



wwPDB EM Validation Summary Report ⓘ

Apr 1, 2025 – 10:52 pm BST

PDB ID : 6YNX / pdb_00006ynx
EMDB ID : EMD-10859
Title : Cryo-EM structure of Tetrahymena thermophila mitochondrial ATP synthase
- Fo-subcomplex
Authors : Kock Flygaard, R.; Muhleip, A.; Amunts, A.
Deposited on : 2020-04-14
Resolution : 2.50 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:

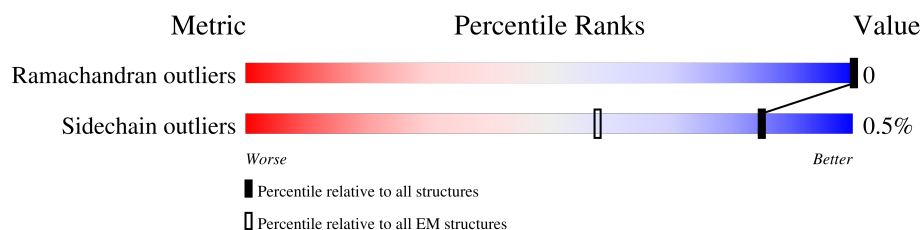
EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

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 2.50 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.













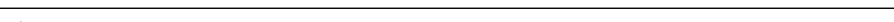

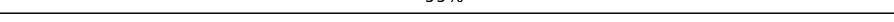
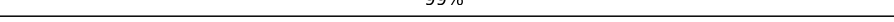
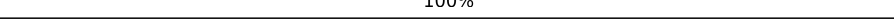
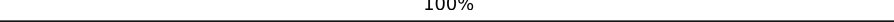




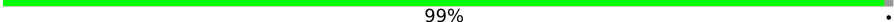
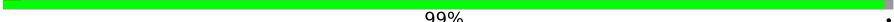



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	446	97% .
1	a	446	96% ..
2	B	381	42% . 58%
2	b	381	42% 58%
3	D	234	47% 53%
3	d	234	47% 53%
4	F	204	98% .
4	f	204	98% .
5	I	209	99% .








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Mol	Chain	Length	Quality of chain
5	i	209	 100%
6	K	179	 99%
6	k	179	 99%
7	C	100	 95%
7	c	100	 94%
8	G	286	 89%
8	g	286	 89%
9	H	268	 86%
9	h	268	 86%
10	J	273	 99%
10	j	273	 99%
11	L	247	 99%
11	l	247	 99%
12	M	221	 100%
12	m	221	 100%
13	N	179	 66%
13	n	179	 66%
14	O	154	 64%
14	o	154	 64%
15	P	152	 99%
15	p	152	 99%
16	Q	152	 71%
16	q	152	 71%
17	R	149	 93%
17	r	149	 97%

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Mol	Chain	Length	Quality of chain
18	S	145	
18	s	145	
19	E	480	
19	e	480	
20	i1	108	
20	i2	108	
21	t	460	

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 139915 atoms, of which 70075 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called subunit a.

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

- Molecule 2 is a protein called subunit b.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	b	161	Total	C	H	N	O	S	0	0
			2678	903	1310	223	232	10		
2	B	161	Total	C	H	N	O	S	0	0
			2675	903	1307	223	232	10		

- Molecule 3 is a protein called subunit d.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	d	110	Total	C	H	N	O	S	0	0
			1764	591	846	147	176	4		
3	D	110	Total	C	H	N	O	S	0	0
			1764	591	846	147	176	4		

- Molecule 4 is a protein called subunit f.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	i	209	Total	C	H	N	O	S	0	0
			3461	1121	1741	304	285	10		
5	I	209	Total	C	H	N	O	S	0	0
			3461	1121	1741	304	285	10		

- Molecule 6 is a protein called subunit k.

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

- Molecule 7 is a protein called subunit 8.

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

- Molecule 8 is a protein called ATPTT3.

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

- Molecule 9 is a protein called ATPTT4.

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

- Molecule 10 is a protein called ATPTT5.

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

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Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	269	Total	C	H	N	O	S	0	0
			4344	1381	2145	406	404	8		

- Molecule 11 is a protein called ATPTT6.

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

- Molecule 12 is a protein called ATPTT7.

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

- Molecule 13 is a protein called ATPTT8.

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

- Molecule 14 is a protein called ATPTT9.

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

- Molecule 15 is a protein called ATPTT10.

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

- Molecule 16 is a protein called ATPTT11.

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

- Molecule 17 is a protein called ATPTT12.

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

- Molecule 18 is a protein called ATPTT13.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	s	105	Total	C	H	N	O	S	0	0
			1714	552	849	148	160	5		
18	S	106	Total	C	H	N	O	S	0	0
			1728	556	856	149	162	5		

- Molecule 19 is a protein called ATPTT1.

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

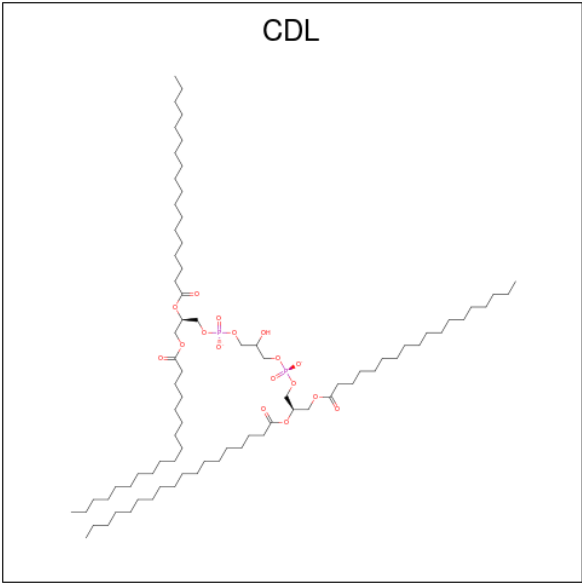
- Molecule 20 is a protein called Inhibitor of F1 (IF1).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	i1	28	Total	C	H	N	O	0	0
			474	154	236	39	45		
20	i2	32	Total	C	H	N	O	0	0
			529	171	262	45	51		

- Molecule 21 is a protein called ATPTT2.

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

- Molecule 22 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



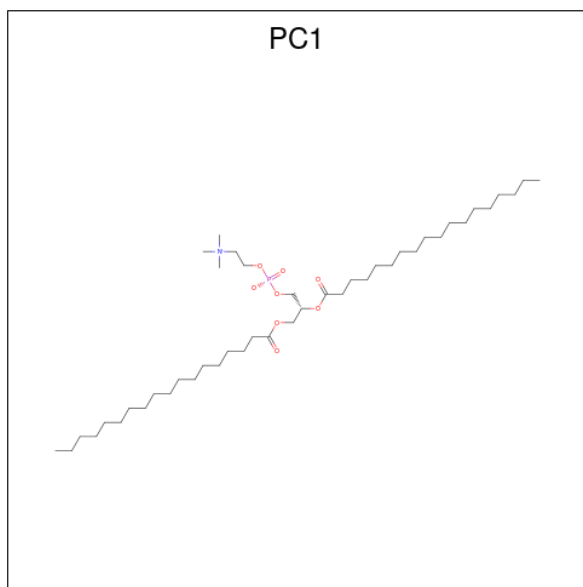
Mol	Chain	Residues	Atoms					AltConf
22	a	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	b	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	b	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	f	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	f	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	f	1	Total	C	H	O	P	0
			256	81	156	17	2	
22	i	1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

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

- Molecule 23 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



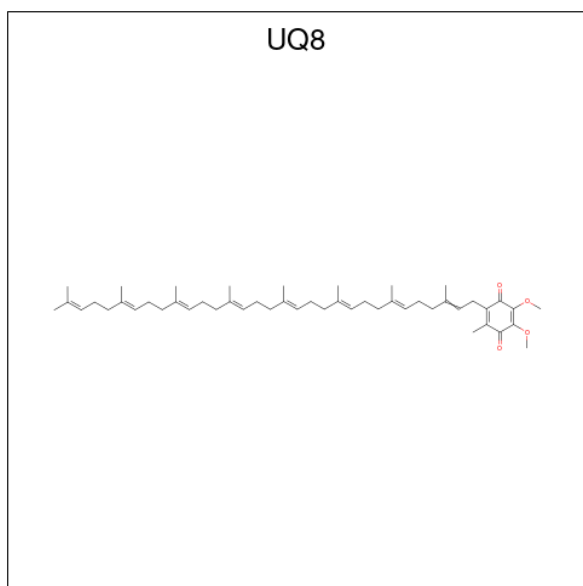
Mol	Chain	Residues	Atoms						AltConf
23	d	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
23	i	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
23	g	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
23	D	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
23	G	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
23	G	1	Total	C	H	N	O	P	0
			142	44	88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

- Molecule 24 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



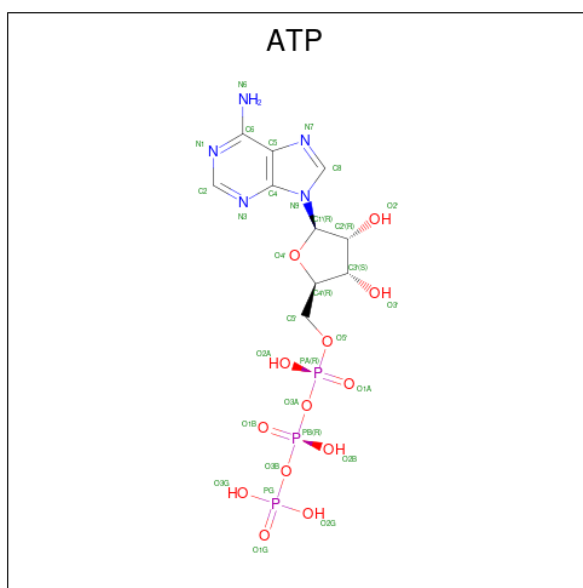
Mol	Chain	Residues	Atoms			AltConf
24	f	1	Total	O	P	0
			5	4	1	
24	F	1	Total	O	P	0
			5	4	1	

- Molecule 25 is Ubiquinone-8 (CCD ID: UQ8) (formula: $C_{49}H_{74}O_4$).



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

- Molecule 26 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

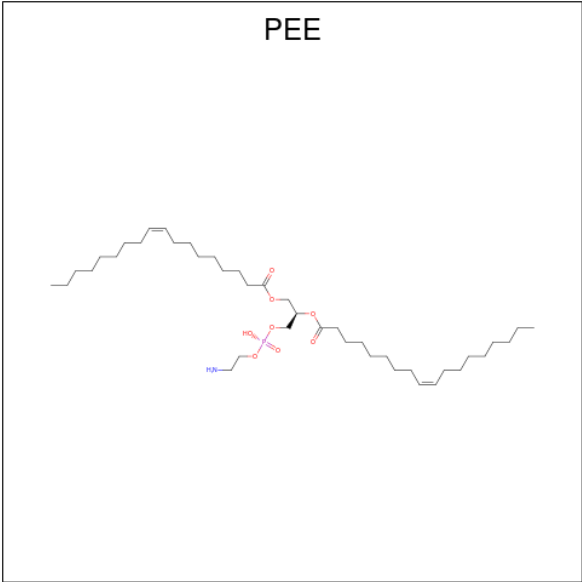


Mol	Chain	Residues	Atoms						AltConf
26	g	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	
26	G	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	

- Molecule 27 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

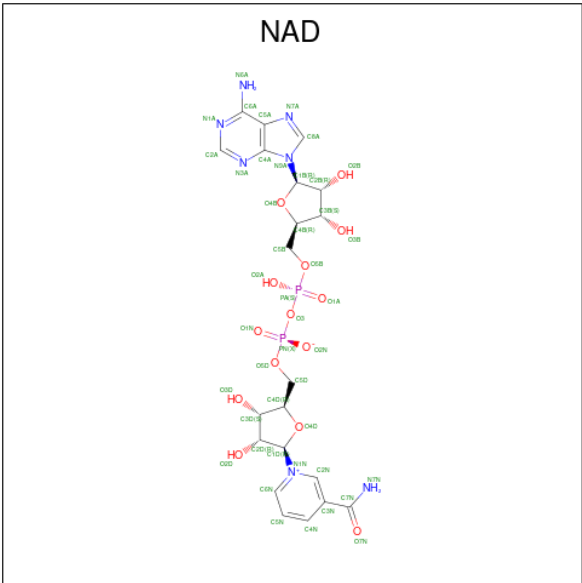
Mol	Chain	Residues	Atoms		AltConf
27	g	1	Total	Mg	0
			1	1	
27	G	1	Total	Mg	0
			1	1	

- Molecule 28 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



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

- Molecule 29 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

LEU LYS GLY THR LEU ASP LYS LYS ALA GLU VAL VAL ALA ARG SER LEU SER SER ALA ALA ILE ASP GLY LEU PHE LEU LYS LYS GLY TYR MET TYR ASP GLN ASN ASP PRO LYS LEU ASN ILE PRO LEU ILE SER ILE LEU SER LYS ILE ILE LEU ALA ASN VAL LYS LYS ILE THR THR LEU SER ALA GLN GLU GLN ALA THR LYS

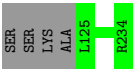
GLY LEU THR ALA LEU GLN LYS LEU SER ILE LYS VAL ASP ASN ARG ALA ARG LYS GLY PHE LEU LYS SER GLN TYR ASP LEU ASN ASP LEU LYS ASN ILE PRO GLU SER ILE VAL LYS SER LYS ILE ILE LEU ALA THR TRP GLY LYS

• Molecule 3: subunit d



MET SER MET LEU ALA LYS ILE ALA ASN VAL VAL THR THR GLN ALA LEU LYS ASN ILE LYS THR THR PRO SER PHE GLN ALA PRO GLY ASN GLN LYS ILE ILE LYS LYS TRP ILE SER SER THR SER LYS THR SER ASN THR THR GLU ARG GLN TYR CYS THR SER LEU ILE

SER SER LEU VAL SER PHE TYR ASN LYS GLN HIS VAL VAL GLU GLN ILE PRO THR ILE ILE ASP PHE ASN THR TRP ALA LYS SER VAL ILE SER PHE THR GLN GLY LEU VAL ASN GLN LYS VAL LYS GLU ASN TYR THR THR ASP ILE SER GLU GLN TYR THR THR ALA ILE SER ARG LYS GLN ILE SER SER ALA



• Molecule 3: subunit d

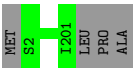


MET SER MET LEU ALA LYS ILE ALA ASN VAL VAL THR THR GLN ALA LEU LYS ASN ILE LYS THR THR PRO SER PHE GLN ALA PRO GLY ASN GLN LYS ILE ILE LYS LYS TRP ILE SER SER THR SER LYS THR SER ASN THR THR GLU ARG GLN TYR CYS THR SER LEU ILE

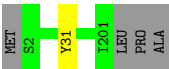
SER SER LEU VAL SER PHE TYR ASN LYS GLN HIS VAL VAL GLU GLN ILE PRO THR ILE ILE ASP PHE ASN THR TRP ALA LYS SER VAL ILE SER PHE THR GLN GLY LEU VAL ASN GLN LYS VAL LYS GLU ASN TYR THR THR ASP ILE SER GLU GLN TYR THR THR ALA ILE SER ARG LYS GLN ILE SER SER ALA



• Molecule 4: subunit f



• Molecule 4: subunit f



• Molecule 5: subunit i/j



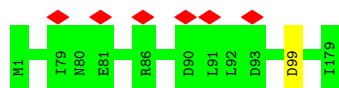
• Molecule 5: subunit i/j

Chain I:  99%



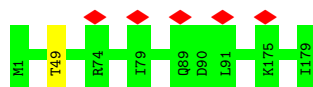
- Molecule 6: subunit k

Chain k:  99%



- Molecule 6: subunit k

Chain K:  99%



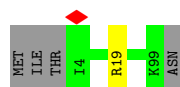
- Molecule 7: subunit 8

Chain c:  94%




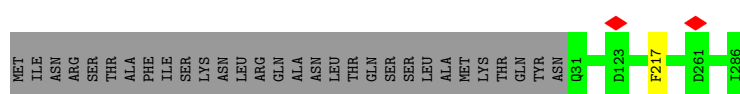
- Molecule 7: subunit 8

Chain C:  95%



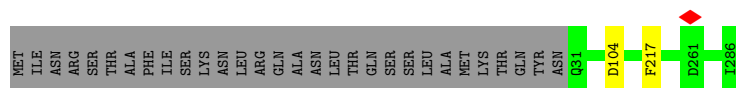
- Molecule 8: ATPTT3

Chain g:  89%




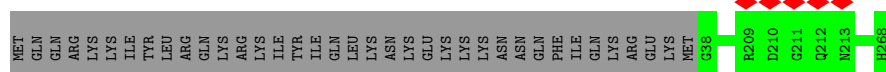
- Molecule 8: ATPTT3

Chain G:  89%




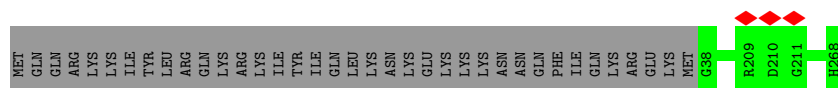
- Molecule 9: ATPTT4

Chain h:  86% 14%



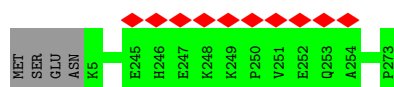
• Molecule 9: ATPTT4

Chain H:  86% 14%



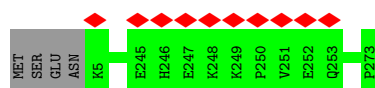
• Molecule 10: ATPTT5

Chain j:  99%



• Molecule 10: ATPTT5

Chain J:  99%



• Molecule 11: ATPTT6

Chain l:  99%



• Molecule 11: ATPTT6

Chain L:  99%



• Molecule 12: ATPTT7

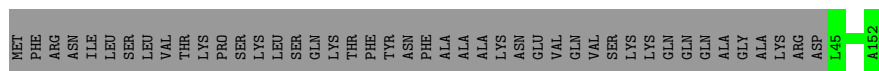
Chain m:  100%

There are no outlier residues recorded for this chain.

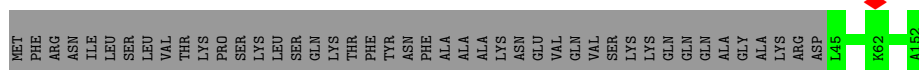
• Molecule 12: ATPTT7

Chain M:  100%

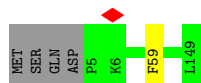
• Molecule 16: ATPTT11

Chain q:  71% 29%

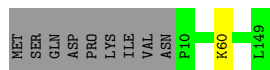
• Molecule 16: ATPTT11

Chain Q:  71% 29%

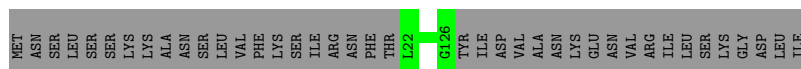
• Molecule 17: ATPTT12

Chain r:  97% ..

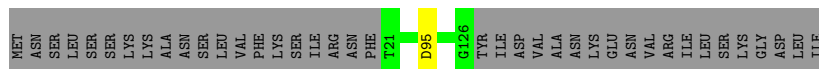
• Molecule 17: ATPTT12

Chain R:  93% • 6%


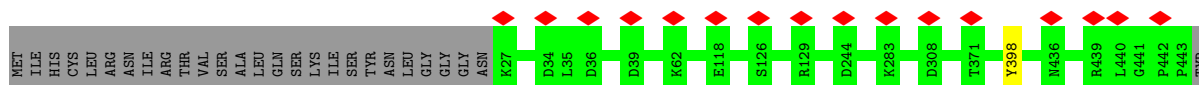
• Molecule 18: ATPTT13

Chain s:  72% 28%

• Molecule 18: ATPTT13


Chain S:  72% • 27%

• Molecule 19: ATPTT1

Chain e:  87% 13%

HIS
LYS
VAL
HIS
LEU
LYS
SER
PHE
PRO
GLU
LEU
PRO
GLY
SER
PRO
GLU
SER
GLN
GLN
SER
SER
GLY
SER
SER
GLY
TYR
PHE
PRO
THR
LYS
THR
GLU
ASN
LYS
ALA
ALA
HIS

• Molecule 19: ATPTT1

Chain E:  86% 13%

MET
ILE
HIS
CYS
LEU
SER
ARG
ASN
ILE
SER
THR
VAL
SER
GLY
ALA
LEU
GLN
SER
SER
LYS
ILE
SER
TYR
ASN
K27
D34
L35
D36
D56
K57
D58
K62
Y63
K64
I115
E118
G127
K309
Q368
T371
Y398
D433
K436
R439
L440

F443
TYR
HIS
VAL
LEU
LYS
SER
PHE
THR
PRO
GLY
LEU
PRO
GLY
GLN
PRO
GLY
ILE
SER
GLN
TYR
PHE
PRO
THR
LYS
THR
THR
ASN
LYS
ALA
ALA
HIS

• Molecule 20: Inhibitor of F1 (IF1)

Chain i1:  8% 25% 74%

MET
ASN
ARG
THR
SER
VAL
ASN
ILE
ALA
LYS
ASN
ASN
LEU
ILE
THR
TYR
ALA
GLN
MET
SER
VAL
GLN
SER
ARG
PHE
ALA
PHE
SER
THR
ARG
GLY
GLY
TRP
ASP
LYS
ARG
THR
LYS
SER
GLN
GLY
VAL
TTR
PHE
ASP
GLN
ASP
ARG
MET
MET
ARG
LEU
LEU
LYS

LEU
ASN
THR
THR
SER
LYS
PHE
VAL
GLY
ASP
SER
GLY
TYR
LEU
ALA
GLN
ASN
L79
E80
I90
N91
Q94
D98
D102
T105
G106
LYS
ASN


• Molecule 20: Inhibitor of F1 (IF1)

Chain i2:  7% 30% 70%

MET
ASN
ARG
THR
SER
VAL
ASN
ILE
ALA
LYS
ASN
ASN
LEU
ILE
THR
TYR
ALA
GLN
MET
SER
VAL
GLN
SER
ARG
PHE
ALA
PHE
SER
THR
ARG
GLY
GLY
TRP
ASP
LYS
ARG
THR
LYS
SER
GLN
GLY
VAL
TTR
PHE
ASP
GLN
ASP
ARG
LYS
ALA
MET
LYS
ARG
LEU
LEU
GLY
GLN

LEU
ASN
THR
THR
SER
LYS
PHE
VAL
GLY
ASP
SER
GLY
TYR
LEU
L75
L79
L85
K86
H89
I90
N91
D102
G106
LYS
ASN

• Molecule 21: ATPTT2

Chain t:  78% 21%

MET
LYS
MET
GLY
TTR
LEU
GLN
SER
GLY
GLY
LYS
LYS
ASP
ALA
ILE
ASN
THR
ARG
LYS
ILE
HIS
LYS
GLY
GLY
GLY
GLY
GLY
GLY
GLY
ILE
ILE
ILE
ASN
GLN
LYS
LYS
LYS
TTR
ILE
GLY
ALA
GLN
GLN
LYS
LYS
GLN

ILE
GLN
SER
LYS
ASN
GLN
ARG
LYS
TTR
ILE
ASN
THR
ARG
LYS
GLN
VAL
PHE
LYS
CYS
LEU
TRP
GLY
ALA
GLN
PRO
ALA
TYR
ASN
PHE
S94
H99
L100
R101
R173
N287
A288
K289
T290
R407
M458
GLY
GLN

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	61157	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	165000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.159	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	498.0, 498.0, 498.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, PO4, ATP, PEE, PC1, UQ8, CDL, MG

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	0.40	0/3752	0.41	0/5109
1	a	0.40	0/3752	0.41	0/5109
2	B	0.41	0/1417	0.42	0/1915
2	b	0.41	0/1417	0.40	0/1915
3	D	0.40	0/944	0.40	0/1278
3	d	0.39	0/944	0.41	0/1278
4	F	0.40	0/1733	0.44	0/2327
4	f	0.40	0/1733	0.43	0/2327
5	I	0.39	0/1771	0.43	0/2394
5	i	0.39	0/1771	0.44	0/2394
6	K	0.33	0/1508	0.42	0/2024
6	k	0.33	0/1508	0.41	0/2024
7	C	0.39	0/866	0.43	0/1176
7	c	0.40	0/866	0.43	0/1176
8	G	0.39	0/2302	0.44	0/3115
8	g	0.39	0/2302	0.43	0/3115
9	H	0.38	0/2006	0.43	0/2704
9	h	0.37	0/2006	0.42	0/2704
10	J	0.38	0/2256	0.43	0/3069
10	j	0.38	0/2256	0.44	0/3069
11	L	0.40	0/2140	0.42	0/2903
11	l	0.39	0/2140	0.42	0/2903
12	M	0.40	0/1912	0.40	0/2598
12	m	0.40	0/1912	0.40	0/2598
13	N	0.42	0/1030	0.44	0/1393
13	n	0.42	0/1030	0.45	0/1393
14	O	0.34	0/821	0.42	0/1104
14	o	0.33	0/821	0.43	0/1104
15	P	0.31	0/1249	0.39	0/1695
15	p	0.31	0/1249	0.40	0/1695
16	Q	0.35	0/888	0.41	0/1200
16	q	0.35	0/888	0.42	0/1200

