



wwPDB EM Validation Summary Report ⓘ

Mar 28, 2026 – 01:45 PM UTC

PDB ID : 6TDV / pdb_00006tdv
EMDB ID : EMD-10468
Title : Cryo-EM structure of Euglena gracilis mitochondrial ATP synthase, membrane region
Authors : Muhleip, A.; Amunts, A.
Deposited on : 2019-11-10
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

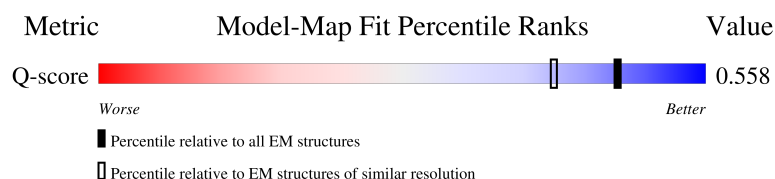
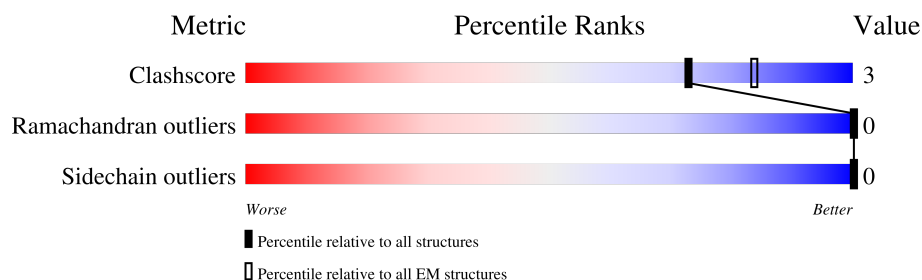
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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.



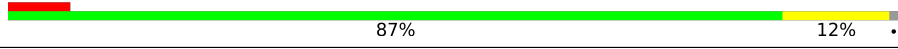
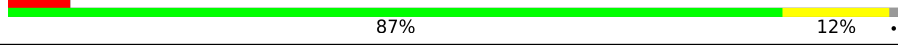
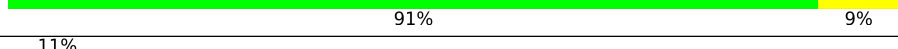
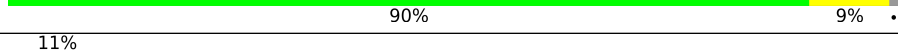
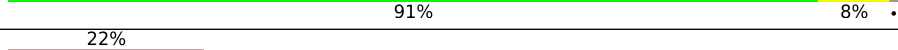
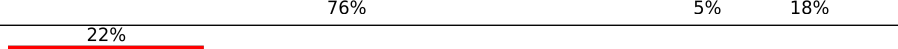
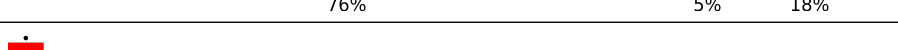
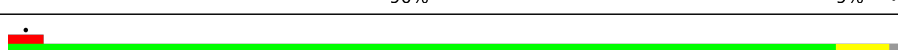
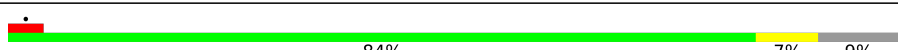
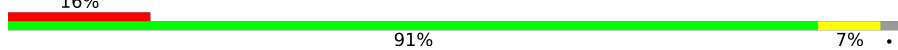
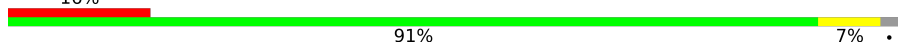
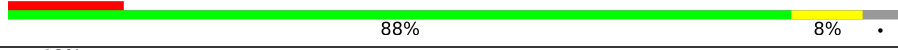
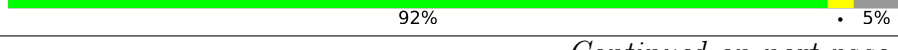
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	487	7% 93% 7%
1	a	487	7% 92% 7%
2	B	338	8% 9% 91%
2	b	338	8% 9% 91%

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Mol	Chain	Length	Quality of chain
3	D	187	
3	d	187	
4	E	97	
4	e	97	
5	F	274	
5	f	274	
6	G	112	
6	g	112	
7	H	476	
7	h	476	
8	I	98	
8	i	98	
9	J	104	
9	j	104	
10	K	113	
10	k	113	
11	L	57	
11	l	57	
12	M	169	
12	m	169	
13	N	137	
13	n	137	
14	O	116	
14	o	116	
15	P	120	

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Mol	Chain	Length	Quality of chain
15	p	120	
16	Q	90	
16	q	90	
17	R	78	
17	r	78	
18	S	74	
18	s	74	
19	T	66	
19	t	66	

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 95420 atoms, of which 47674 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 ATPTB1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	486	Total	C	H	N	O	S	0	0
			7864	2525	3919	677	733	10		
1	a	486	Total	C	H	N	O	S	0	0
			7864	2525	3919	677	733	10		

- Molecule 2 is a protein called ATPTB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	31	Total	C	H	N	O	0	0
			494	153	243	44	54		
2	b	31	Total	C	H	N	O	0	0
			494	153	243	44	54		

- Molecule 3 is a protein called ATPTB6.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	186	Total	C	H	N	O	S	0	0
			3040	977	1519	269	267	8		
3	d	186	Total	C	H	N	O	S	0	0
			3040	977	1519	269	267	8		

- Molecule 4 is a protein called ATPTB12.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	96	Total	C	H	N	O	S	0	0
			1574	509	777	144	141	3		
4	e	96	Total	C	H	N	O	S	0	0
			1577	510	779	144	141	3		

- Molecule 5 is a protein called subunit a.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	274	Total	C	H	N	O	S	0	0
			4639	1566	2327	341	391	14		
5	f	274	Total	C	H	N	O	S	0	0
			4642	1566	2329	342	391	14		

- Molecule 6 is a protein called subunit b.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	G	111	Total	C	H	N	O	S	0	0
			1803	566	924	160	146	7		
6	g	111	Total	C	H	N	O	S	0	0
			1803	566	924	160	146	7		

- Molecule 7 is a protein called subunit d.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	H	388	Total	C	H	N	O	S	0	0
			6165	1987	3059	512	598	9		
7	h	388	Total	C	H	N	O	S	0	0
			6165	1987	3059	512	598	9		

- Molecule 8 is a protein called subunit f.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	I	97	Total	C	H	N	O	S	0	0
			1553	504	771	140	135	3		
8	i	97	Total	C	H	N	O	S	0	0
			1553	504	771	140	135	3		

- Molecule 9 is a protein called subunit i/j.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	J	103	Total	C	H	N	O	S	0	0
			1734	581	853	151	146	3		
9	j	103	Total	C	H	N	O	S	0	0
			1734	581	853	151	146	3		

- Molecule 10 is a protein called subunit k.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	K	103	Total	C	H	N	O	S	0	0
			1637	530	821	136	144	6		

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Mol	Chain	Residues	Atoms						AltConf	Trace
10	k	103	Total	C	H	N	O	S	0	0
			1637	530	821	136	144	6		

- Molecule 11 is a protein called subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	L	57	Total	C	H	N	O		0	0
			1008	350	507	69	82			
11	l	57	Total	C	H	N	O		0	0
			1008	350	507	69	82			

- Molecule 12 is a protein called ATPEG1.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	M	166	Total	C	H	N	O	S	0	0
			2717	887	1354	228	240	8		
12	m	166	Total	C	H	N	O	S	0	0
			2717	887	1354	228	240	8		

- Molecule 13 is a protein called ATPEG2.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	N	131	Total	C	H	N	O	S	0	0
			2167	714	1070	198	182	3		
13	n	131	Total	C	H	N	O	S	0	0
			2167	714	1070	198	182	3		

- Molecule 14 is a protein called ATPEG3.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	O	100	Total	C	H	N	O	S	0	0
			1652	556	803	146	145	2		
14	o	100	Total	C	H	N	O	S	0	0
			1652	556	803	146	145	2		

- Molecule 15 is a protein called ATPEG4.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	P	114	Total	C	H	N	O	S	0	0
			1838	601	912	159	160	6		
15	p	114	Total	C	H	N	O	S	0	0
			1838	601	912	159	160	6		

- Molecule 16 is a protein called ATPEG5.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	Q	89	Total	C	H	N	O	S	0	0
			1476	475	723	137	137	4		
16	q	89	Total	C	H	N	O	S	0	0
			1476	475	723	137	137	4		

- Molecule 17 is a protein called ATPEG6.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	R	69	Total	C	H	N	O	S	0	0
			1160	374	581	106	97	2		
17	r	69	Total	C	H	N	O	S	0	0
			1160	374	581	106	97	2		

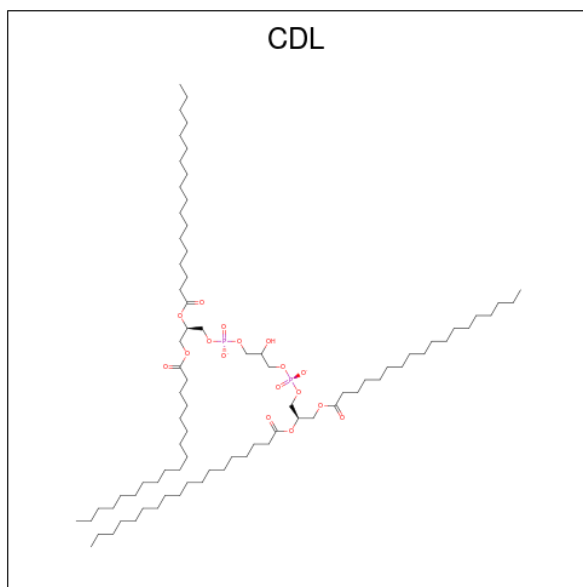
- Molecule 18 is a protein called ATPEG7.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	S	65	Total	C	H	N	O	S	0	0
			1092	371	541	90	89	1		
18	s	65	Total	C	H	N	O	S	0	0
			1092	371	541	90	89	1		

- Molecule 19 is a protein called ATPEG8.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	T	66	Total	C	H	N	O	S	0	0
			1080	349	552	95	83	1		
19	t	66	Total	C	H	N	O	S	0	0
			1080	349	552	95	83	1		

- Molecule 20 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



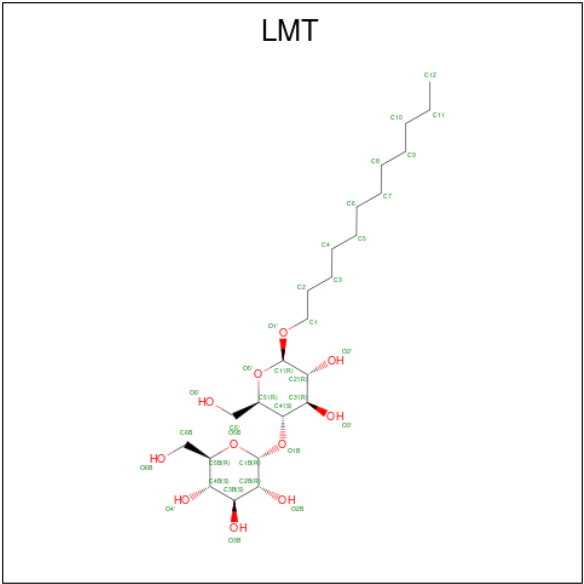
Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	H	O	P	0
			183	62	102	17	2	
20	A	1	Total	C	H	O	P	0
			170	62	89	17	2	
20	A	1	Total	C	H	O	P	0
			184	63	102	17	2	
20	A	1	Total	C	H	O	P	0
			99	44	36	17	2	
20	D	1	Total	C	H	O	P	0
			228	72	137	17	2	
20	D	1	Total	C	H	O	P	0
			184	67	98	17	2	
20	E	1	Total	C	H	O	P	0
			95	44	32	17	2	
20	M	1	Total	C	H	O	P	0
			152	58	75	17	2	
20	M	1	Total	C	H	O	P	0
			80	34	27	17	2	
20	O	1	Total	C	H	O	P	0
			124	46	59	17	2	
20	P	1	Total	C	H	O	P	0
			75	29	27	17	2	
20	R	1	Total	C	H	O	P	0
			150	57	74	17	2	
20	a	1	Total	C	H	O	P	0
			183	62	102	17	2	
20	a	1	Total	C	H	O	P	0
			170	62	89	17	2	

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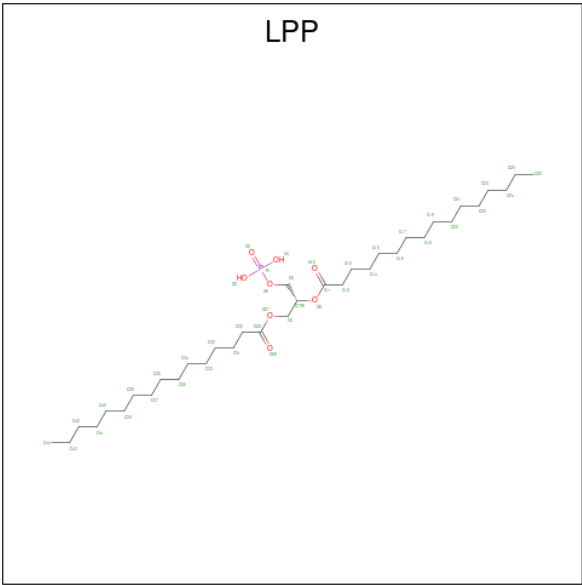
Mol	Chain	Residues	Atoms					AltConf
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			184	63	102	17	2	
20	a	1	Total	C	H	O	P	0
			99	44	36	17	2	
20	d	1	Total	C	H	O	P	0
			228	72	137	17	2	
20	d	1	Total	C	H	O	P	0
			184	67	98	17	2	
20	e	1	Total	C	H	O	P	0
			95	44	32	17	2	
20	m	1	Total	C	H	O	P	0
			152	58	75	17	2	
20	m	1	Total	C	H	O	P	0
			80	34	27	17	2	
20	o	1	Total	C	H	O	P	0
			124	46	59	17	2	
20	p	1	Total	C	H	O	P	0
			244	79	146	17	2	
20	p	1	Total	C	H	O	P	0
			75	29	27	17	2	
20	r	1	Total	C	H	O	P	0
			150	57	74	17	2	

- Molecule 21 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms				AltConf
21	D	1	Total	C	H	O	0
			81	24	46	11	
21	F	1	Total	C	H	O	0
			81	24	46	11	
21	N	1	Total	C	H	O	0
			81	24	46	11	
21	Q	1	Total	C	H	O	0
			81	24	46	11	
21	d	1	Total	C	H	O	0
			81	24	46	11	
21	f	1	Total	C	H	O	0
			81	24	46	11	
21	n	1	Total	C	H	O	0
			81	24	46	11	
21	q	1	Total	C	H	O	0
			81	24	46	11	

- Molecule 22 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (CCD ID: LPP) (formula: C₃₅H₆₉O₈P) (labeled as "Ligand of Interest" by depositor).



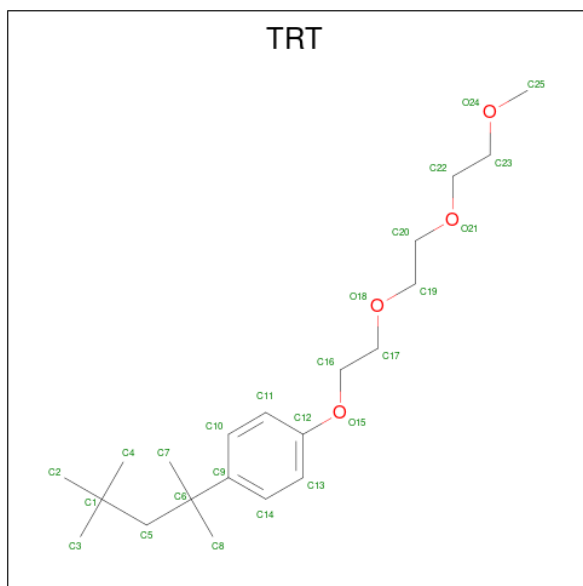
Mol	Chain	Residues	Atoms					AltConf
22	F	1	Total	C	H	O	P	0
			41	15	17	8	1	
22	I	1	Total	C	H	O	P	0
			111	35	67	8	1	
22	N	1	Total	C	H	O	P	0
			43	17	17	8	1	

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Mol	Chain	Residues	Atoms					AltConf
22	O	1	Total	C	H	O	P	0
			40	14	17	8	1	
22	O	1	Total	C	H	O	P	0
			73	23	41	8	1	
22	P	1	Total	C	H	O	P	0
			43	17	17	8	1	
22	R	1	Total	C	H	O	P	0
			48	22	17	8	1	
22	f	1	Total	C	H	O	P	0
			41	15	17	8	1	
22	i	1	Total	C	H	O	P	0
			111	35	67	8	1	
22	o	1	Total	C	H	O	P	0
			40	14	17	8	1	
22	o	1	Total	C	H	O	P	0
			73	23	41	8	1	
22	r	1	Total	C	H	O	P	0
			48	22	17	8	1	

- Molecule 23 is FRAGMENT OF TRITON X-100 (CCD ID: TRT) (formula: $C_{21}H_{36}O_4$).

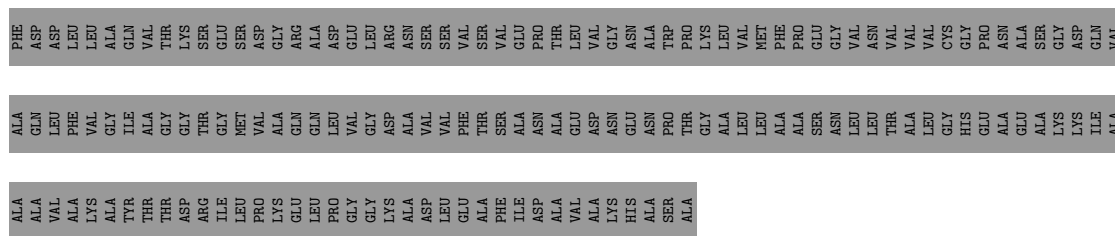


Mol	Chain	Residues	Atoms					AltConf
23	G	1	Total	C	H	O		0
			61	21	36	4		
23	G	1	Total	C	H	O		0
			61	21	36	4		

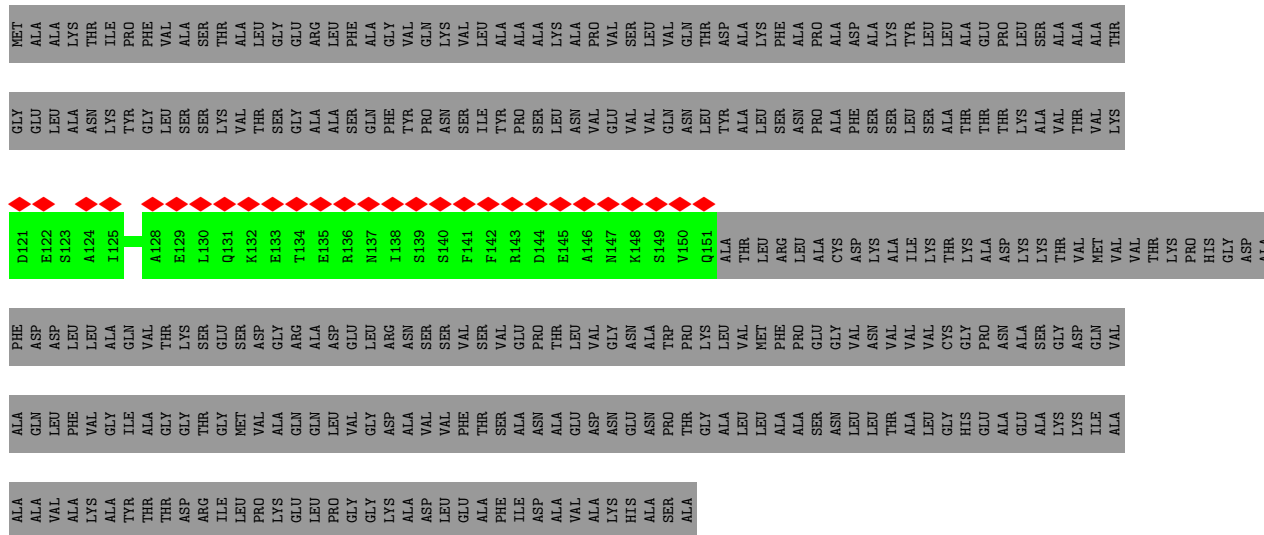
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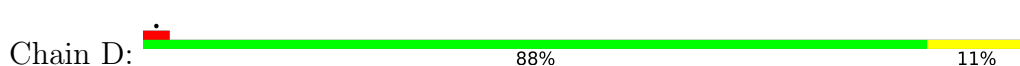
Mol	Chain	Residues	Atoms				AltConf
23	M	1	Total 61	C 21	H 36	O 4	0
23	M	1	Total 61	C 21	H 36	O 4	0
23	N	1	Total 61	C 21	H 36	O 4	0
23	N	1	Total 61	C 21	H 36	O 4	0
23	P	1	Total 61	C 21	H 36	O 4	0
23	R	1	Total 61	C 21	H 36	O 4	0
23	g	1	Total 61	C 21	H 36	O 4	0
23	g	1	Total 61	C 21	H 36	O 4	0
23	m	1	Total 61	C 21	H 36	O 4	0
23	m	1	Total 61	C 21	H 36	O 4	0
23	n	1	Total 61	C 21	H 36	O 4	0
23	n	1	Total 61	C 21	H 36	O 4	0
23	p	1	Total 61	C 21	H 36	O 4	0
23	r	1	Total 61	C 21	H 36	O 4	0



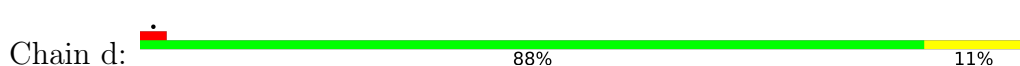
- Molecule 2: ATPTB3



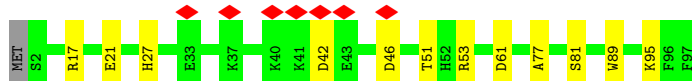
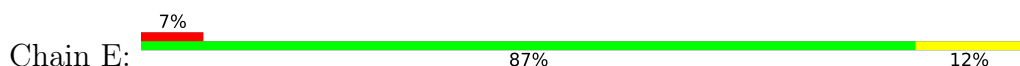
- Molecule 3: ATPTB6



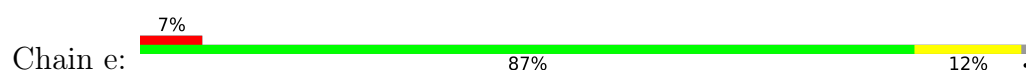
- Molecule 3: ATPTB6



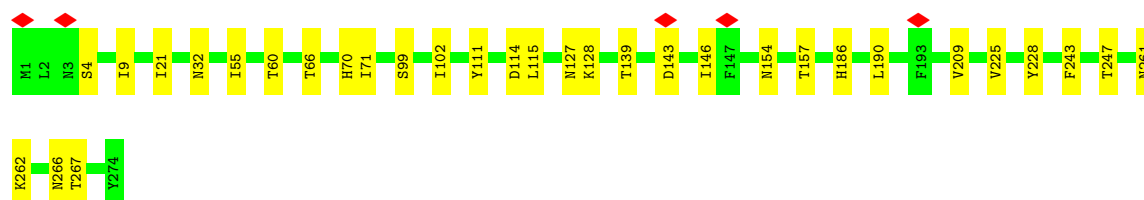
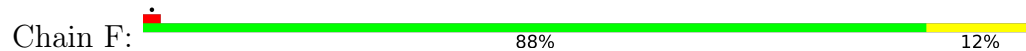
- Molecule 4: ATPB12



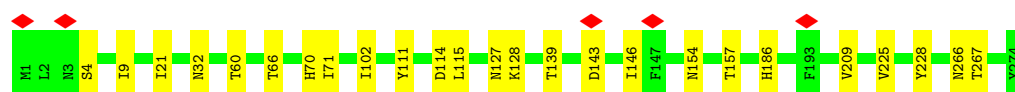
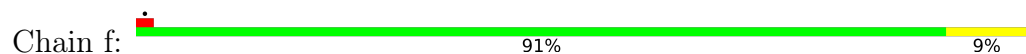
- Molecule 4: ATPB12



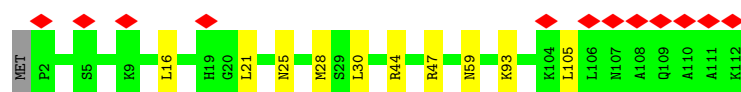
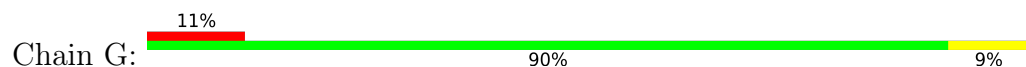
- Molecule 5: subunit a



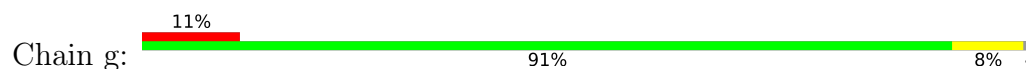
- Molecule 5: subunit a



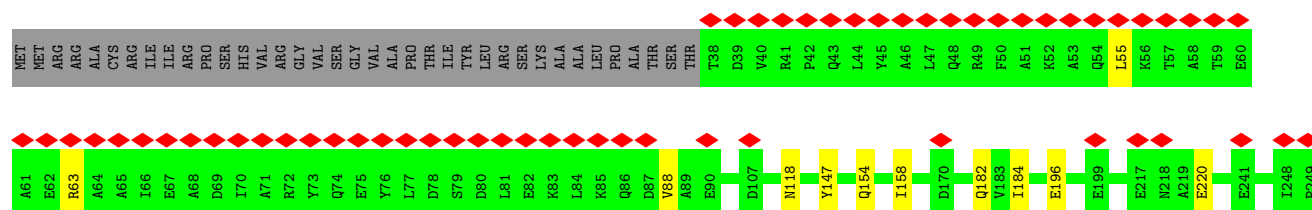
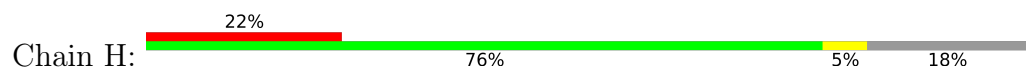
- Molecule 6: subunit b

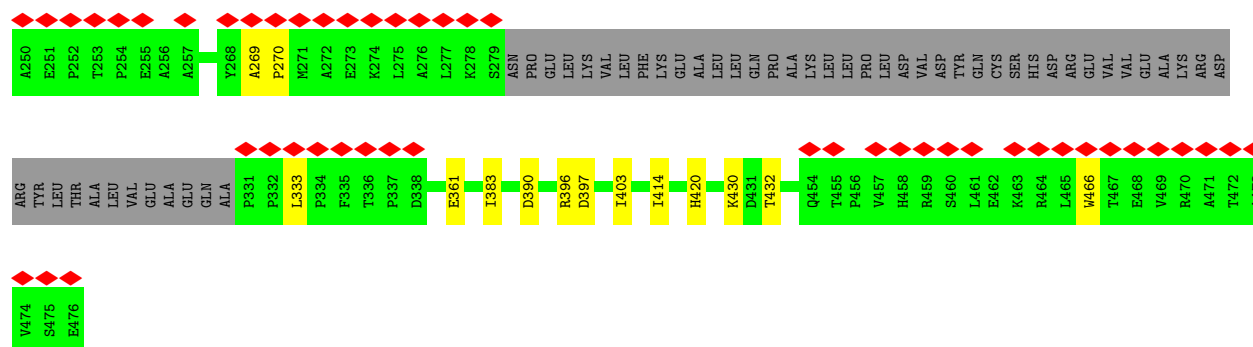


- Molecule 6: subunit b

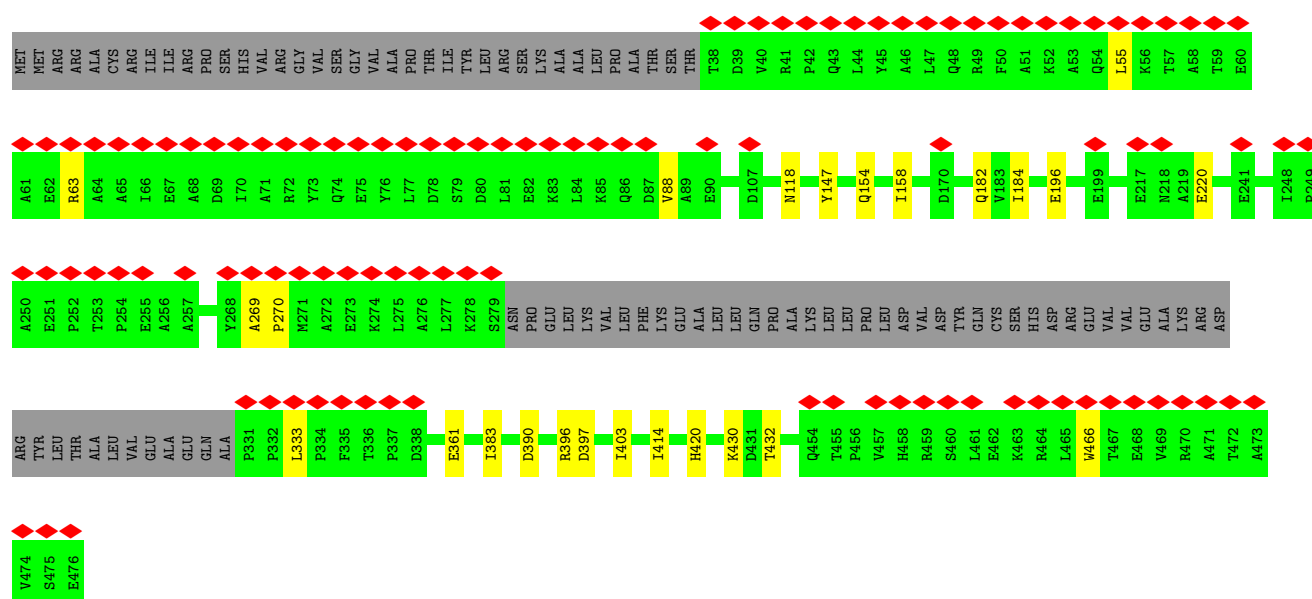
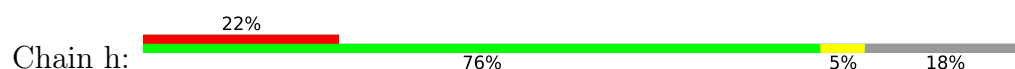


