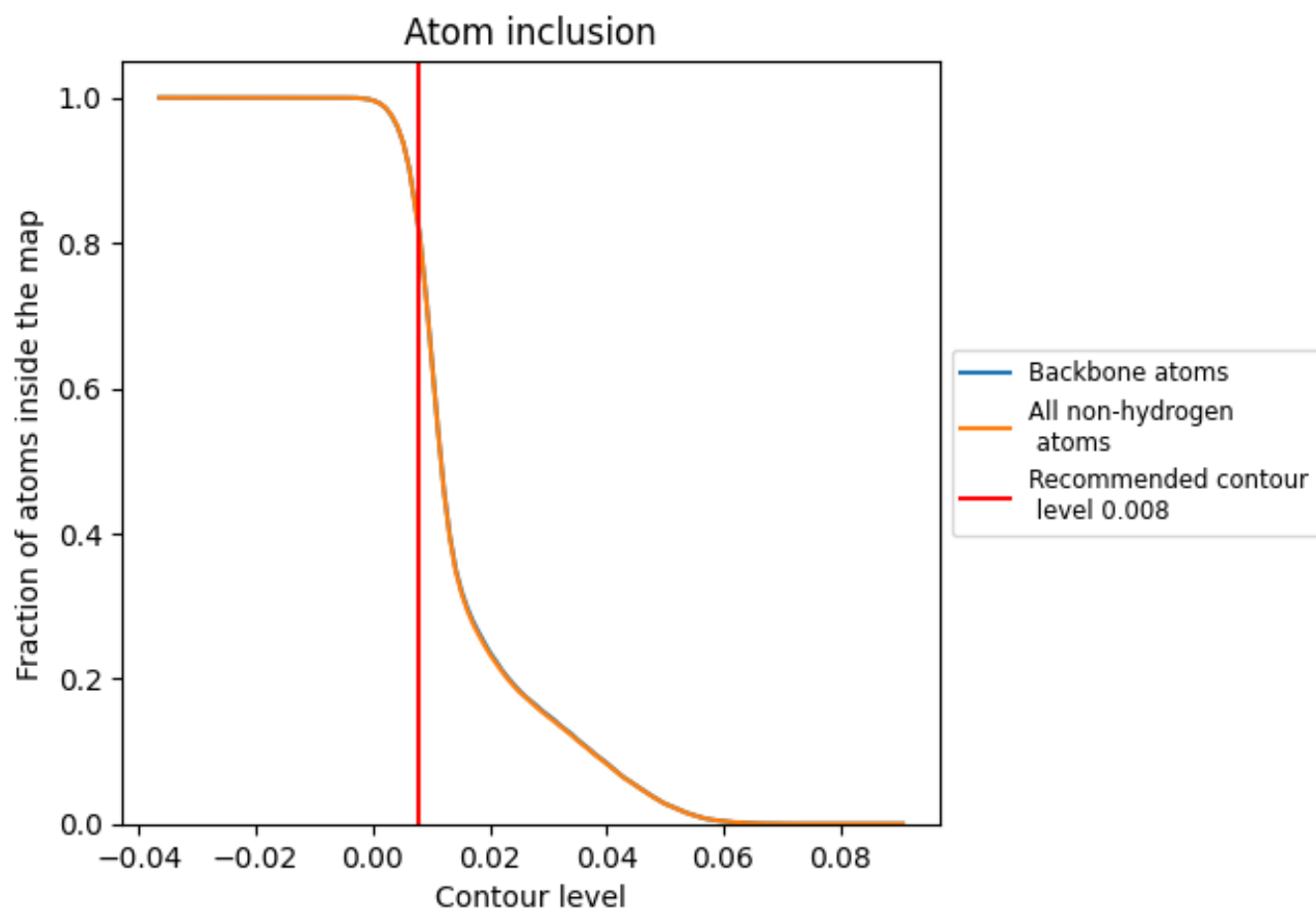
This section was not generated.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	0.8126
A	0.9541
A1	0.7552
A2	0.7545
B1	0.8002
B2	0.7972
C	0.9153
C1	0.7772
C2	0.7742
D	0.8587
D1	0.7226
D2	0.7188
E	0.9366
E1	0.7712
E2	0.7688
F	0.9257
F1	0.7609
F2	0.7582
G	0.8080
G1	0.7240
G2	0.7257
H	0.8267
H1	0.7545
H2	0.7569
I	0.9604
I1	0.7171
I2	0.7190
J	0.9176
J1	0.5971
J2	0.5948
K	0.9350
K1	0.7159
K2	0.7105
L	0.8636
L1	0.6484







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Chain	Atom inclusion
L2	0.6491
M	0.9177
M1	0.7596
M2	0.7574
N	0.9751
O	0.9483
O1	0.8164
O2	0.8164
P	0.9357
P1	0.8414
P2	0.8360
Q	0.9292
Q1	0.7950
Q2	0.7932
R	0.9444
R1	0.8360
R2	0.8342
S1	0.8592
S2	0.8538
T1	0.8360
T2	0.8378
U1	0.8414
U2	0.8467
V1	0.7897
V2	0.7950
W1	0.8039
W2	0.8057
X1	0.8235
X2	0.8271
a	0.9556
c	0.9092
d	0.8572
e	0.9355
f	0.9242
g	0.8085
h	0.8277
i	0.9604
j	0.9140
k	0.9338
l	0.8555
m	0.9150
n	0.9734

Continued on next page...

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Chain	Atom inclusion
o	 0.9470
p	 0.9297
q	 0.9316
r	 0.9479