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	R	0.40	0/1185	0.41	0/1594
17	r	0.40	0/1225	0.41	0/1649
18	S	0.37	0/892	0.45	0/1209
18	s	0.38	0/885	0.45	0/1199
19	E	0.29	0/3492	0.42	0/4720
19	e	0.30	0/3492	0.42	0/4720
20	i1	0.45	0/242	0.50	0/328
20	i2	0.25	0/272	0.36	0/370
21	t	0.37	0/3103	0.44	1/4200 (0.0%)
All	All	0.38	0/67978	0.42	1/91997 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	t	101	ARG	NE-CZ-NH2	5.96	123.28	120.30

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	431/446 (97%)	425 (99%)	6 (1%)	0	100	100
1	a	431/446 (97%)	425 (99%)	6 (1%)	0	100	100
2	B	159/381 (42%)	153 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	159/381 (42%)	154 (97%)	5 (3%)	0	100	100
3	D	108/234 (46%)	106 (98%)	2 (2%)	0	100	100
3	d	108/234 (46%)	107 (99%)	1 (1%)	0	100	100
4	F	198/204 (97%)	197 (100%)	1 (0%)	0	100	100
4	f	198/204 (97%)	196 (99%)	2 (1%)	0	100	100
5	I	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
5	i	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
6	K	177/179 (99%)	169 (96%)	8 (4%)	0	100	100
6	k	177/179 (99%)	168 (95%)	9 (5%)	0	100	100
7	C	94/100 (94%)	90 (96%)	4 (4%)	0	100	100
7	c	94/100 (94%)	91 (97%)	3 (3%)	0	100	100
8	G	254/286 (89%)	246 (97%)	8 (3%)	0	100	100
8	g	254/286 (89%)	243 (96%)	11 (4%)	0	100	100
9	H	229/268 (85%)	223 (97%)	6 (3%)	0	100	100
9	h	229/268 (85%)	227 (99%)	2 (1%)	0	100	100
10	J	267/273 (98%)	259 (97%)	8 (3%)	0	100	100
10	j	267/273 (98%)	259 (97%)	8 (3%)	0	100	100
11	L	244/247 (99%)	239 (98%)	5 (2%)	0	100	100
11	l	244/247 (99%)	240 (98%)	4 (2%)	0	100	100
12	M	219/221 (99%)	217 (99%)	2 (1%)	0	100	100
12	m	219/221 (99%)	218 (100%)	1 (0%)	0	100	100
13	N	117/179 (65%)	113 (97%)	4 (3%)	0	100	100
13	n	117/179 (65%)	114 (97%)	3 (3%)	0	100	100
14	O	97/154 (63%)	95 (98%)	2 (2%)	0	100	100
14	o	97/154 (63%)	96 (99%)	1 (1%)	0	100	100
15	P	148/152 (97%)	142 (96%)	6 (4%)	0	100	100
15	p	148/152 (97%)	143 (97%)	5 (3%)	0	100	100
16	Q	106/152 (70%)	104 (98%)	2 (2%)	0	100	100
16	q	106/152 (70%)	103 (97%)	3 (3%)	0	100	100
17	R	138/149 (93%)	135 (98%)	3 (2%)	0	100	100
17	r	143/149 (96%)	141 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	S	104/145 (72%)	101 (97%)	3 (3%)	0	100	100
18	s	103/145 (71%)	100 (97%)	3 (3%)	0	100	100
19	E	415/480 (86%)	408 (98%)	7 (2%)	0	100	100
19	e	415/480 (86%)	406 (98%)	9 (2%)	0	100	100
20	i1	26/108 (24%)	26 (100%)	0	0	100	100
20	i2	30/108 (28%)	30 (100%)	0	0	100	100
21	t	363/460 (79%)	356 (98%)	7 (2%)	0	100	100
All	All	7847/9594 (82%)	7667 (98%)	180 (2%)	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	397/409 (97%)	395 (100%)	2 (0%)	86	95
1	a	397/409 (97%)	394 (99%)	3 (1%)	79	91
2	B	143/331 (43%)	141 (99%)	2 (1%)	62	83
2	b	143/331 (43%)	143 (100%)	0	100	100
3	D	95/206 (46%)	95 (100%)	0	100	100
3	d	95/206 (46%)	95 (100%)	0	100	100
4	F	175/178 (98%)	174 (99%)	1 (1%)	84	94
4	f	175/178 (98%)	175 (100%)	0	100	100
5	I	182/182 (100%)	179 (98%)	3 (2%)	58	80
5	i	182/182 (100%)	181 (100%)	1 (0%)	86	95
6	K	152/152 (100%)	151 (99%)	1 (1%)	81	93
6	k	152/152 (100%)	151 (99%)	1 (1%)	81	93
7	C	93/97 (96%)	92 (99%)	1 (1%)	70	87
7	c	93/97 (96%)	91 (98%)	2 (2%)	47	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	G	235/262 (90%)	233 (99%)	2 (1%)	75	90
8	g	235/262 (90%)	234 (100%)	1 (0%)	89	96
9	H	208/245 (85%)	208 (100%)	0	100	100
9	h	208/245 (85%)	208 (100%)	0	100	100
10	J	235/239 (98%)	235 (100%)	0	100	100
10	j	235/239 (98%)	235 (100%)	0	100	100
11	L	219/220 (100%)	218 (100%)	1 (0%)	86	95
11	l	219/220 (100%)	218 (100%)	1 (0%)	86	95
12	M	202/202 (100%)	201 (100%)	1 (0%)	86	95
12	m	202/202 (100%)	202 (100%)	0	100	100
13	N	104/162 (64%)	104 (100%)	0	100	100
13	n	104/162 (64%)	104 (100%)	0	100	100
14	O	89/142 (63%)	89 (100%)	0	100	100
14	o	89/142 (63%)	89 (100%)	0	100	100
15	P	131/133 (98%)	131 (100%)	0	100	100
15	p	131/133 (98%)	131 (100%)	0	100	100
16	Q	97/135 (72%)	97 (100%)	0	100	100
16	q	97/135 (72%)	97 (100%)	0	100	100
17	R	120/129 (93%)	119 (99%)	1 (1%)	79	91
17	r	125/129 (97%)	124 (99%)	1 (1%)	79	91
18	S	95/131 (72%)	94 (99%)	1 (1%)	70	87
18	s	94/131 (72%)	94 (100%)	0	100	100
19	E	359/414 (87%)	357 (99%)	2 (1%)	84	94
19	e	359/414 (87%)	358 (100%)	1 (0%)	91	97
20	i1	26/101 (26%)	25 (96%)	1 (4%)	28	53
20	i2	29/101 (29%)	29 (100%)	0	100	100
21	t	325/414 (78%)	321 (99%)	4 (1%)	67	86
All	All	7046/8554 (82%)	7012 (100%)	34 (0%)	85	95

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	E	398	TYR

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Mol	Chain	Res	Type
20	i1	79	LEU
21	t	173	ARG
1	A	247	TYR
1	A	14	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
21	t	170	ASN
21	t	234	GLN
9	H	136	HIS
10	J	130	GLN
12	M	74	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](#)

Of 50 ligands modelled in this entry, 2 are monoatomic - leaving 48 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
22	CDL	B	402	-	99,99,99	0.88	8 (8%)	105,111,111	1.06	4 (3%)
22	CDL	B	404	-	99,99,99	0.89	8 (8%)	105,111,111	0.95	4 (3%)
22	CDL	i	302	-	99,99,99	0.89	8 (8%)	105,111,111	0.94	4 (3%)
28	PEE	J	303	10	47,47,50	1.18	6 (12%)	50,52,55	1.13	4 (8%)
22	CDL	I	301	5	99,99,99	0.88	6 (6%)	105,111,111	0.95	3 (2%)
22	CDL	K	202	-	99,99,99	0.88	7 (7%)	105,111,111	1.07	5 (4%)
22	CDL	f	303	-	99,99,99	0.89	8 (8%)	105,111,111	1.12	5 (4%)
22	CDL	l	304	-	99,99,99	0.89	7 (7%)	105,111,111	1.04	4 (3%)
28	PEE	J	304	-	50,50,50	1.16	6 (12%)	53,55,55	1.12	3 (5%)
22	CDL	a	501	-	99,99,99	0.89	7 (7%)	105,111,111	1.02	3 (2%)
29	NAD	E	900	-	42,48,48	3.83	19 (45%)	50,73,73	2.10	6 (12%)
25	UQ8	i	303	-	53,53,53	1.80	7 (13%)	64,67,67	1.60	15 (23%)
22	CDL	L	301	-	99,99,99	0.89	8 (8%)	105,111,111	0.99	4 (3%)
23	PC1	g	303	8	53,53,53	0.97	3 (5%)	59,61,61	1.04	2 (3%)
22	CDL	J	302	-	99,99,99	0.87	7 (7%)	105,111,111	0.99	4 (3%)
22	CDL	l	301	-	99,99,99	0.88	7 (7%)	105,111,111	1.02	4 (3%)
22	CDL	J	301	-	99,99,99	0.89	6 (6%)	105,111,111	1.07	4 (3%)
22	CDL	B	401	-	99,99,99	0.89	8 (8%)	105,111,111	0.99	5 (4%)
23	PC1	d	301	3	53,53,53	0.93	4 (7%)	59,61,61	1.08	3 (5%)
23	PC1	G	303	-	53,53,53	0.97	4 (7%)	59,61,61	0.94	2 (3%)
23	PC1	G	304	8	53,53,53	0.97	3 (5%)	59,61,61	1.04	2 (3%)
24	PO4	f	301	-	4,4,4	1.06	0	6,6,6	0.42	0
22	CDL	k	202	-	99,99,99	0.89	7 (7%)	105,111,111	1.04	5 (4%)
22	CDL	A	501	-	99,99,99	0.88	7 (7%)	105,111,111	1.01	5 (4%)
22	CDL	k	203	-	99,99,99	0.89	7 (7%)	105,111,111	0.99	4 (3%)
22	CDL	r	201	-	99,99,99	0.87	5 (5%)	105,111,111	0.97	4 (3%)
22	CDL	b	402	-	99,99,99	0.89	7 (7%)	105,111,111	0.93	4 (3%)
22	CDL	B	405	2	99,99,99	0.88	8 (8%)	105,111,111	1.10	5 (4%)
28	PEE	l	302	-	47,47,50	1.18	6 (12%)	50,52,55	1.09	3 (6%)
22	CDL	k	201	-	99,99,99	0.89	8 (8%)	105,111,111	1.08	5 (4%)
22	CDL	f	304	4	99,99,99	0.88	8 (8%)	105,111,111	1.05	4 (3%)
22	CDL	I	302	-	99,99,99	0.89	8 (8%)	105,111,111	0.99	4 (3%)
26	ATP	G	301	27	26,33,33	4.75	7 (26%)	31,52,52	2.46	7 (22%)
22	CDL	K	201	-	99,99,99	0.89	8 (8%)	105,111,111	1.01	4 (3%)
23	PC1	D	301	3	53,53,53	0.95	4 (7%)	59,61,61	1.10	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CDL	j	301	-	99,99,99	0.89	7 (7%)	105,111,111	1.07	4 (3%)
22	CDL	B	403	2	99,99,99	0.87	7 (7%)	105,111,111	1.09	4 (3%)
25	UQ8	I	303	-	53,53,53	1.81	7 (13%)	64,67,67	1.57	13 (20%)
24	PO4	F	900	-	4,4,4	1.06	0	6,6,6	0.46	0
22	CDL	p	201	-	99,99,99	0.88	8 (8%)	105,111,111	1.00	4 (3%)
28	PEE	l	303	-	50,50,50	1.15	6 (12%)	53,55,55	1.13	3 (5%)
23	PC1	i	301	-	53,53,53	0.96	4 (7%)	59,61,61	0.96	2 (3%)
29	NAD	e	900	-	42,48,48	3.83	19 (45%)	50,73,73	2.17	7 (14%)
22	CDL	f	302	4	99,99,99	0.88	8 (8%)	105,111,111	1.07	4 (3%)
22	CDL	b	401	-	99,99,99	0.88	8 (8%)	105,111,111	0.98	4 (3%)
22	CDL	j	302	-	99,99,99	0.87	7 (7%)	105,111,111	1.02	4 (3%)
22	CDL	P	201	-	99,99,99	0.88	8 (8%)	105,111,111	1.03	5 (4%)
26	ATP	g	301	27	26,33,33	4.76	7 (26%)	31,52,52	2.45	7 (22%)

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
22	CDL	B	402	-	-	53/110/110/110	-
22	CDL	B	404	-	-	40/110/110/110	-
22	CDL	i	302	-	-	41/110/110/110	-
28	PEE	J	303	10	-	23/51/51/54	-
22	CDL	I	301	5	-	50/110/110/110	-
22	CDL	K	202	-	-	39/110/110/110	-
22	CDL	f	303	-	-	42/110/110/110	-
22	CDL	l	304	-	-	41/110/110/110	-
28	PEE	J	304	-	-	24/54/54/54	-
22	CDL	a	501	-	-	47/110/110/110	-
29	NAD	E	900	-	-	7/26/62/62	0/5/5/5
25	UQ8	i	303	-	-	8/51/75/75	0/1/1/1
22	CDL	L	301	-	-	44/110/110/110	-
23	PC1	g	303	8	-	17/57/57/57	-
22	CDL	J	302	-	-	36/110/110/110	-
22	CDL	l	301	-	-	37/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CDL	J	301	-	-	35/110/110/110	-
22	CDL	B	401	-	-	52/110/110/110	-
23	PC1	d	301	3	-	17/57/57/57	-
23	PC1	G	303	-	-	16/57/57/57	-
23	PC1	G	304	8	-	19/57/57/57	-
22	CDL	k	202	-	-	44/110/110/110	-
22	CDL	A	501	-	-	51/110/110/110	-
22	CDL	k	203	-	-	45/110/110/110	-
22	CDL	r	201	-	-	47/110/110/110	-
22	CDL	b	402	-	-	43/110/110/110	-
22	CDL	B	405	2	-	40/110/110/110	-
28	PEE	l	302	-	-	26/51/51/54	-
22	CDL	k	201	-	-	35/110/110/110	-
22	CDL	f	304	4	-	59/110/110/110	-
22	CDL	I	302	-	-	41/110/110/110	-
26	ATP	G	301	27	-	0/18/38/38	0/3/3/3
22	CDL	K	201	-	-	33/110/110/110	-
23	PC1	D	301	3	-	14/57/57/57	-
22	CDL	j	301	-	-	41/110/110/110	-
22	CDL	B	403	2	-	43/110/110/110	-
25	UQ8	I	303	-	-	11/51/75/75	0/1/1/1
22	CDL	p	201	-	-	34/110/110/110	-
28	PEE	l	303	-	-	24/54/54/54	-
23	PC1	i	301	-	-	16/57/57/57	-
29	NAD	e	900	-	-	8/26/62/62	0/5/5/5
22	CDL	f	302	4	-	43/110/110/110	-
22	CDL	b	401	-	-	55/110/110/110	-
22	CDL	j	302	-	-	37/110/110/110	-
22	CDL	P	201	-	-	39/110/110/110	-
26	ATP	g	301	27	-	0/18/38/38	0/3/3/3

The worst 5 of 333 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	g	301	ATP	C2'-C1'	-17.21	1.27	1.53
26	G	301	ATP	C2'-C1'	-17.05	1.27	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	301	ATP	O4'-C1'	11.06	1.56	1.41
26	g	301	ATP	O4'-C1'	10.92	1.56	1.41
29	e	900	NAD	O4D-C1D	-9.81	1.27	1.41

The worst 5 of 207 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	e	900	NAD	C1B-N9A-C4A	-8.37	111.94	126.64
29	E	900	NAD	C1B-N9A-C4A	-8.11	112.38	126.64
29	e	900	NAD	C5A-C6A-N6A	8.10	132.67	120.35
29	E	900	NAD	C5A-C6A-N6A	7.92	132.39	120.35
26	G	301	ATP	C5-C6-N6	7.45	131.68	120.35

There are no chirality outliers.

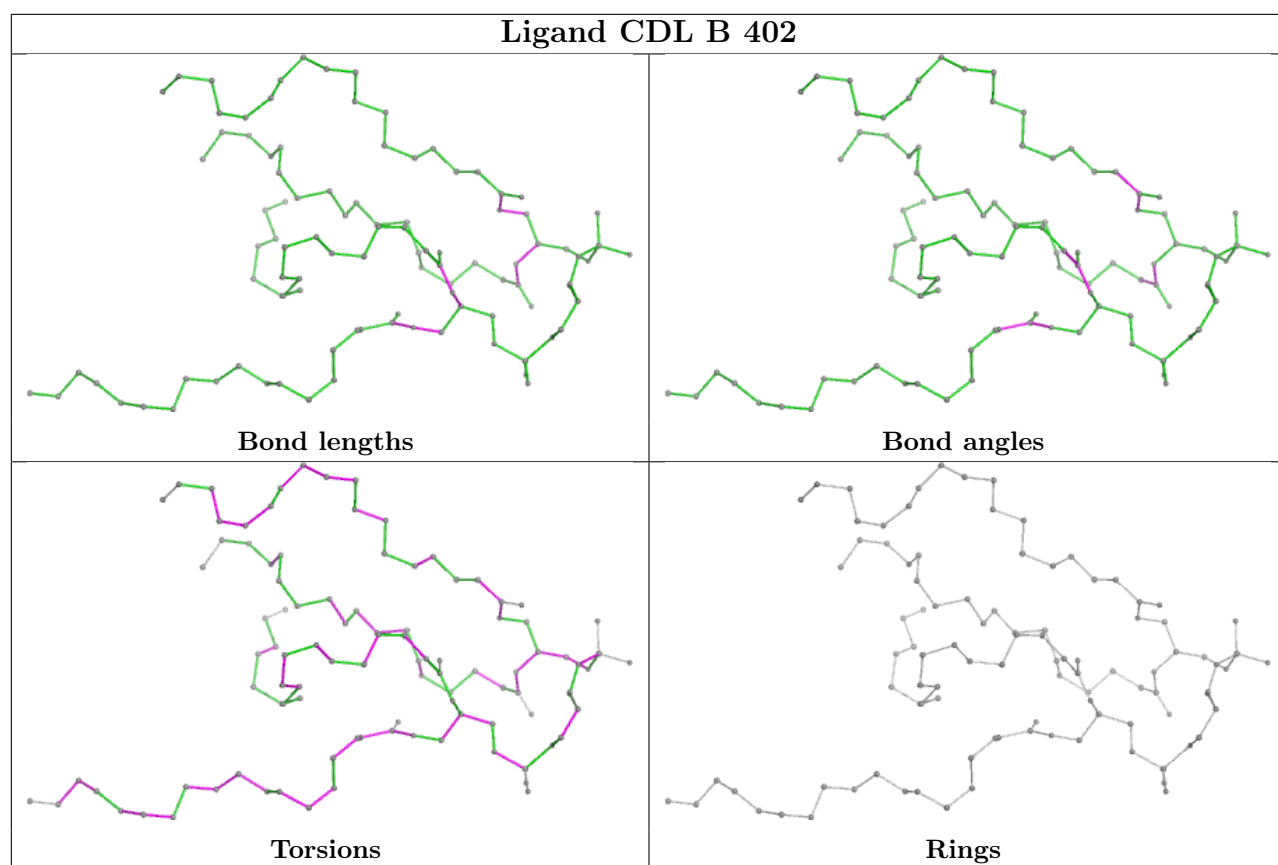
5 of 1517 torsion outliers are listed below:

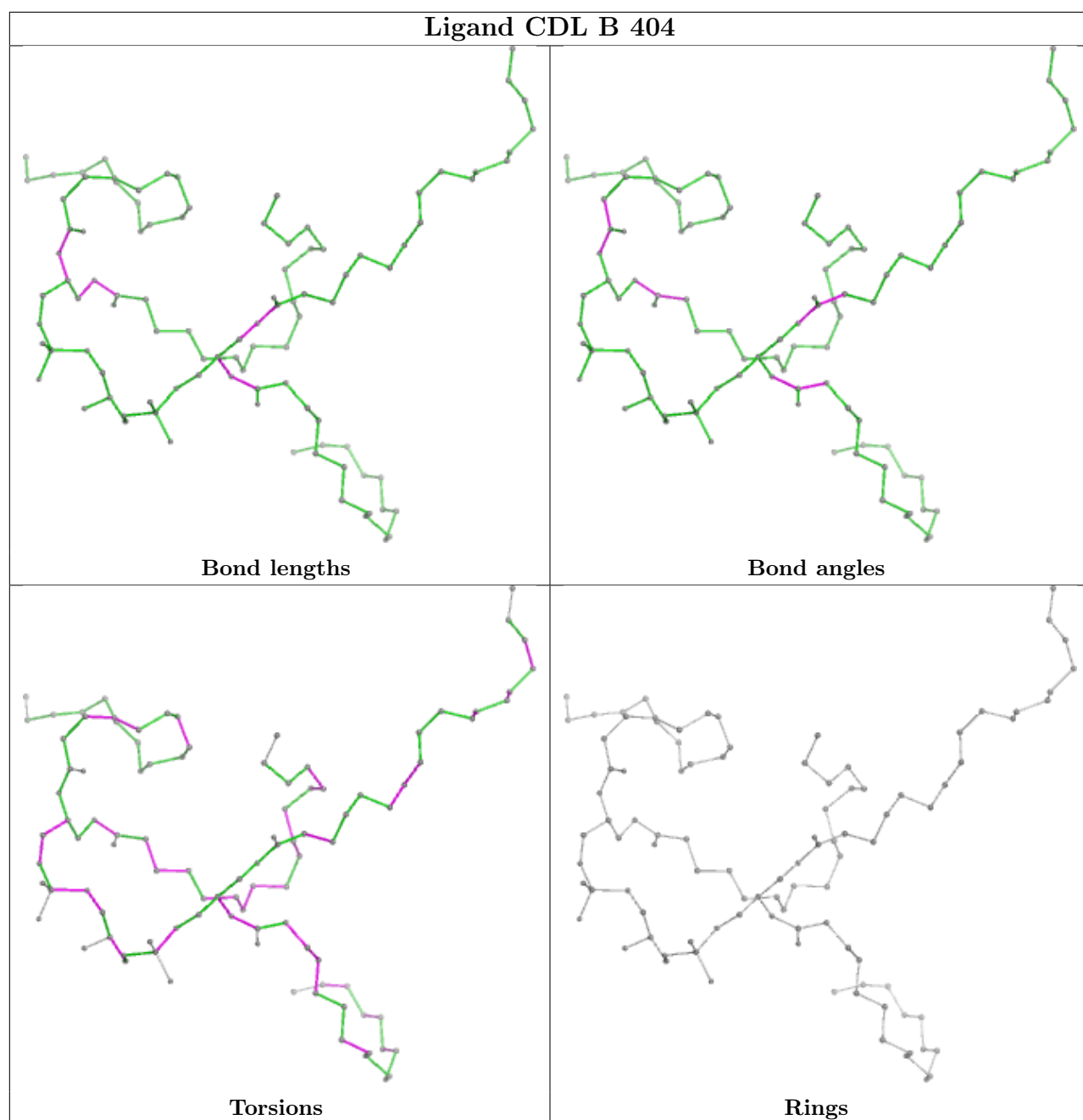
Mol	Chain	Res	Type	Atoms
22	a	501	CDL	CB3-OB5-PB2-OB3
22	a	501	CDL	CB3-OB5-PB2-OB4
22	a	501	CDL	OB7-CB5-OB6-CB4
22	a	501	CDL	C51-CB5-OB6-CB4
22	b	401	CDL	C1-CA2-OA2-PA1

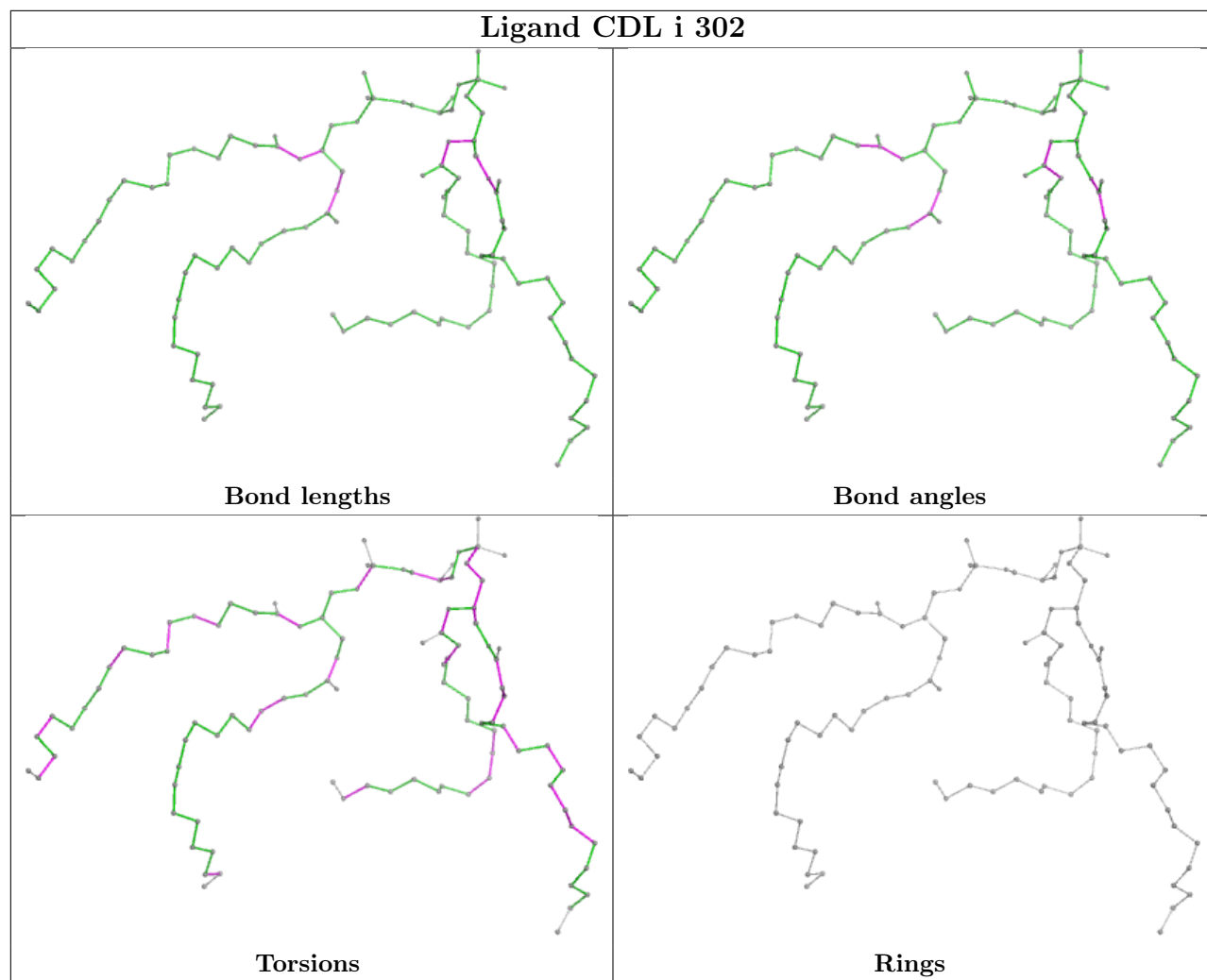
There are no ring outliers.