- Molecule 7: subunit d

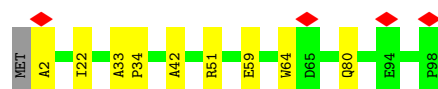
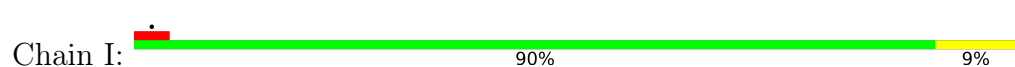




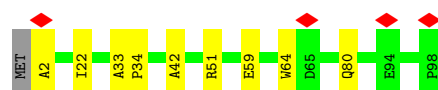
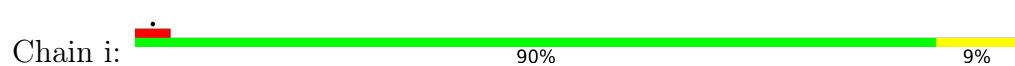
- Molecule 7: subunit d



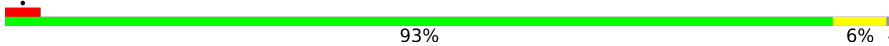
- Molecule 8: subunit f



- Molecule 8: subunit f

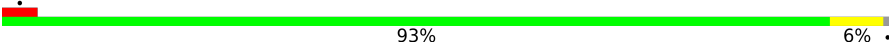


- Molecule 9: subunit i/j

Chain J:  93% 6%



- Molecule 9: subunit i/j

Chain j:  93% 6%



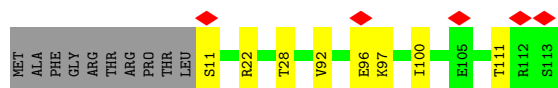
- Molecule 10: subunit k

Chain K:  84% 7% 9%

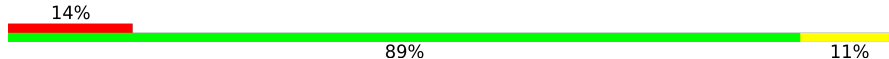


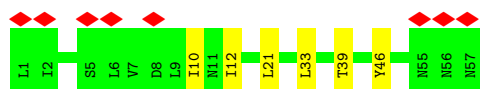
- Molecule 10: subunit k

Chain k:  84% 7% 9%



- Molecule 11: subunit 8

Chain L:  14% 89% 11%

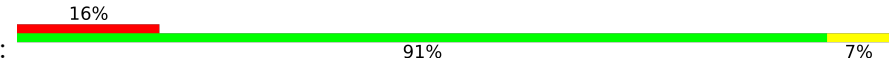


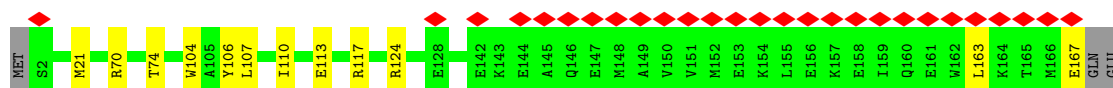
- Molecule 11: subunit 8

Chain l:  12% 89% 11%

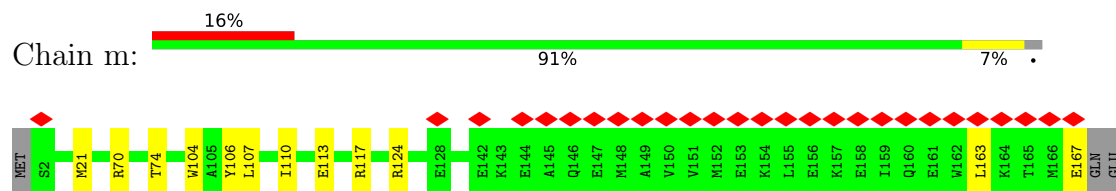


- Molecule 12: ATPEG1

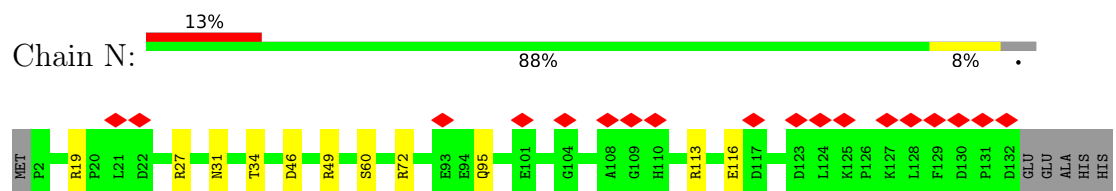
Chain M:  16% 91% 7%



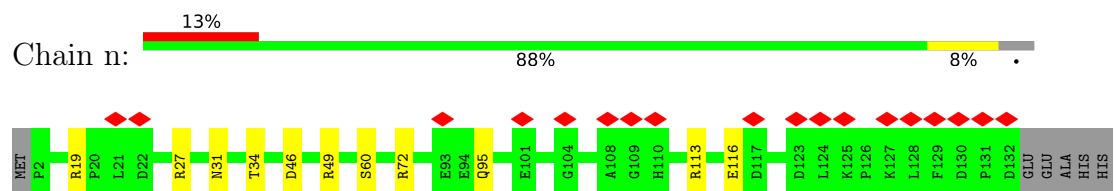
- Molecule 12: ATPEG1



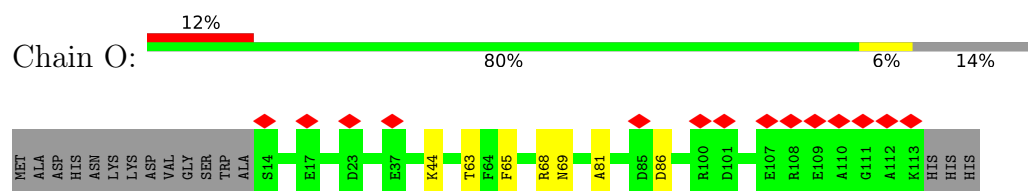
- Molecule 13: ATPEG2



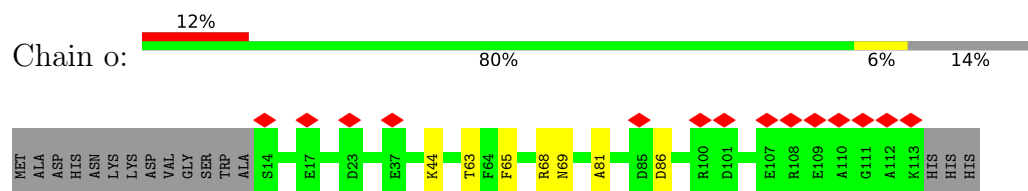
- Molecule 13: ATPEG2



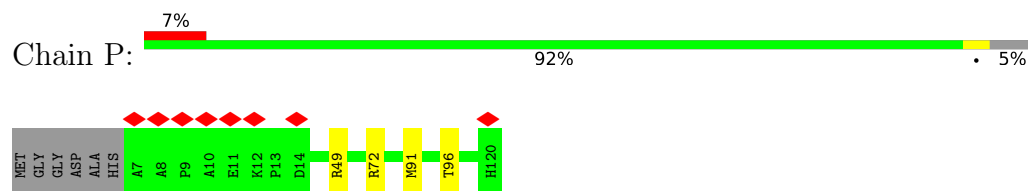
- Molecule 14: ATPEG3



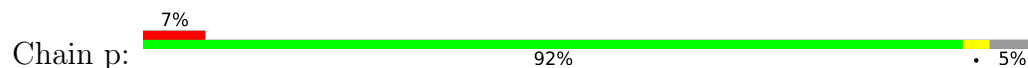
- Molecule 14: ATPEG3

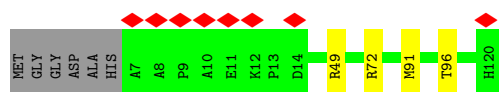


- Molecule 15: ATPEG4

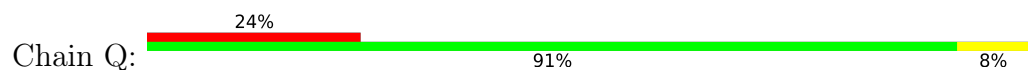


- Molecule 15: ATPEG4

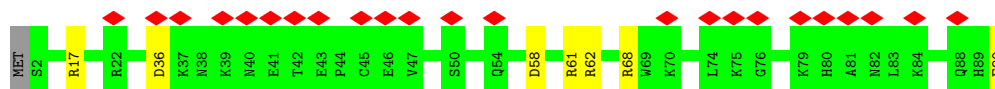
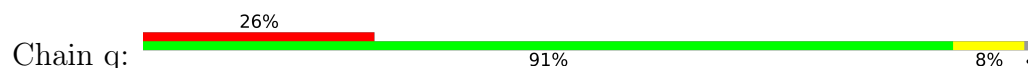




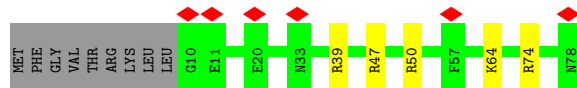
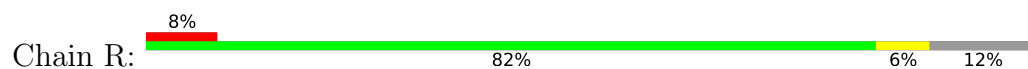
- Molecule 16: ATPEG5



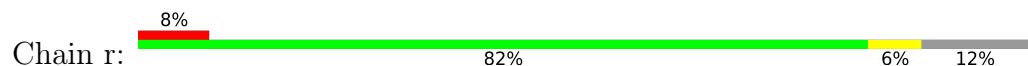
- Molecule 16: ATPEG5



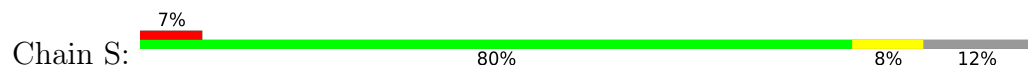
- Molecule 17: ATPEG6



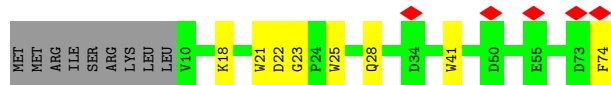
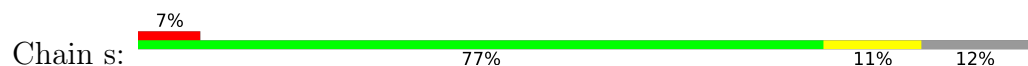
- Molecule 17: ATPEG6



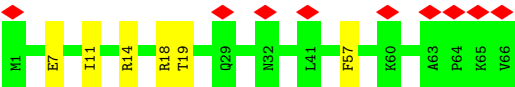
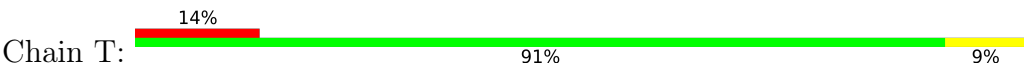
- Molecule 18: ATPEG7



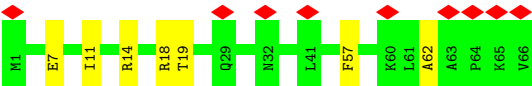
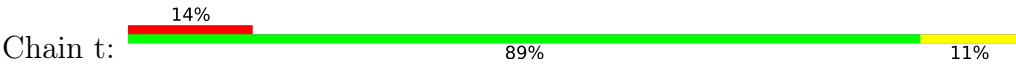
- Molecule 18: ATPEG7



- Molecule 19: ATPEG8



● Molecule 19: ATPEG8



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	150242	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 ($e^-/\text{\AA}^2$)	36.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.133	Depositor
Minimum map value	-0.061	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	461.99997, 461.99997, 461.99997	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, TRT, CDL, LPP

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	0.27	0/4047	0.38	0/5500
1	a	0.27	0/4047	0.38	0/5500
2	B	0.15	0/252	0.30	0/335
2	b	0.15	0/252	0.30	0/335
3	D	0.25	0/1559	0.37	0/2106
3	d	0.25	0/1559	0.37	0/2106
4	E	0.22	0/819	0.35	0/1096
4	e	0.22	0/821	0.35	0/1100
5	F	0.27	0/2377	0.38	0/3228
5	f	0.26	0/2379	0.38	0/3233
6	G	0.26	0/901	0.41	0/1218
6	g	0.26	0/901	0.41	0/1218
7	H	0.24	0/3185	0.34	0/4352
7	h	0.24	0/3185	0.34	0/4352
8	I	0.26	0/804	0.38	0/1084
8	i	0.26	0/804	0.38	0/1084
9	J	0.24	0/918	0.36	0/1255
9	j	0.25	0/918	0.36	0/1255
10	K	0.23	0/839	0.33	0/1135
10	k	0.23	0/839	0.33	0/1135
11	L	0.25	0/518	0.37	0/711
11	l	0.26	0/518	0.37	0/711
12	M	0.24	0/1399	0.35	0/1895
12	m	0.24	0/1399	0.35	0/1895
13	N	0.24	0/1137	0.31	0/1540
13	n	0.24	0/1137	0.31	0/1540
14	O	0.23	0/881	0.34	0/1193
14	o	0.23	0/881	0.34	0/1193
15	P	0.26	0/955	0.36	0/1292
15	p	0.27	0/955	0.36	0/1292
16	Q	0.20	0/774	0.40	0/1040
16	q	0.20	0/774	0.40	0/1040

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	R	0.21	0/594	0.38	0/798
17	r	0.21	0/594	0.38	0/798
18	S	0.24	0/575	0.37	0/785
18	s	0.24	0/575	0.37	0/785
19	T	0.23	0/543	0.35	0/730
19	t	0.23	0/543	0.35	0/730
All	All	0.25	0/46158	0.36	0/62595

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 ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3945	3919	3919	22	0
1	a	3945	3919	3919	25	0
2	B	251	243	243	0	0
2	b	251	243	243	0	0
3	D	1521	1519	1519	15	0
3	d	1521	1519	1519	15	0
4	E	797	777	777	9	0
4	e	798	779	779	9	0
5	F	2312	2327	2327	23	0
5	f	2313	2329	2329	19	0
6	G	879	924	924	12	0
6	g	879	924	924	11	0
7	H	3106	3059	3059	19	0
7	h	3106	3059	3059	20	0
8	I	782	771	771	8	0
8	i	782	771	771	8	0
9	J	881	853	852	8	0
9	j	881	853	852	7	0
10	K	816	821	821	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	k	816	821	821	7	0
11	L	501	507	507	6	0
11	l	501	507	507	6	0
12	M	1363	1354	1354	7	0
12	m	1363	1354	1354	7	0
13	N	1097	1070	1070	8	0
13	n	1097	1070	1070	8	0
14	O	849	803	803	6	0
14	o	849	803	803	6	0
15	P	926	912	912	4	0
15	p	926	912	912	4	0
16	Q	753	723	723	5	0
16	q	753	723	723	5	0
17	R	579	581	581	7	0
17	r	579	581	581	7	0
18	S	551	541	541	6	0
18	s	551	541	541	7	0
19	T	528	552	552	6	0
19	t	528	552	552	7	0
20	A	307	329	395	8	0
20	D	177	235	255	6	0
20	E	63	32	73	6	0
20	M	130	102	151	4	0
20	O	65	59	77	4	0
20	P	48	27	40	1	0
20	R	76	74	99	2	0
20	a	307	329	395	7	0
20	d	177	235	255	6	0
20	e	63	32	73	7	0
20	m	130	102	151	1	0
20	o	65	59	77	3	0
20	p	146	173	189	1	0
20	r	76	74	99	2	0
21	D	35	46	44	0	0
21	F	35	46	44	2	0
21	N	35	46	44	0	0
21	Q	35	46	45	0	0
21	d	35	46	45	0	0
21	f	35	46	44	2	0
21	n	35	46	44	0	0
21	q	35	46	45	0	0
22	F	24	17	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	I	44	67	67	2	0
22	N	26	17	25	2	0
22	O	55	58	59	0	0
22	P	26	17	25	2	0
22	R	31	17	35	1	0
22	f	24	17	21	0	0
22	i	44	67	67	2	0
22	o	55	58	59	0	0
22	r	31	17	35	1	0
23	G	50	72	72	6	0
23	M	50	72	72	2	0
23	N	50	72	72	8	0
23	P	25	36	36	0	0
23	R	25	36	36	0	0
23	g	50	72	72	6	0
23	m	50	72	72	2	0
23	n	50	72	72	7	0
23	p	25	36	36	0	0
23	r	25	36	36	0	0
All	All	47746	47674	48188	317	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 317 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:68:TYR:O	3:D:77:ARG:NH1	2.19	0.75
3:d:68:TYR:O	3:d:77:ARG:NH1	2.19	0.75
1:a:156:LEU:O	1:a:312:ARG:NH2	2.22	0.73
1:A:156:LEU:O	1:A:312:ARG:NH2	2.22	0.71
10:k:11:SER:OG	19:t:7:GLU:OE1	2.09	0.70

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	484/487 (99%)	467 (96%)	17 (4%)	0	100	100
1	a	484/487 (99%)	467 (96%)	17 (4%)	0	100	100
2	B	29/338 (9%)	29 (100%)	0	0	100	100
2	b	29/338 (9%)	29 (100%)	0	0	100	100
3	D	184/187 (98%)	180 (98%)	4 (2%)	0	100	100
3	d	184/187 (98%)	180 (98%)	4 (2%)	0	100	100
4	E	94/97 (97%)	91 (97%)	3 (3%)	0	100	100
4	e	94/97 (97%)	91 (97%)	3 (3%)	0	100	100
5	F	270/274 (98%)	262 (97%)	8 (3%)	0	100	100
5	f	272/274 (99%)	264 (97%)	8 (3%)	0	100	100
6	G	109/112 (97%)	108 (99%)	1 (1%)	0	100	100
6	g	109/112 (97%)	108 (99%)	1 (1%)	0	100	100
7	H	384/476 (81%)	380 (99%)	4 (1%)	0	100	100
7	h	384/476 (81%)	380 (99%)	4 (1%)	0	100	100
8	I	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
8	i	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
9	J	101/104 (97%)	99 (98%)	2 (2%)	0	100	100
9	j	101/104 (97%)	99 (98%)	2 (2%)	0	100	100
10	K	101/113 (89%)	99 (98%)	2 (2%)	0	100	100
10	k	101/113 (89%)	99 (98%)	2 (2%)	0	100	100
11	L	55/57 (96%)	51 (93%)	4 (7%)	0	100	100
11	l	55/57 (96%)	51 (93%)	4 (7%)	0	100	100
12	M	164/169 (97%)	164 (100%)	0	0	100	100
12	m	164/169 (97%)	164 (100%)	0	0	100	100
13	N	129/137 (94%)	124 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	n	129/137 (94%)	124 (96%)	5 (4%)	0	100	100
14	O	98/116 (84%)	95 (97%)	3 (3%)	0	100	100
14	o	98/116 (84%)	95 (97%)	3 (3%)	0	100	100
15	P	112/120 (93%)	109 (97%)	3 (3%)	0	100	100
15	p	112/120 (93%)	109 (97%)	3 (3%)	0	100	100
16	Q	87/90 (97%)	80 (92%)	7 (8%)	0	100	100
16	q	87/90 (97%)	80 (92%)	7 (8%)	0	100	100
17	R	67/78 (86%)	66 (98%)	1 (2%)	0	100	100
17	r	67/78 (86%)	66 (98%)	1 (2%)	0	100	100
18	S	63/74 (85%)	61 (97%)	2 (3%)	0	100	100
18	s	63/74 (85%)	61 (97%)	2 (3%)	0	100	100
19	T	64/66 (97%)	63 (98%)	1 (2%)	0	100	100
19	t	64/66 (97%)	63 (98%)	1 (2%)	0	100	100
All	All	5382/6386 (84%)	5241 (97%)	141 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/427 (100%)	426 (100%)	0	100	100
1	a	426/427 (100%)	426 (100%)	0	100	100
2	B	28/259 (11%)	28 (100%)	0	100	100
2	b	28/259 (11%)	28 (100%)	0	100	100
3	D	159/160 (99%)	159 (100%)	0	100	100
3	d	159/160 (99%)	159 (100%)	0	100	100
4	E	80/82 (98%)	80 (100%)	0	100	100
4	e	81/82 (99%)	81 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	258/259 (100%)	258 (100%)	0	100	100
5	f	259/259 (100%)	259 (100%)	0	100	100
6	G	98/99 (99%)	98 (100%)	0	100	100
6	g	98/99 (99%)	98 (100%)	0	100	100
7	H	339/414 (82%)	339 (100%)	0	100	100
7	h	339/414 (82%)	339 (100%)	0	100	100
8	I	82/83 (99%)	82 (100%)	0	100	100
8	i	82/83 (99%)	82 (100%)	0	100	100
9	J	94/95 (99%)	94 (100%)	0	100	100
9	j	94/95 (99%)	94 (100%)	0	100	100
10	K	89/97 (92%)	89 (100%)	0	100	100
10	k	89/97 (92%)	89 (100%)	0	100	100
11	L	56/56 (100%)	56 (100%)	0	100	100
11	l	56/56 (100%)	56 (100%)	0	100	100
12	M	137/140 (98%)	137 (100%)	0	100	100
12	m	137/140 (98%)	137 (100%)	0	100	100
13	N	114/119 (96%)	114 (100%)	0	100	100
13	n	114/119 (96%)	114 (100%)	0	100	100
14	O	90/103 (87%)	90 (100%)	0	100	100
14	o	90/103 (87%)	90 (100%)	0	100	100
15	P	96/99 (97%)	96 (100%)	0	100	100
15	p	96/99 (97%)	96 (100%)	0	100	100
16	Q	82/83 (99%)	82 (100%)	0	100	100
16	q	82/83 (99%)	82 (100%)	0	100	100
17	R	59/67 (88%)	59 (100%)	0	100	100
17	r	59/67 (88%)	59 (100%)	0	100	100
18	S	59/68 (87%)	59 (100%)	0	100	100
18	s	59/68 (87%)	59 (100%)	0	100	100
19	T	54/54 (100%)	54 (100%)	0	100	100
19	t	54/54 (100%)	54 (100%)	0	100	100
All	All	4802/5528 (87%)	4802 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
3	d	3	HIS
16	q	40	ASN
5	f	125	ASN
12	m	130	HIS
4	e	52	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

61 ligands 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	$\# Z > 2$
23	TRT	g	202	-	25,25,25	0.60	0	33,33,33	0.69	0
23	TRT	r	103	-	25,25,25	0.53	0	33,33,33	0.82	1 (3%)
20	CDL	A	504	-	62,62,99	1.11	8 (12%)	68,74,111	1.18	4 (5%)
20	CDL	a	503	-	80,80,99	0.98	8 (10%)	85,91,111	1.06	4 (4%)
21	LMT	n	201	-	36,36,36	1.17	6 (16%)	47,47,47	1.02	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	TRT	G	202	-	25,25,25	0.60	0	33,33,33	0.69	0
23	TRT	p	203	-	25,25,25	1.25	3 (12%)	33,33,33	4.51	8 (24%)
22	LPP	o	203	-	31,31,43	1.28	4 (12%)	34,36,48	1.14	2 (5%)
22	LPP	o	202	-	22,22,43	1.41	3 (13%)	25,27,48	1.21	2 (8%)
23	TRT	N	201	-	25,25,25	0.51	0	33,33,33	0.85	1 (3%)
21	LMT	Q	101	-	36,36,36	1.14	6 (16%)	47,47,47	1.01	2 (4%)
20	CDL	R	101	-	75,75,99	1.01	8 (10%)	81,87,111	1.06	4 (4%)
20	CDL	M	203	-	76,76,99	1.00	8 (10%)	82,88,111	1.10	4 (4%)
20	CDL	A	503	-	80,80,99	0.98	8 (10%)	85,91,111	1.06	4 (4%)
23	TRT	m	204	-	25,25,25	0.55	0	33,33,33	0.78	1 (3%)
20	CDL	D	201	-	90,90,99	0.92	8 (8%)	96,102,111	1.04	4 (4%)
20	CDL	d	202	-	84,84,99	0.96	8 (9%)	90,96,111	1.02	4 (4%)
20	CDL	o	201	-	64,64,99	1.09	8 (12%)	70,76,111	1.08	4 (5%)
22	LPP	r	102	-	30,30,43	1.26	4 (13%)	33,35,48	1.26	2 (6%)
23	TRT	N	202	-	25,25,25	0.61	0	33,33,33	0.64	0
20	CDL	p	202	-	47,47,99	1.25	8 (17%)	53,59,111	1.31	5 (9%)
23	TRT	n	202	-	25,25,25	0.51	0	33,33,33	0.86	1 (3%)
20	CDL	A	502	-	80,80,99	0.99	8 (10%)	86,92,111	1.09	4 (4%)
20	CDL	a	502	-	80,80,99	0.98	8 (10%)	86,92,111	1.09	4 (4%)
21	LMT	q	101	-	36,36,36	1.15	6 (16%)	47,47,47	1.01	2 (4%)
22	LPP	F	301	-	23,23,43	1.39	3 (13%)	26,28,48	1.23	2 (7%)
20	CDL	m	202	-	52,52,99	1.20	8 (15%)	58,64,111	1.26	4 (6%)
23	TRT	G	201	-	25,25,25	0.54	0	33,33,33	0.79	0
23	TRT	g	201	-	25,25,25	0.53	0	33,33,33	0.79	0
23	TRT	P	203	-	25,25,25	1.25	3 (12%)	33,33,33	4.51	8 (24%)
20	CDL	a	501	-	80,80,99	0.98	7 (8%)	86,92,111	1.12	5 (5%)
20	CDL	e	101	-	62,62,99	1.09	8 (12%)	68,74,111	1.13	4 (5%)
22	LPP	I	101	-	43,43,43	1.13	3 (6%)	46,48,48	1.00	2 (4%)
23	TRT	M	201	-	25,25,25	0.55	0	33,33,33	0.68	1 (3%)
23	TRT	M	202	-	25,25,25	0.55	0	33,33,33	0.78	1 (3%)
23	TRT	n	203	-	25,25,25	0.61	0	33,33,33	0.64	0
22	LPP	R	102	-	30,30,43	1.27	4 (13%)	33,35,48	1.25	2 (6%)
21	LMT	F	302	-	36,36,36	1.15	5 (13%)	47,47,47	0.96	2 (4%)
21	LMT	N	204	-	36,36,36	1.17	6 (16%)	47,47,47	1.03	4 (8%)
20	CDL	E	101	-	62,62,99	1.09	8 (12%)	68,74,111	1.12	4 (5%)
20	CDL	A	501	-	80,80,99	0.98	7 (8%)	86,92,111	1.12	5 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	LPP	N	203	-	25,25,43	1.35	3 (12%)	28,30,48	1.28	2 (7%)
23	TRT	m	203	-	25,25,25	0.55	0	33,33,33	0.68	1 (3%)
20	CDL	d	201	-	90,90,99	0.92	8 (8%)	96,102,111	1.05	4 (4%)
22	LPP	i	101	-	43,43,43	1.13	3 (6%)	46,48,48	1.00	2 (4%)
20	CDL	D	202	-	84,84,99	0.96	8 (9%)	90,96,111	1.04	5 (5%)
21	LMT	d	203	-	36,36,36	1.17	6 (16%)	47,47,47	0.92	1 (2%)
20	CDL	r	101	-	75,75,99	1.01	8 (10%)	81,87,111	1.04	4 (4%)
22	LPP	O	203	-	31,31,43	1.28	4 (12%)	34,36,48	1.14	2 (5%)
22	LPP	P	202	-	25,25,43	1.35	3 (12%)	28,30,48	1.27	2 (7%)
22	LPP	f	301	-	23,23,43	1.39	3 (13%)	26,28,48	1.24	2 (7%)
23	TRT	R	103	-	25,25,25	0.53	0	33,33,33	0.82	1 (3%)
20	CDL	m	201	-	76,76,99	1.01	8 (10%)	82,88,111	1.10	4 (4%)
20	CDL	M	204	-	52,52,99	1.21	8 (15%)	58,64,111	1.27	4 (6%)
22	LPP	O	202	-	22,22,43	1.41	3 (13%)	25,27,48	1.21	2 (8%)
20	CDL	a	504	-	62,62,99	1.11	8 (12%)	68,74,111	1.18	4 (5%)
20	CDL	p	201	-	97,97,99	0.91	8 (8%)	103,109,111	1.00	4 (3%)
21	LMT	D	203	-	36,36,36	1.16	5 (13%)	47,47,47	0.92	1 (2%)
21	LMT	f	302	-	36,36,36	1.15	5 (13%)	47,47,47	0.96	2 (4%)
20	CDL	O	201	-	64,64,99	1.09	8 (12%)	70,76,111	1.07	4 (5%)
20	CDL	P	201	-	47,47,99	1.26	8 (17%)	53,59,111	1.32	5 (9%)

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
23	TRT	g	202	-	-	15/23/23/23	0/1/1/1
23	TRT	r	103	-	-	9/23/23/23	0/1/1/1
20	CDL	A	504	-	-	33/73/73/110	-
20	CDL	a	503	-	-	31/89/89/110	-
21	LMT	n	201	-	-	9/21/61/61	0/2/2/2
23	TRT	G	202	-	-	15/23/23/23	0/1/1/1
23	TRT	p	203	-	-	15/23/23/23	0/1/1/1
22	LPP	o	203	-	-	15/33/33/45	-
22	LPP	o	202	-	-	10/24/24/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	TRT	N	201	-	-	7/23/23/23	0/1/1/1
21	LMT	Q	101	-	-	6/21/61/61	0/2/2/2
20	CDL	R	101	-	-	33/86/86/110	-
20	CDL	M	203	-	-	39/87/87/110	-
20	CDL	A	503	-	-	33/89/89/110	-
23	TRT	m	204	-	-	8/23/23/23	0/1/1/1
20	CDL	D	201	-	-	35/101/101/110	-
20	CDL	d	202	-	-	44/95/95/110	-
20	CDL	o	201	-	-	38/75/75/110	-
22	LPP	r	102	-	-	13/32/32/45	-
23	TRT	N	202	-	-	14/23/23/23	0/1/1/1
20	CDL	p	202	-	-	23/57/57/110	-
23	TRT	n	202	-	-	7/23/23/23	0/1/1/1
20	CDL	A	502	-	-	30/91/91/110	-
20	CDL	a	502	-	-	33/91/91/110	-
21	LMT	q	101	-	-	6/21/61/61	0/2/2/2
22	LPP	F	301	-	-	5/25/25/45	-
20	CDL	m	202	-	-	30/63/63/110	-
23	TRT	G	201	-	-	8/23/23/23	0/1/1/1
23	TRT	g	201	-	-	8/23/23/23	0/1/1/1
23	TRT	P	203	-	-	15/23/23/23	0/1/1/1
20	CDL	a	501	-	-	28/91/91/110	-
20	CDL	e	101	-	-	40/73/73/110	-
22	LPP	I	101	-	-	13/45/45/45	-
23	TRT	M	201	-	-	10/23/23/23	0/1/1/1
23	TRT	M	202	-	-	8/23/23/23	0/1/1/1
23	TRT	n	203	-	-	14/23/23/23	0/1/1/1
22	LPP	R	102	-	-	13/32/32/45	-
21	LMT	F	302	-	-	8/21/61/61	0/2/2/2
21	LMT	N	204	-	-	9/21/61/61	0/2/2/2
20	CDL	E	101	-	-	40/73/73/110	-
20	CDL	A	501	-	-	27/91/91/110	-
22	LPP	N	203	-	-	12/27/27/45	-
23	TRT	m	203	-	-	10/23/23/23	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CDL	d	201	-	-	33/101/101/110	-
22	LPP	i	101	-	-	13/45/45/45	-
20	CDL	D	202	-	-	43/95/95/110	-
21	LMT	d	203	-	-	7/21/61/61	0/2/2/2
20	CDL	r	101	-	-	36/86/86/110	-
22	LPP	O	203	-	-	15/33/33/45	-
22	LPP	P	202	-	-	12/27/27/45	-
22	LPP	f	301	-	-	5/25/25/45	-
23	TRT	R	103	-	-	9/23/23/23	0/1/1/1
20	CDL	m	201	-	-	39/87/87/110	-
20	CDL	M	204	-	-	29/63/63/110	-
22	LPP	O	202	-	-	10/24/24/45	-
20	CDL	a	504	-	-	33/73/73/110	-
20	CDL	p	201	-	-	45/108/108/110	-
21	LMT	D	203	-	-	7/21/61/61	0/2/2/2
21	LMT	f	302	-	-	8/21/61/61	0/2/2/2
20	CDL	O	201	-	-	34/75/75/110	-
20	CDL	P	201	-	-	24/57/57/110	-

The worst 5 of 289 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	P	203	TRT	C6-C9	4.13	1.60	1.53
23	p	203	TRT	C6-C9	4.13	1.60	1.53
22	P	202	LPP	O9-C11	3.36	1.43	1.34
22	N	203	LPP	O9-C11	3.34	1.43	1.34
22	I	101	LPP	O9-C11	3.25	1.43	1.34

The worst 5 of 171 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	203	TRT	C7-C6-C8	14.88	152.16	107.26
23	p	203	TRT	C7-C6-C8	14.88	152.14	107.26
23	P	203	TRT	C5-C6-C9	11.75	139.47	112.00
23	p	203	TRT	C5-C6-C9	11.75	139.46	112.00
23	p	203	TRT	C8-C6-C9	-11.22	81.81	110.18

There are no chirality outliers.