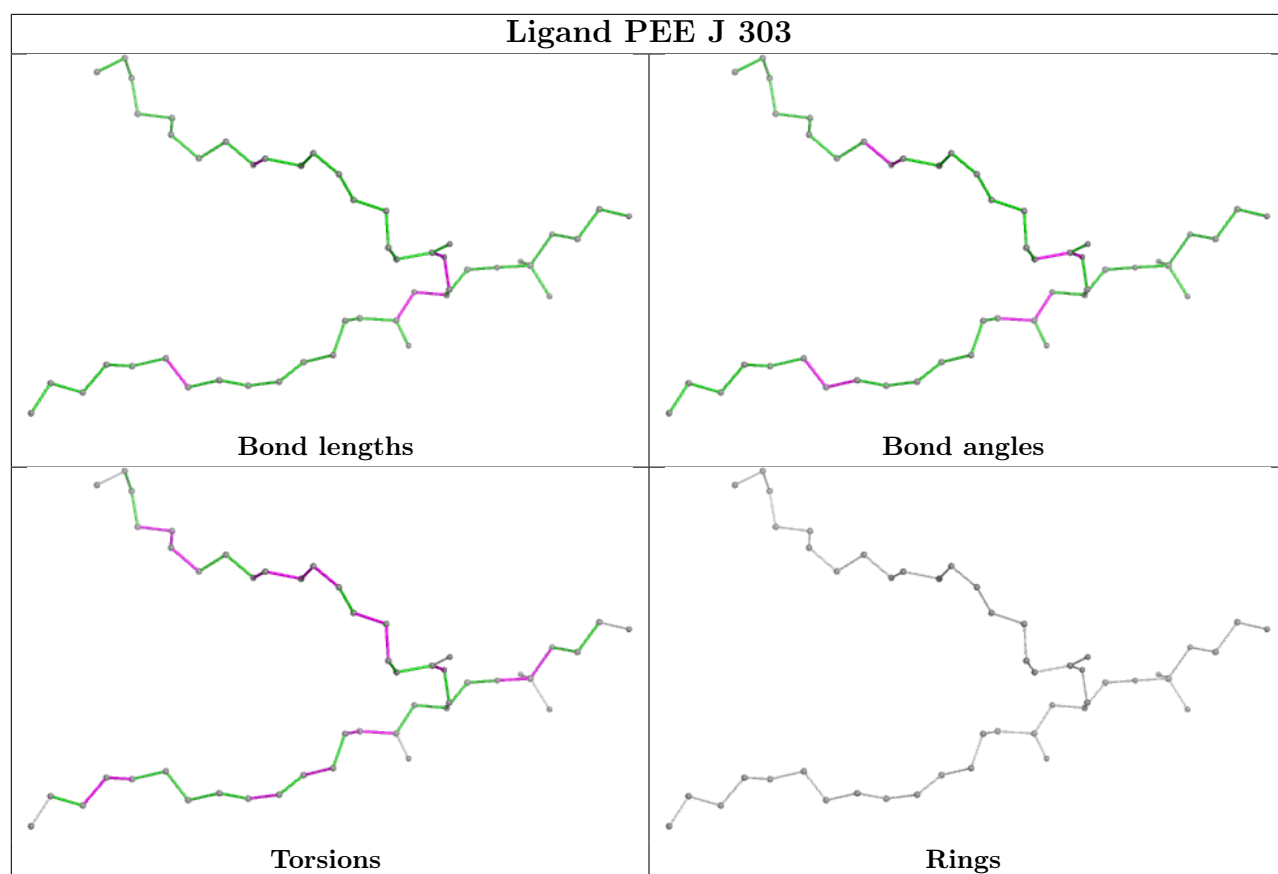
No monomer is involved in short contacts.

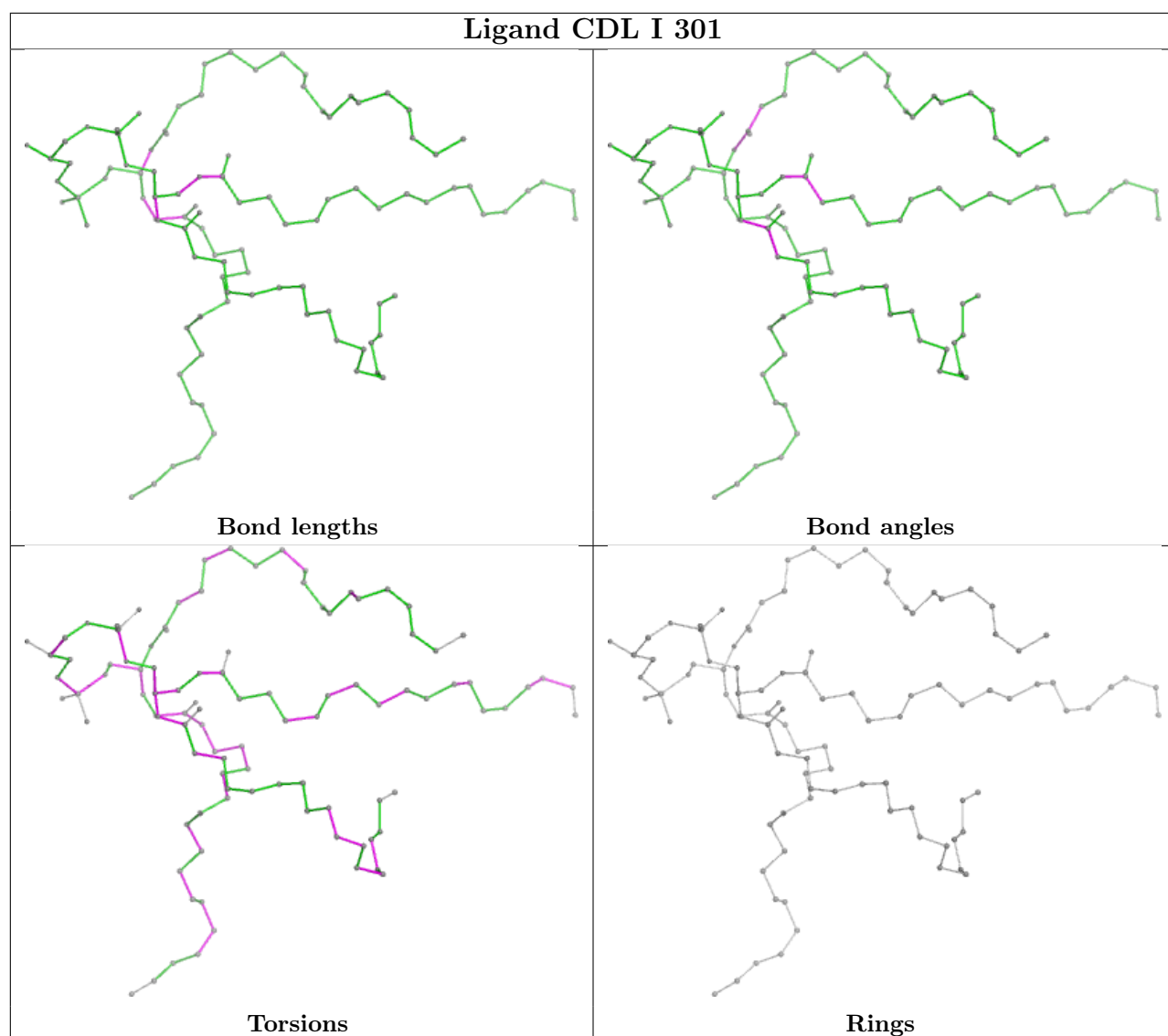
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

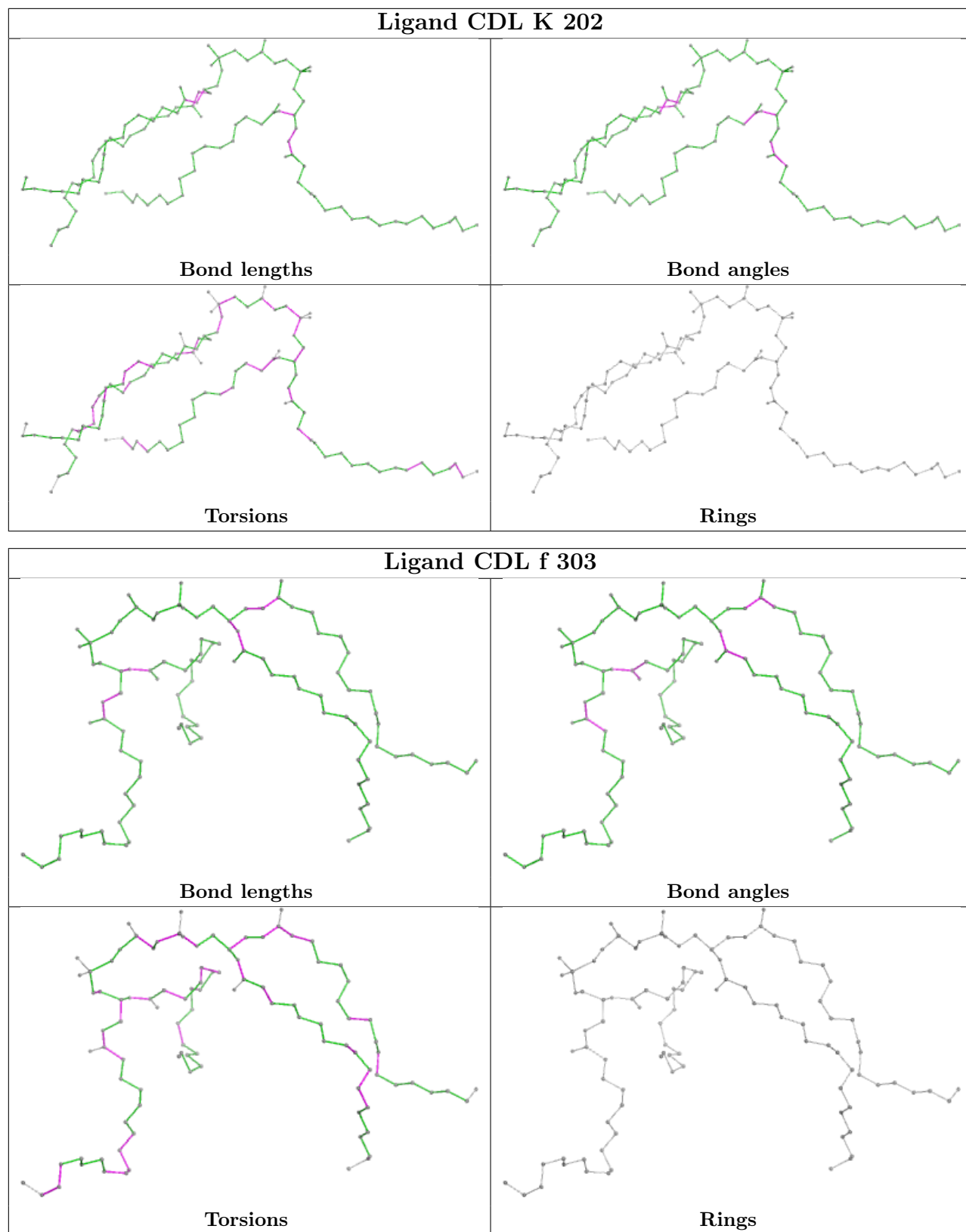


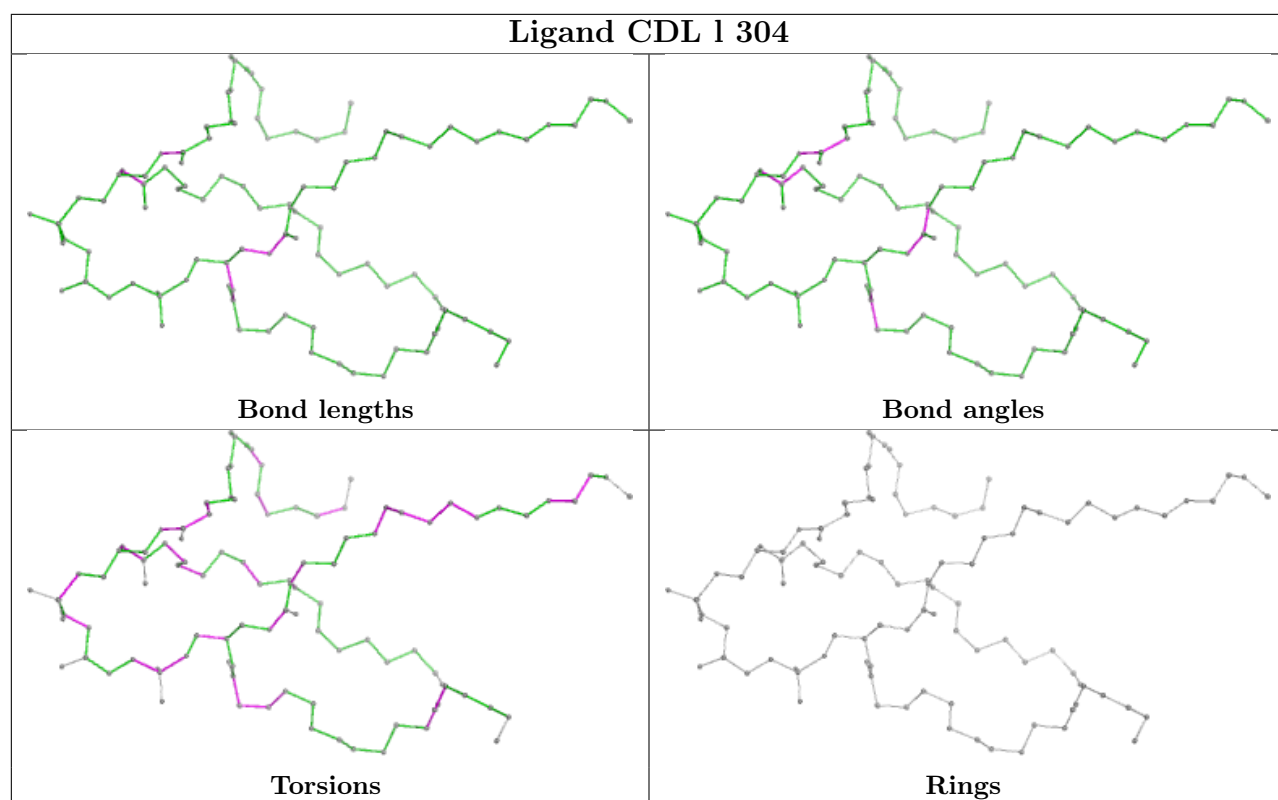


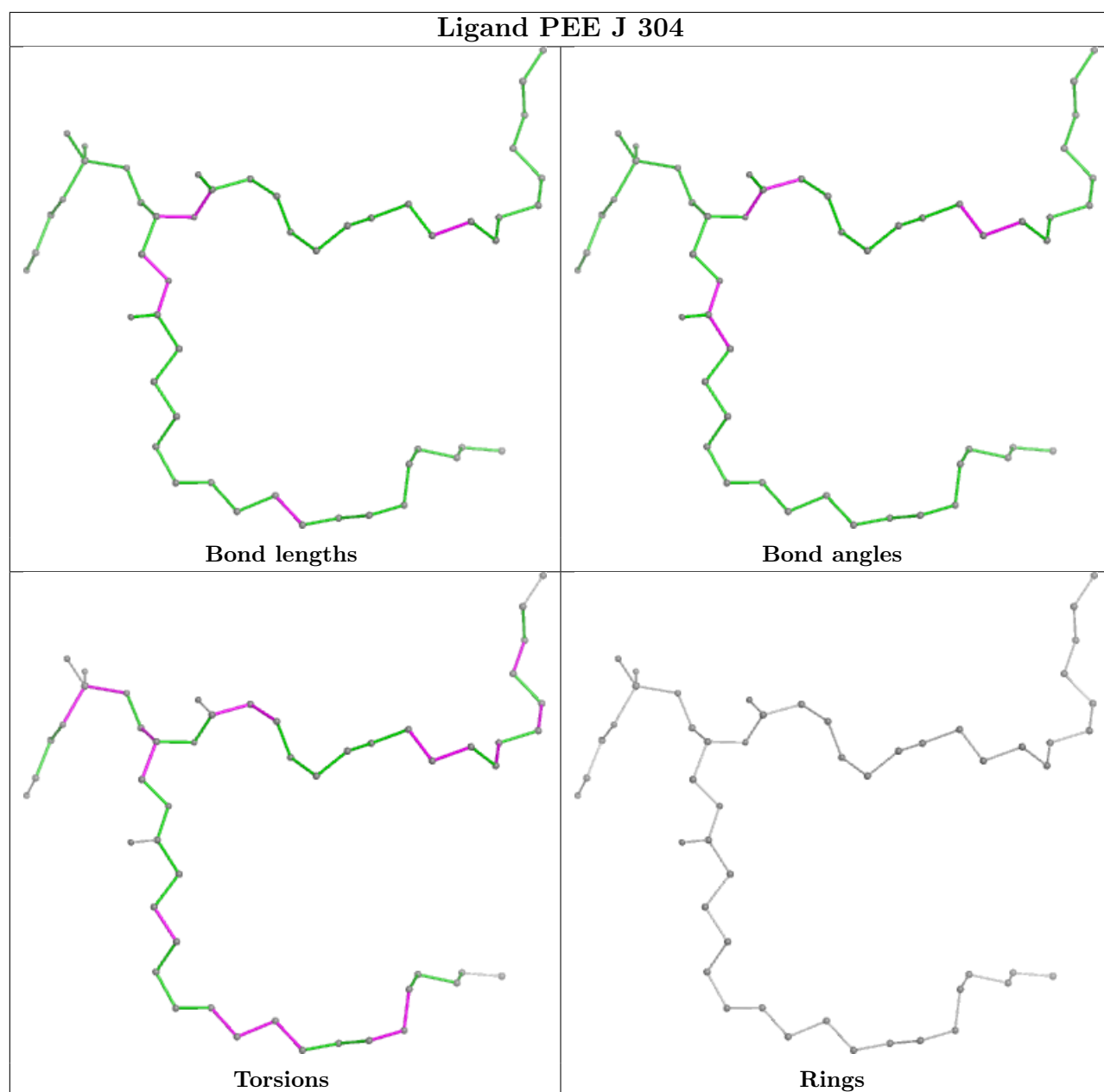


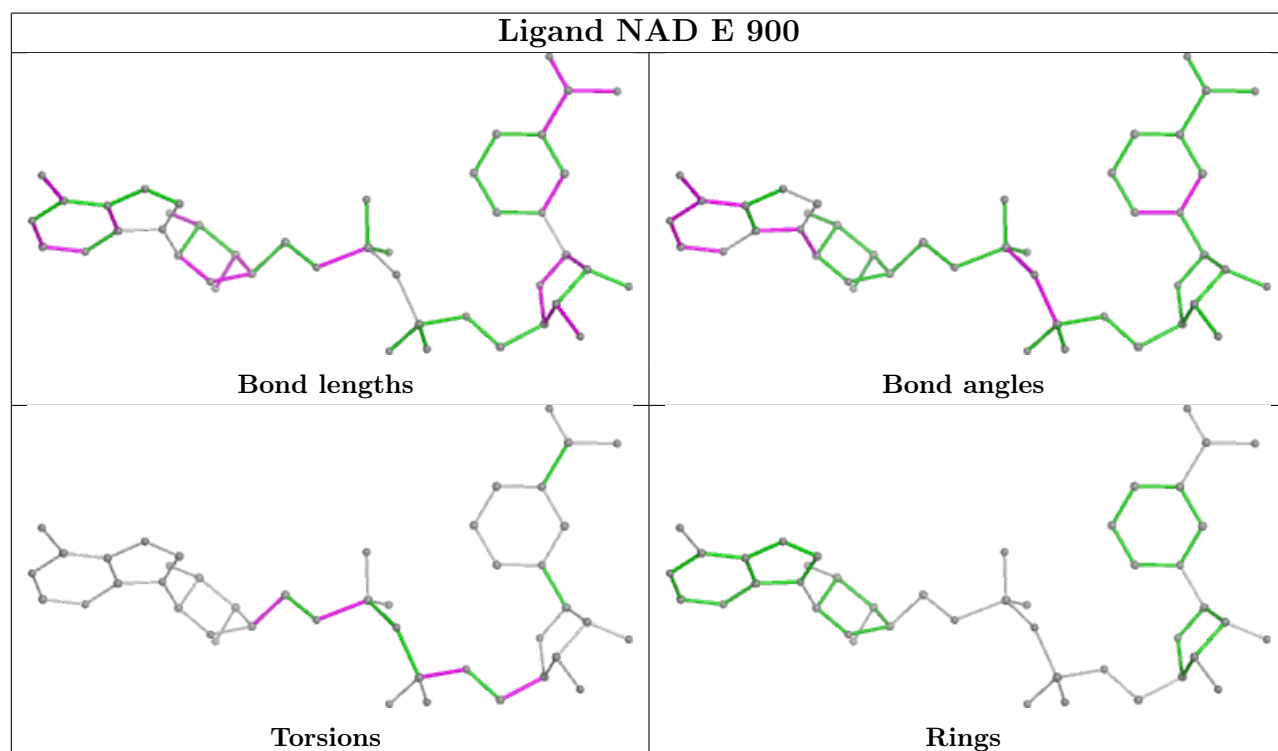
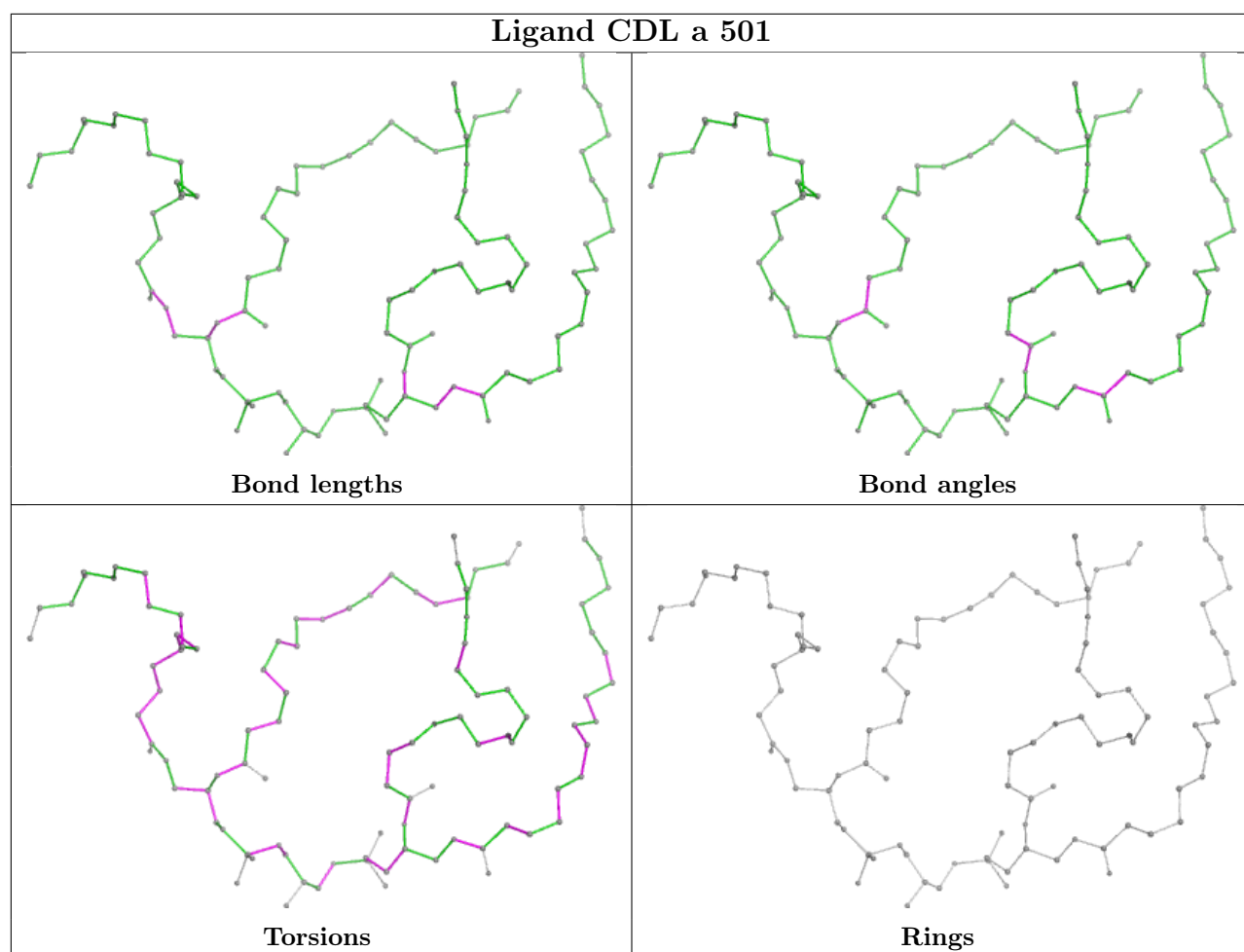


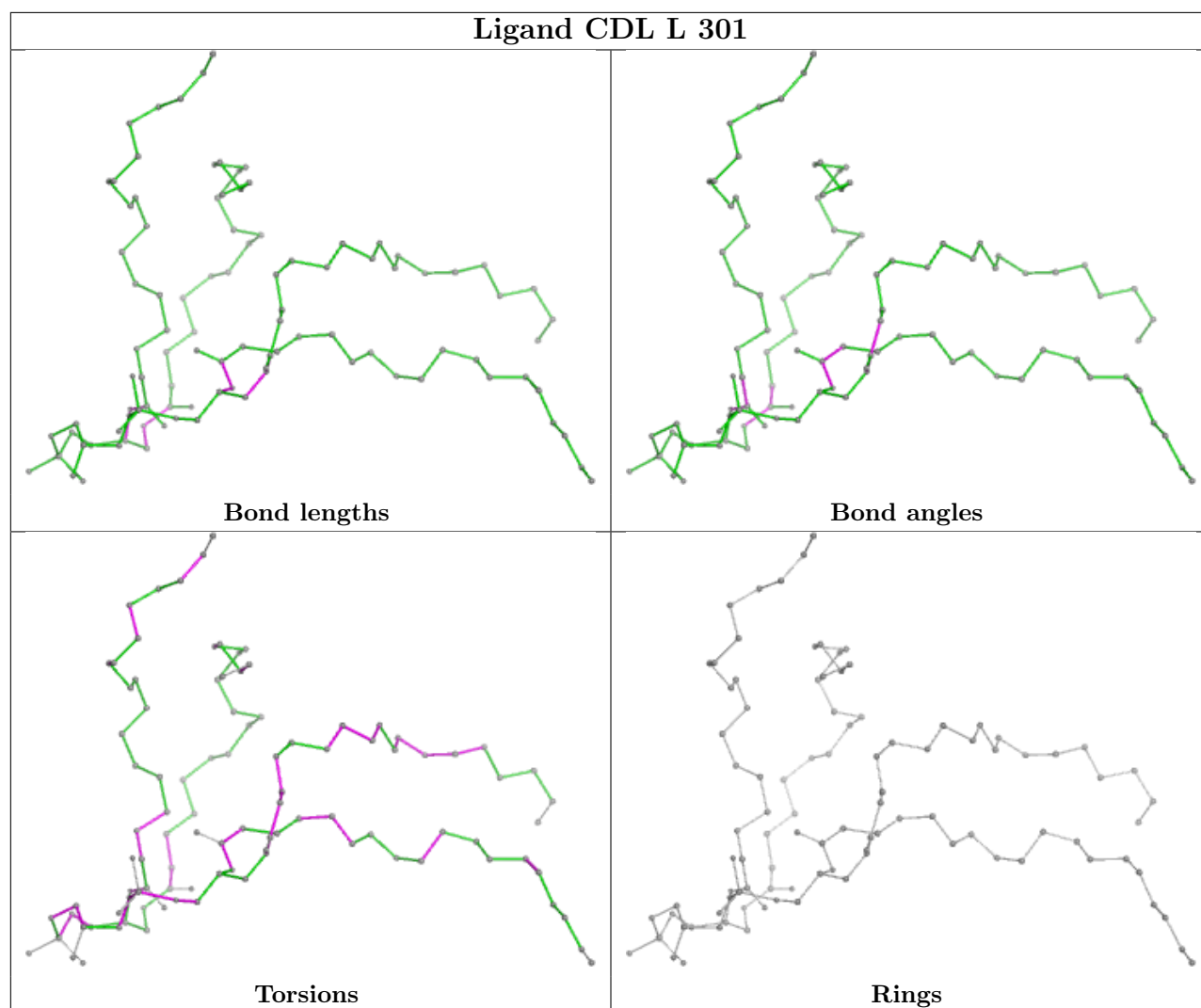
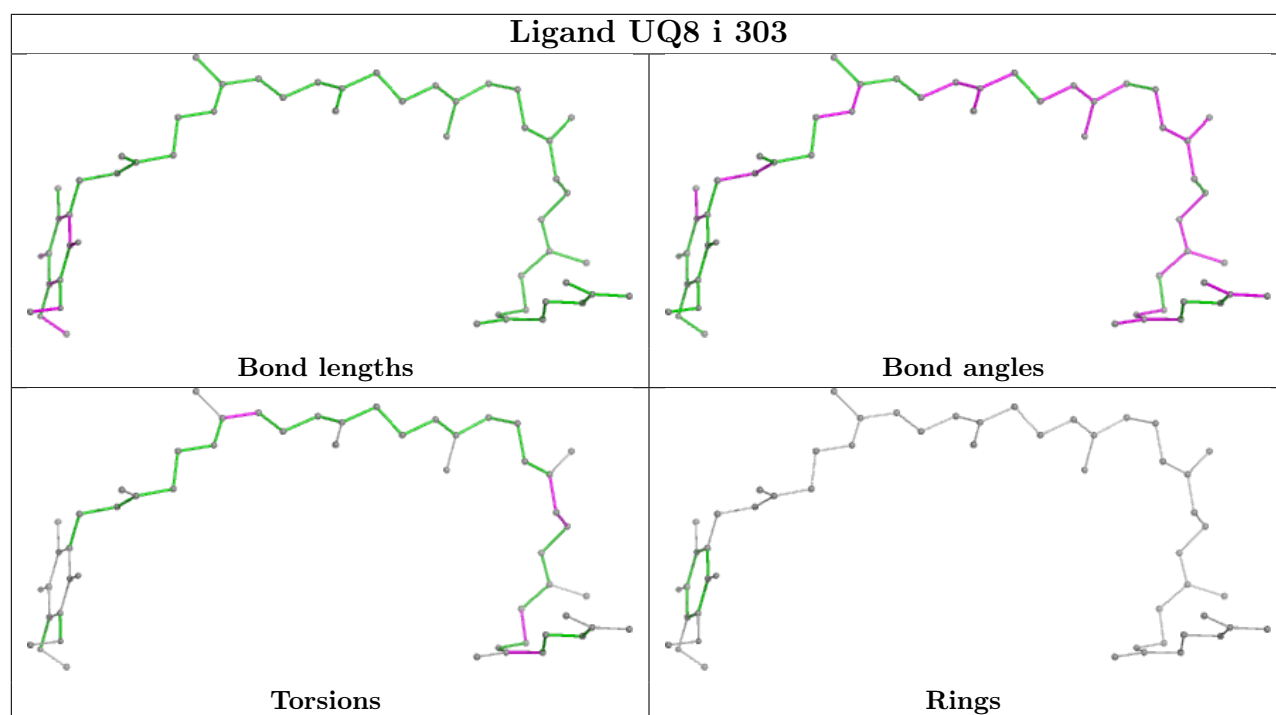


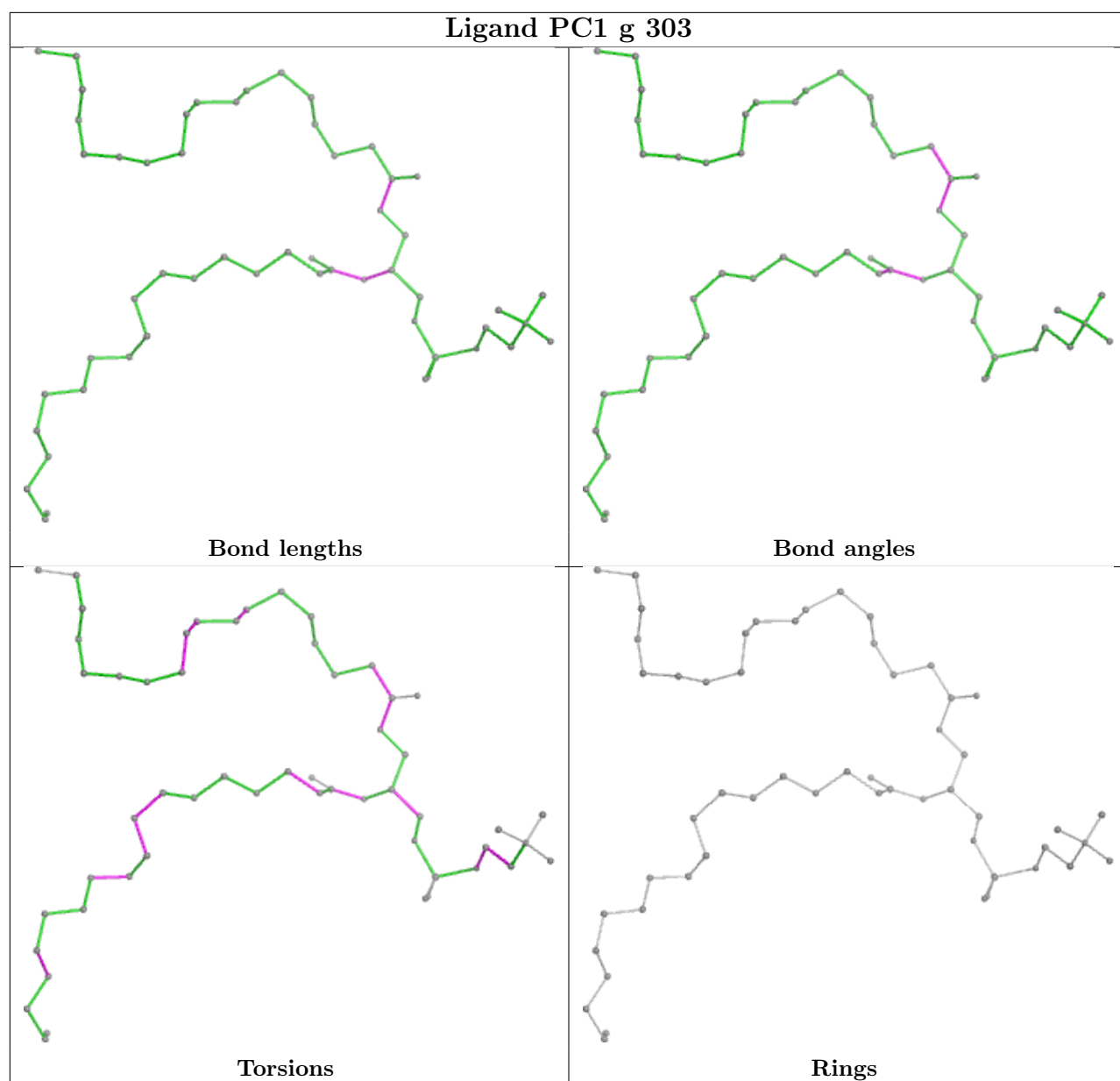


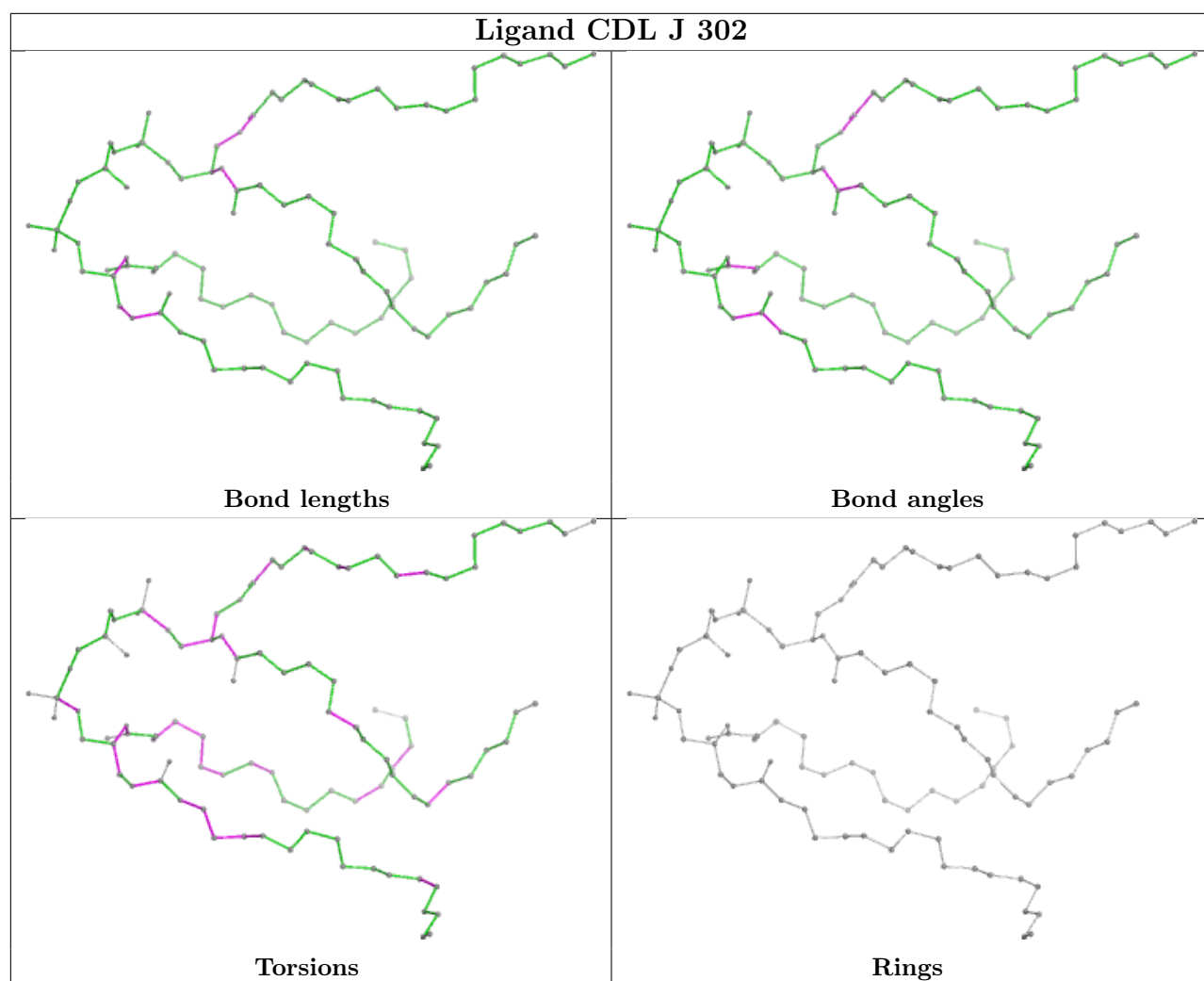


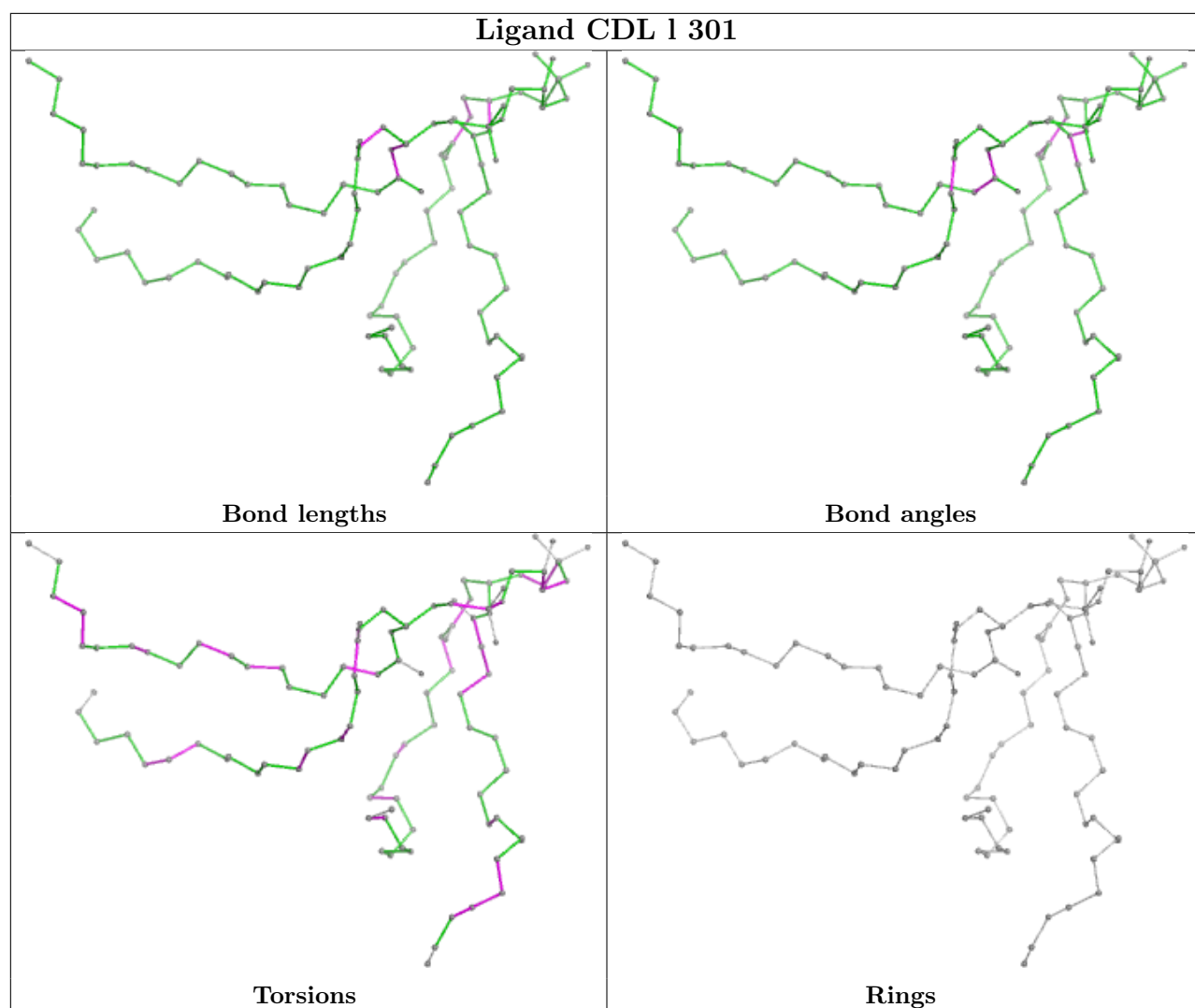


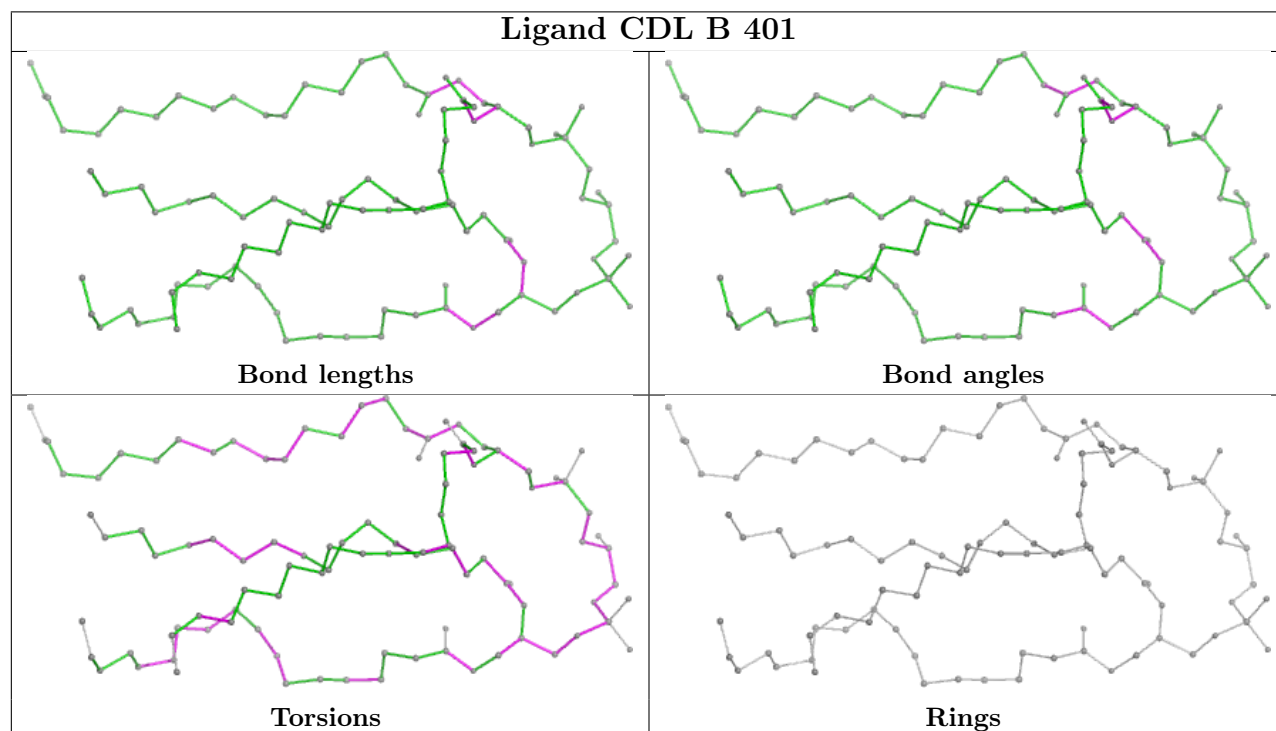
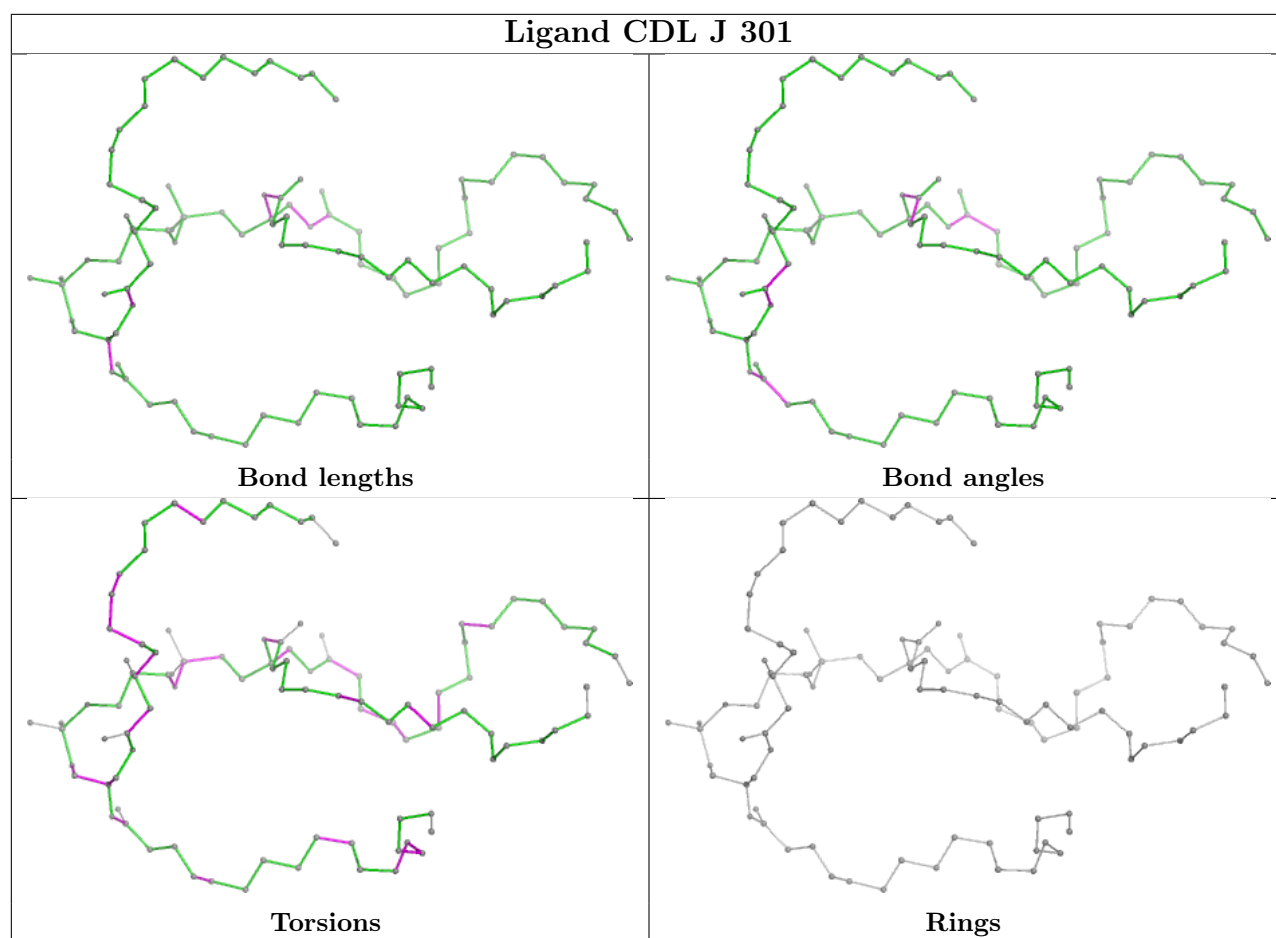