5 of 1221 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	501	CDL	CB2-OB2-PB2-OB3
20	A	501	CDL	CB3-OB5-PB2-OB3
20	A	501	CDL	C51-CB5-OB6-CB4
20	A	502	CDL	O1-C1-CB2-OB2
20	A	502	CDL	CA3-OA5-PA1-OA3

There are no ring outliers.

38 monomers are involved in 93 short contacts:

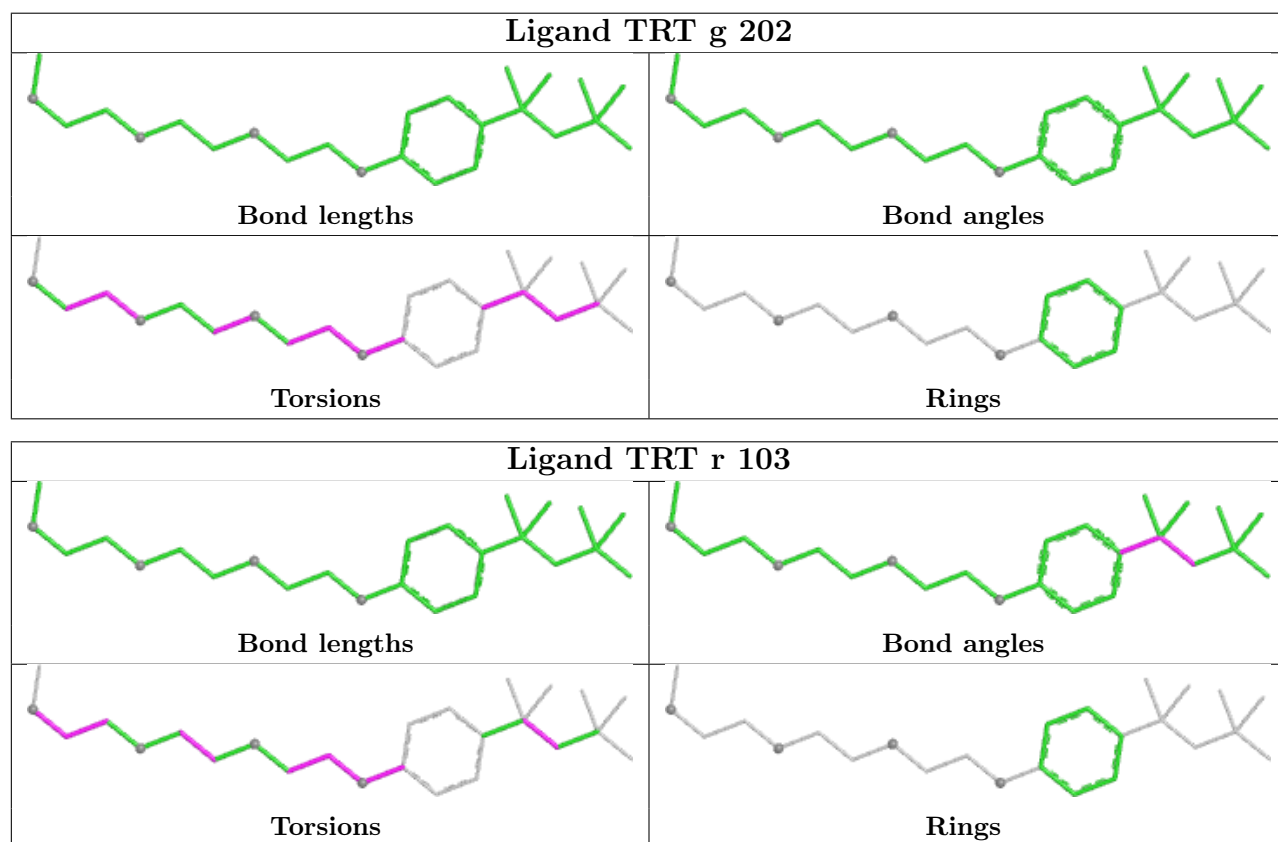
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	g	202	TRT	3	0
20	a	503	CDL	3	0
23	G	202	TRT	3	0
23	N	201	TRT	6	0
20	R	101	CDL	2	0
20	M	203	CDL	3	0
20	A	503	CDL	3	0
23	m	204	TRT	2	0
20	D	201	CDL	2	0
20	d	202	CDL	3	0
20	o	201	CDL	3	0
22	r	102	LPP	1	0
23	N	202	TRT	3	0
20	p	202	CDL	1	0
23	n	202	TRT	5	0
20	A	502	CDL	4	0
20	a	502	CDL	4	0
23	G	201	TRT	3	0
23	g	201	TRT	3	0
20	e	101	CDL	7	0
22	I	101	LPP	2	0
23	M	202	TRT	2	0
23	n	203	TRT	2	0
22	R	102	LPP	1	0
21	F	302	LMT	2	0
20	E	101	CDL	6	0
20	A	501	CDL	1	0
22	N	203	LPP	2	0
20	d	201	CDL	3	0
22	i	101	LPP	2	0
20	D	202	CDL	4	0

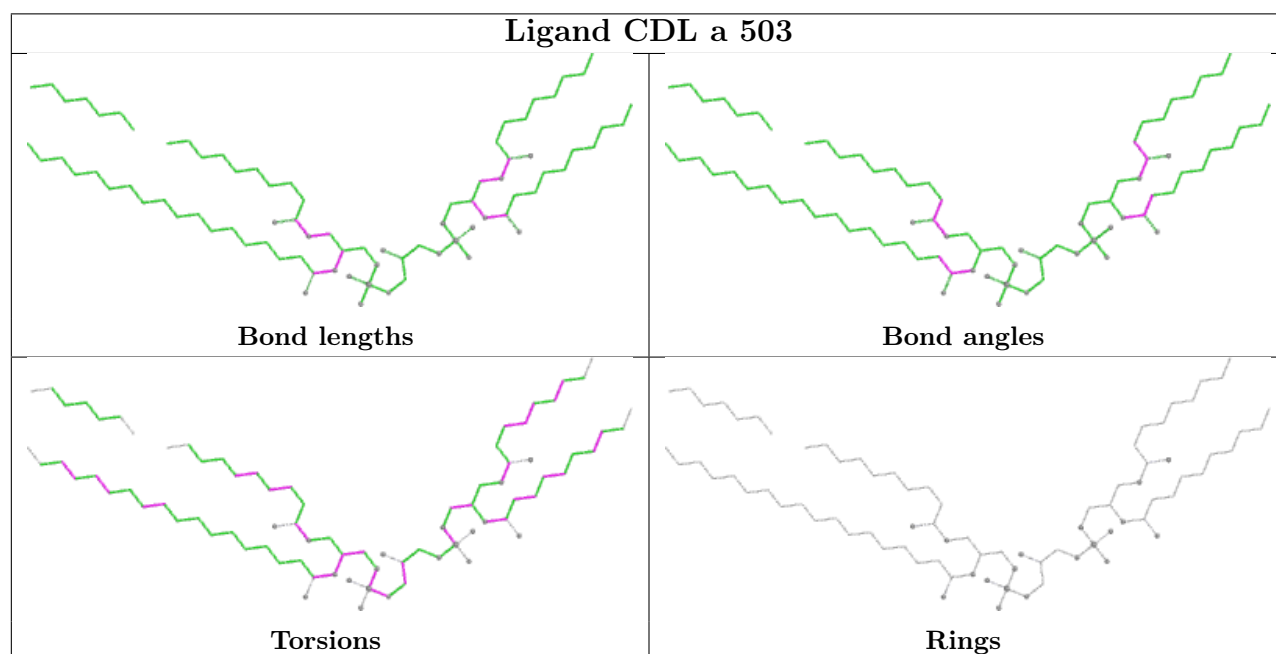
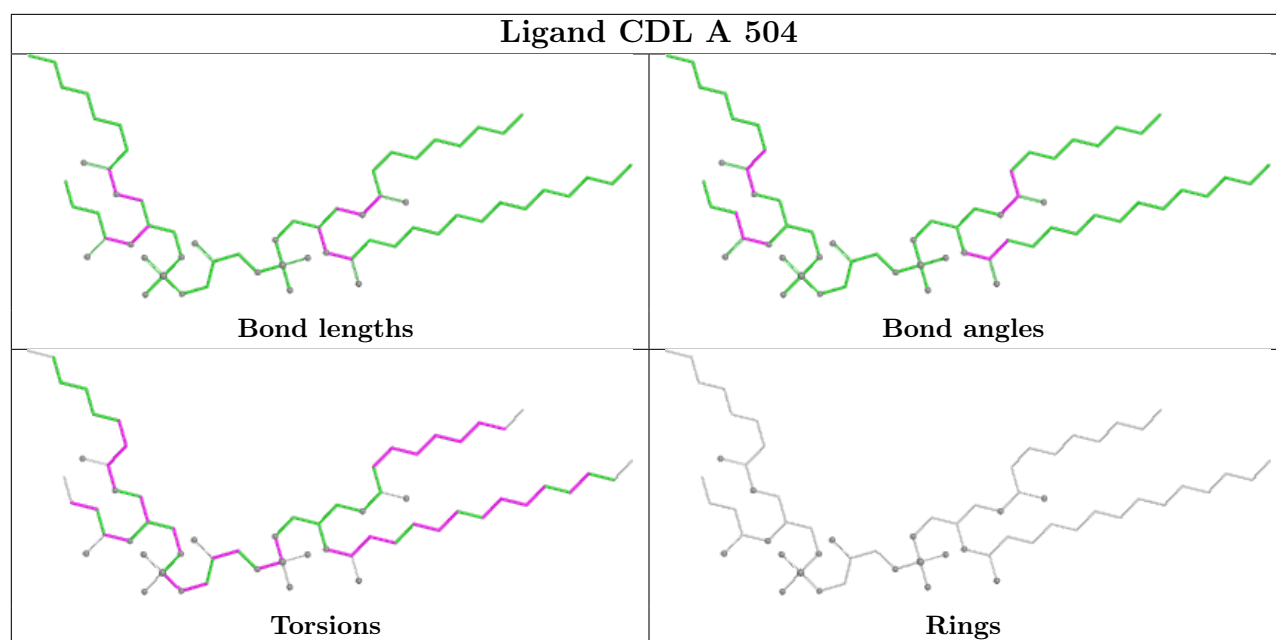
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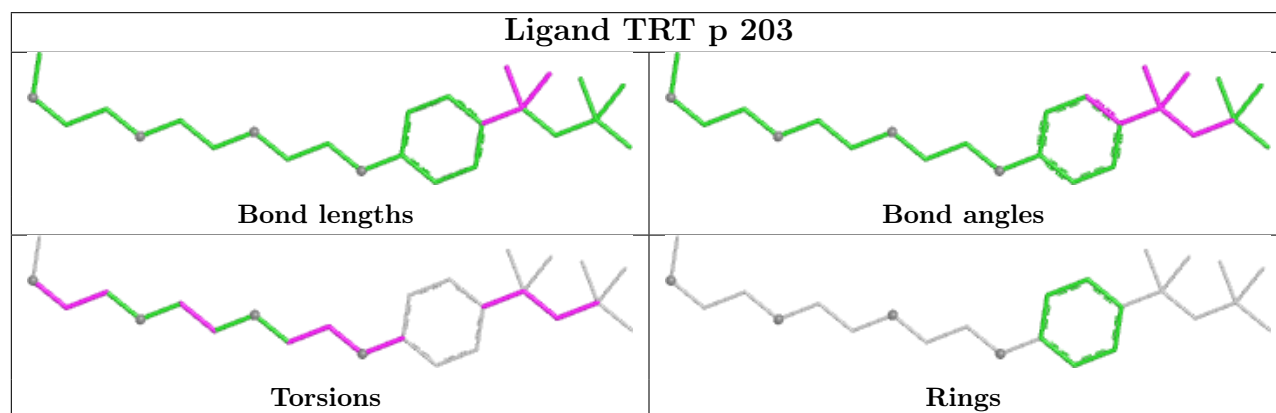
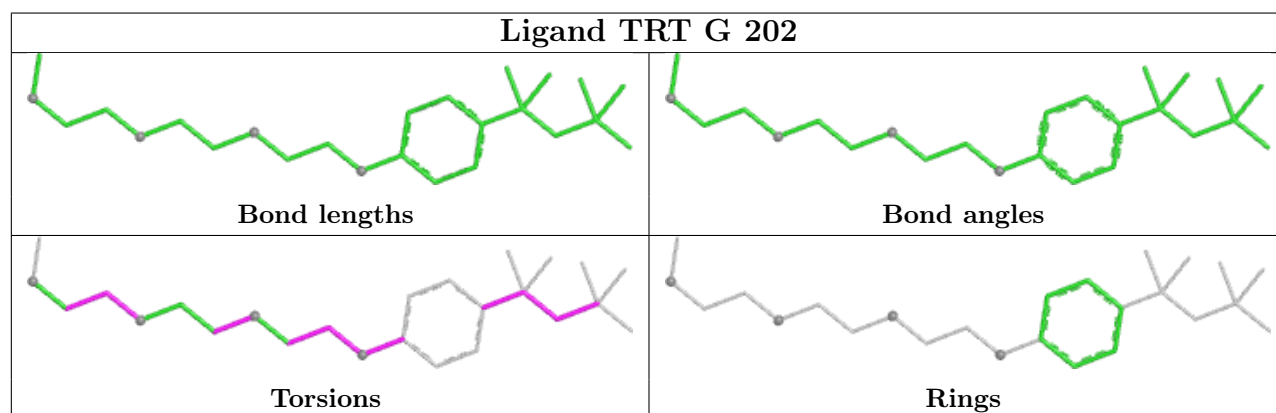
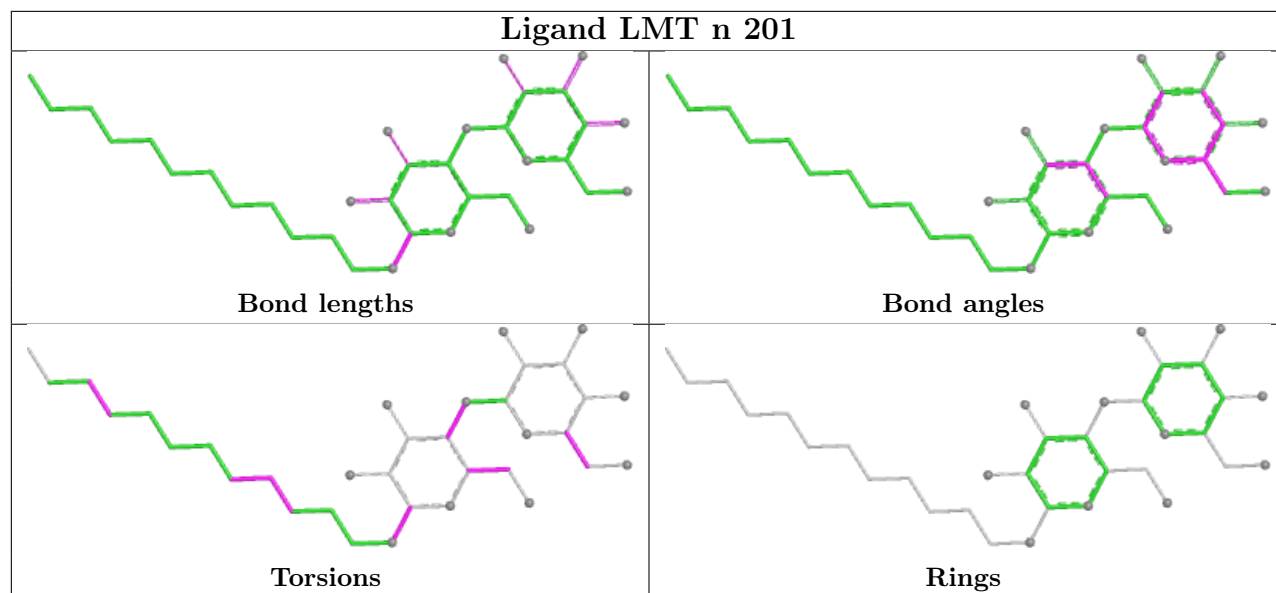
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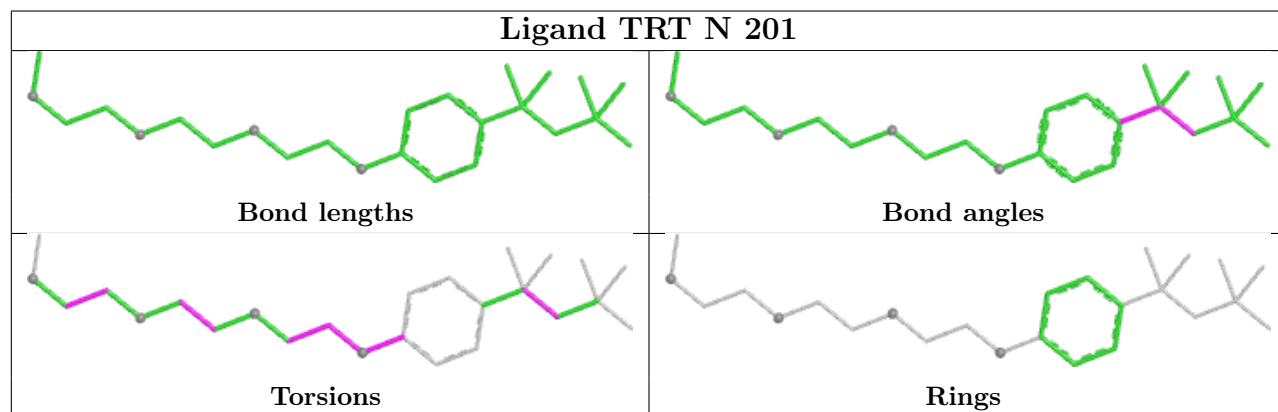
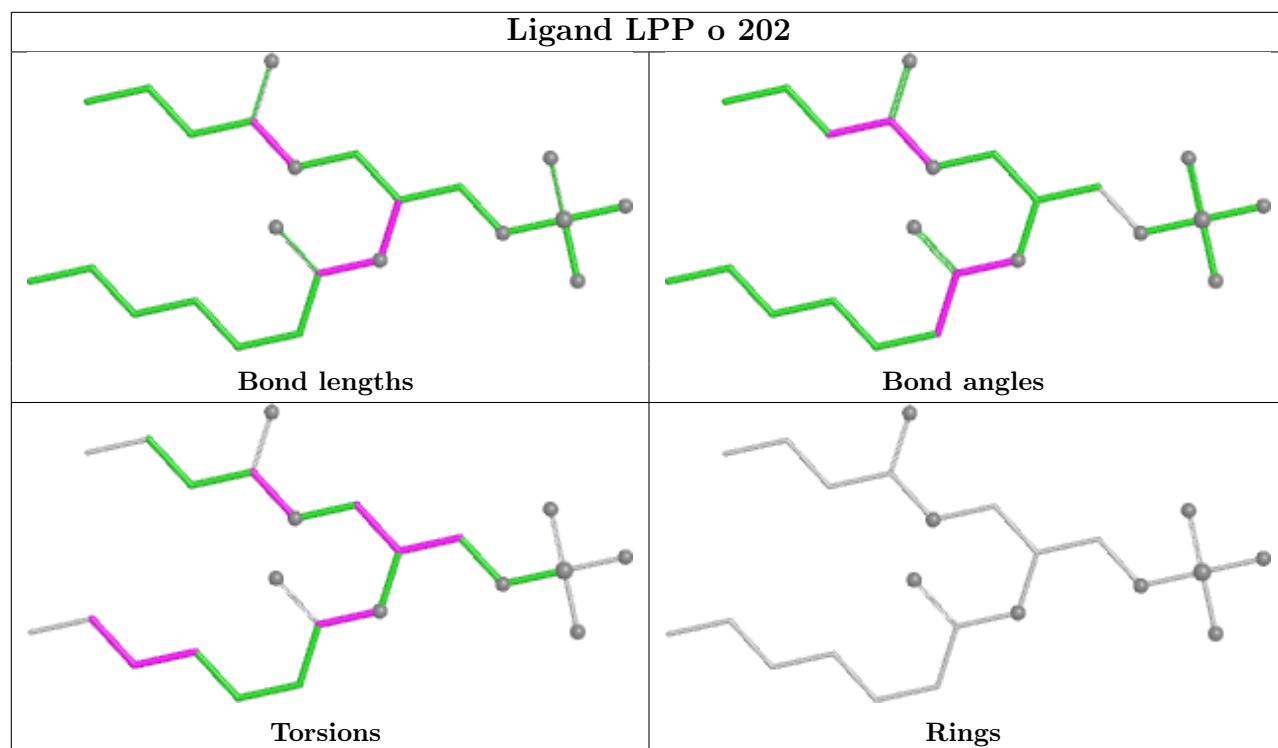
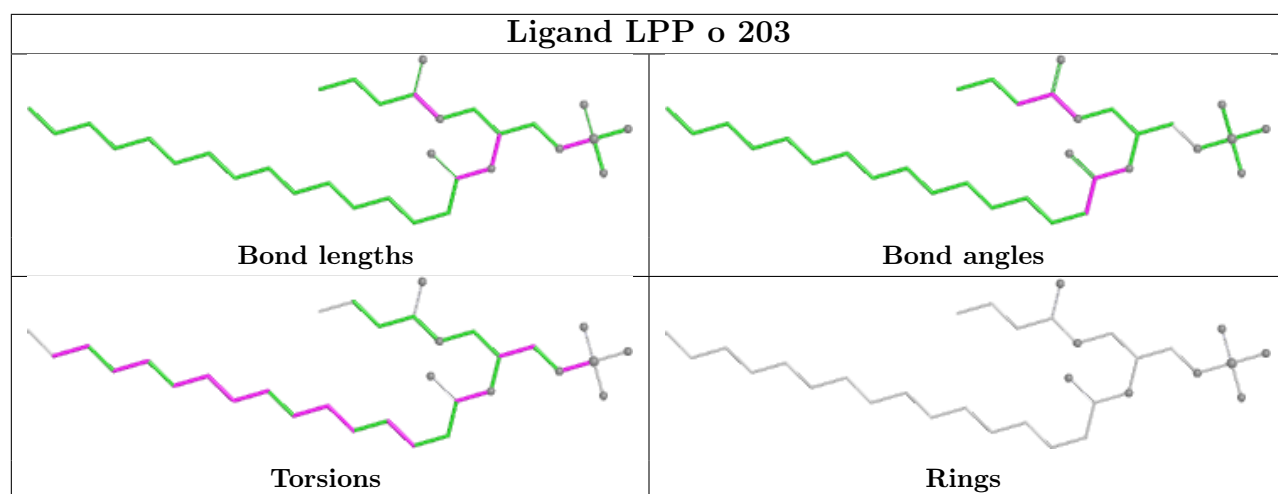
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	r	101	CDL	2	0
22	P	202	LPP	2	0
20	m	201	CDL	1	0
20	M	204	CDL	1	0
21	f	302	LMT	2	0
20	O	201	CDL	4	0
20	P	201	CDL	1	0

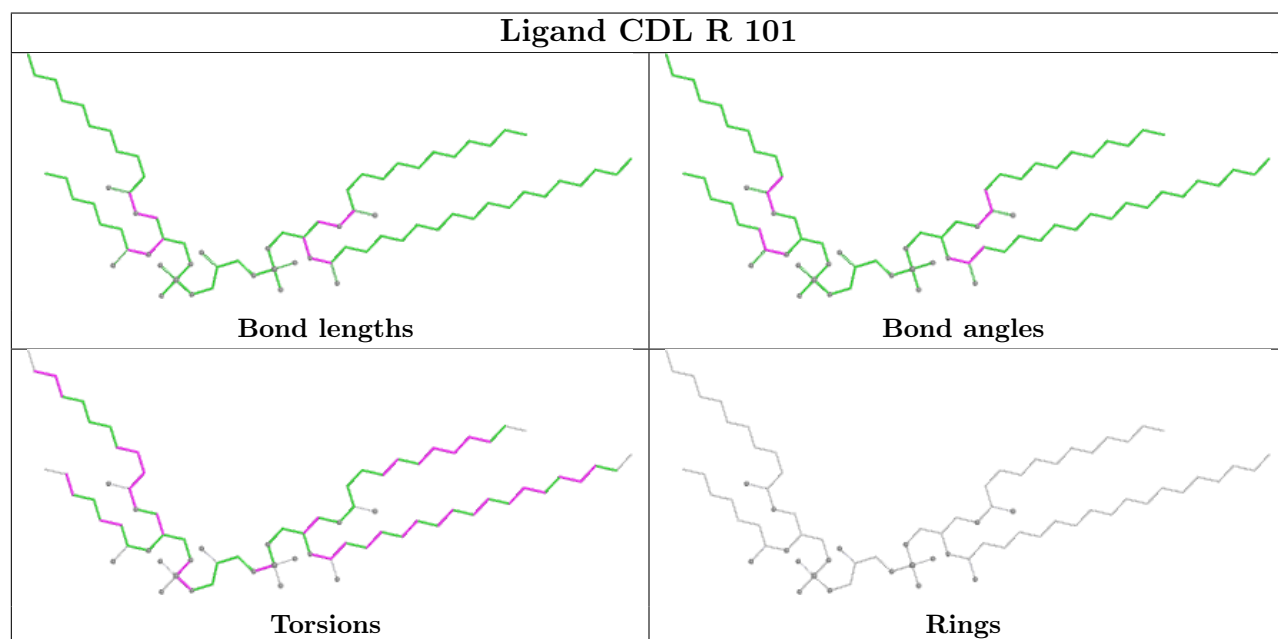
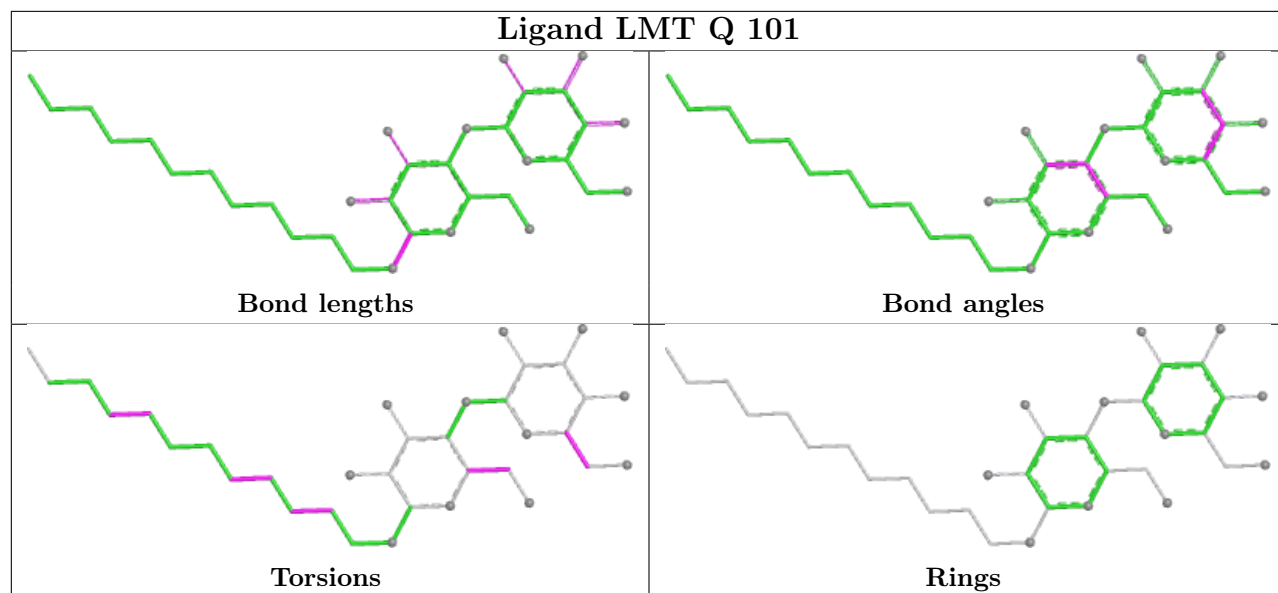
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

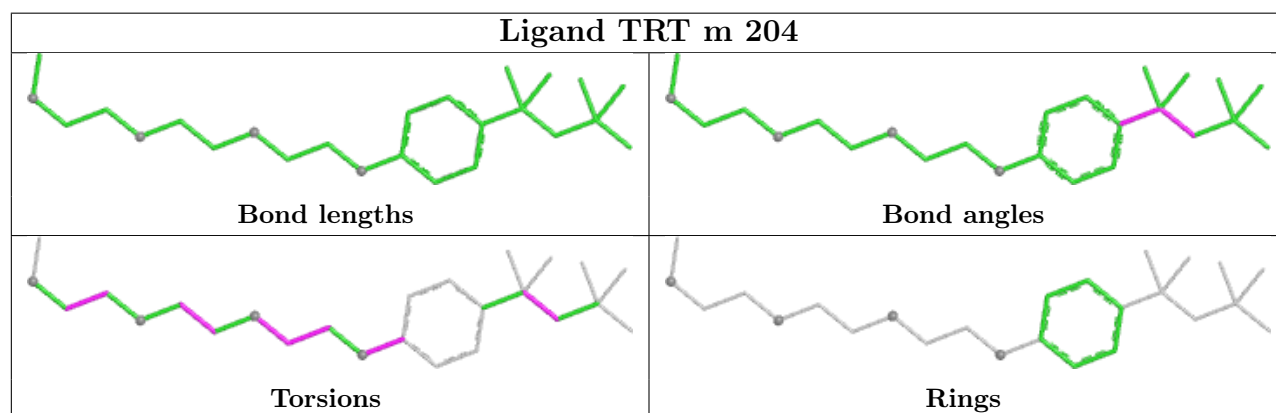
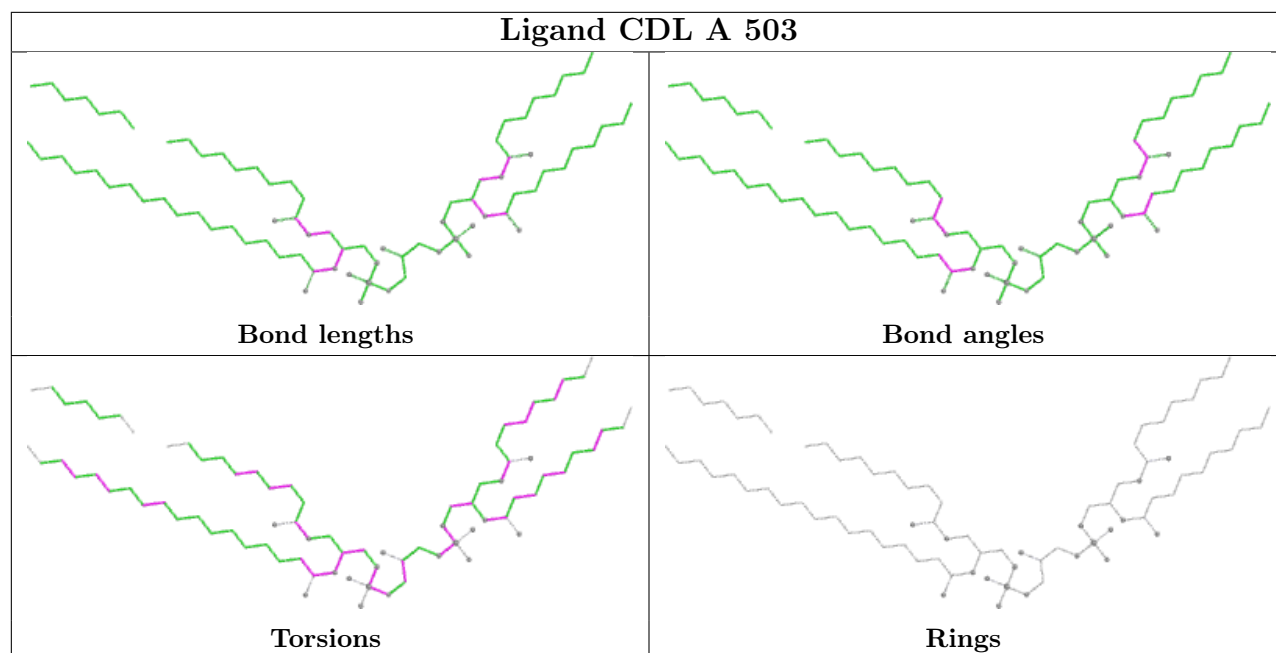
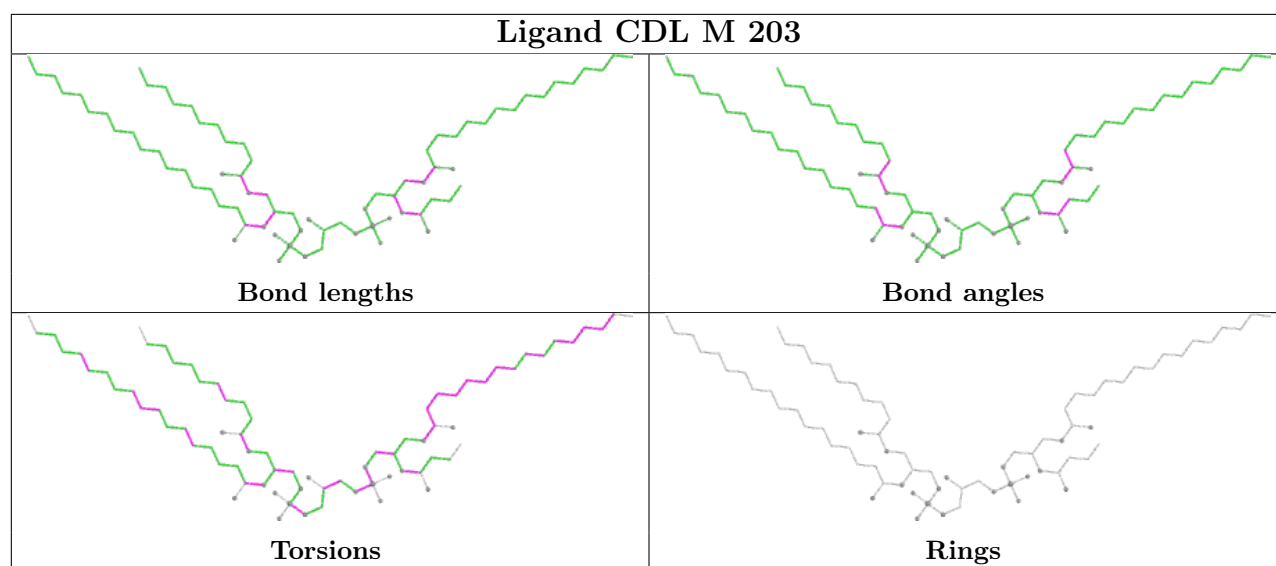


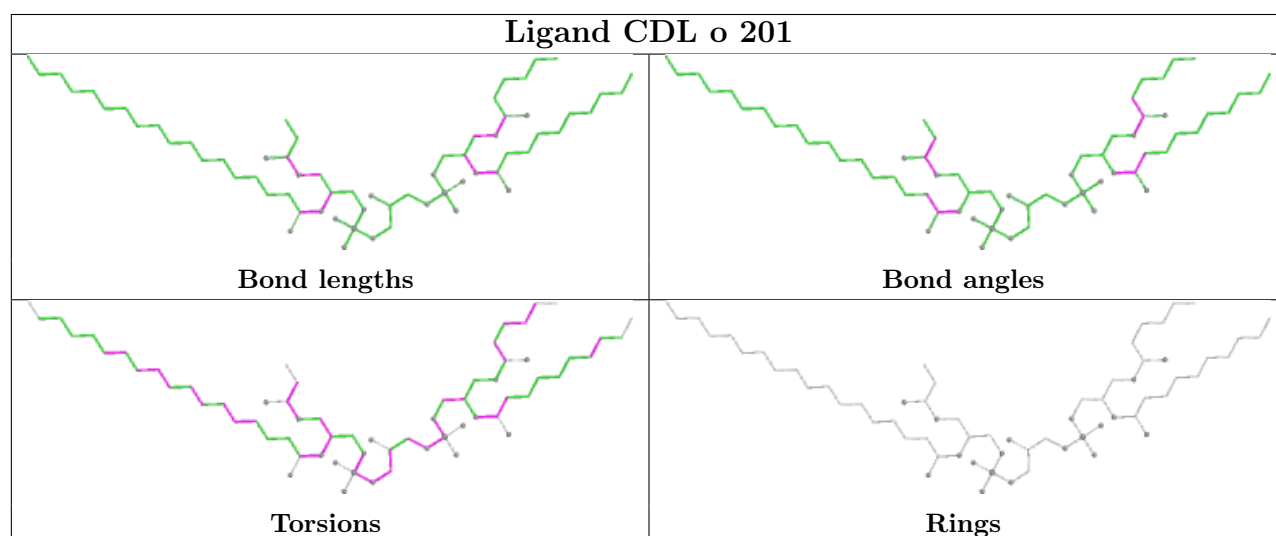
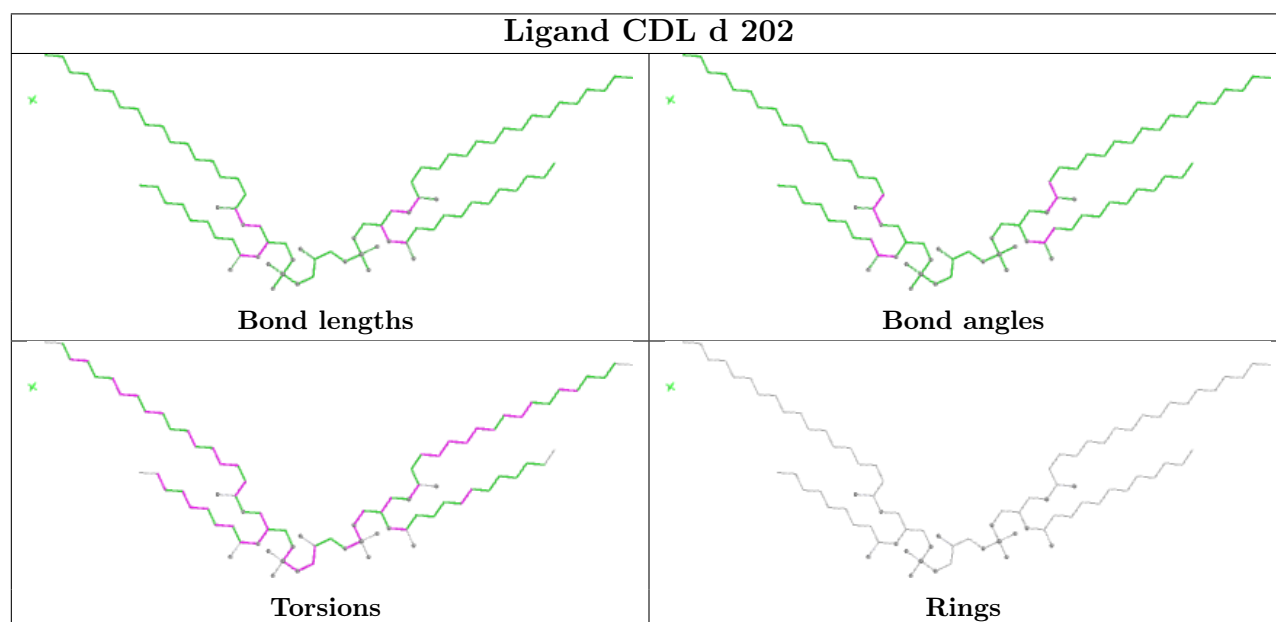
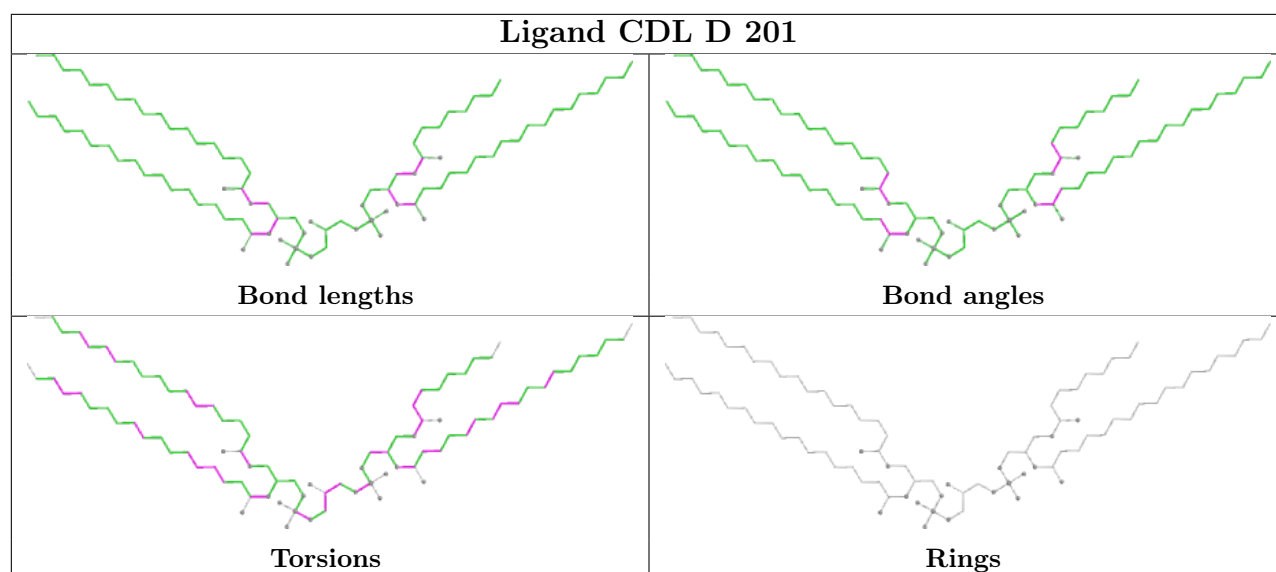


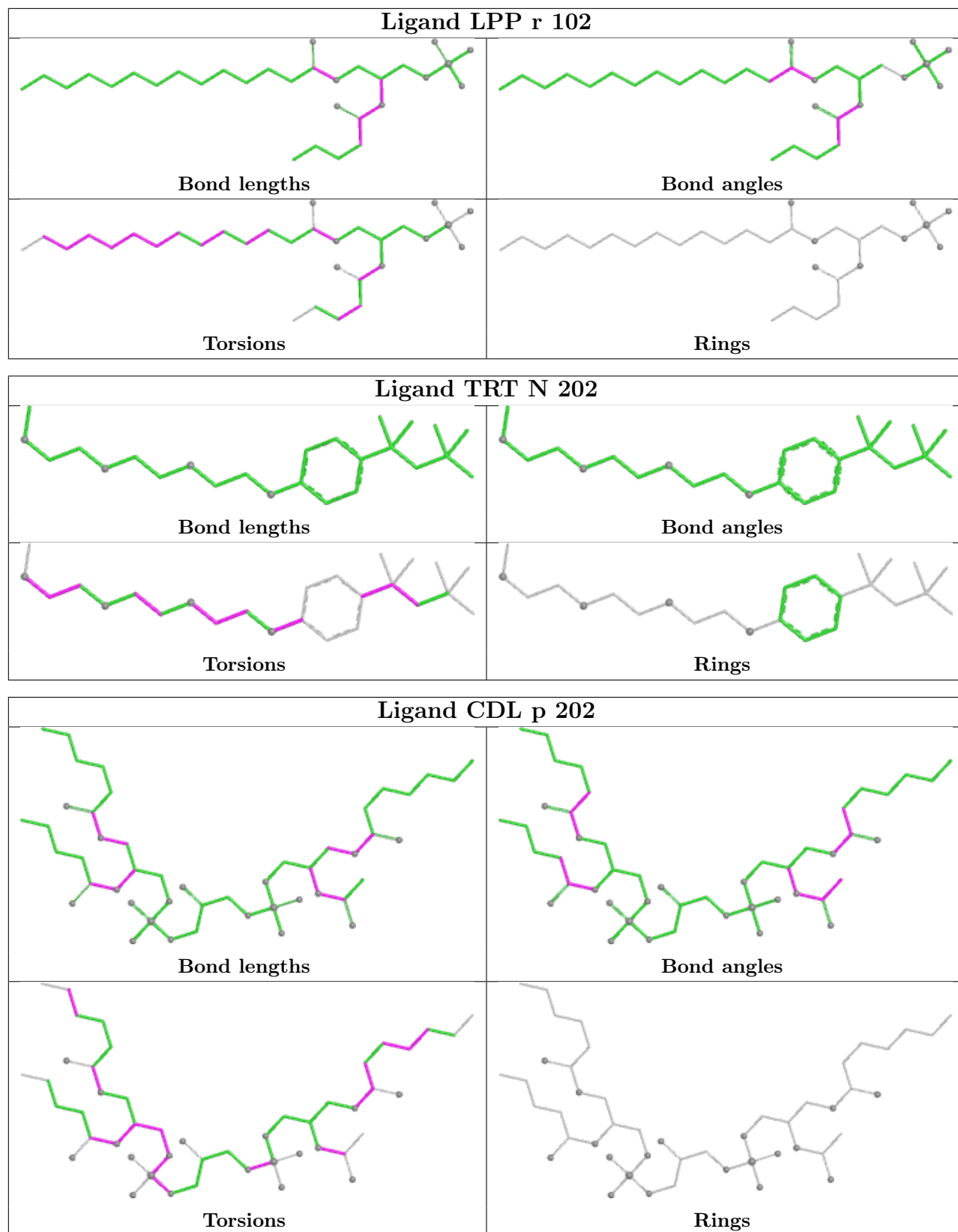


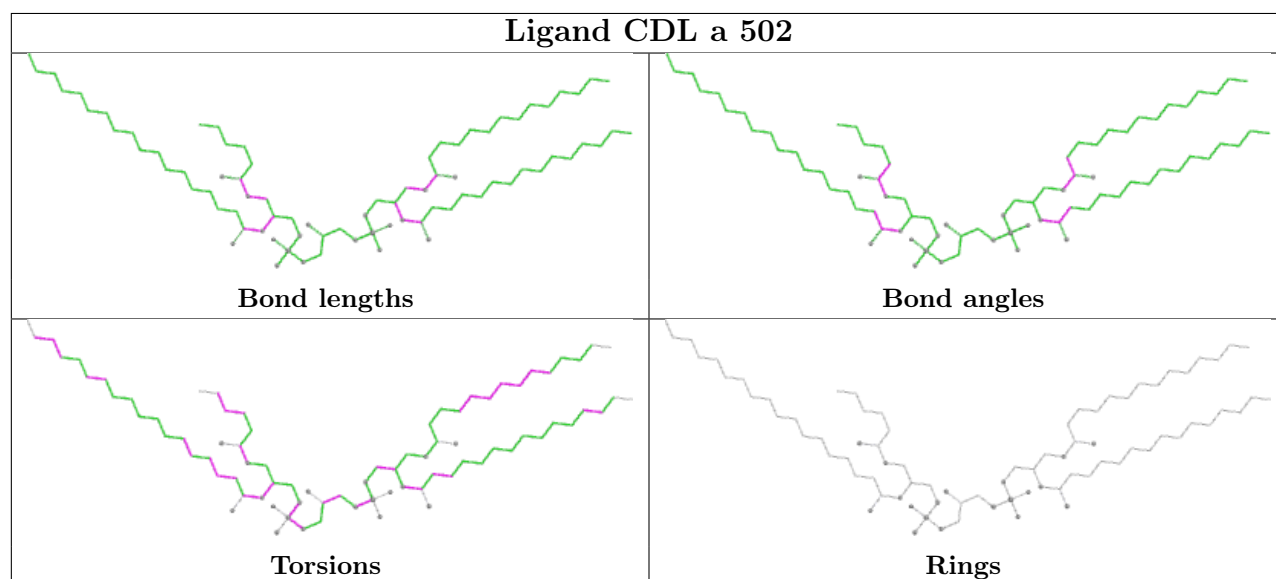
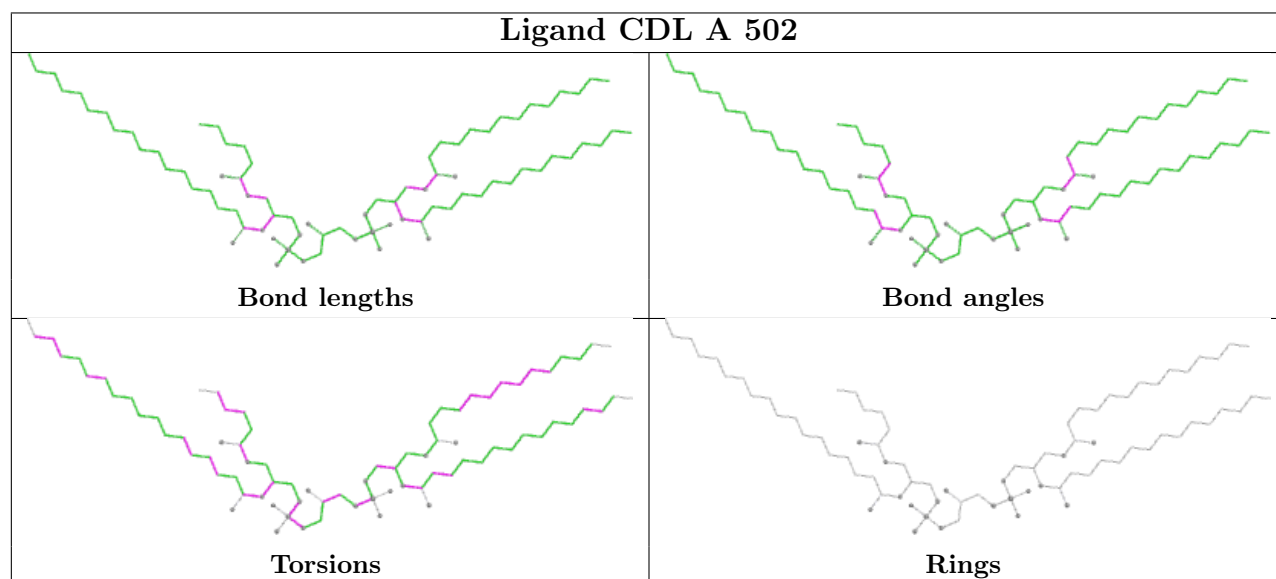
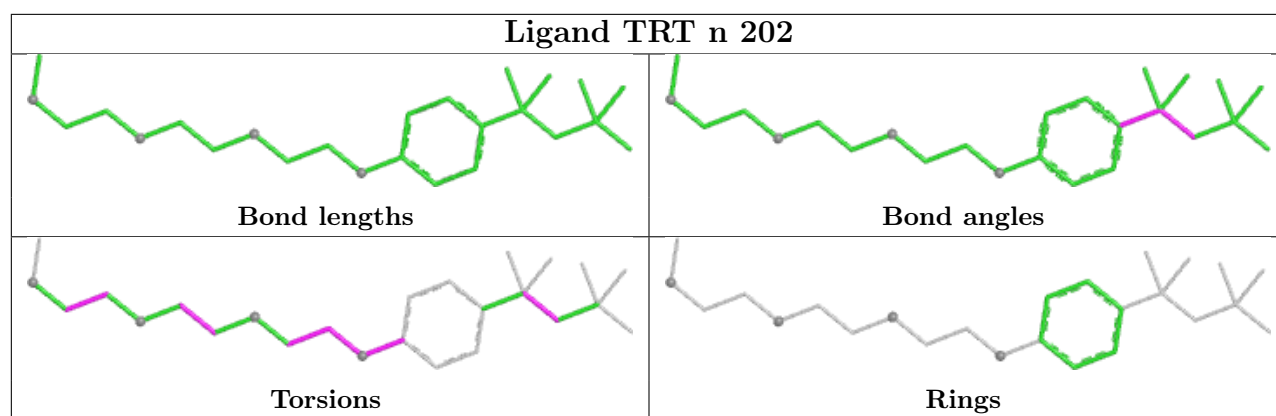