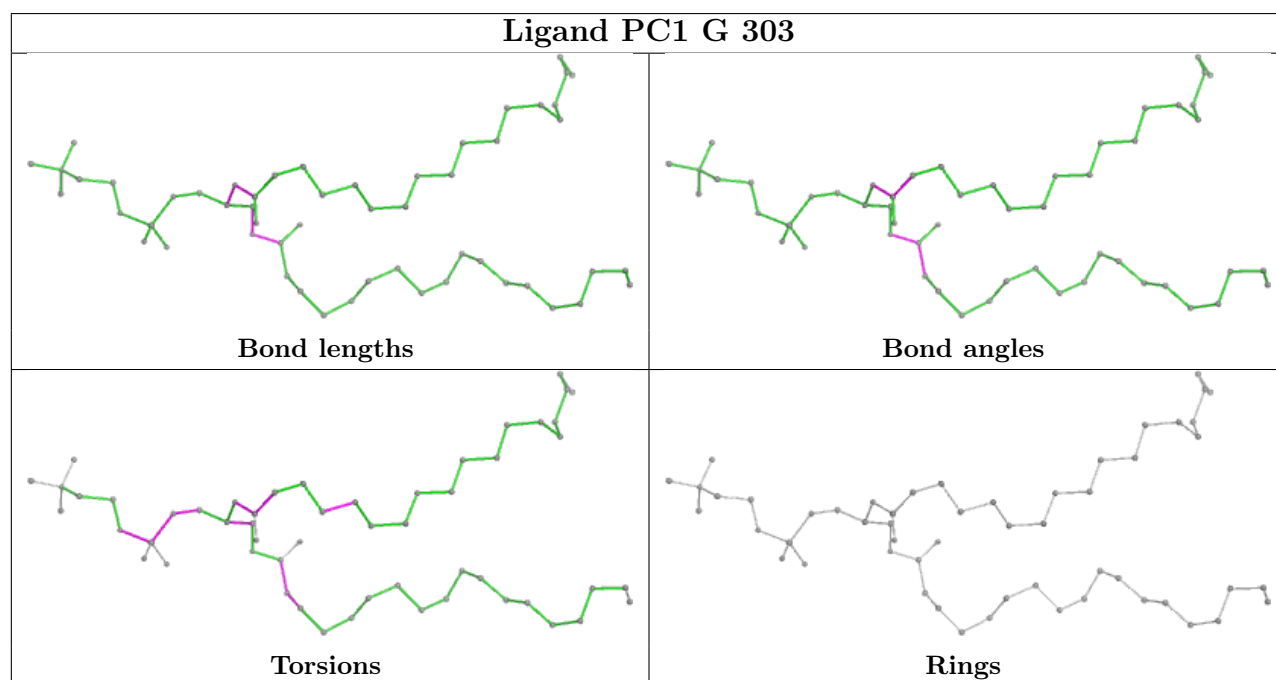
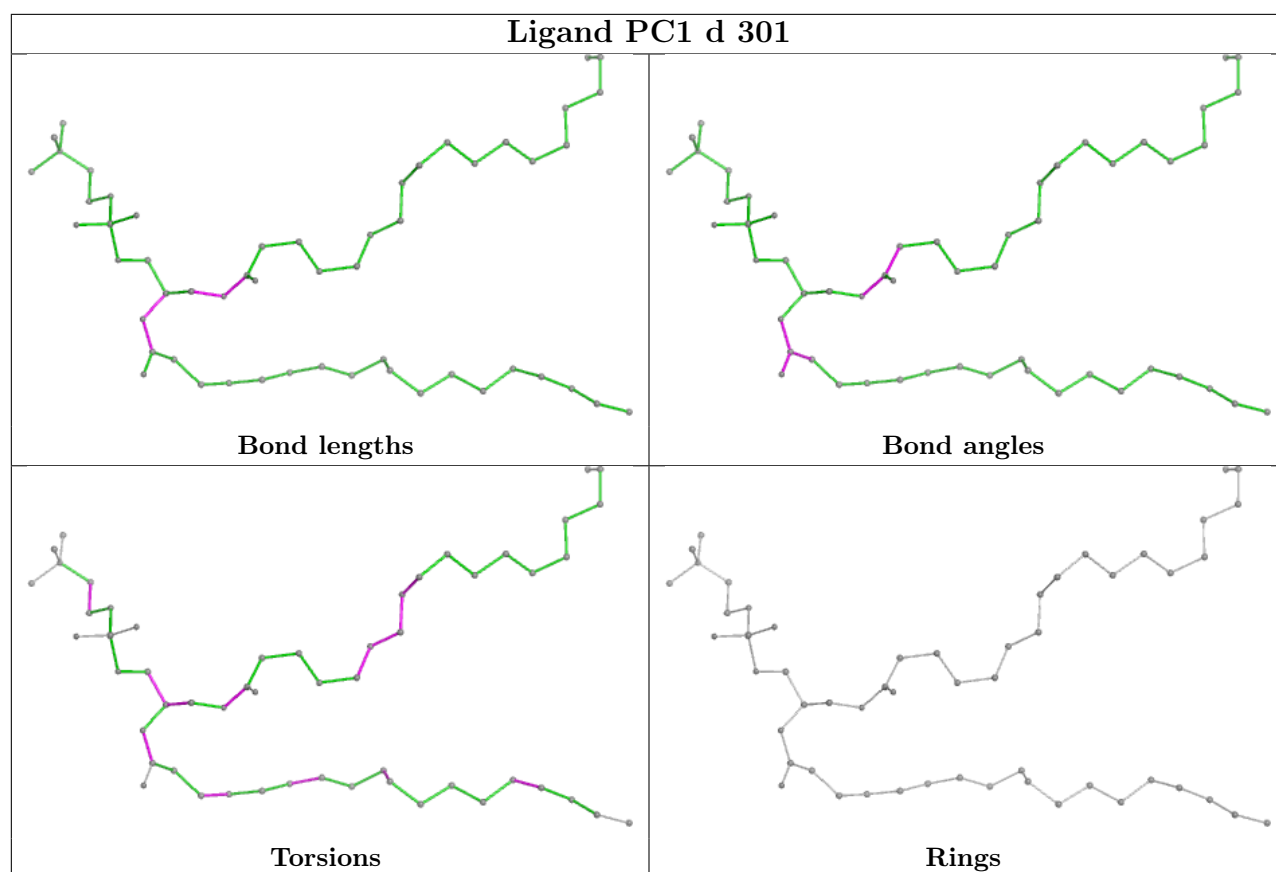


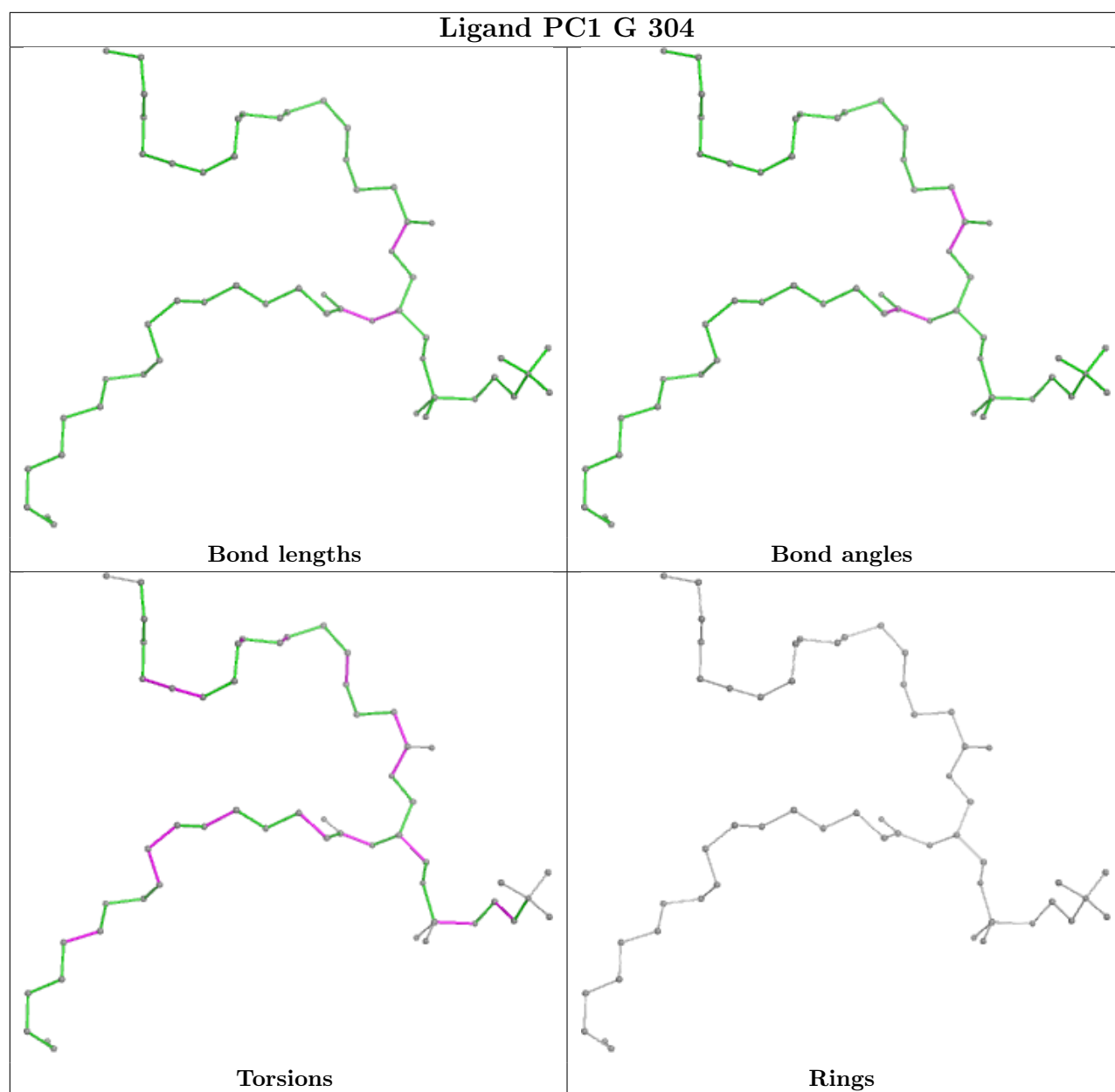


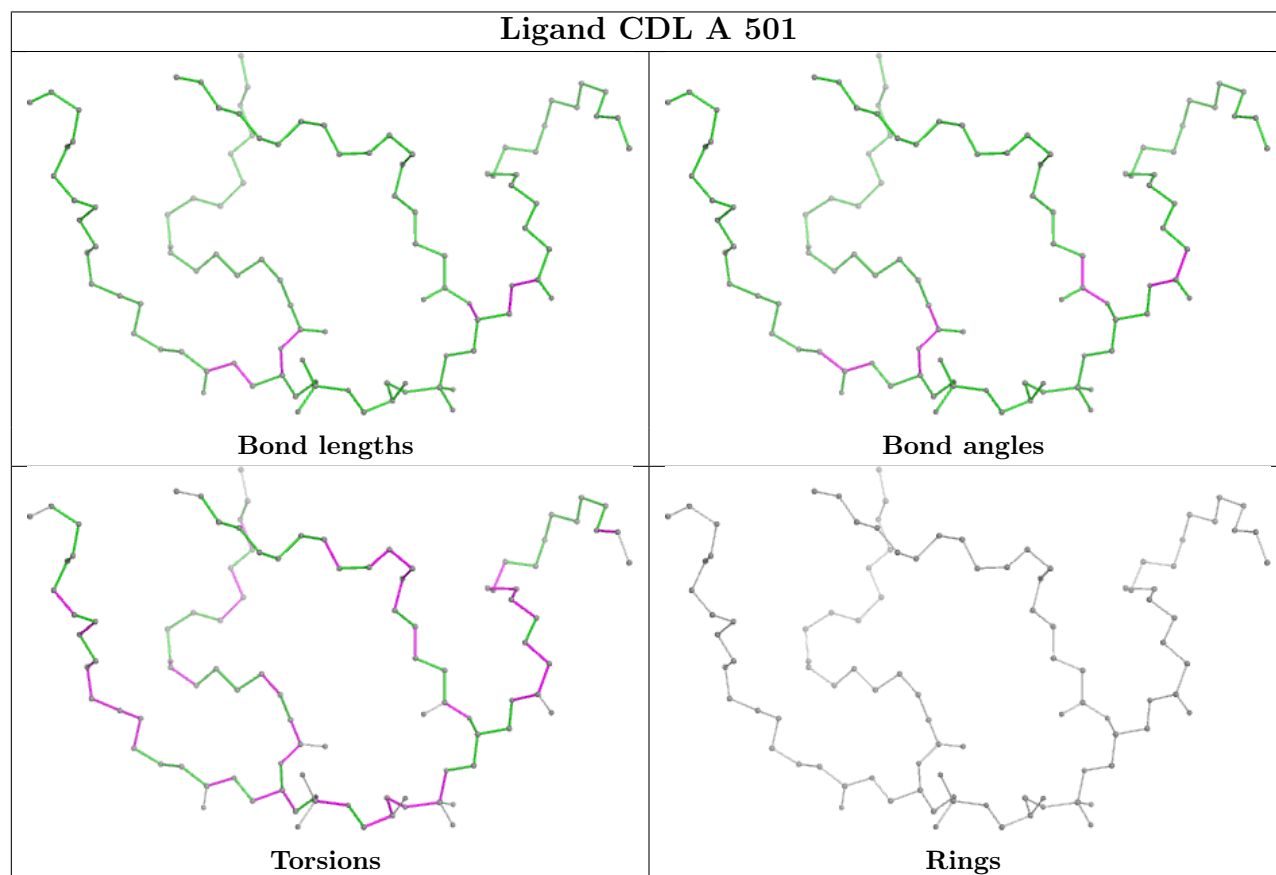
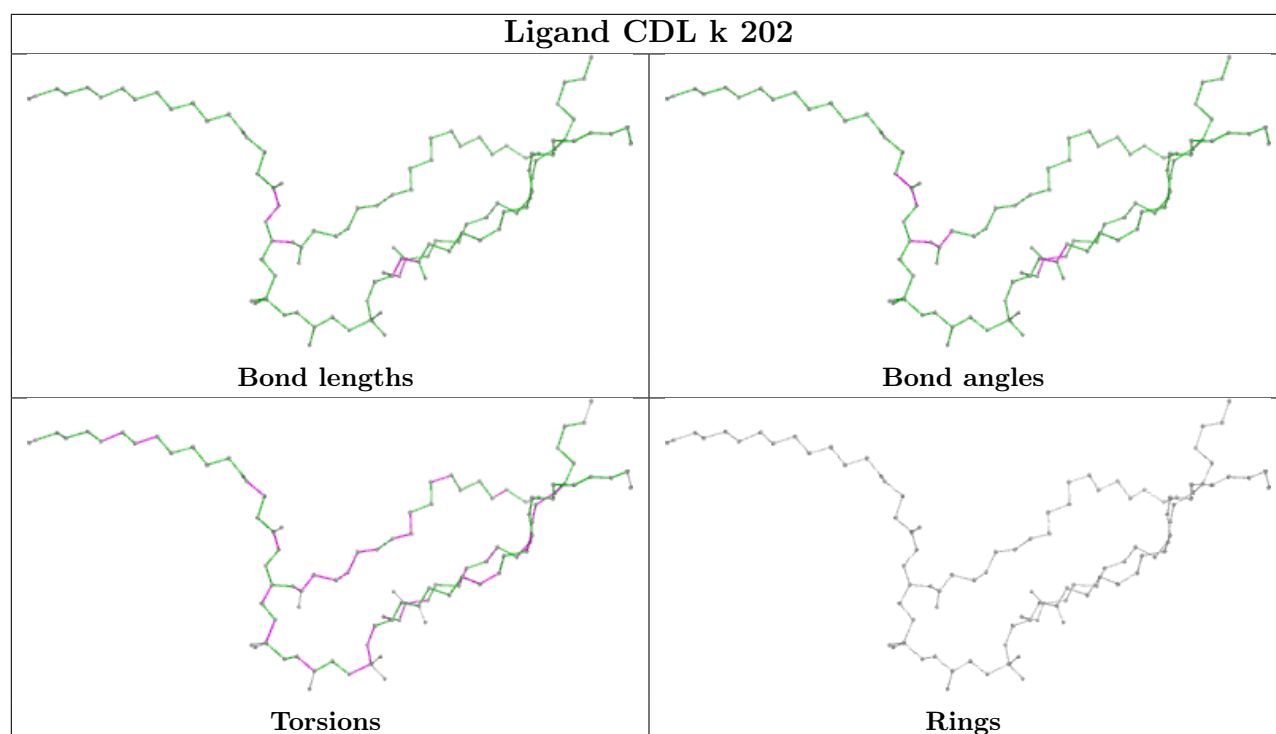


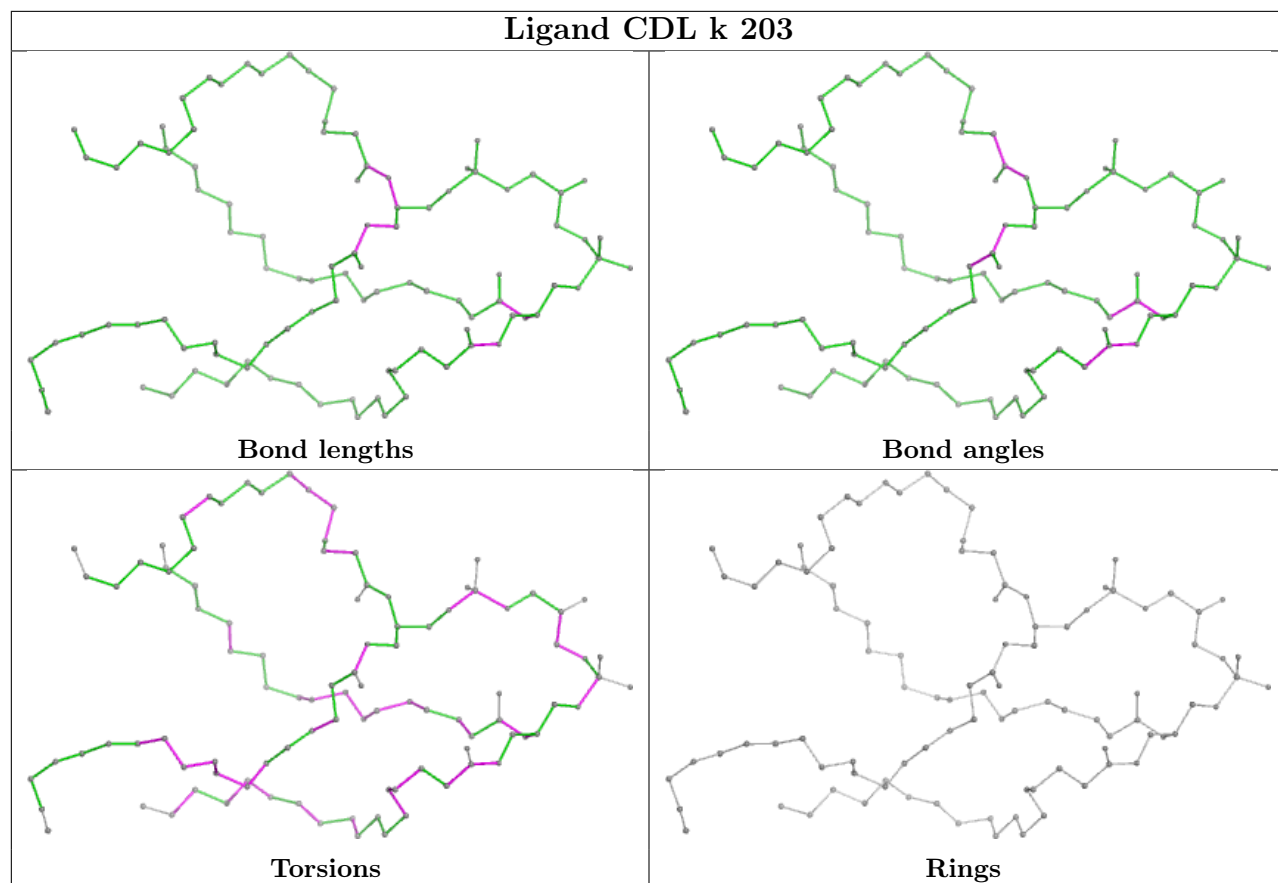


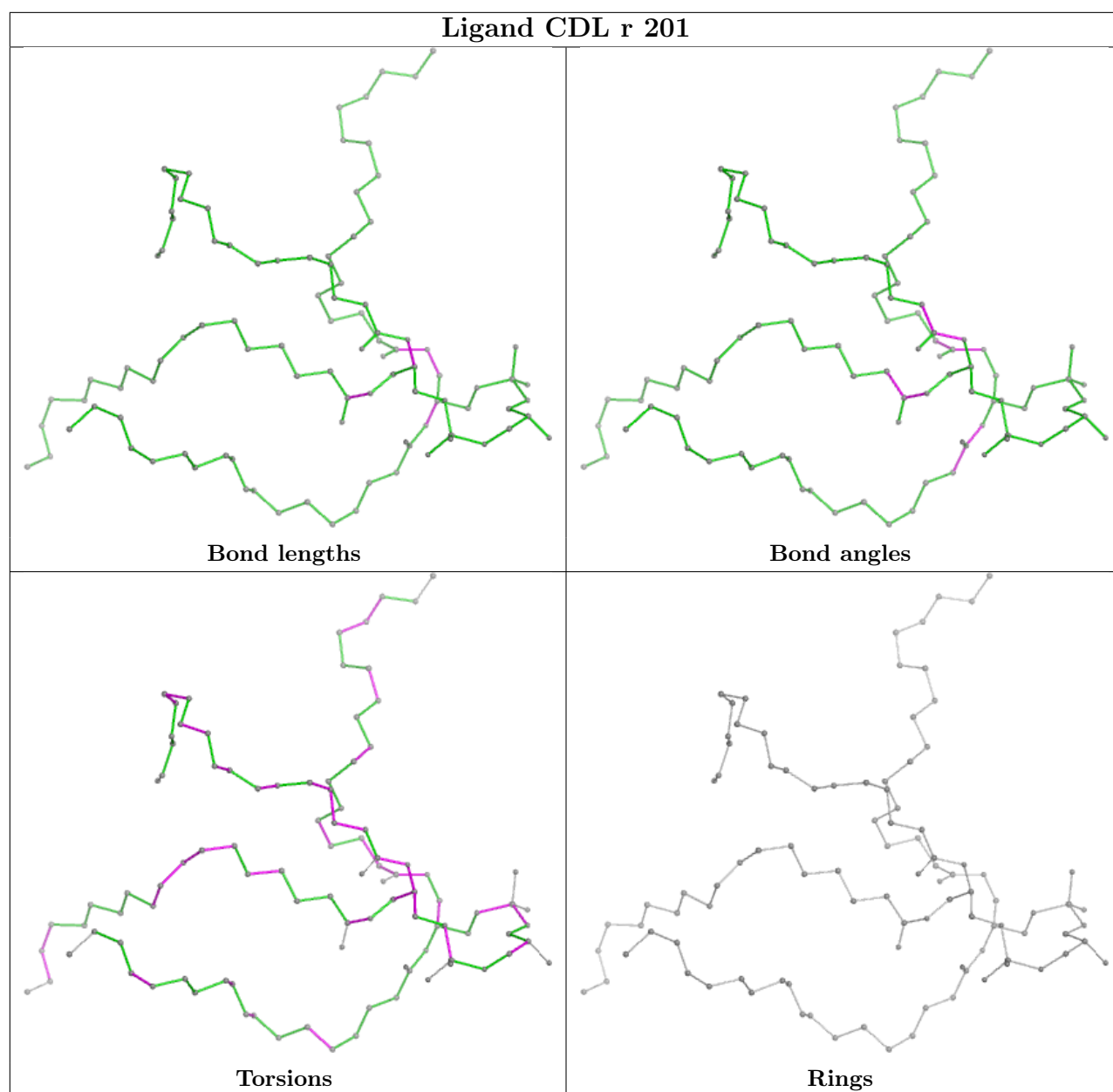


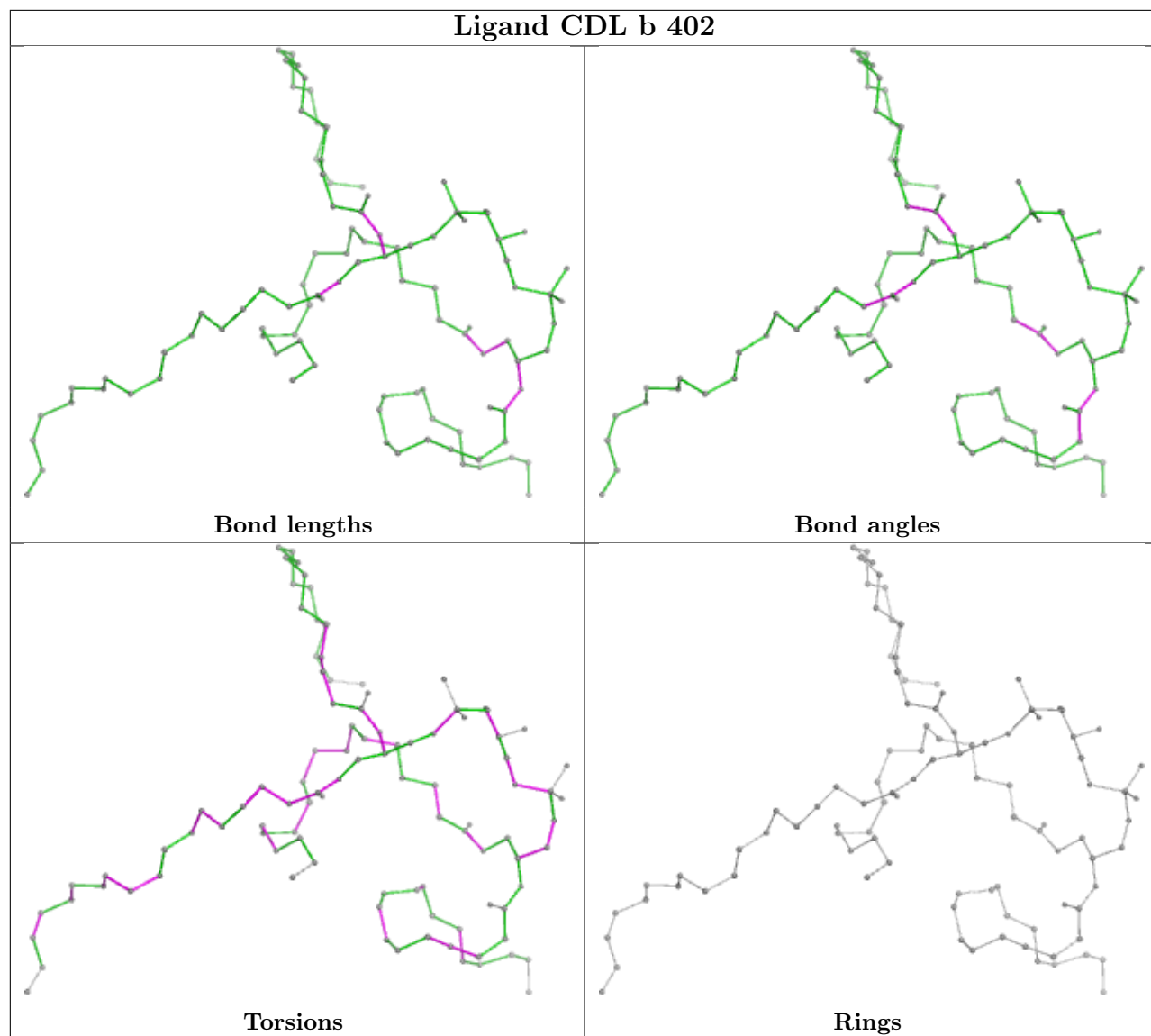


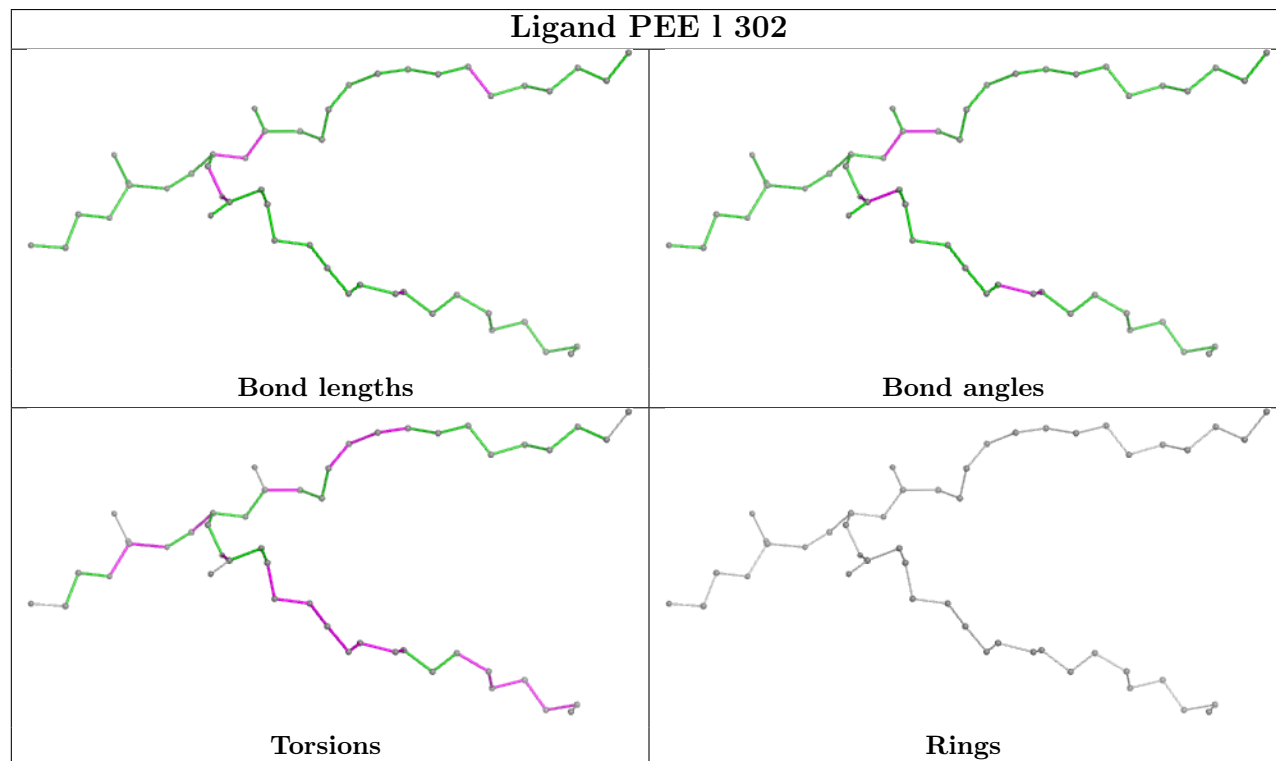
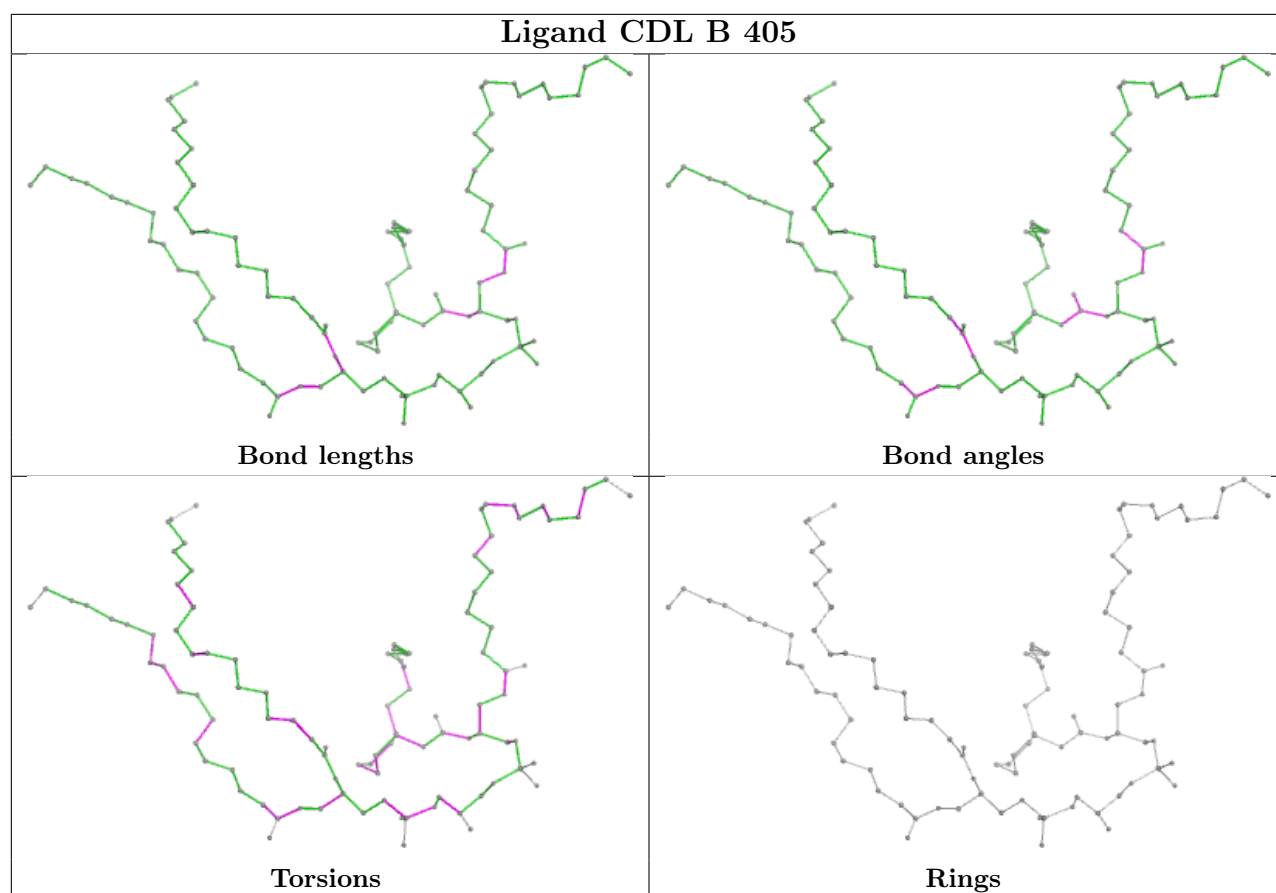