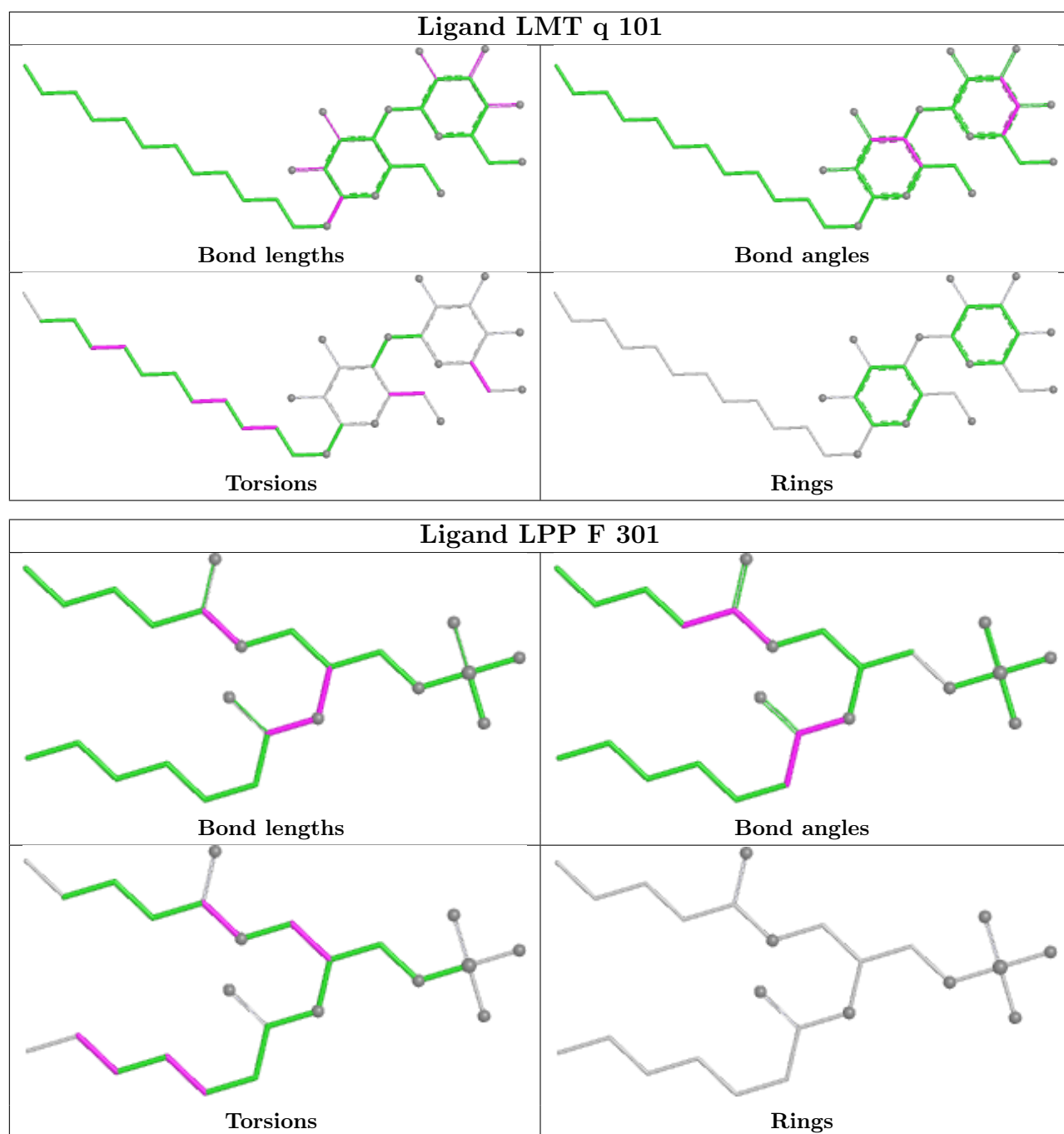


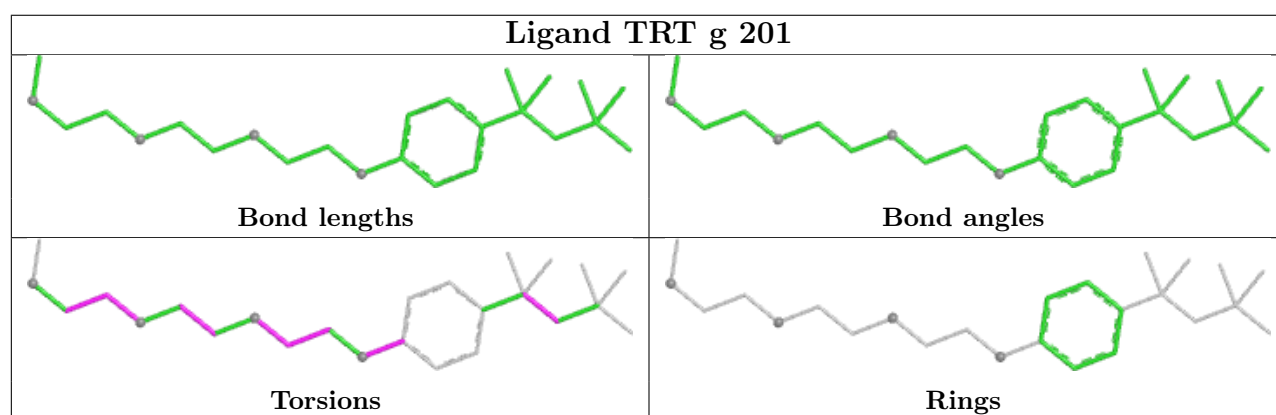
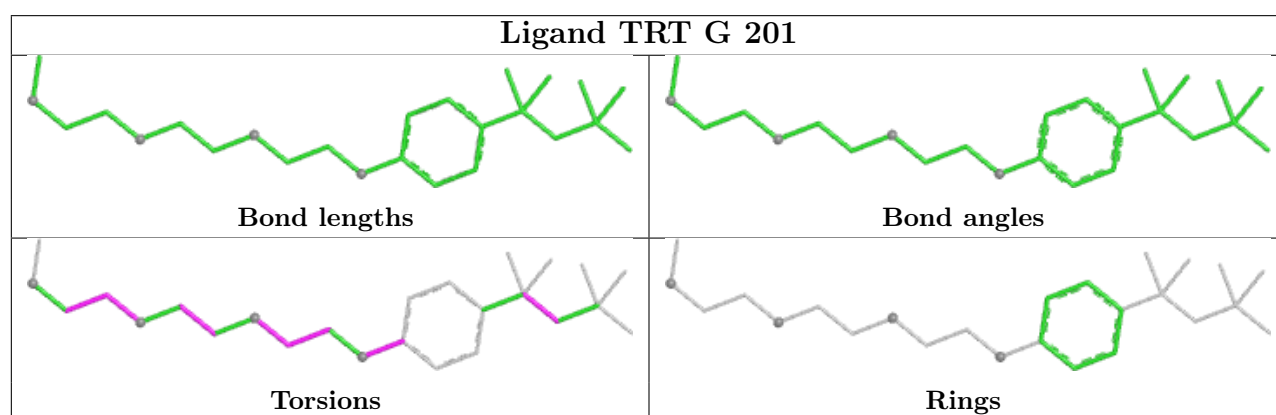
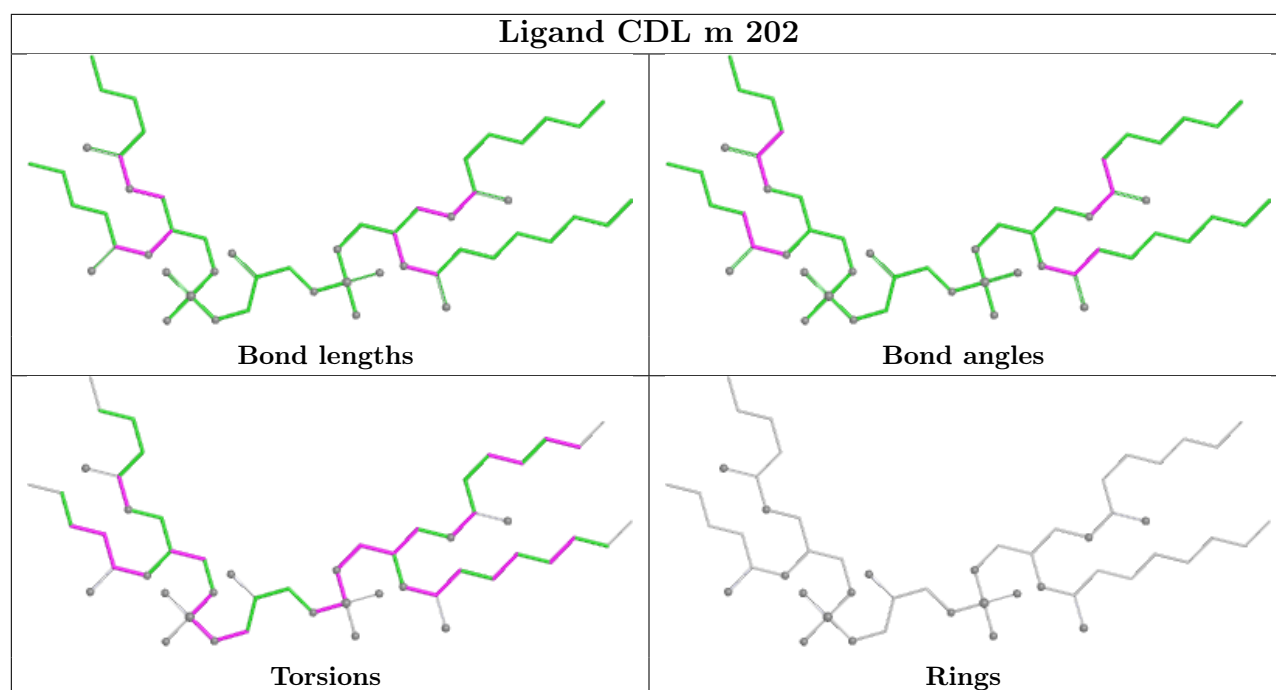


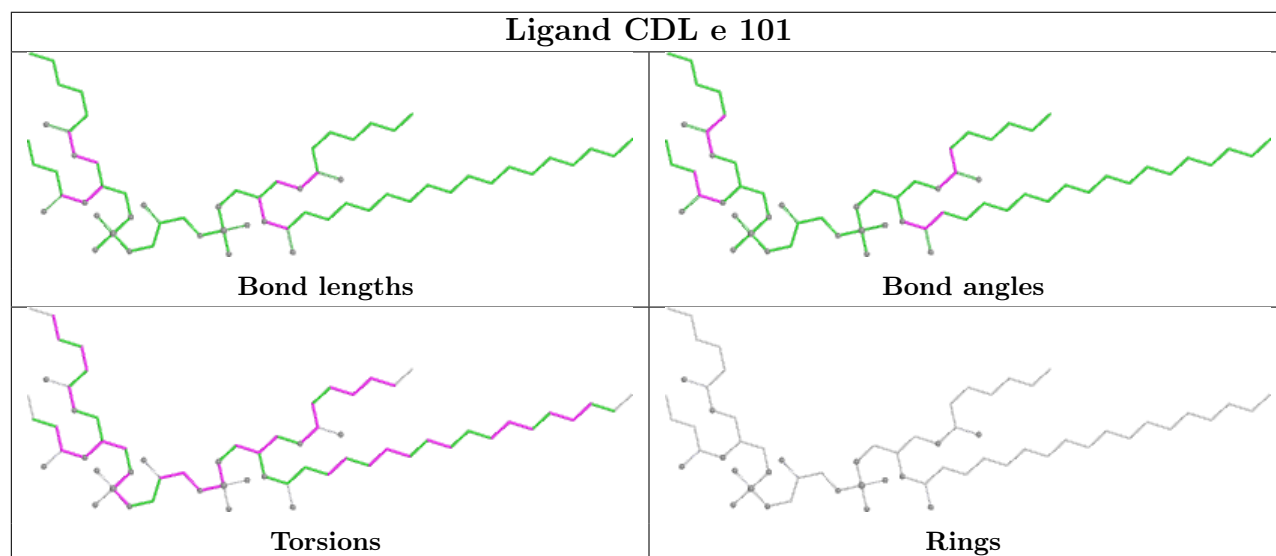
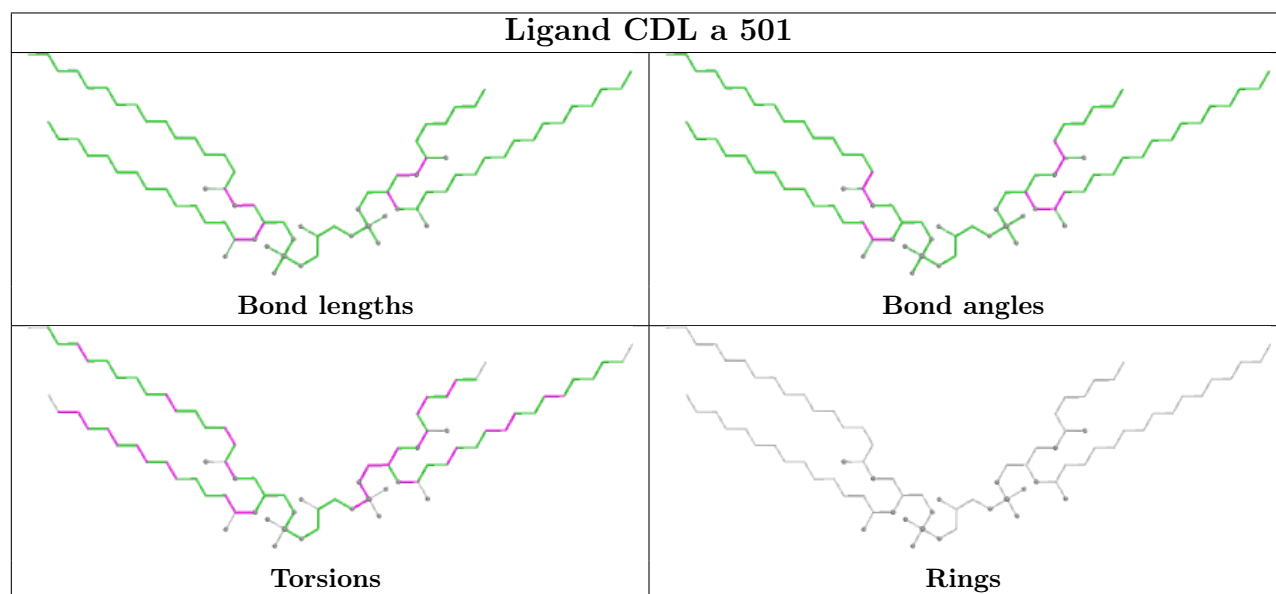
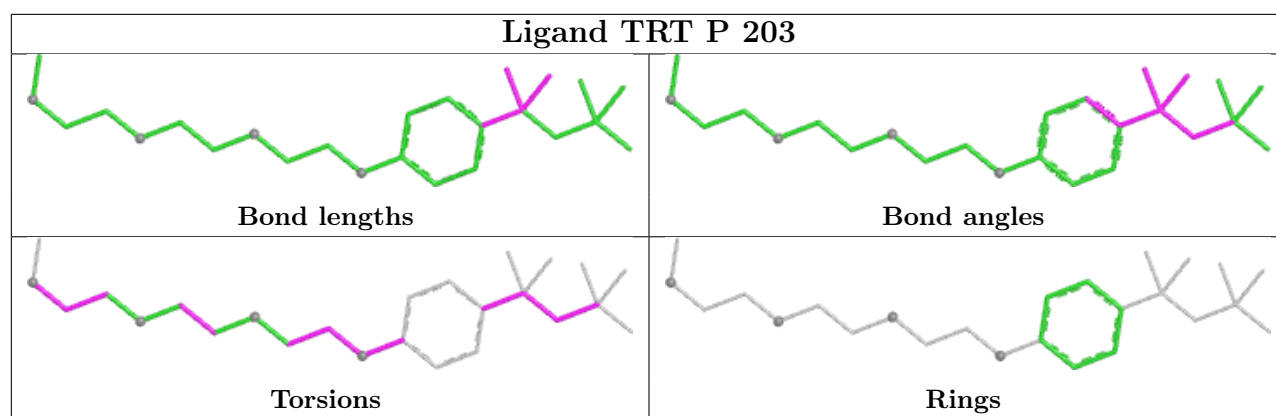


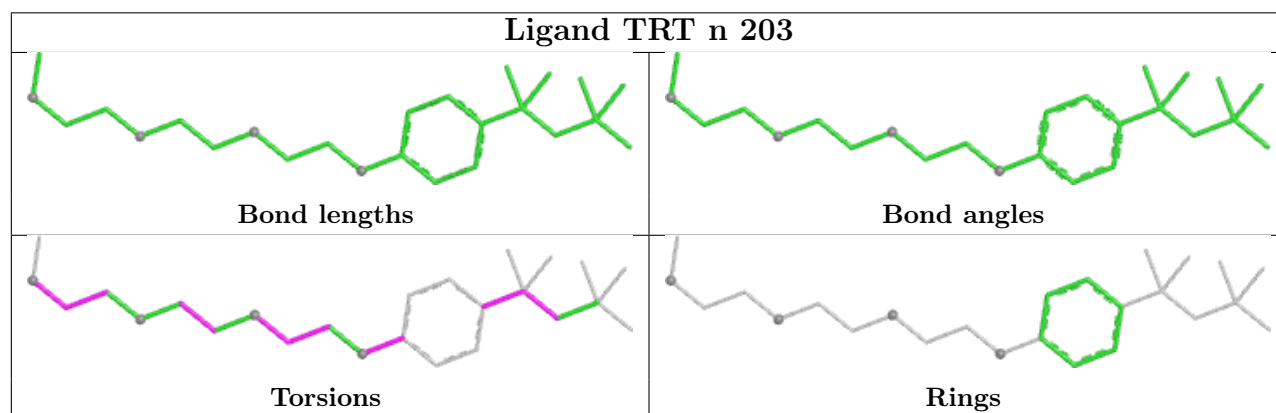
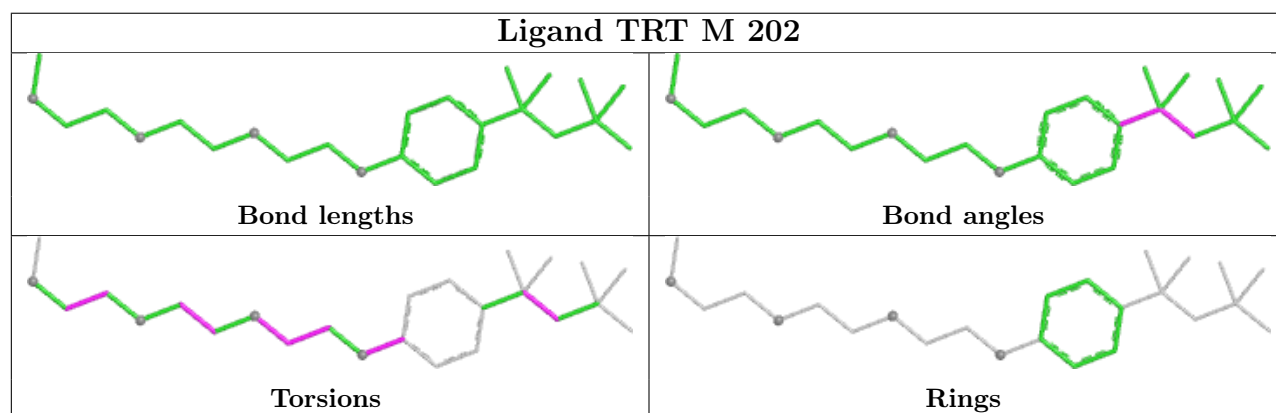
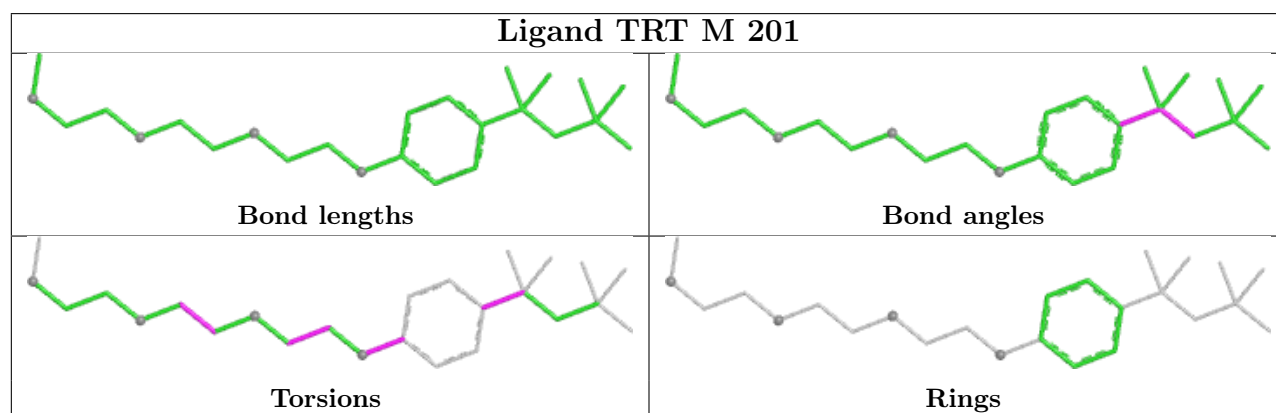
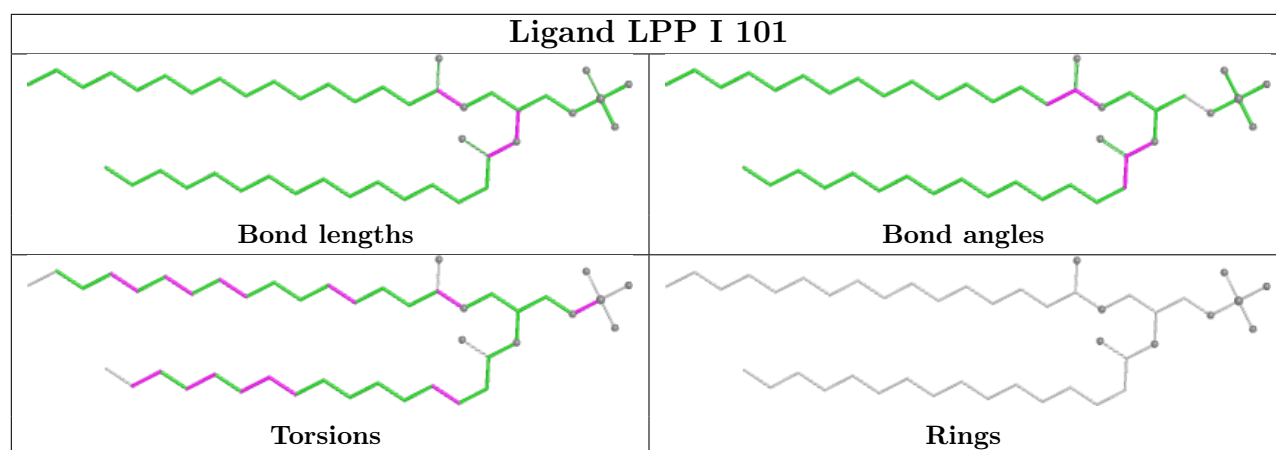


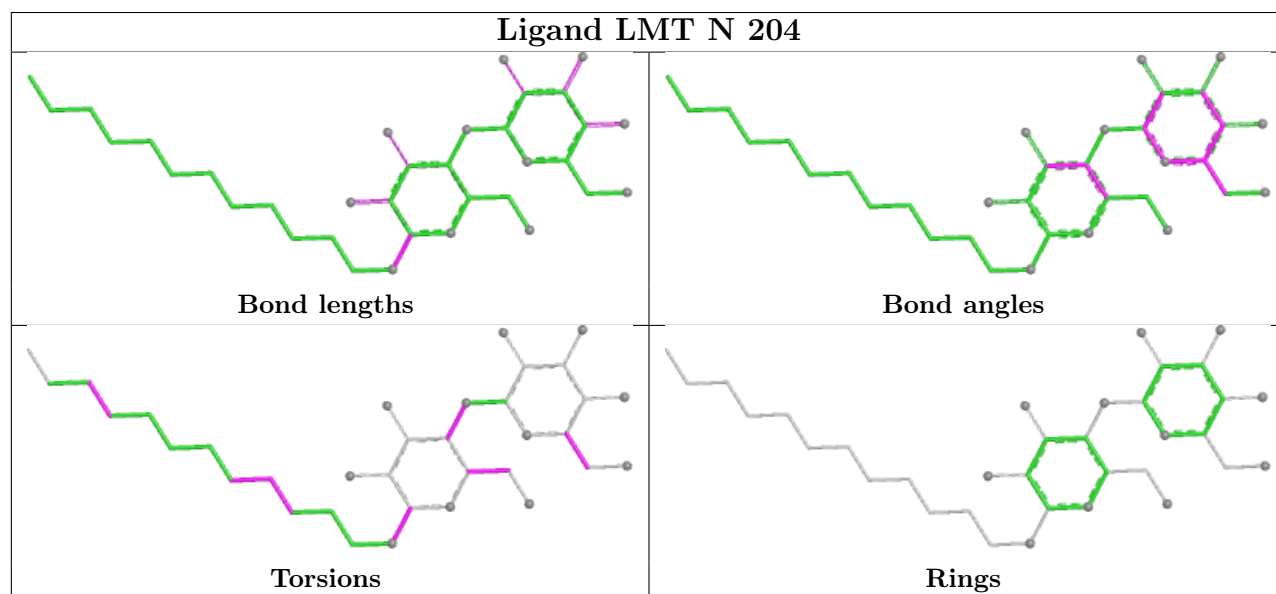
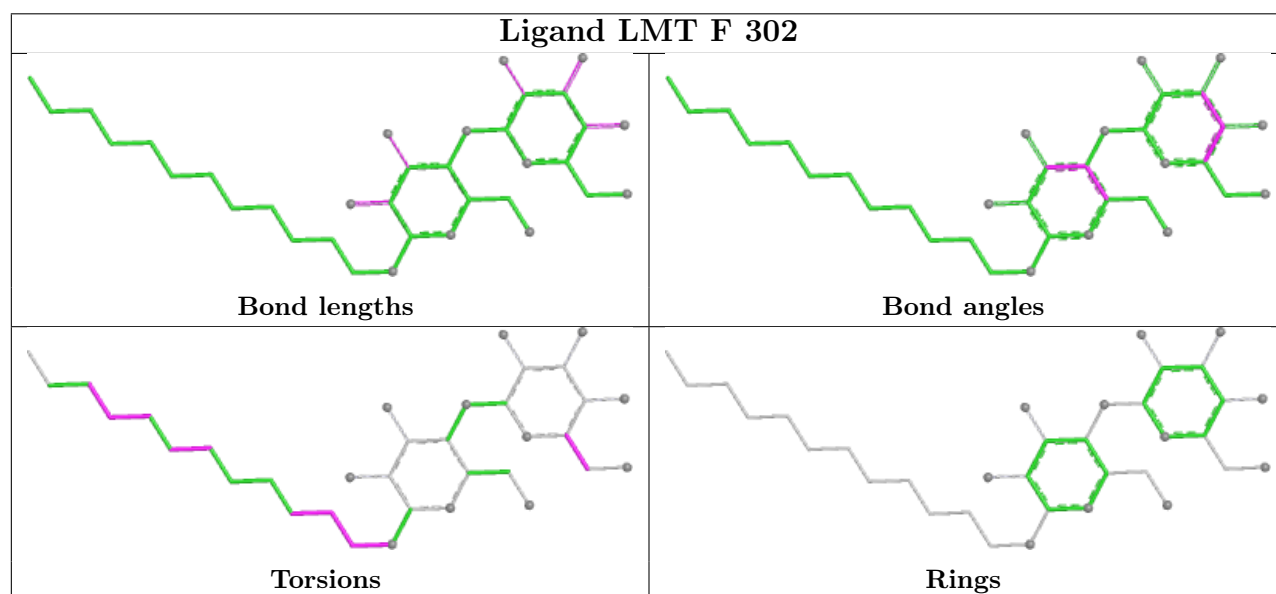
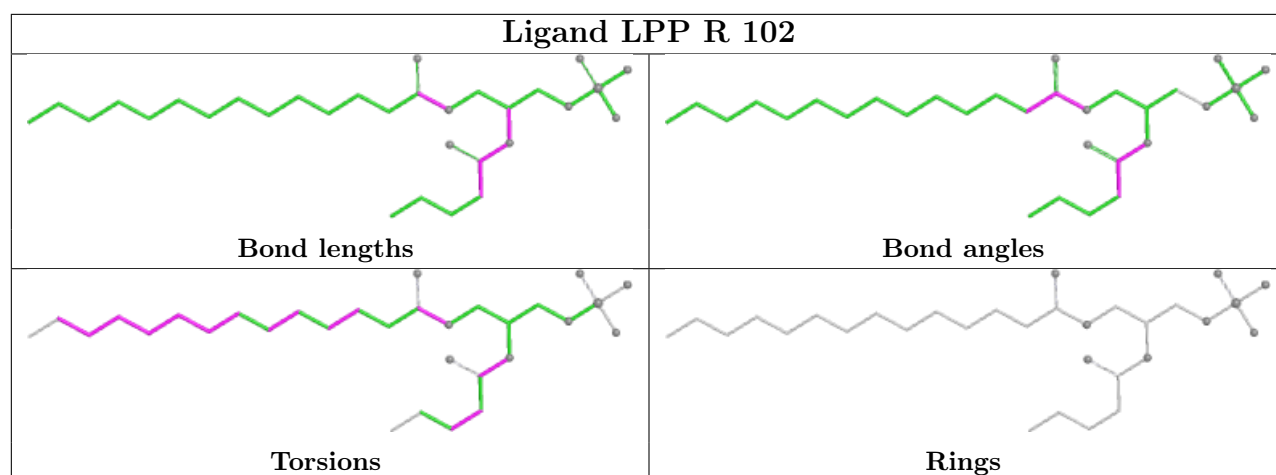