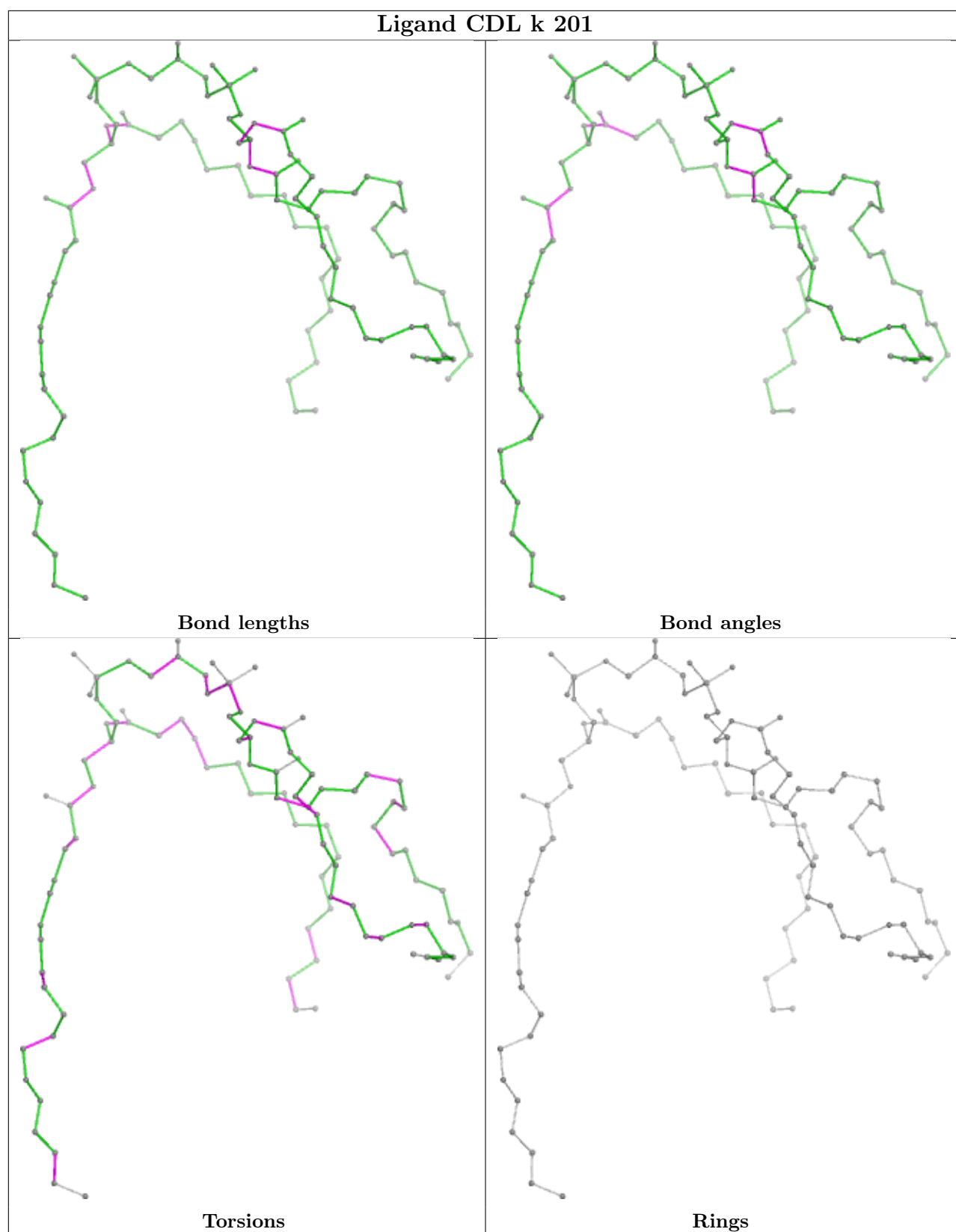


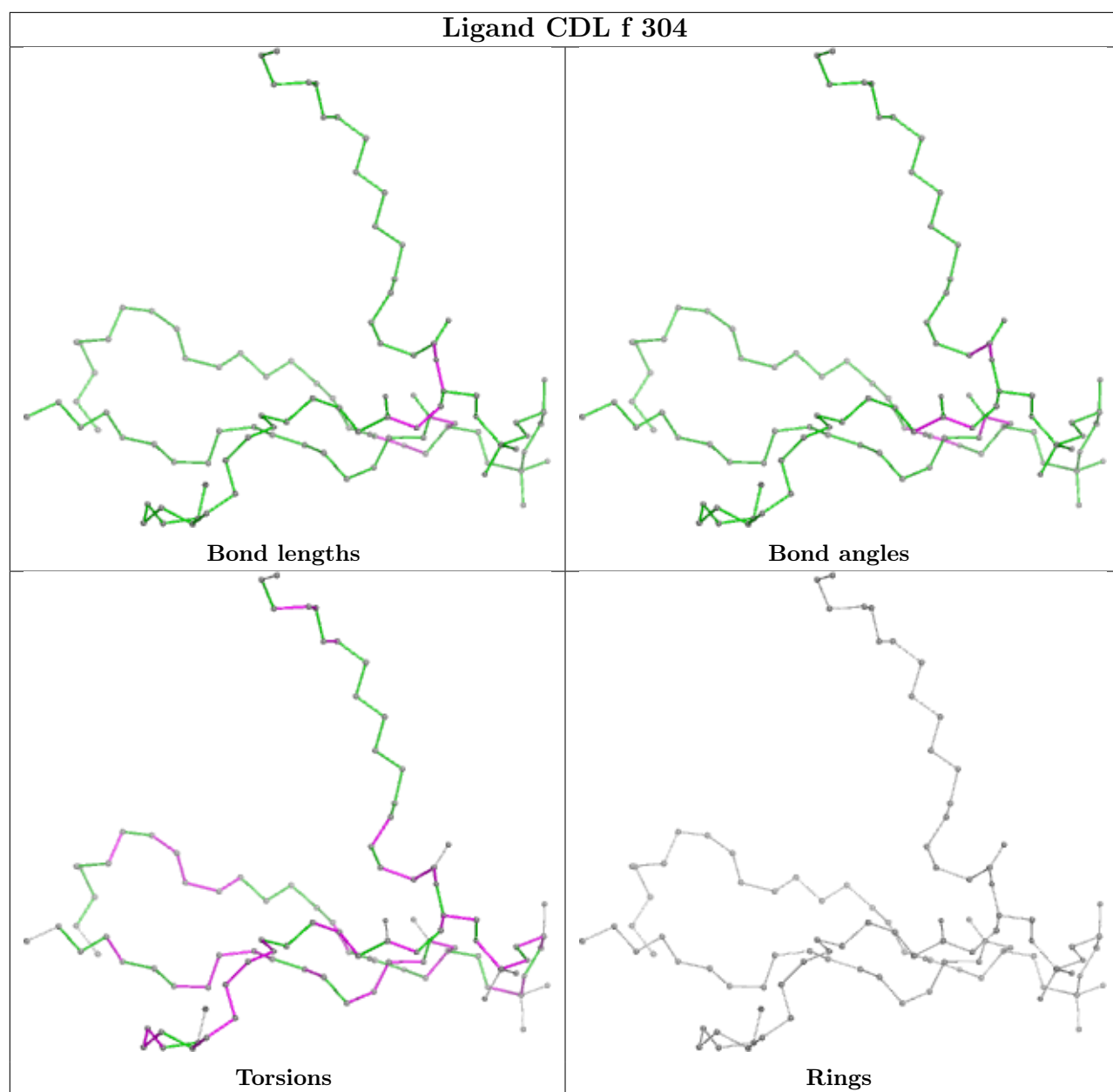


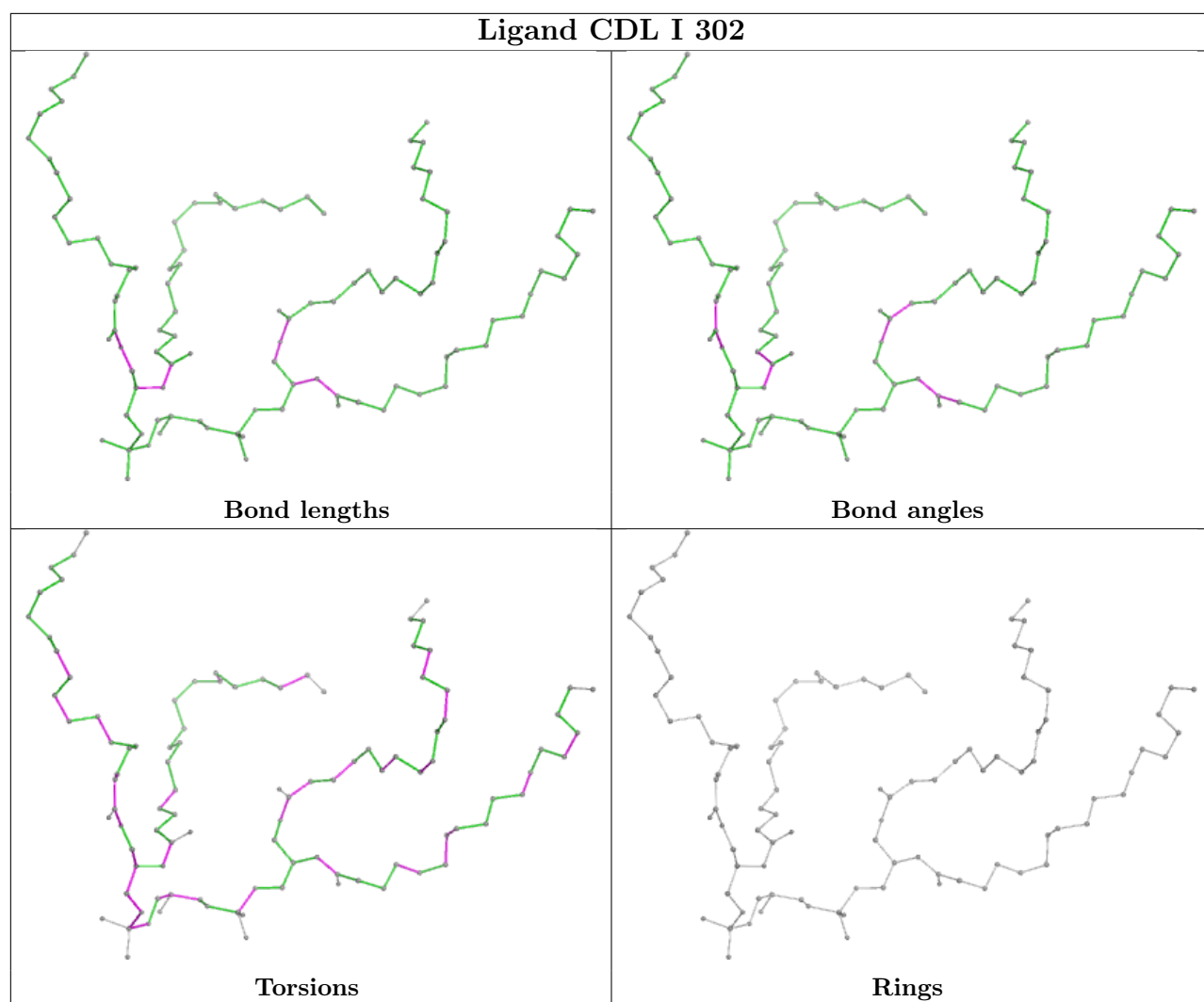


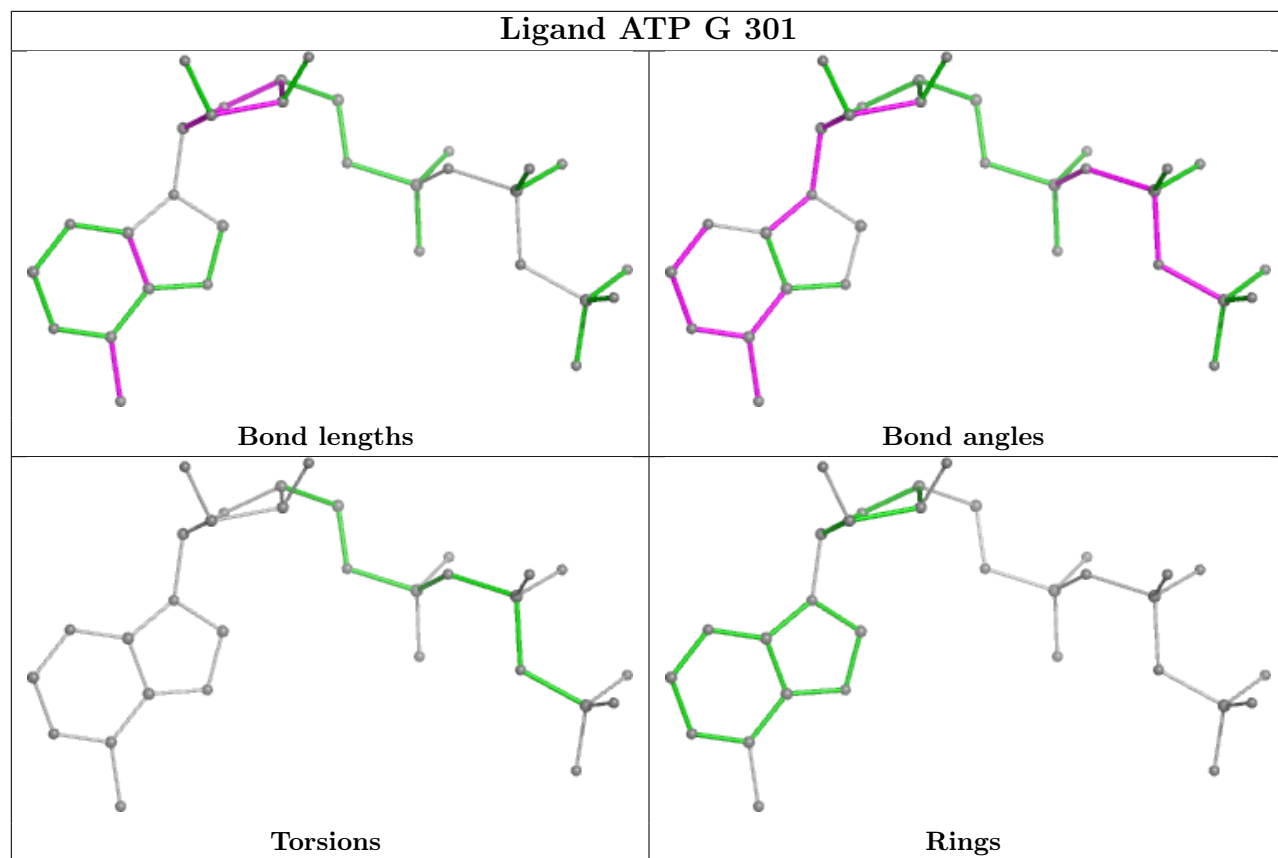


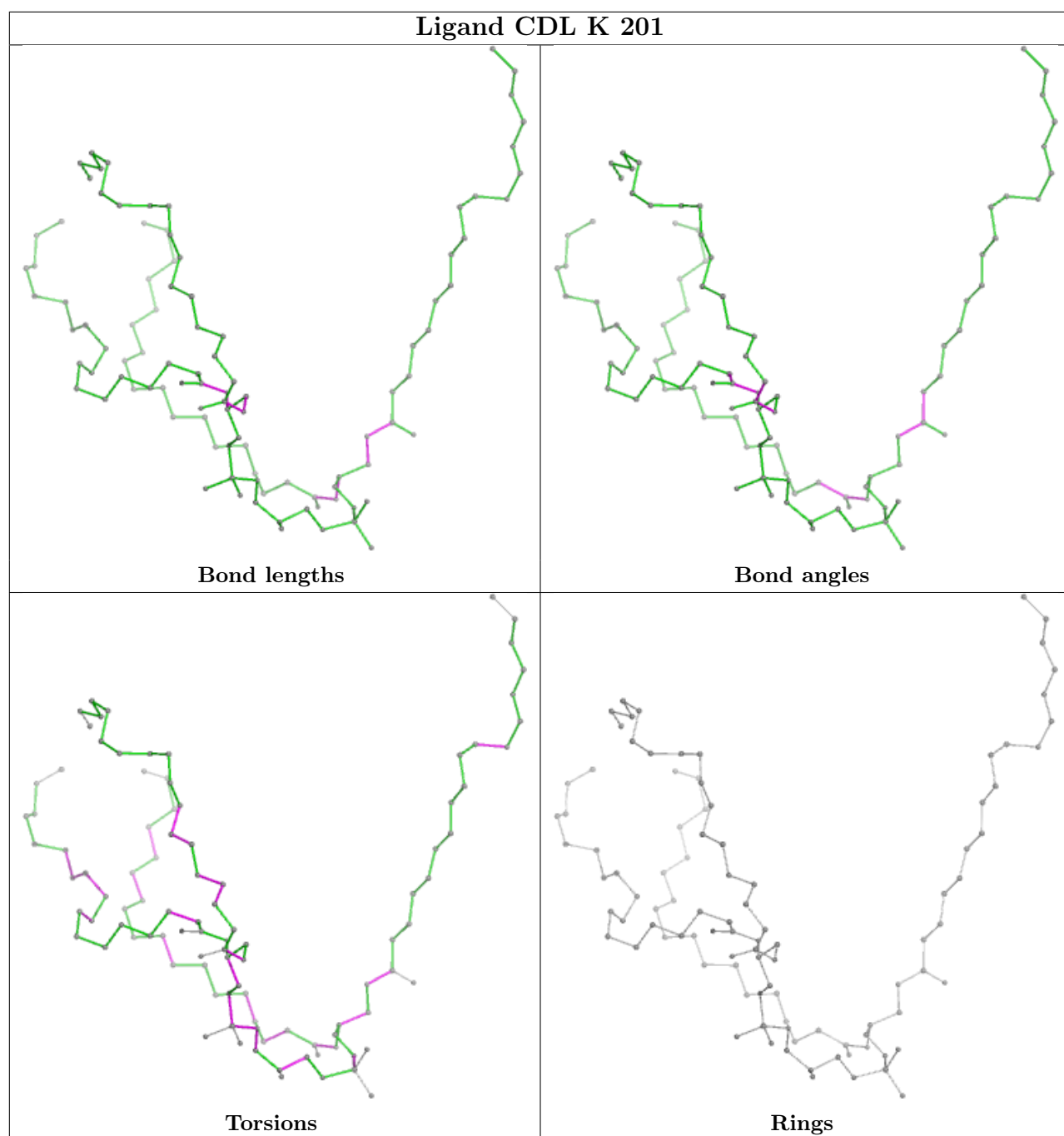


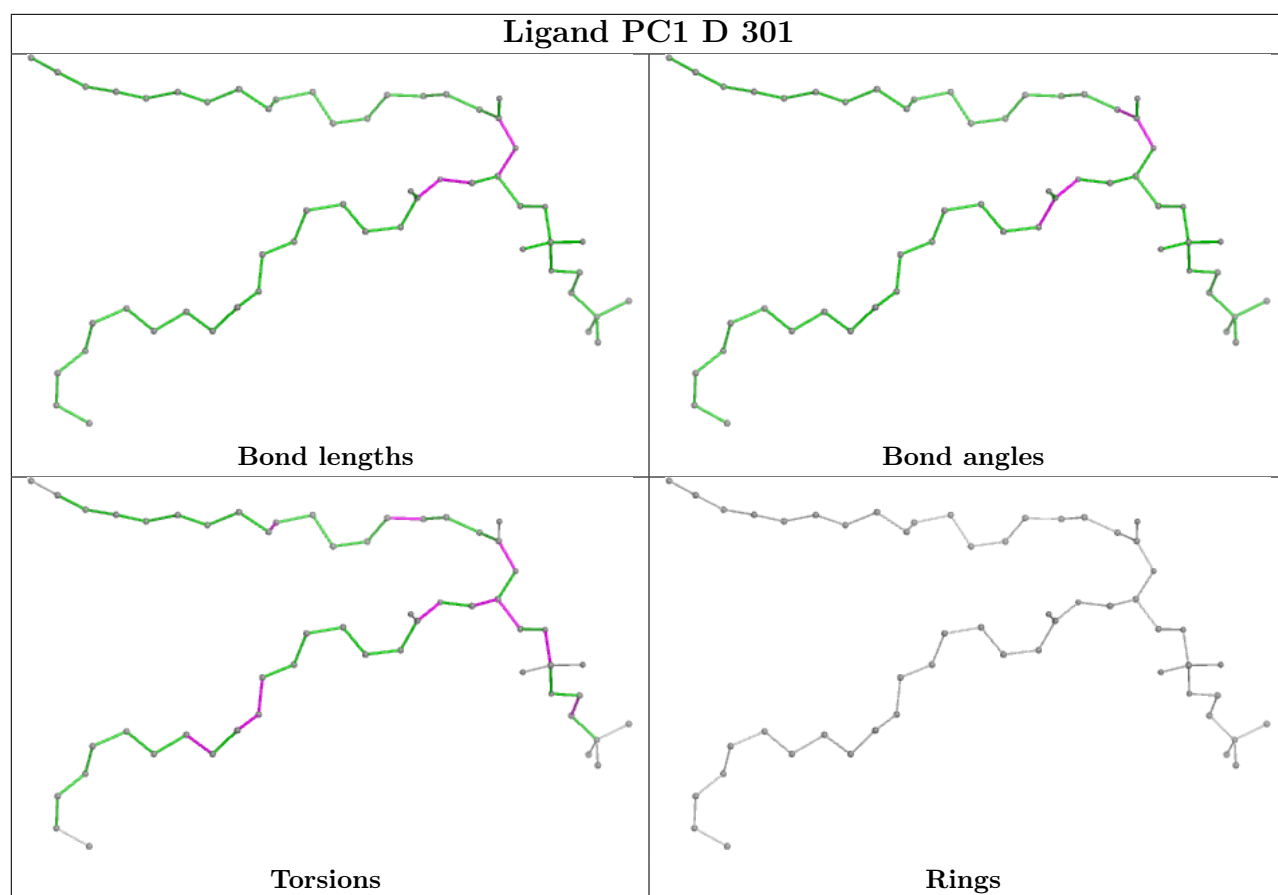


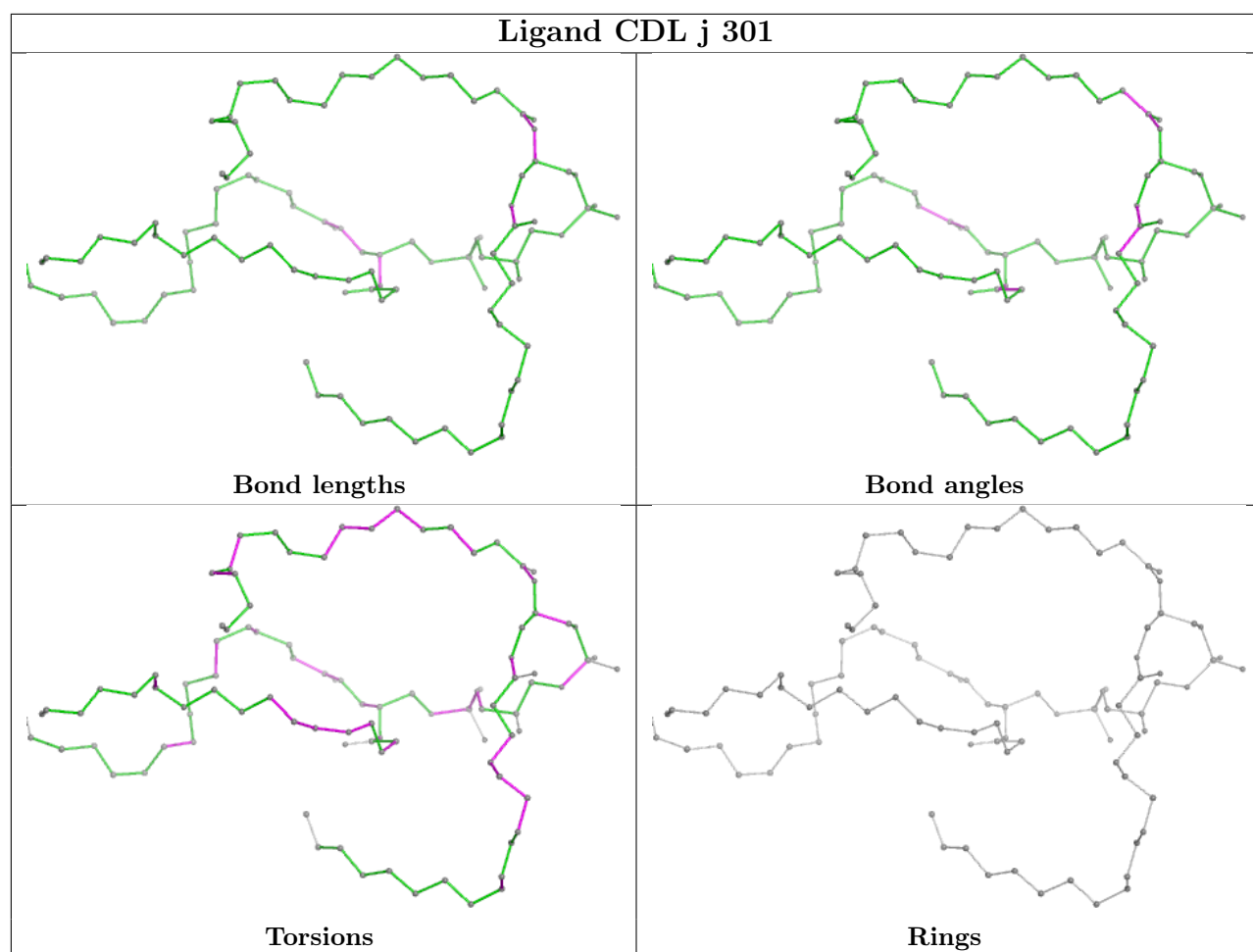


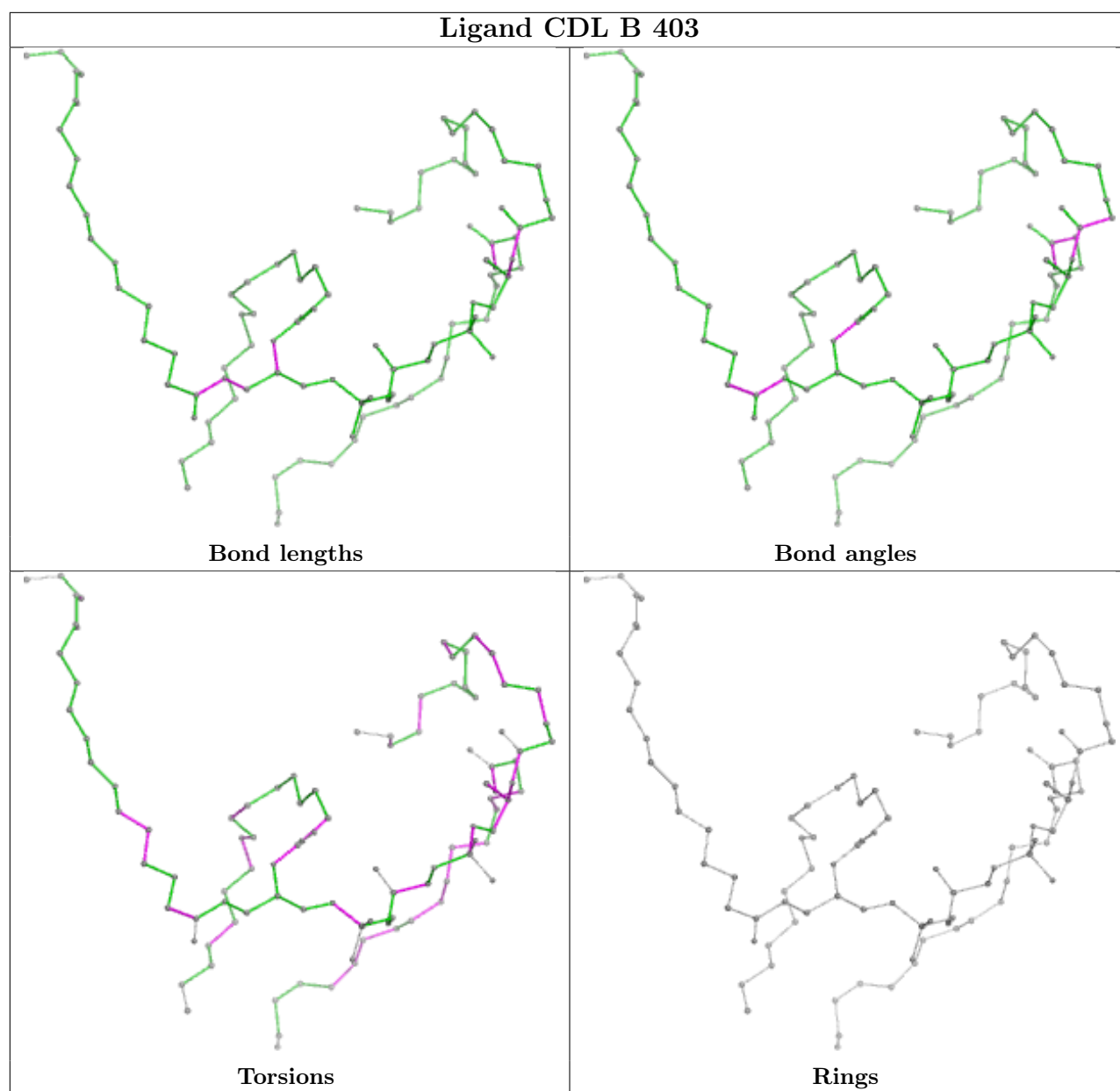


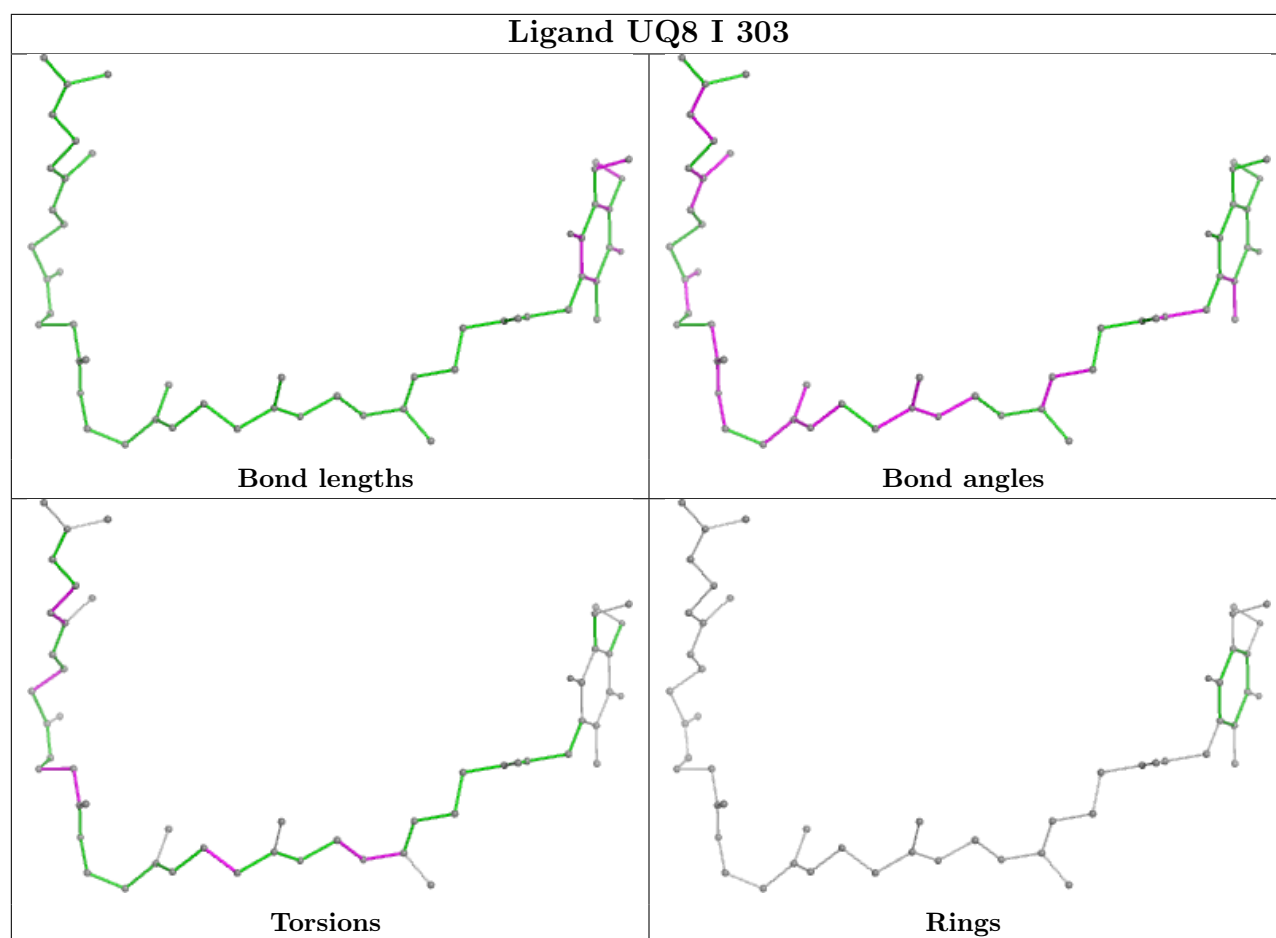