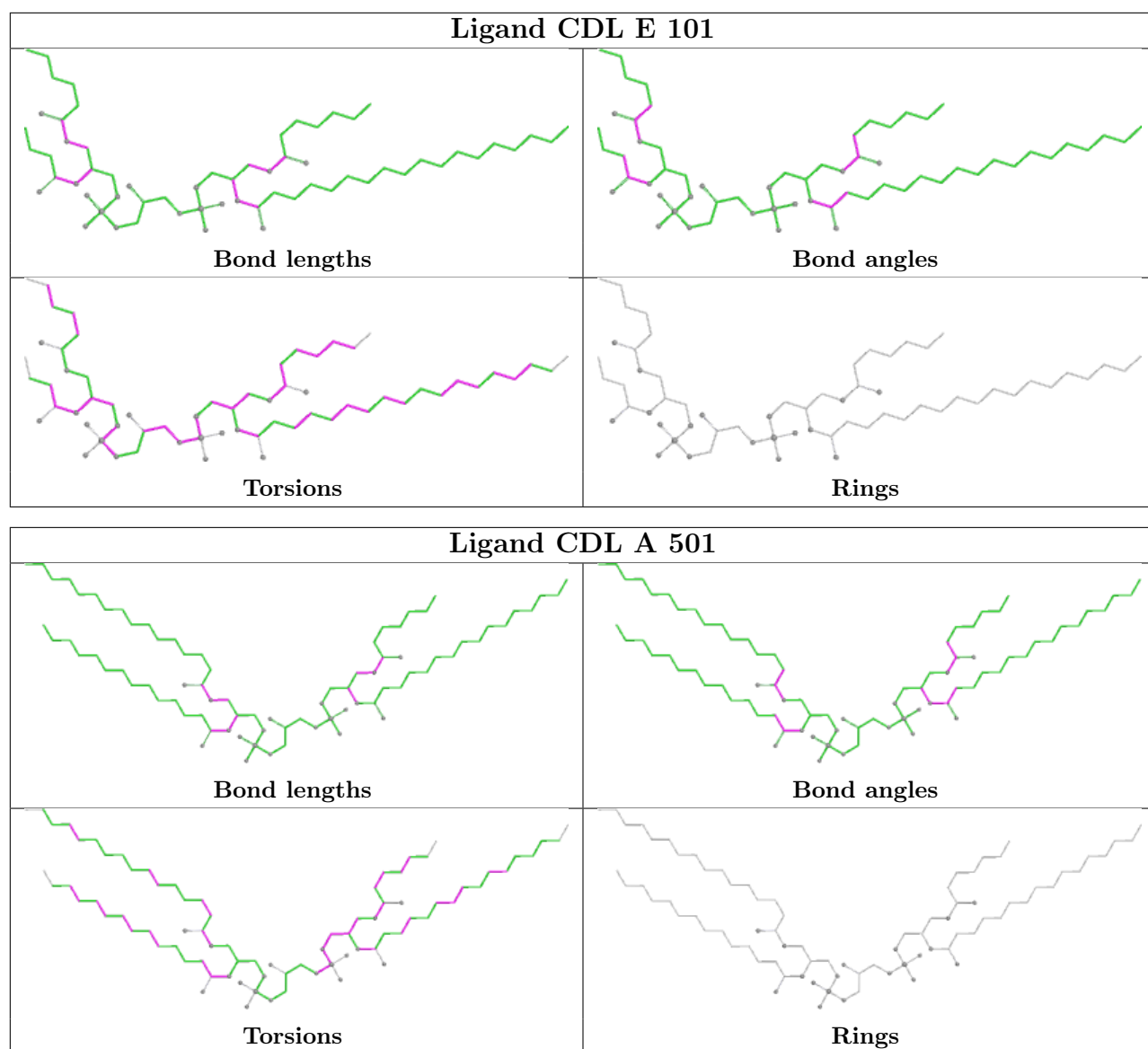


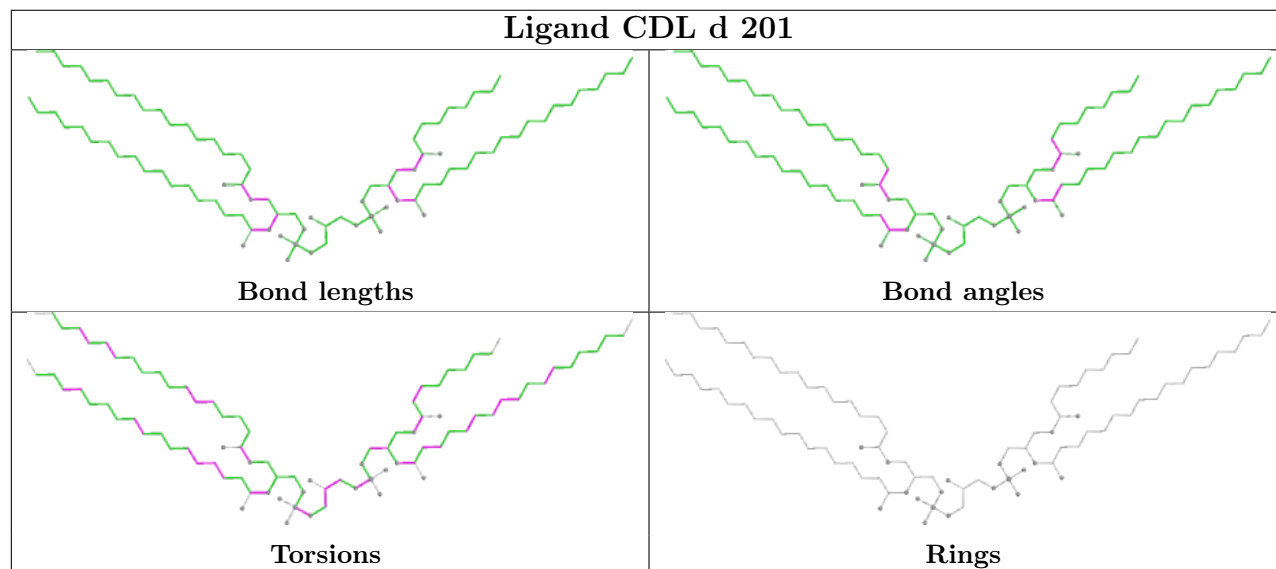
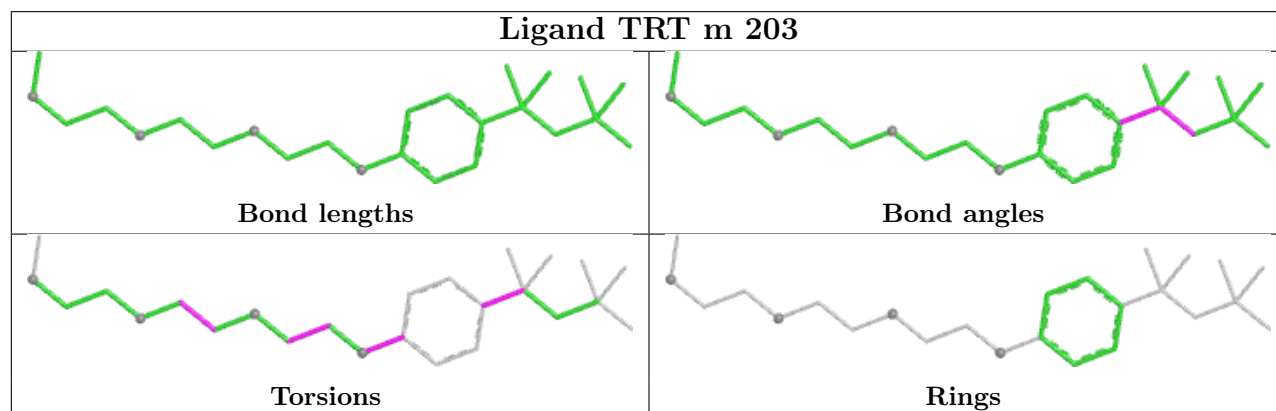
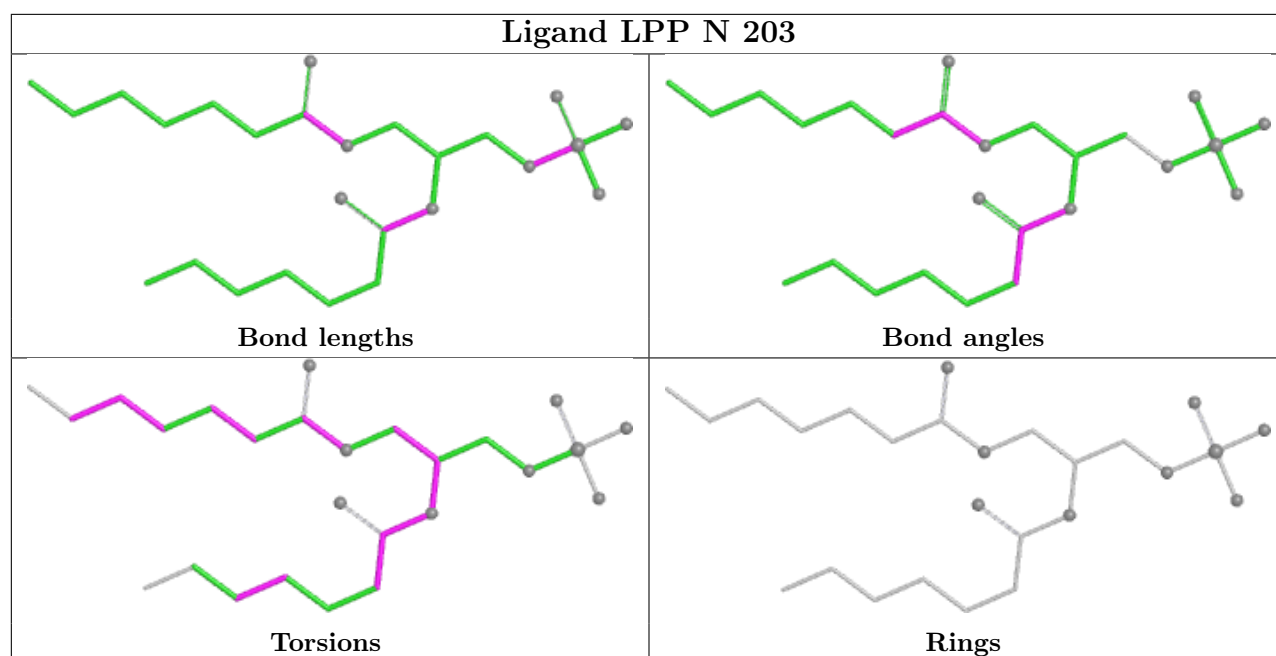


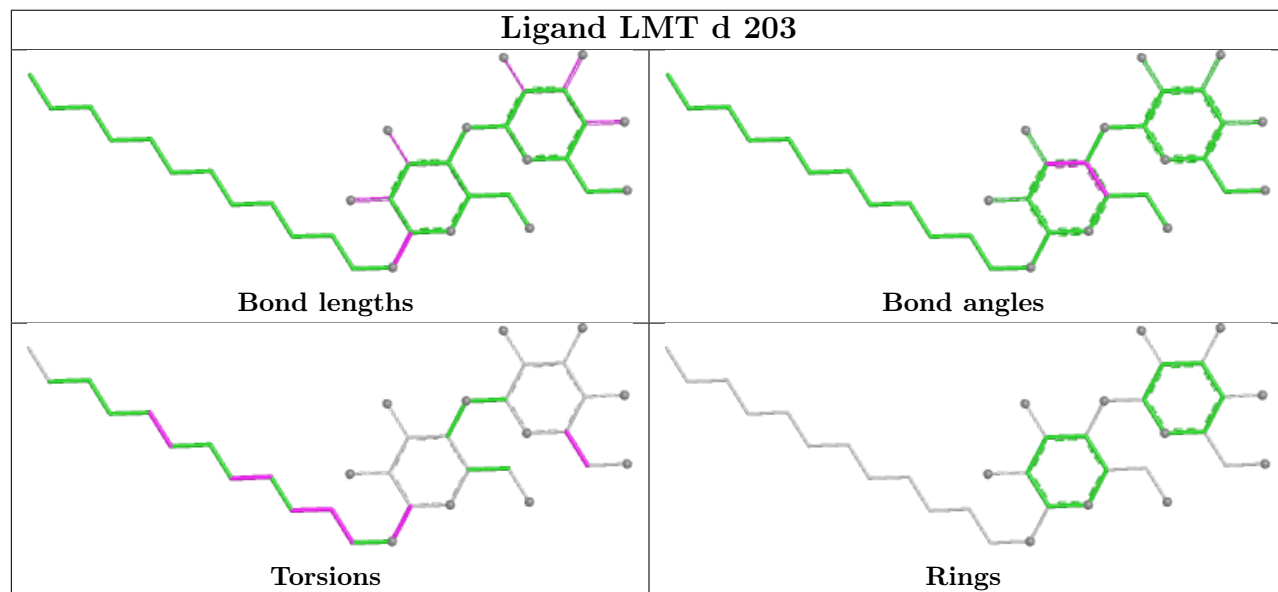
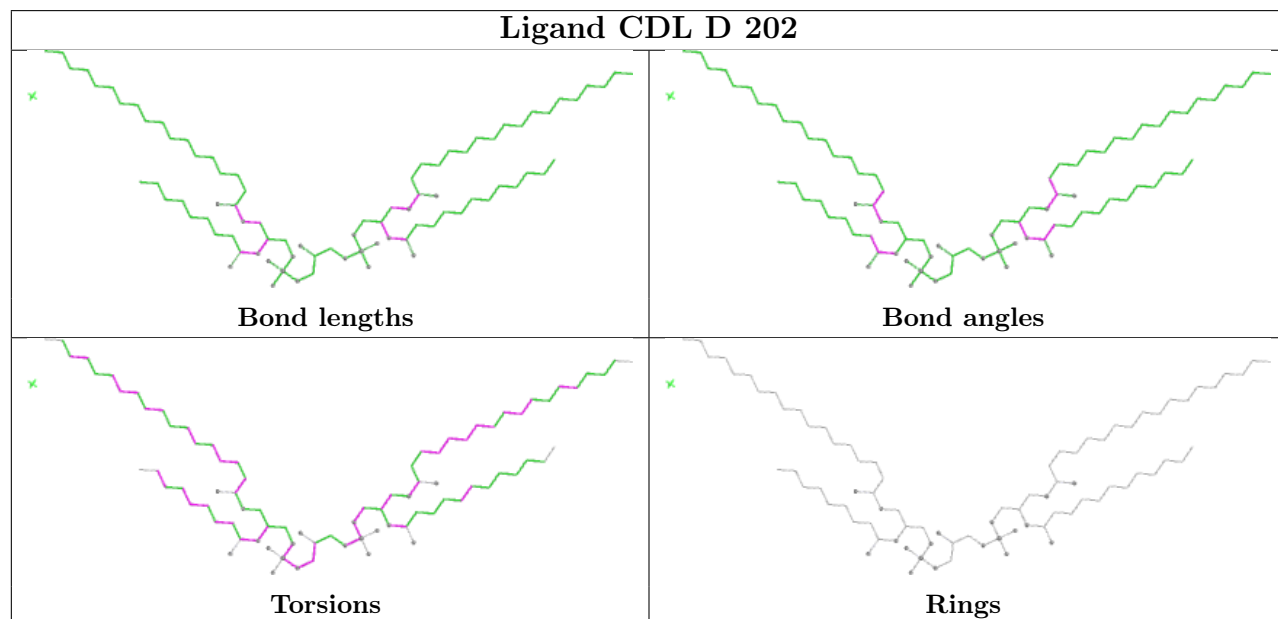
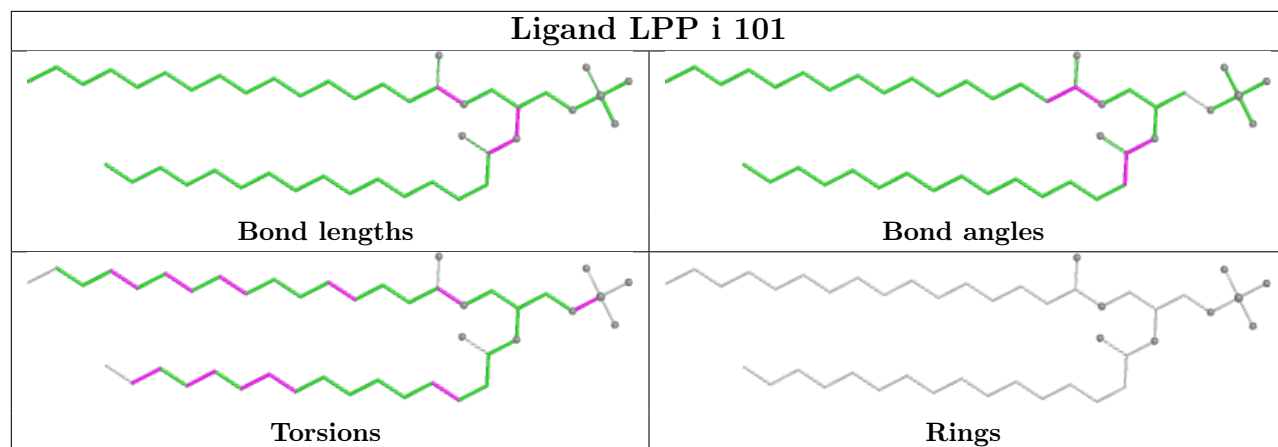


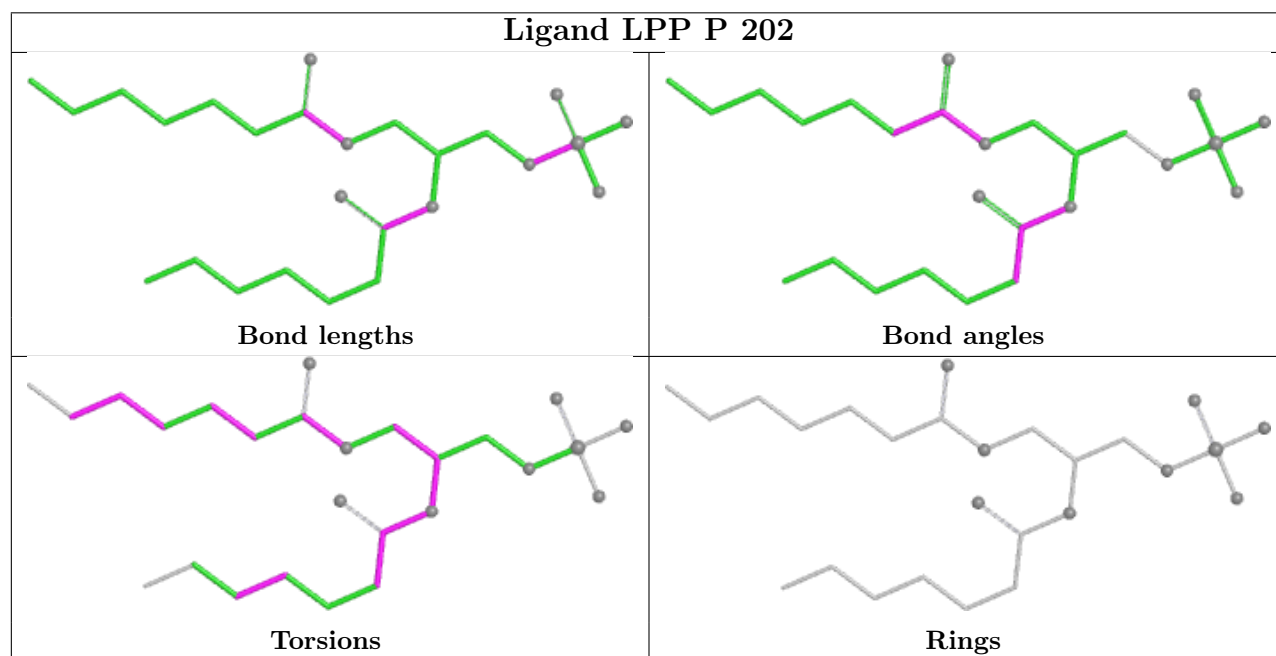
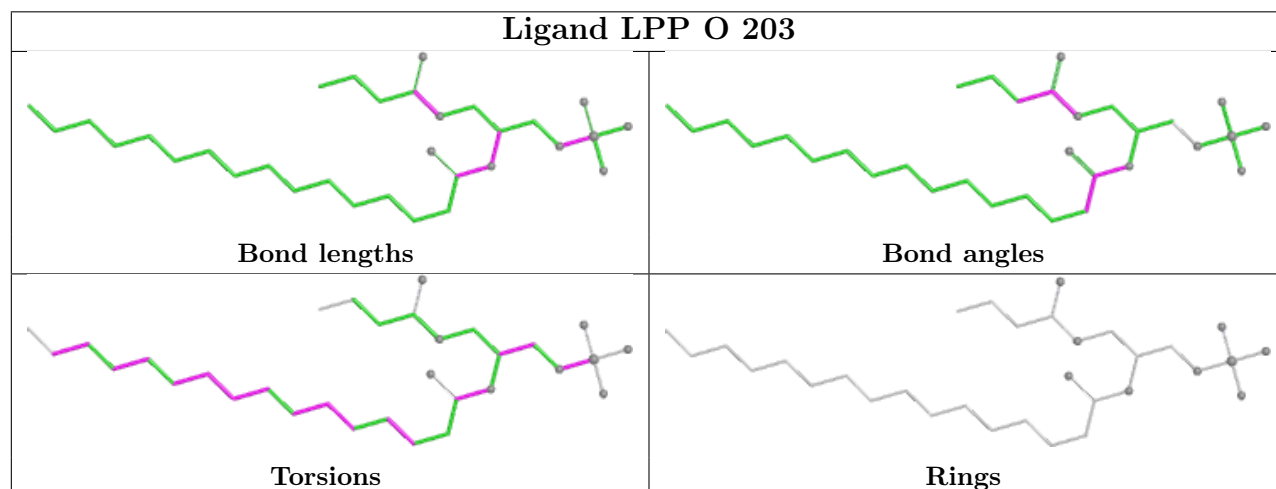
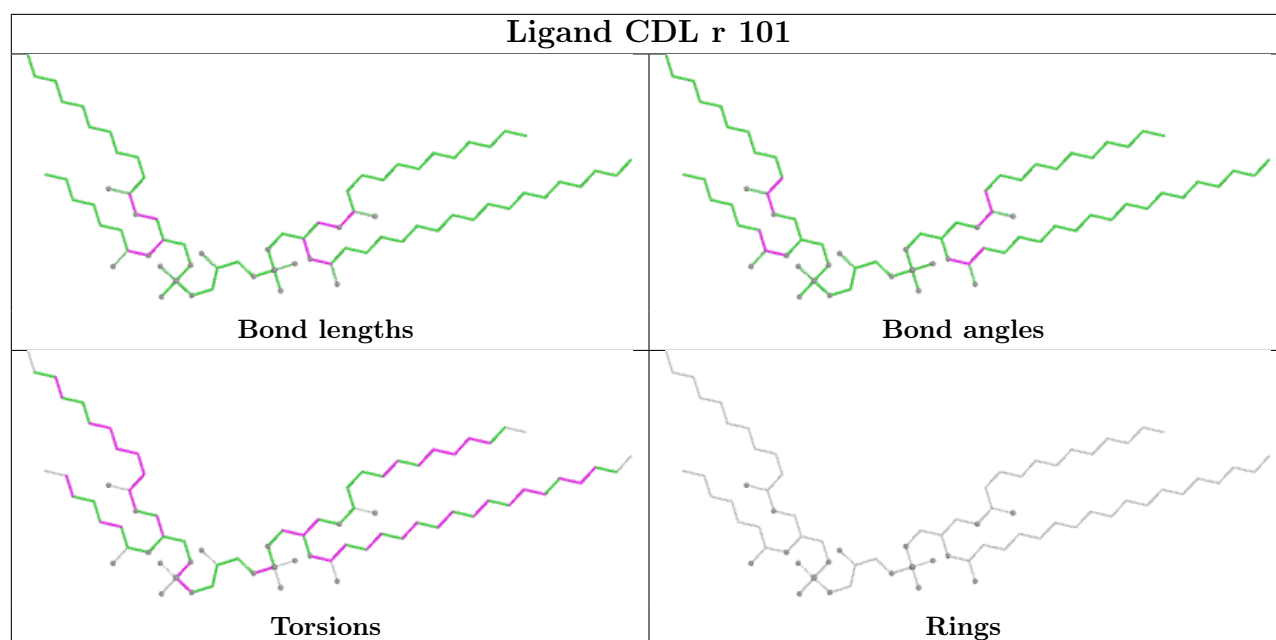


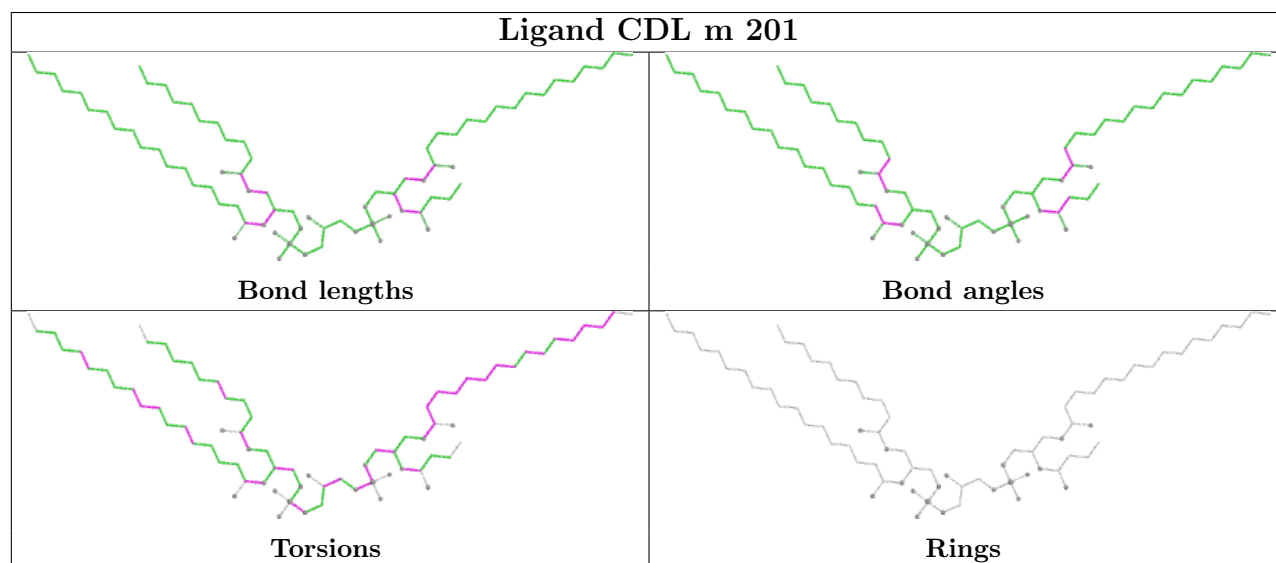
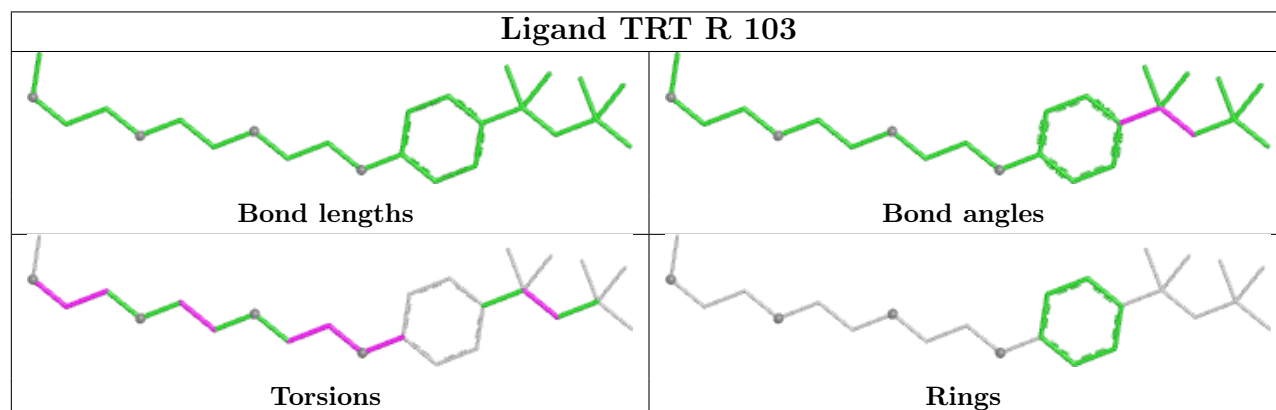
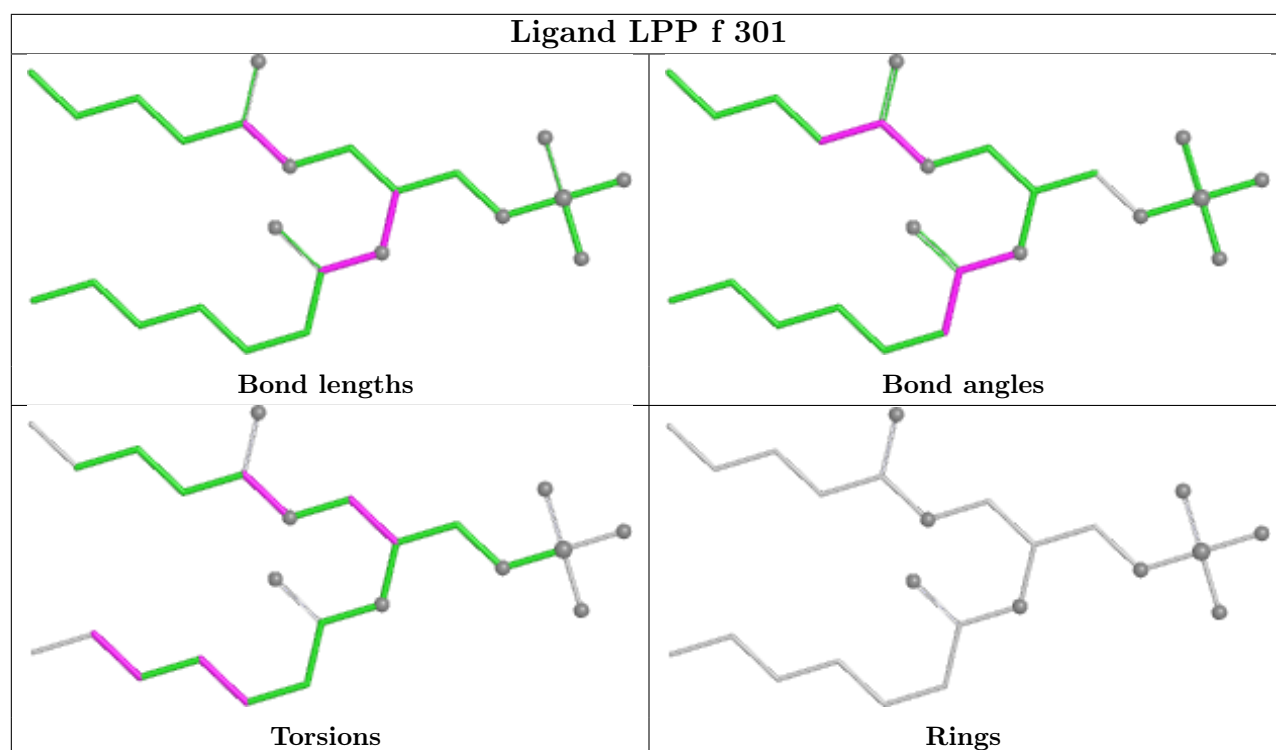


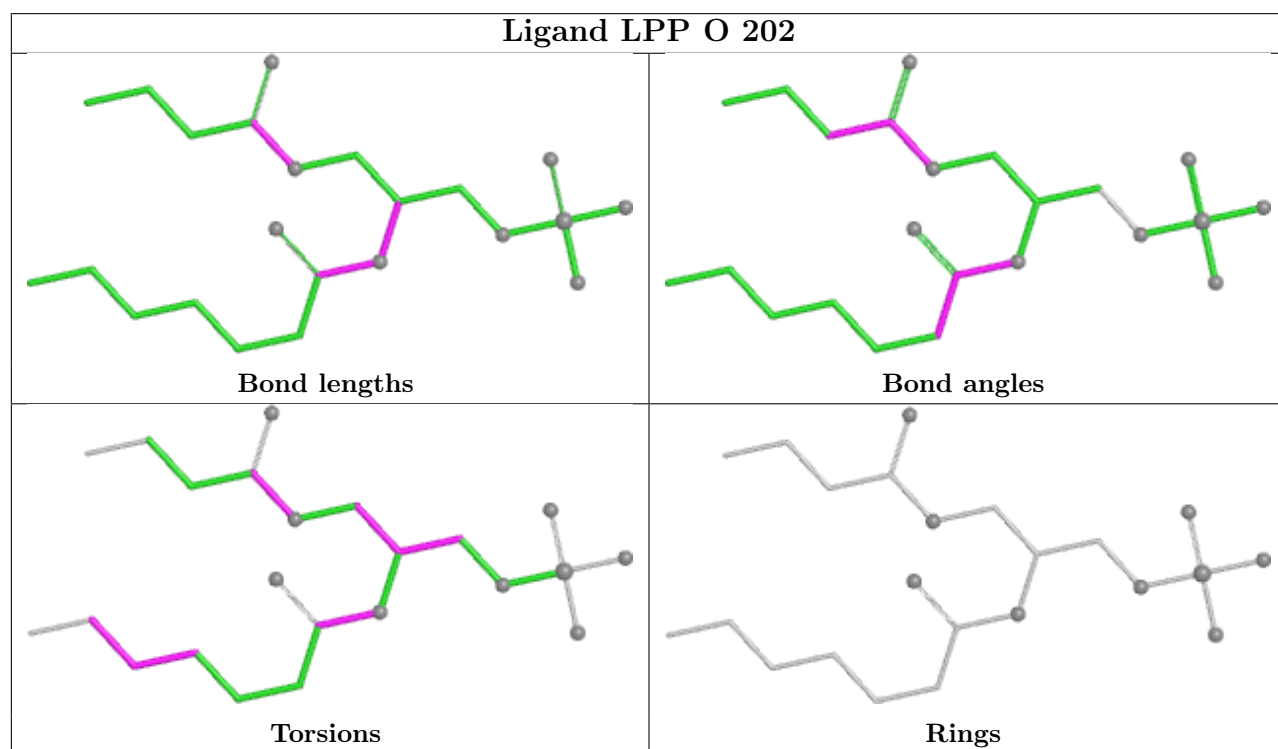
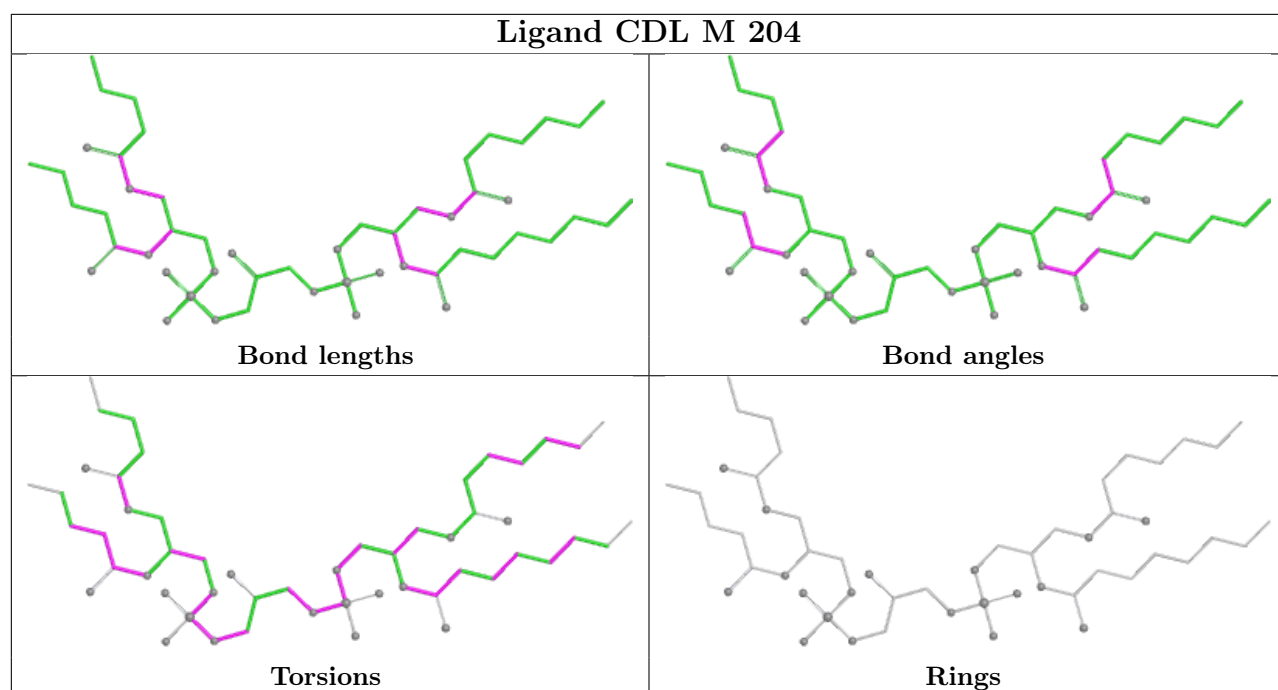


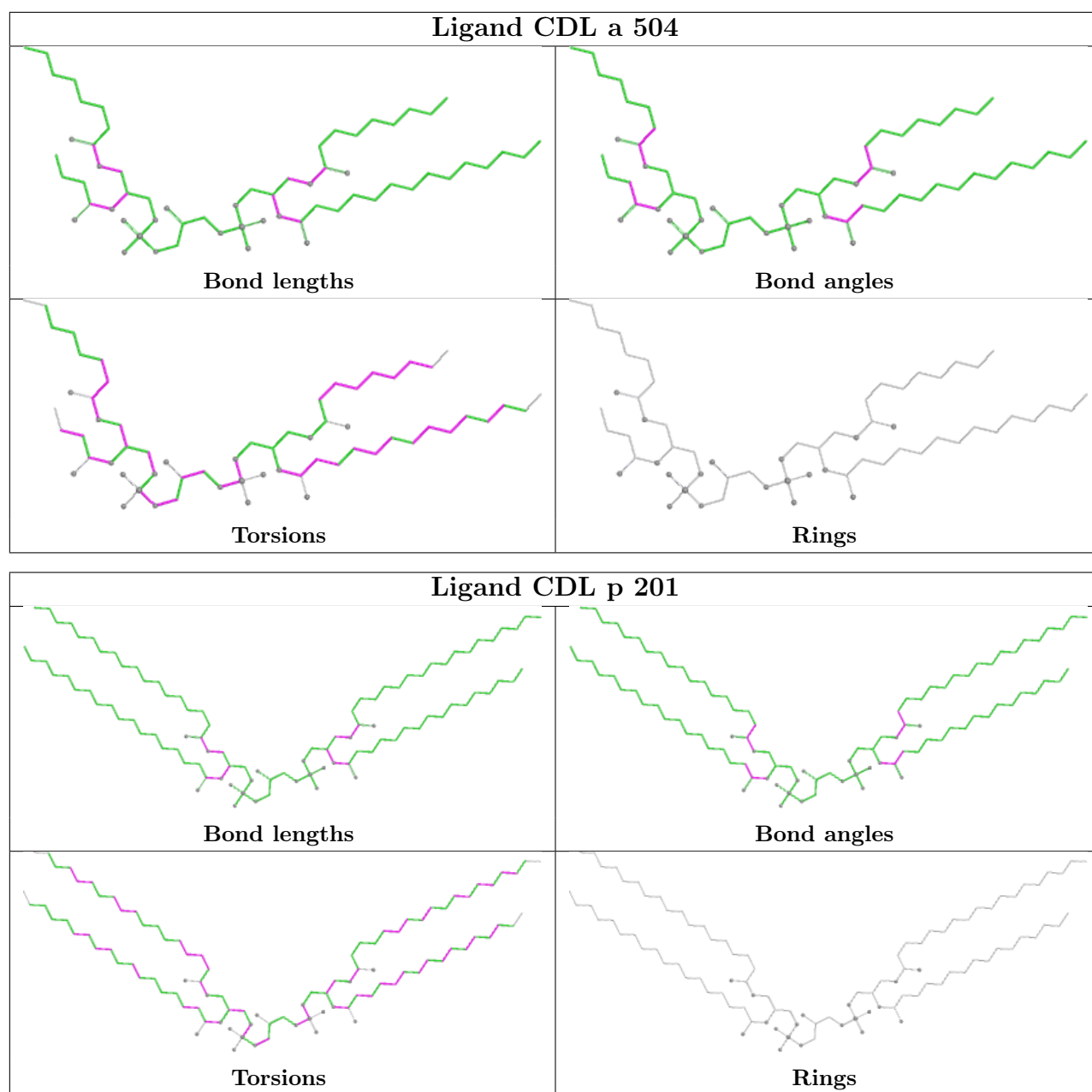


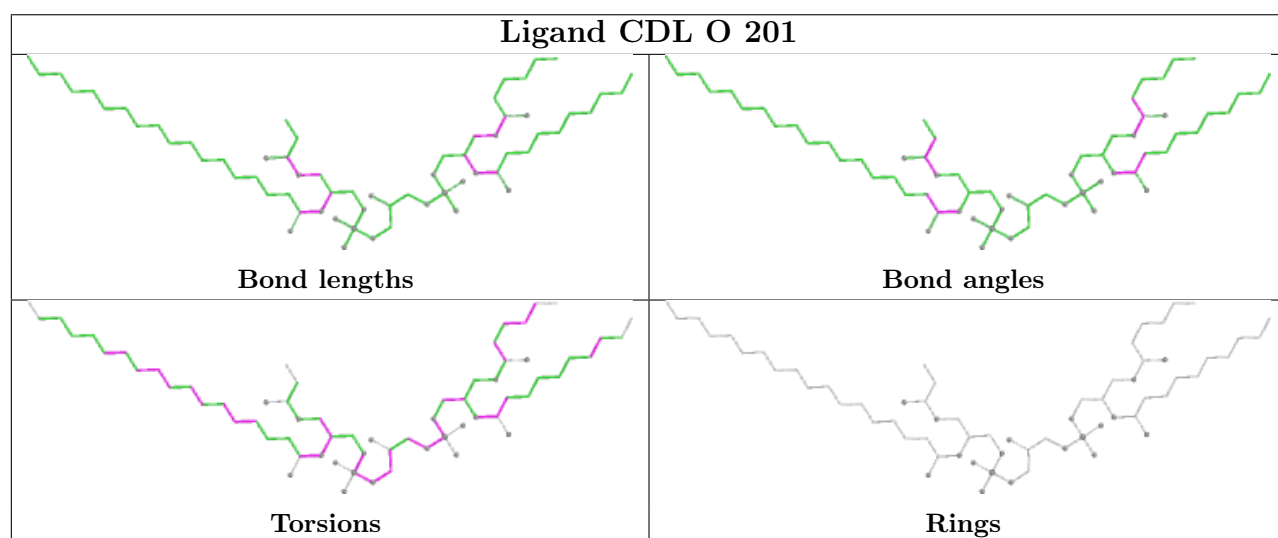
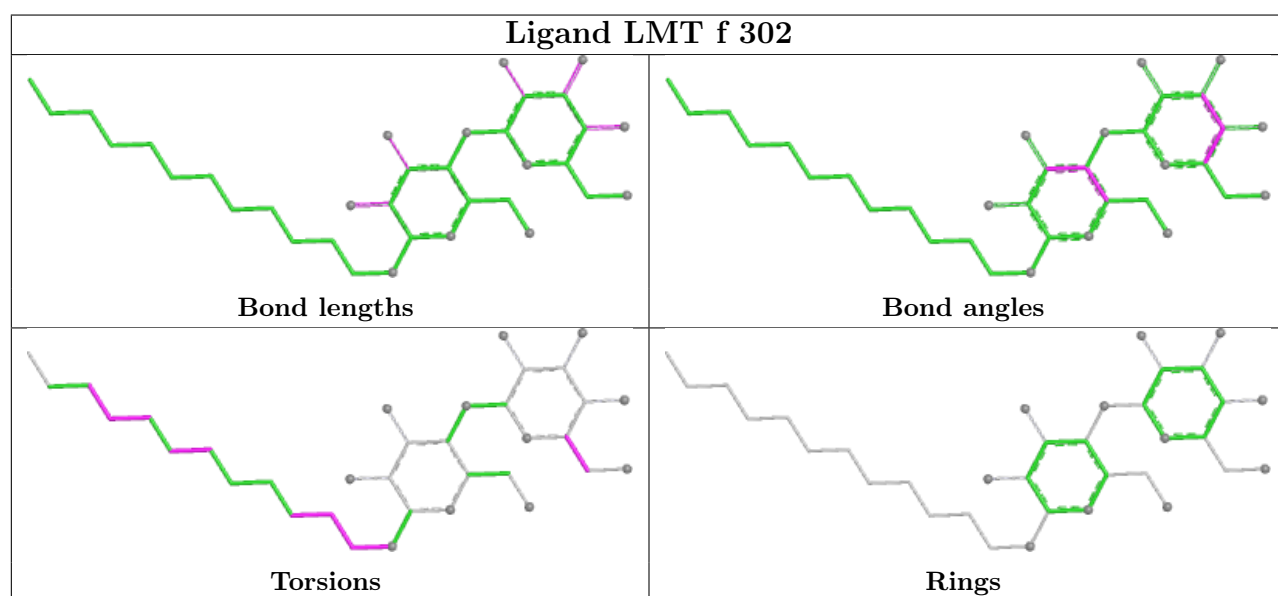
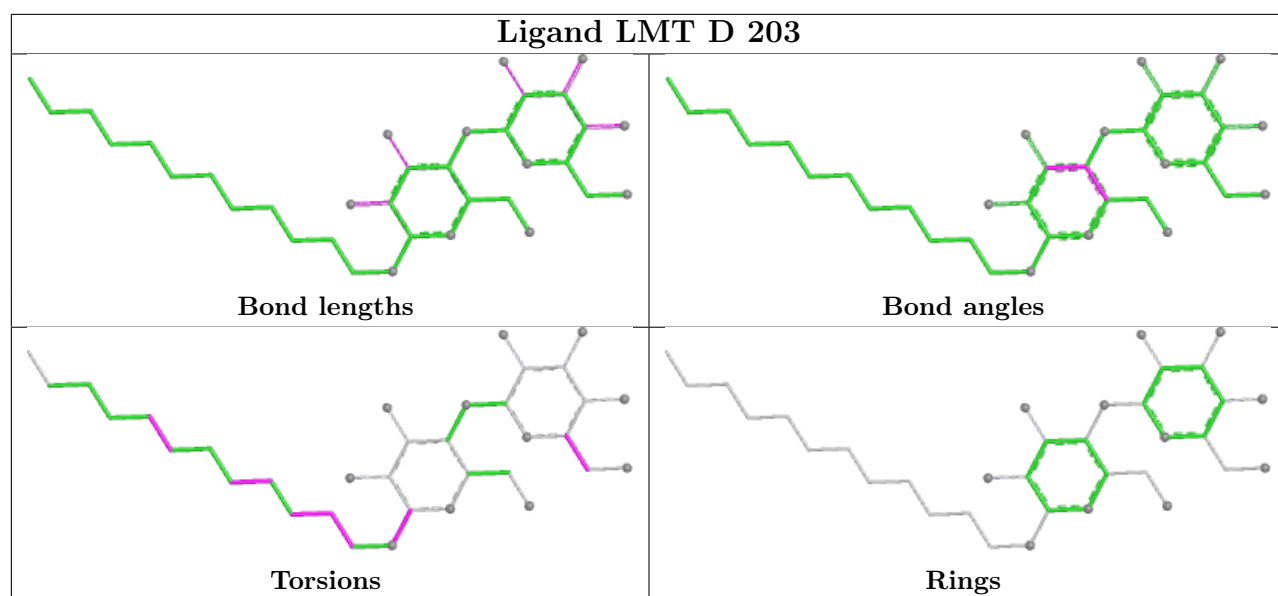


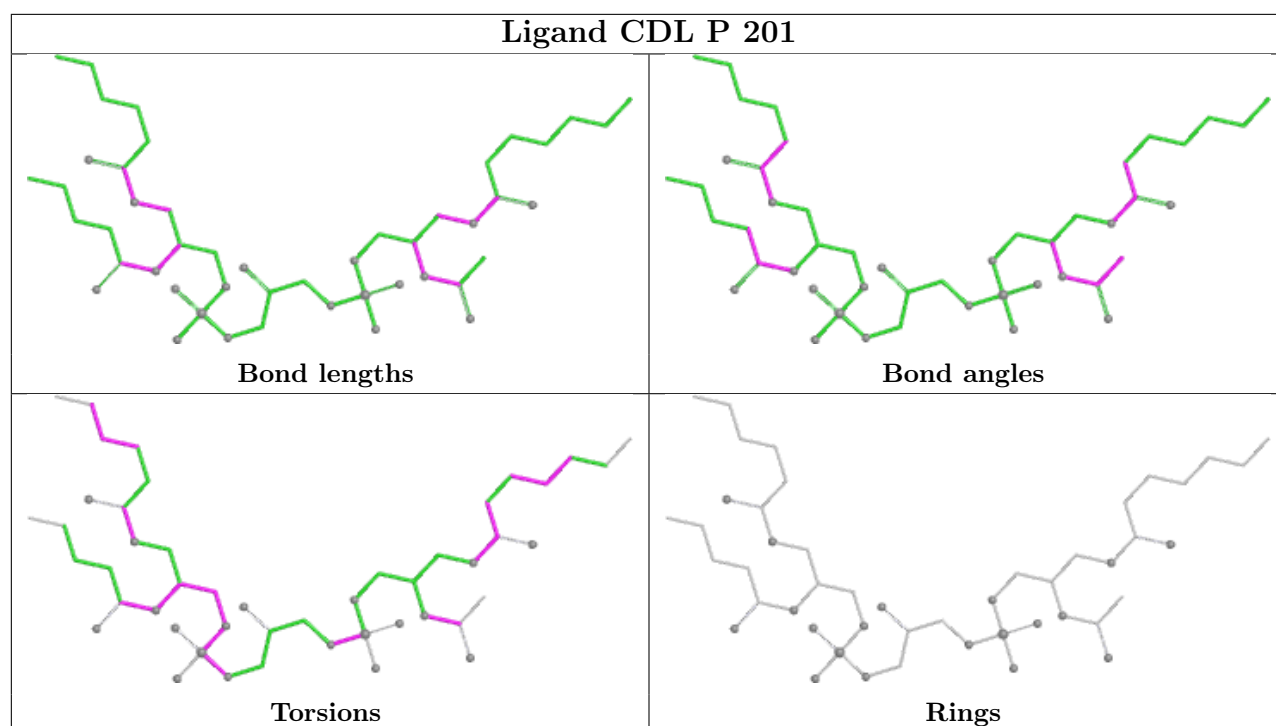












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

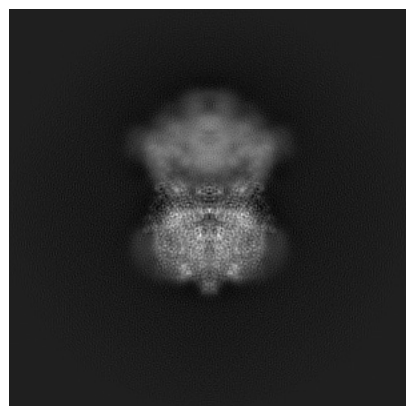
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10468. These allow visual inspection of the internal detail of the map and identification of artifacts.

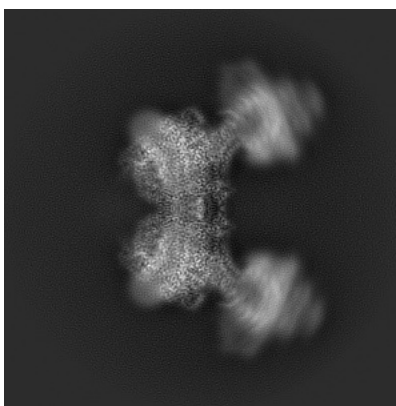
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

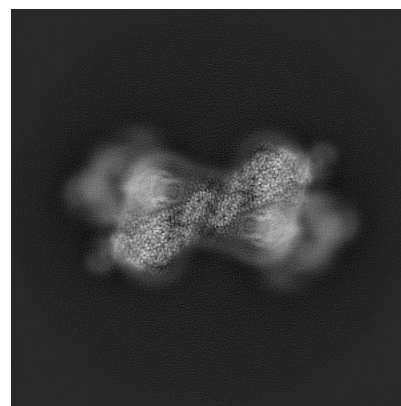
6.1.1 Primary map



X

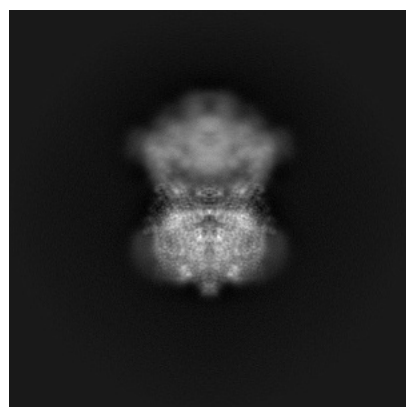


Y

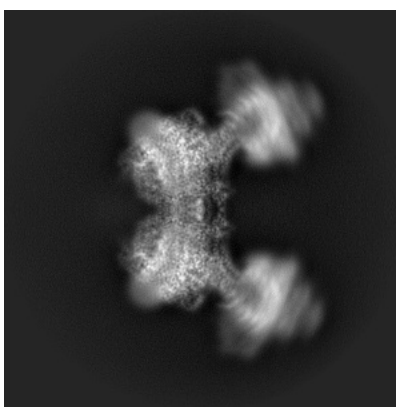


Z

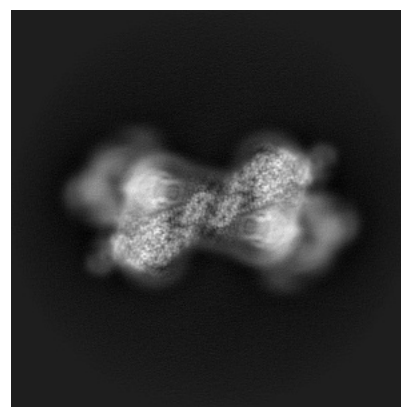
6.1.2 Raw map



X



Y

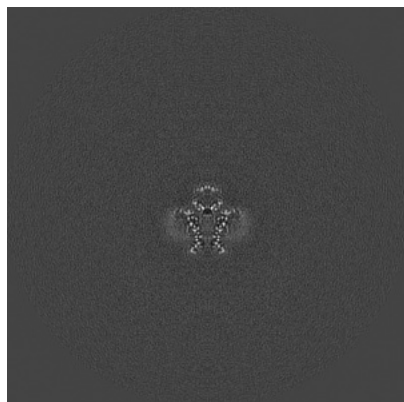


Z

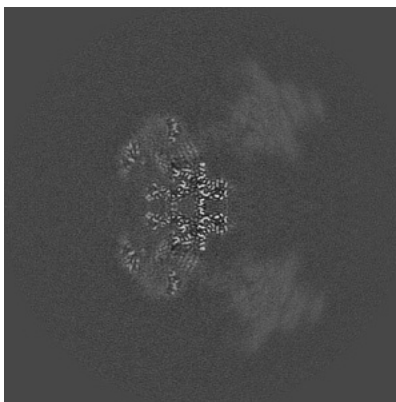
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

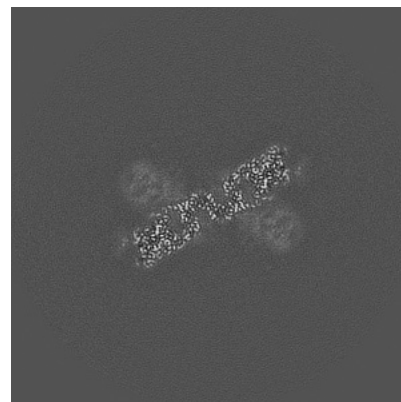
6.2.1 Primary map



X Index: 220

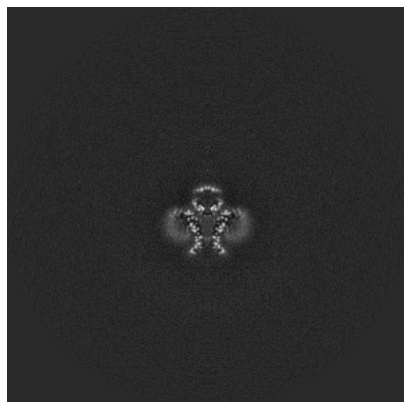


Y Index: 220

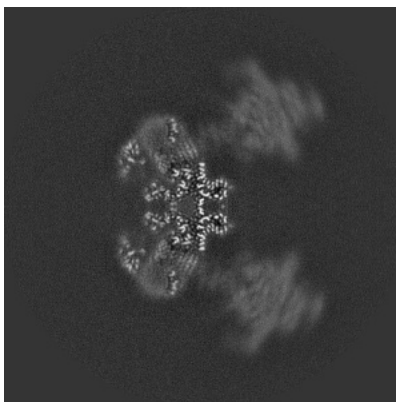


Z Index: 220

6.2.2 Raw map



X Index: 220



Y Index: 220

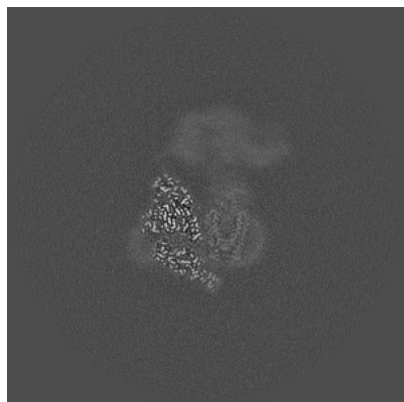


Z Index: 220

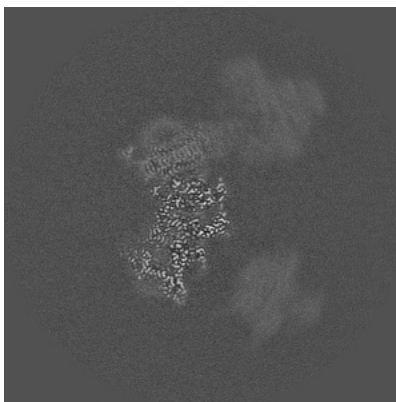
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

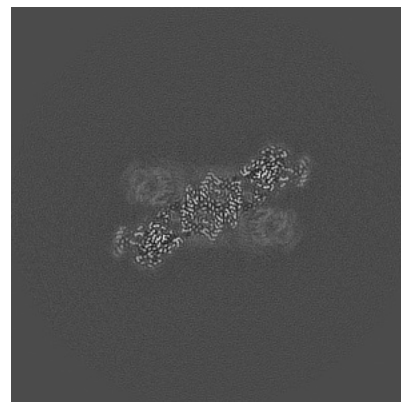
6.3.1 Primary map



X Index: 158

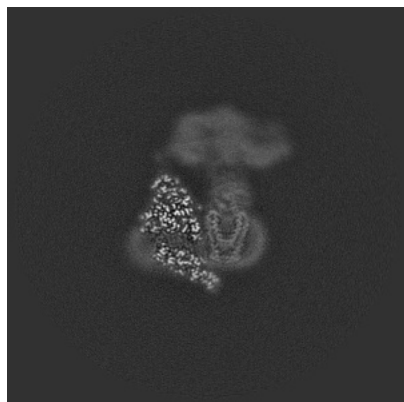


Y Index: 210

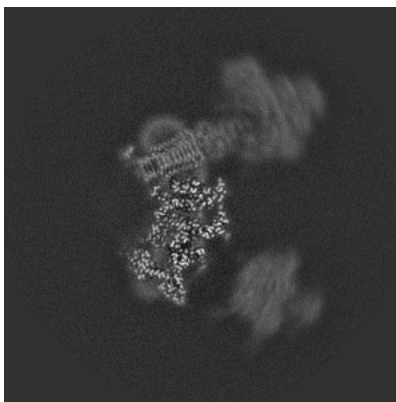


Z Index: 214

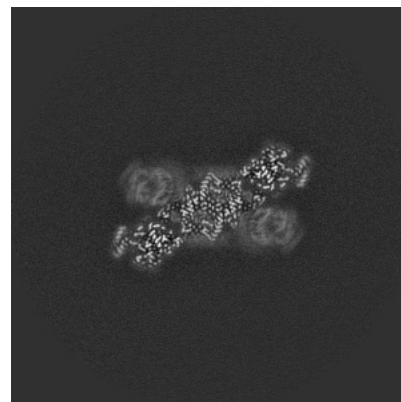
6.3.2 Raw map



X Index: 157



Y Index: 209

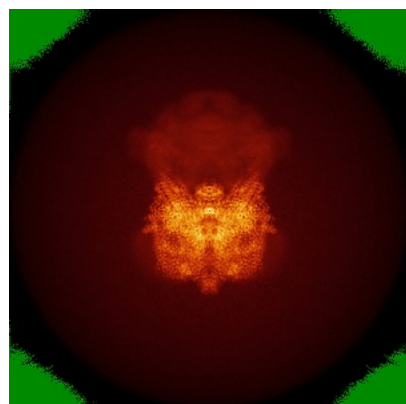


Z Index: 214

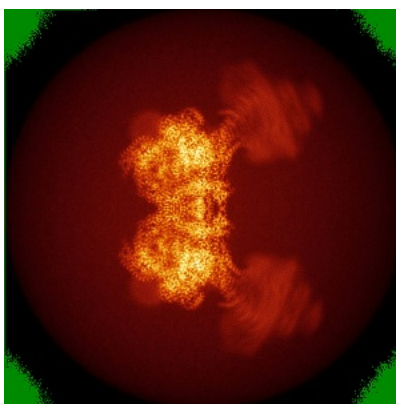
The images above show the largest variance slices of the map in three orthogonal directions.

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

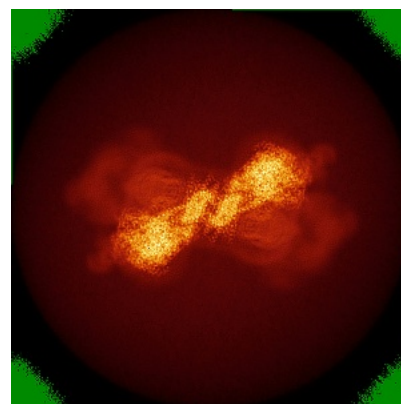
6.4.1 Primary map



X



Y



Z

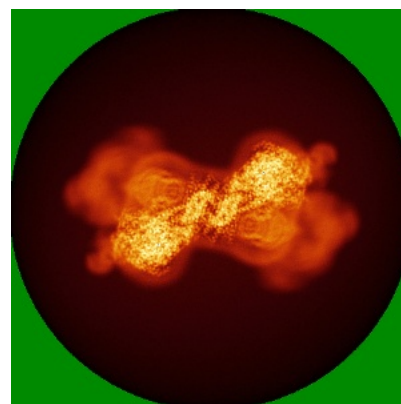
6.4.2 Raw map



X



Y

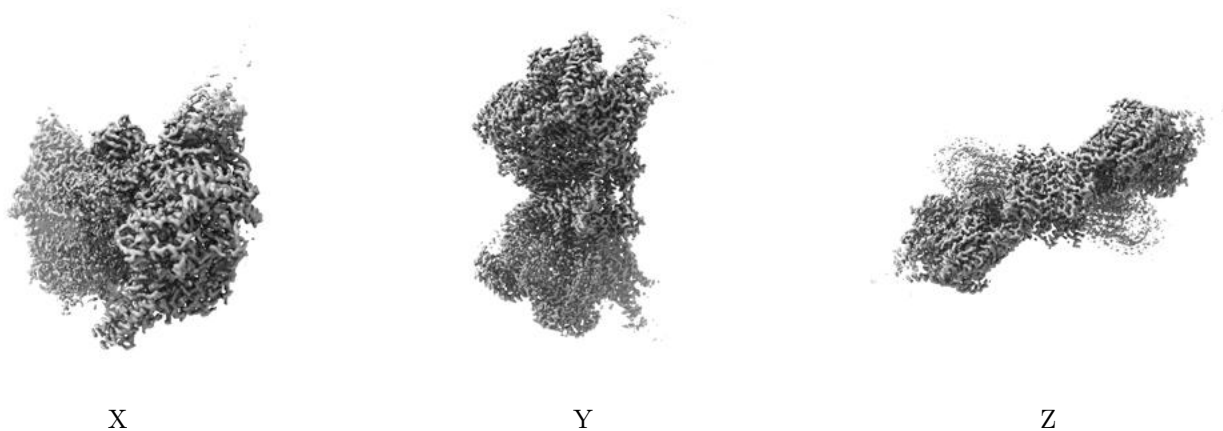


Z

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

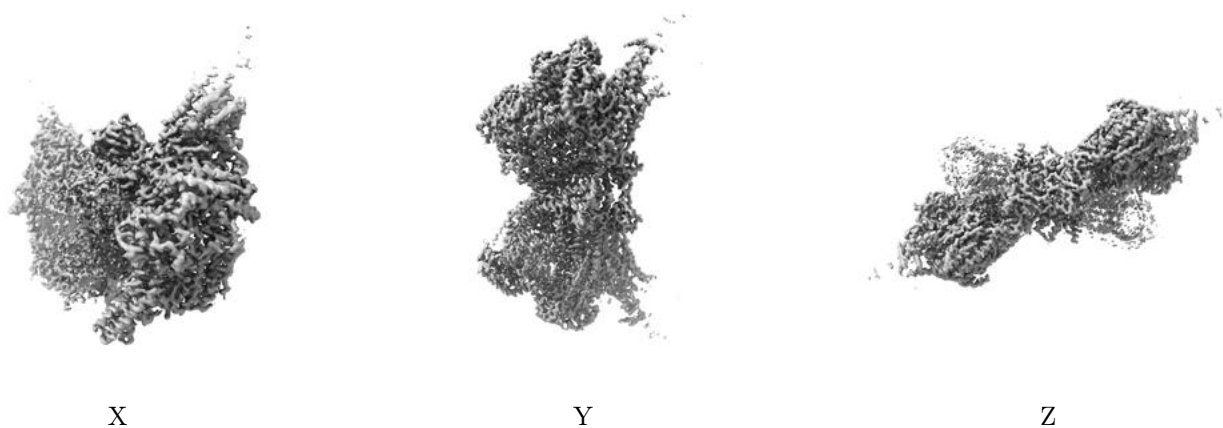
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

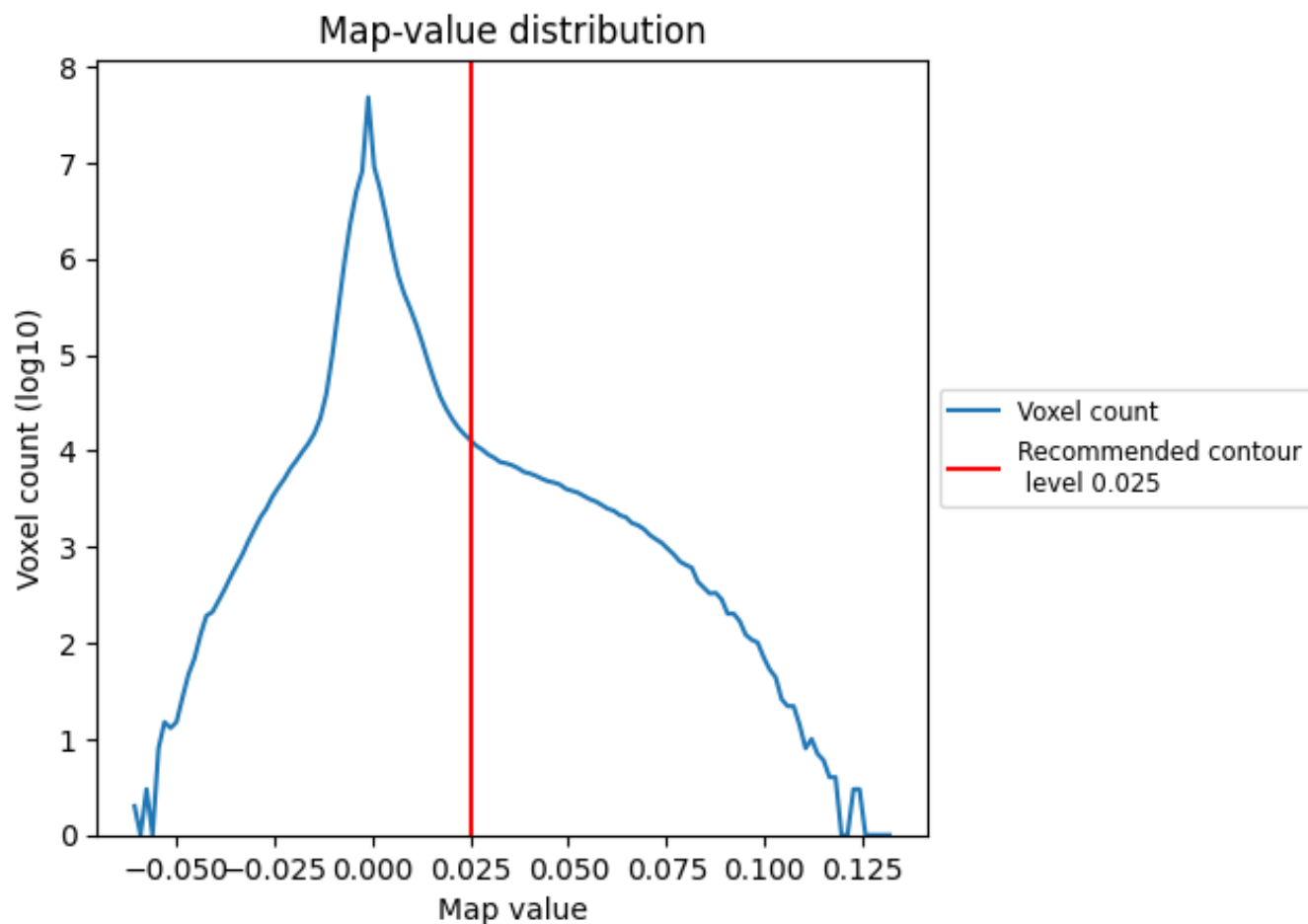
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

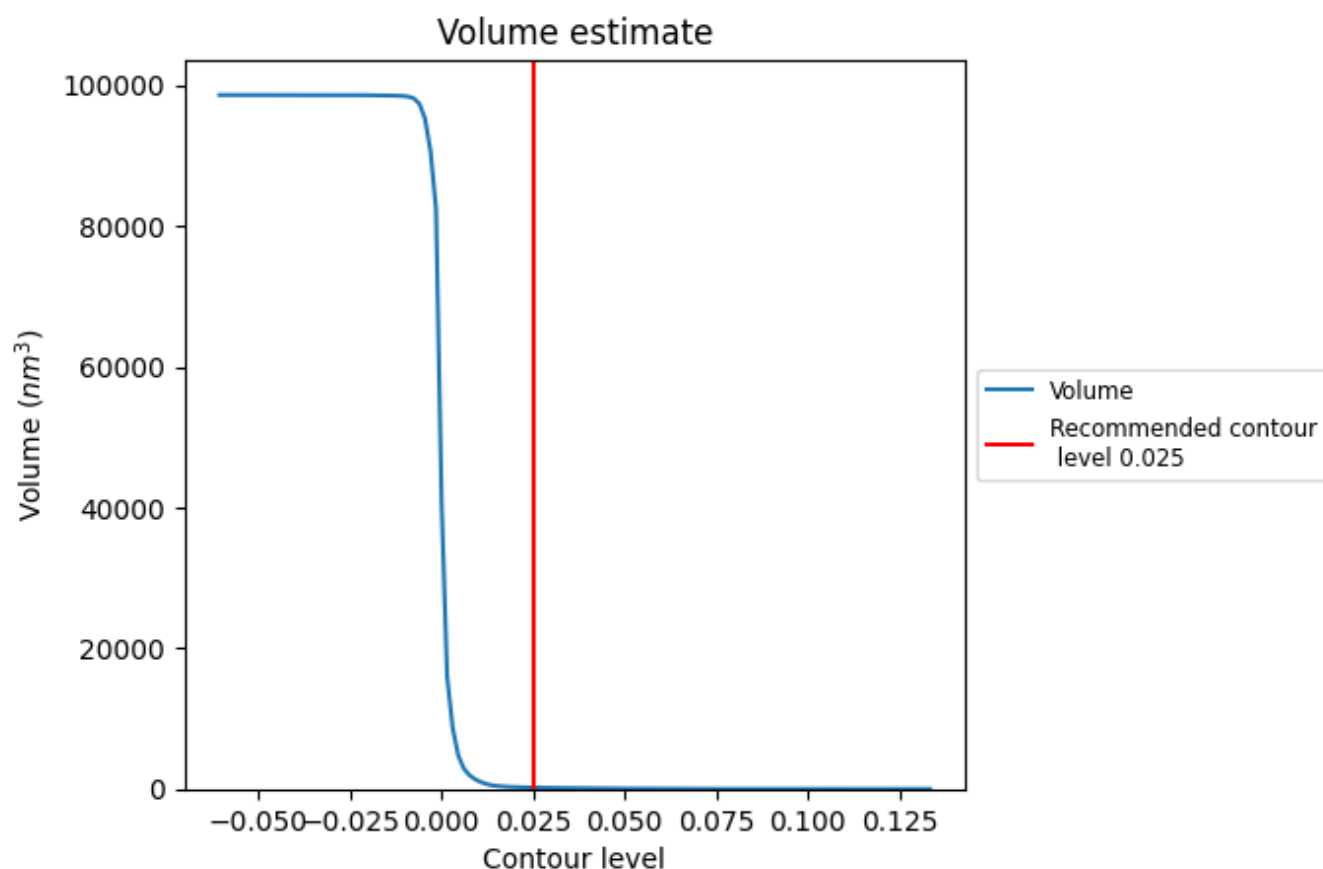
This section contains the results of statistical analysis of the map.

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.

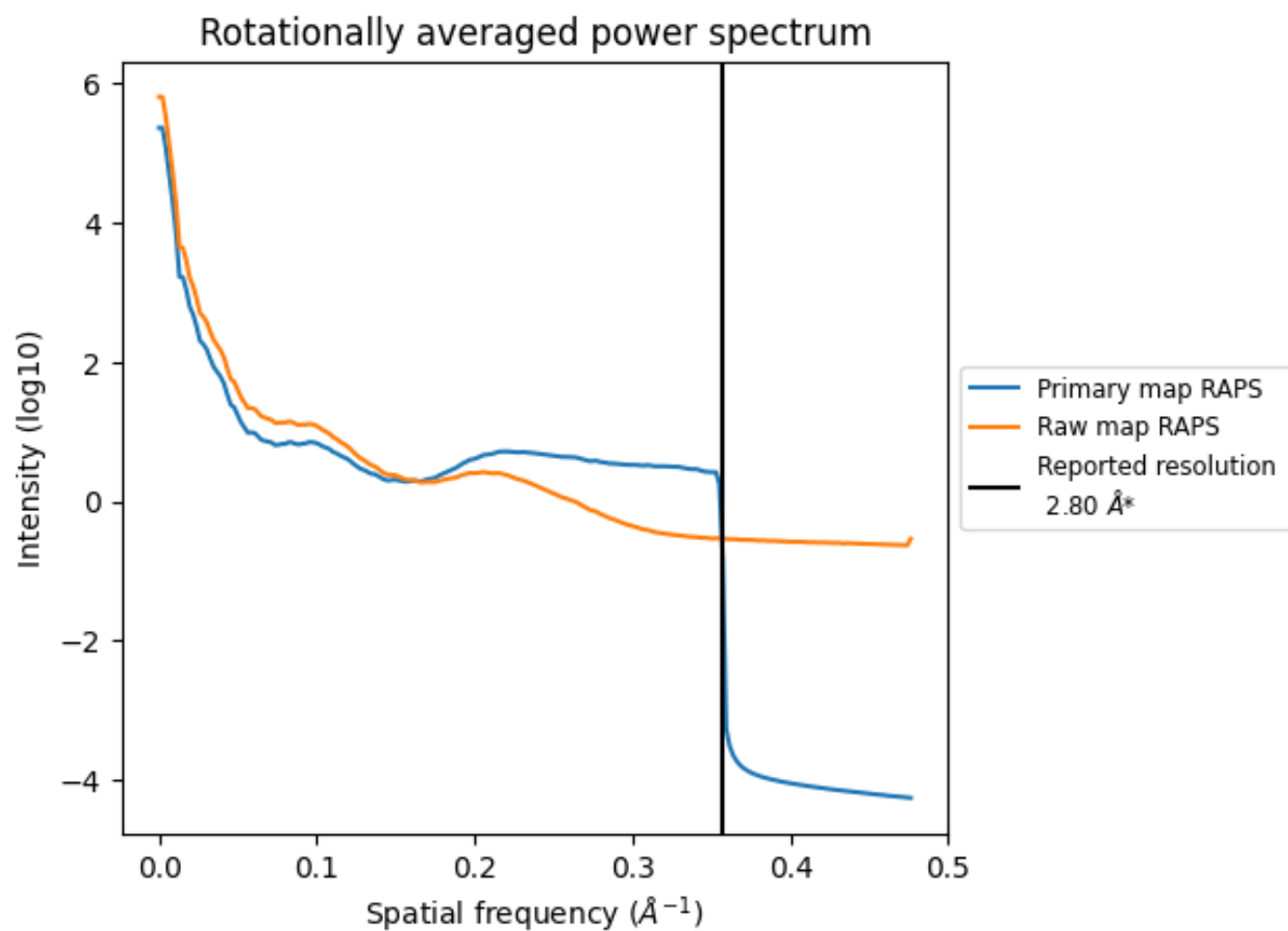
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 192 nm³; this corresponds to an approximate mass of 173 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

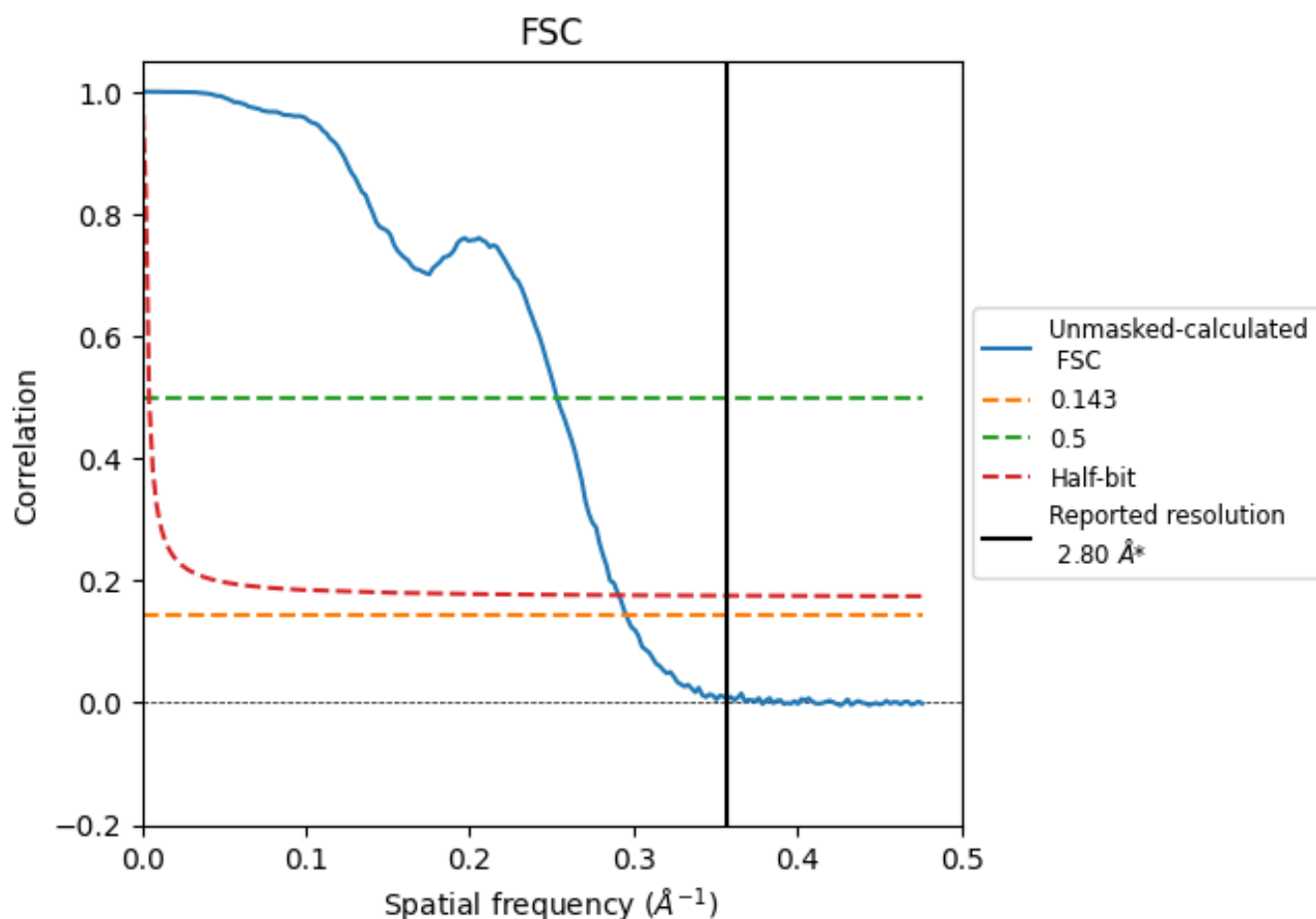


*Reported resolution corresponds to spatial frequency of 0.357 $\text{\AA}^{-1}$

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 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

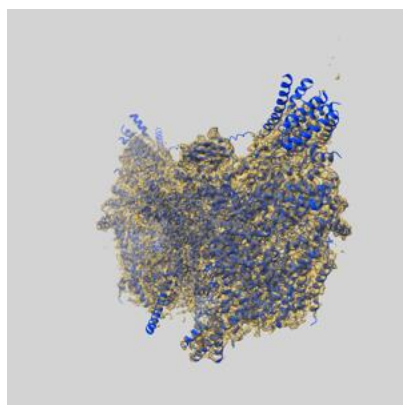
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.38	3.95	3.44

*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 3.38 differs from the reported value 2.8 by more than 10 %

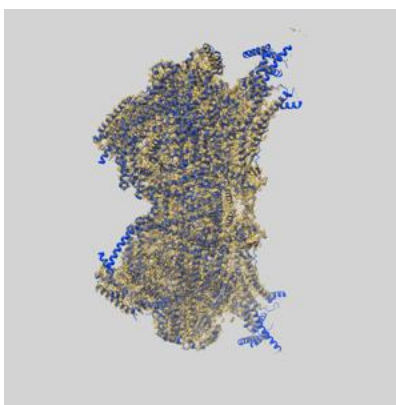
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10468 and PDB model 6TDV. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

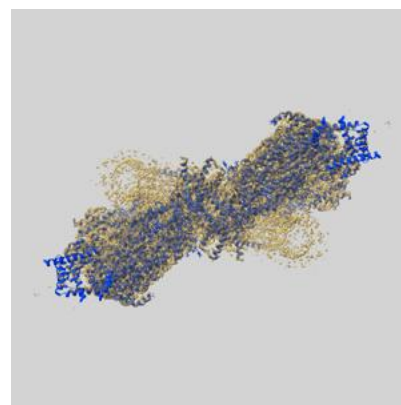
9.1 Map-model overlay [i](#)



X



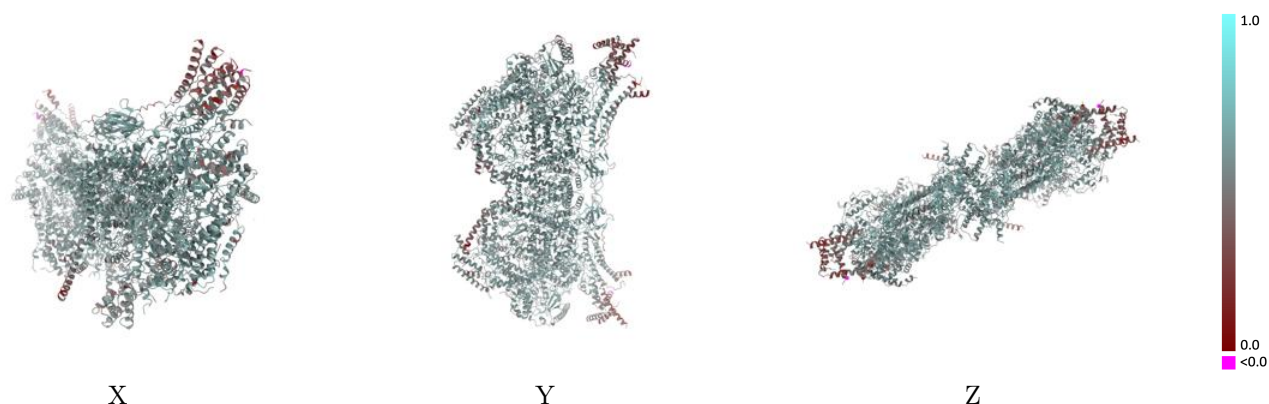
Y



Z

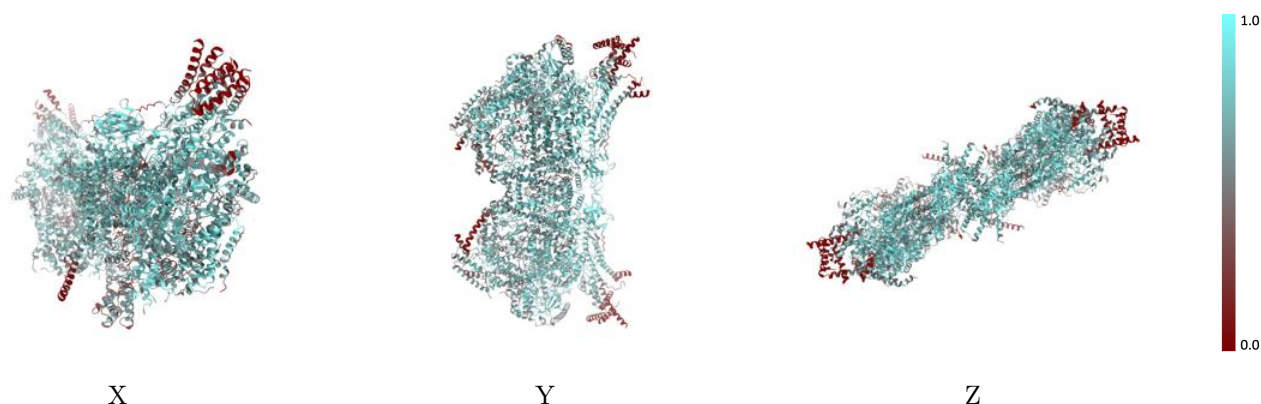
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



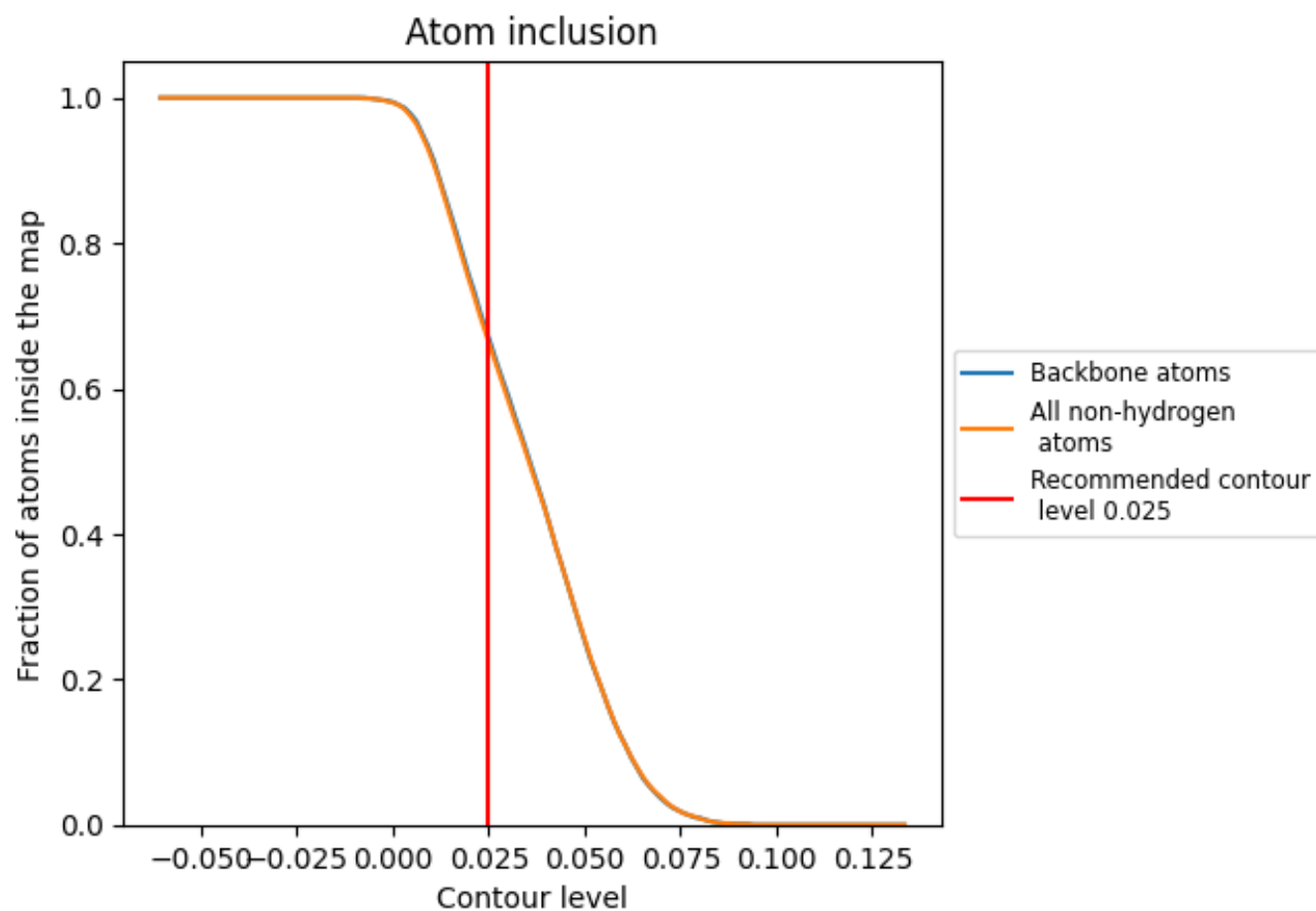
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 66% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6640	 0.5580
A	 0.6970	 0.5680
B	 0.1210	 0.3190
D	 0.7070	 0.5750
E	 0.6790	 0.5630
F	 0.7500	 0.5880
G	 0.6710	 0.5580
H	 0.5710	 0.5090
I	 0.7140	 0.5740
J	 0.7450	 0.5960
K	 0.7150	 0.5700
L	 0.7070	 0.5760
M	 0.6170	 0.5500
N	 0.6530	 0.5720
O	 0.6210	 0.5540
P	 0.7080	 0.5750
Q	 0.5480	 0.4960
R	 0.6090	 0.5520
S	 0.7360	 0.5960
T	 0.7060	 0.5710
a	 0.6970	 0.5700
b	 0.1210	 0.3130
d	 0.7080	 0.5750
e	 0.6780	 0.5630
f	 0.7500	 0.5880
g	 0.6710	 0.5580
h	 0.5730	 0.5080
i	 0.7140	 0.5770
j	 0.7450	 0.5930
k	 0.7140	 0.5740
l	 0.7070	 0.5750
m	 0.6220	 0.5480
n	 0.6570	 0.5760
o	 0.6210	 0.5540
p	 0.6640	 0.5740



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Chain	Atom inclusion	Q-score
q	 0.5480	 0.4990
r	 0.6090	 0.5530
s	 0.7340	 0.5990
t	 0.7120	 0.5730