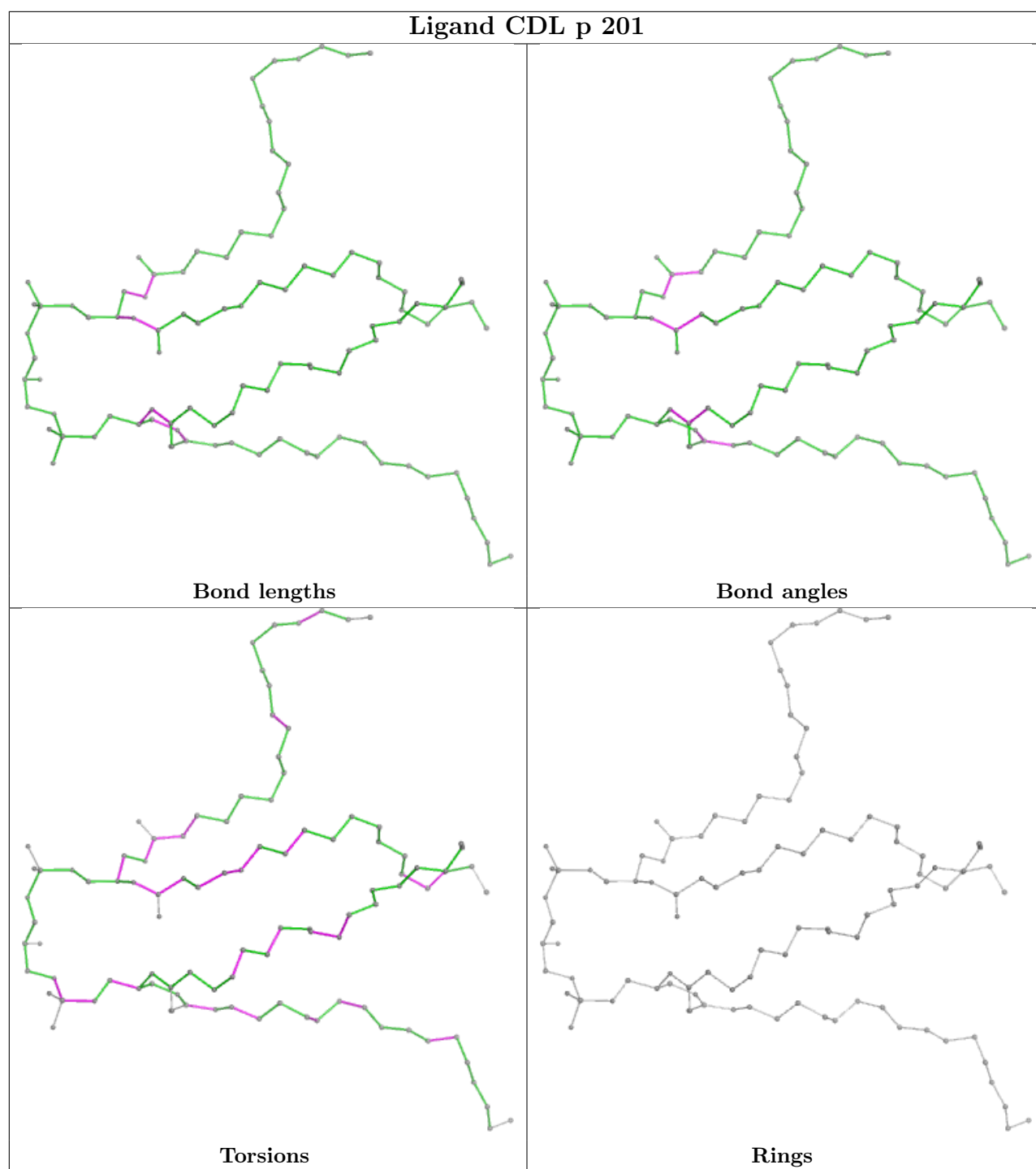


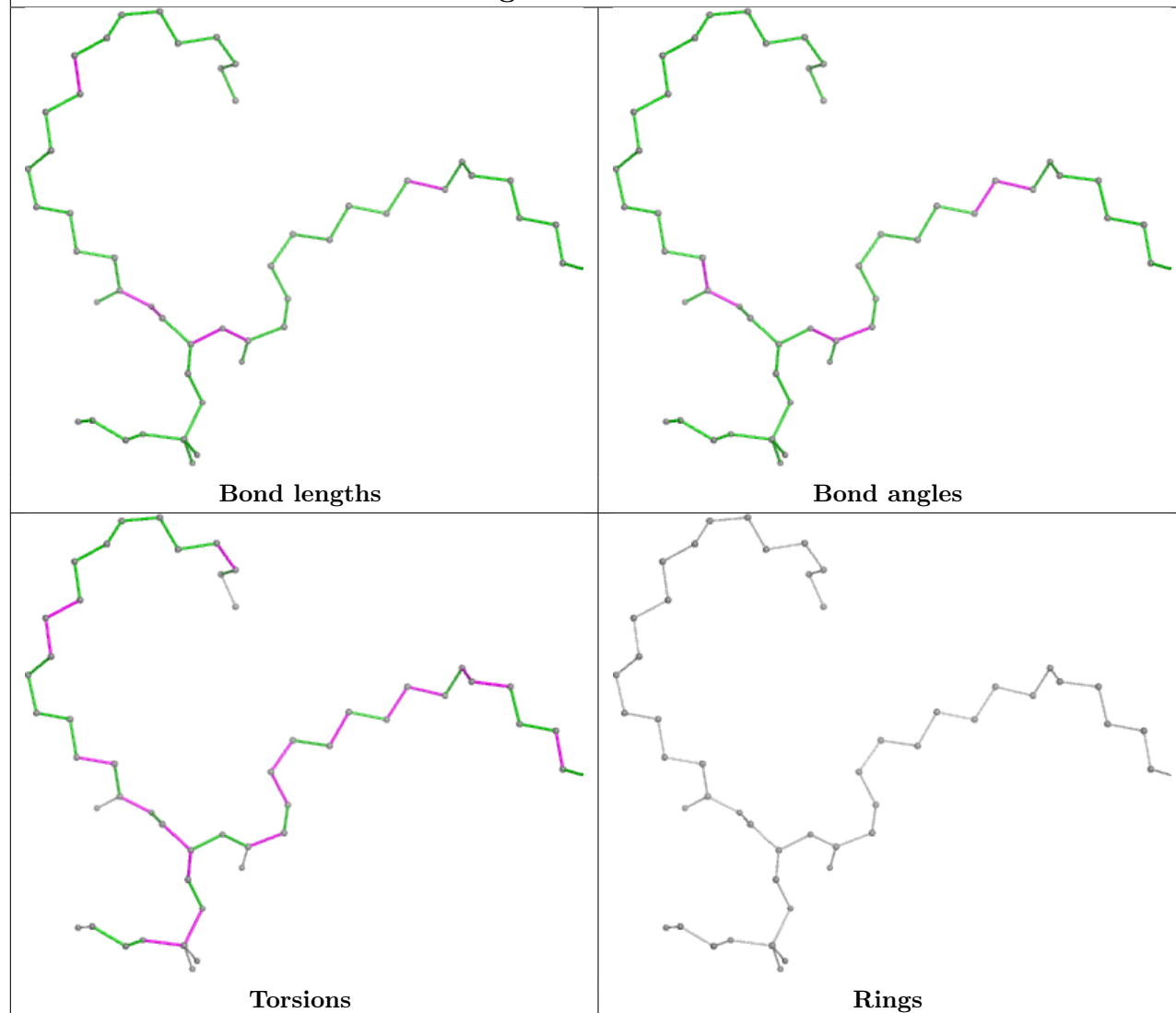
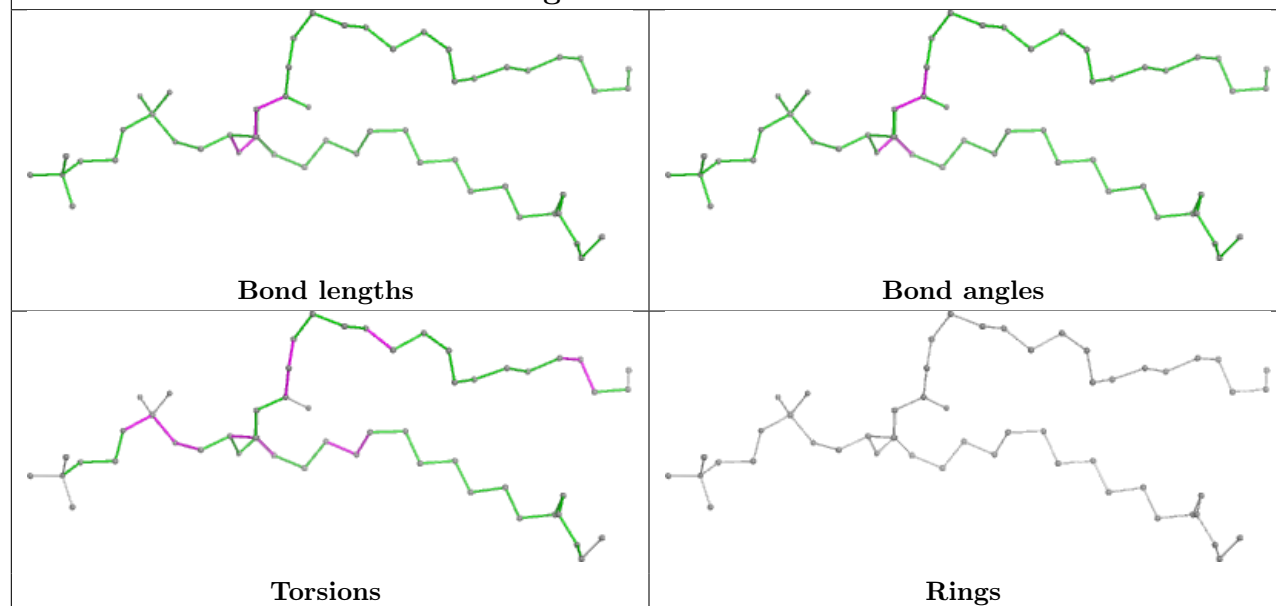


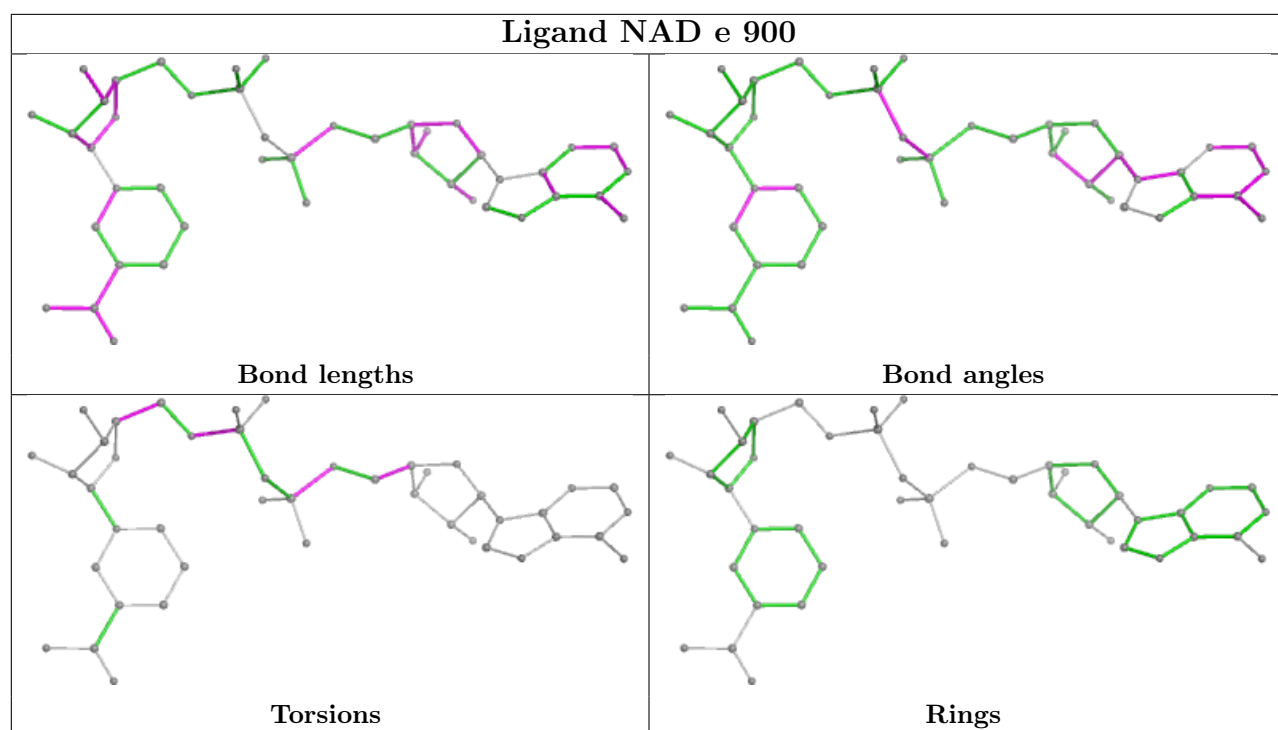


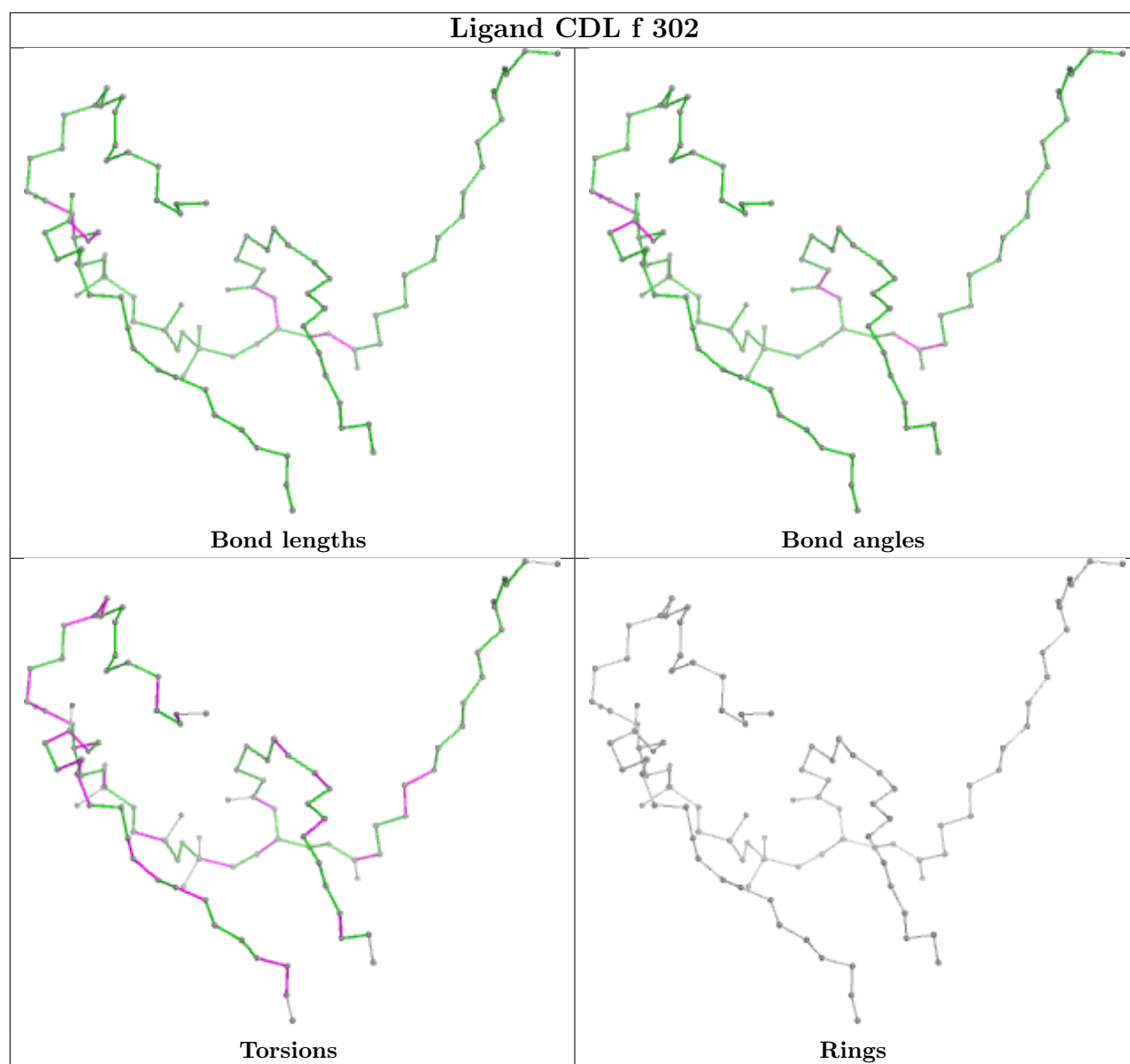


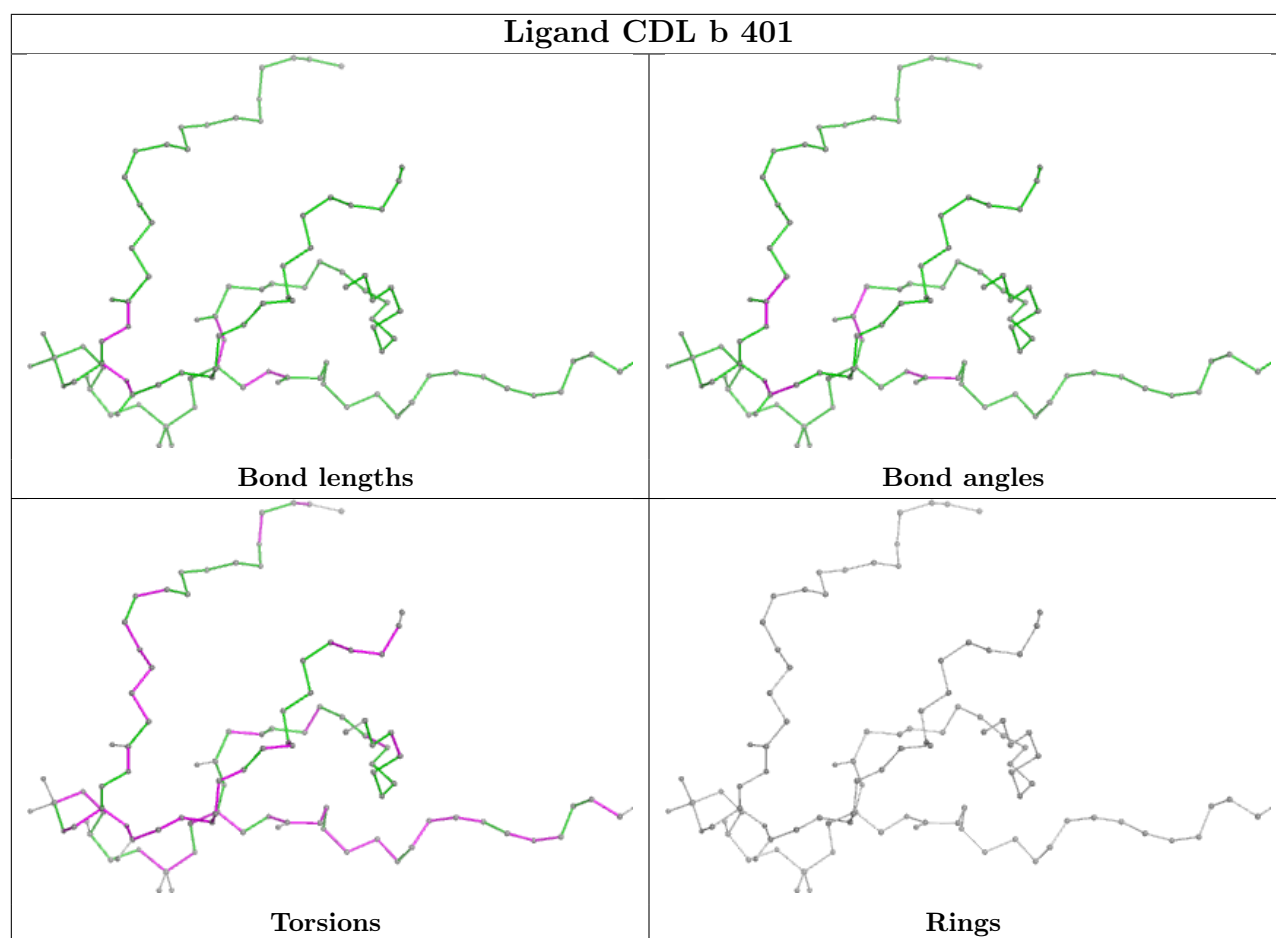


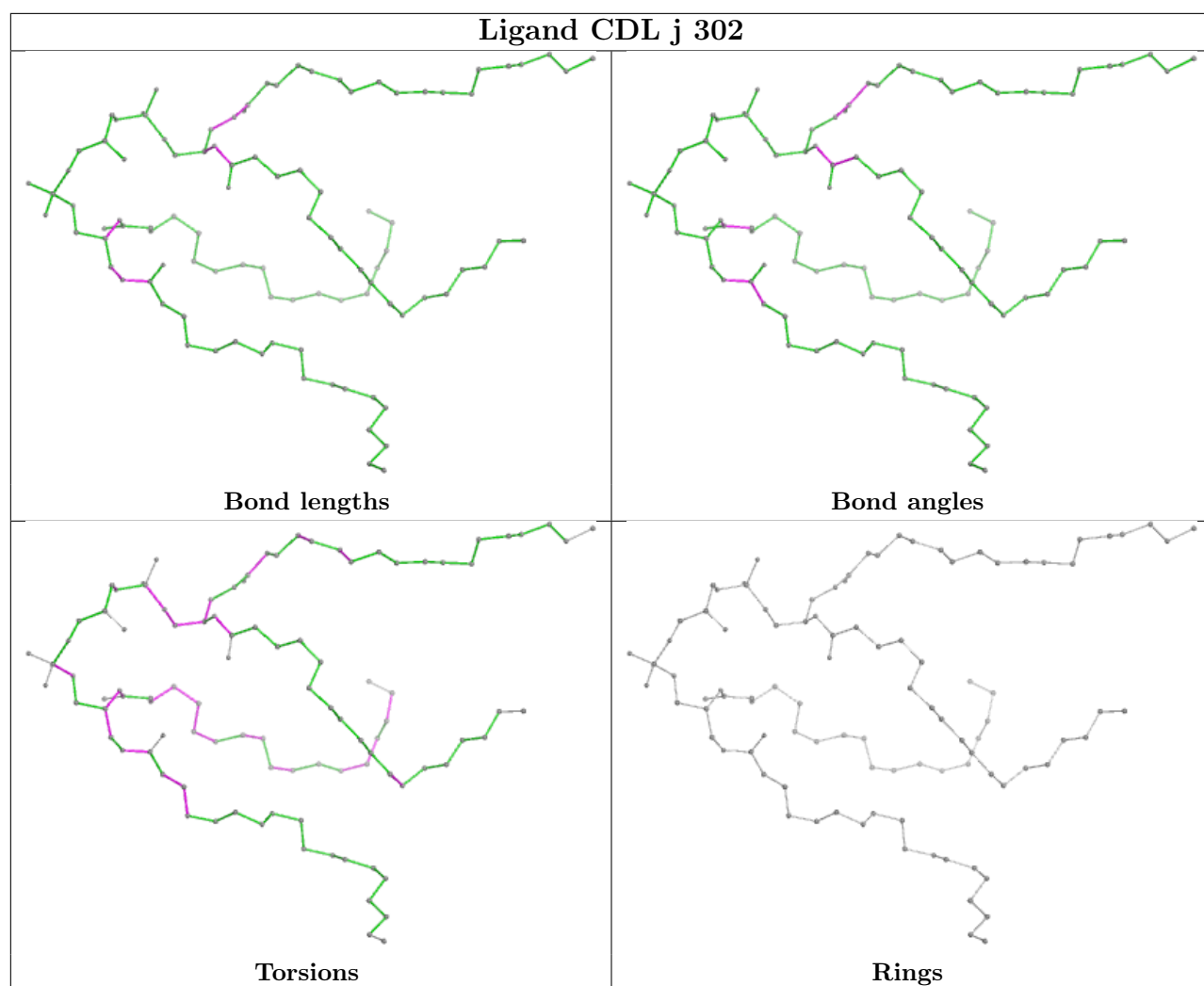


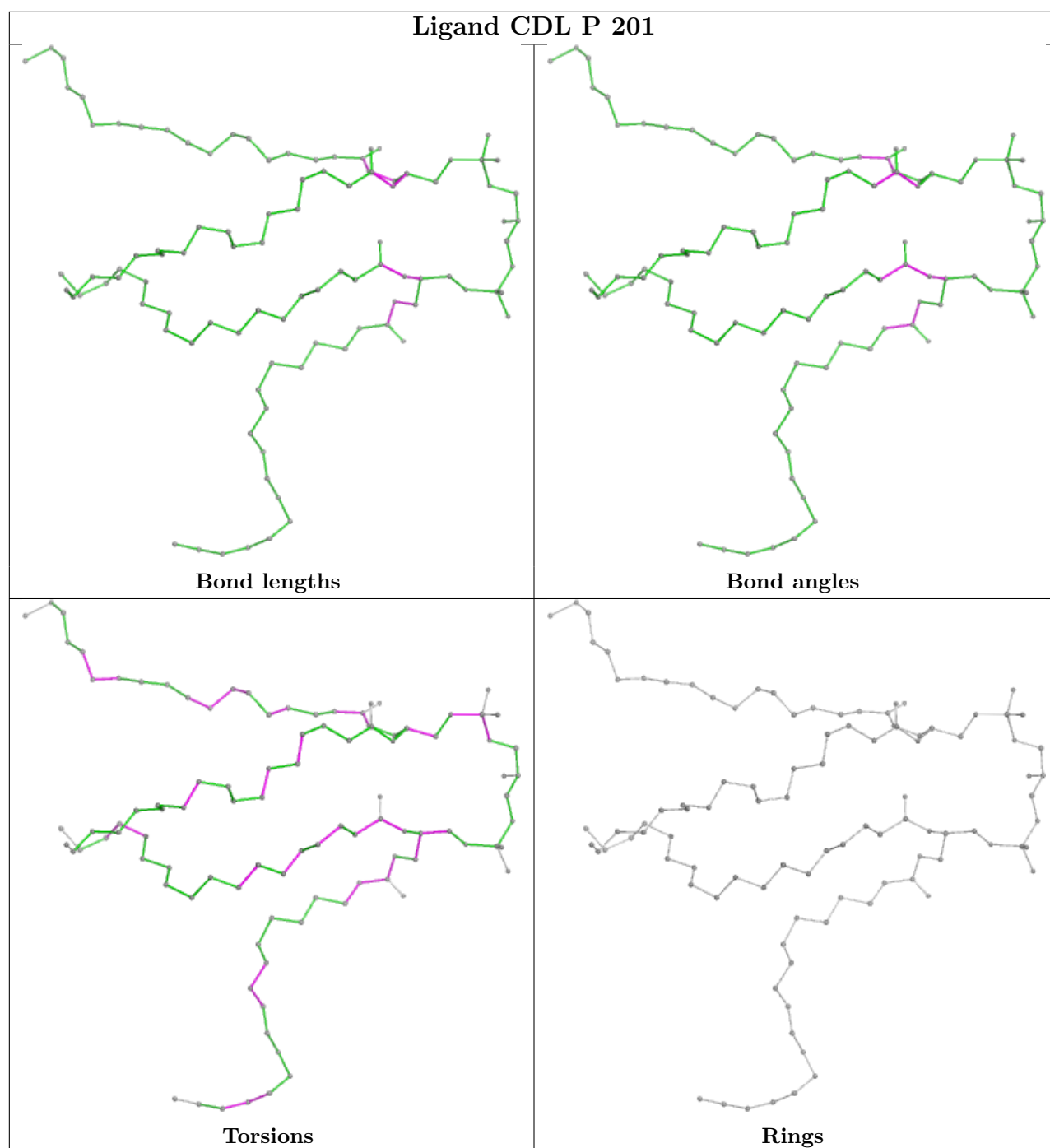
Ligand PEE 1 303**Ligand PC1 i 301**

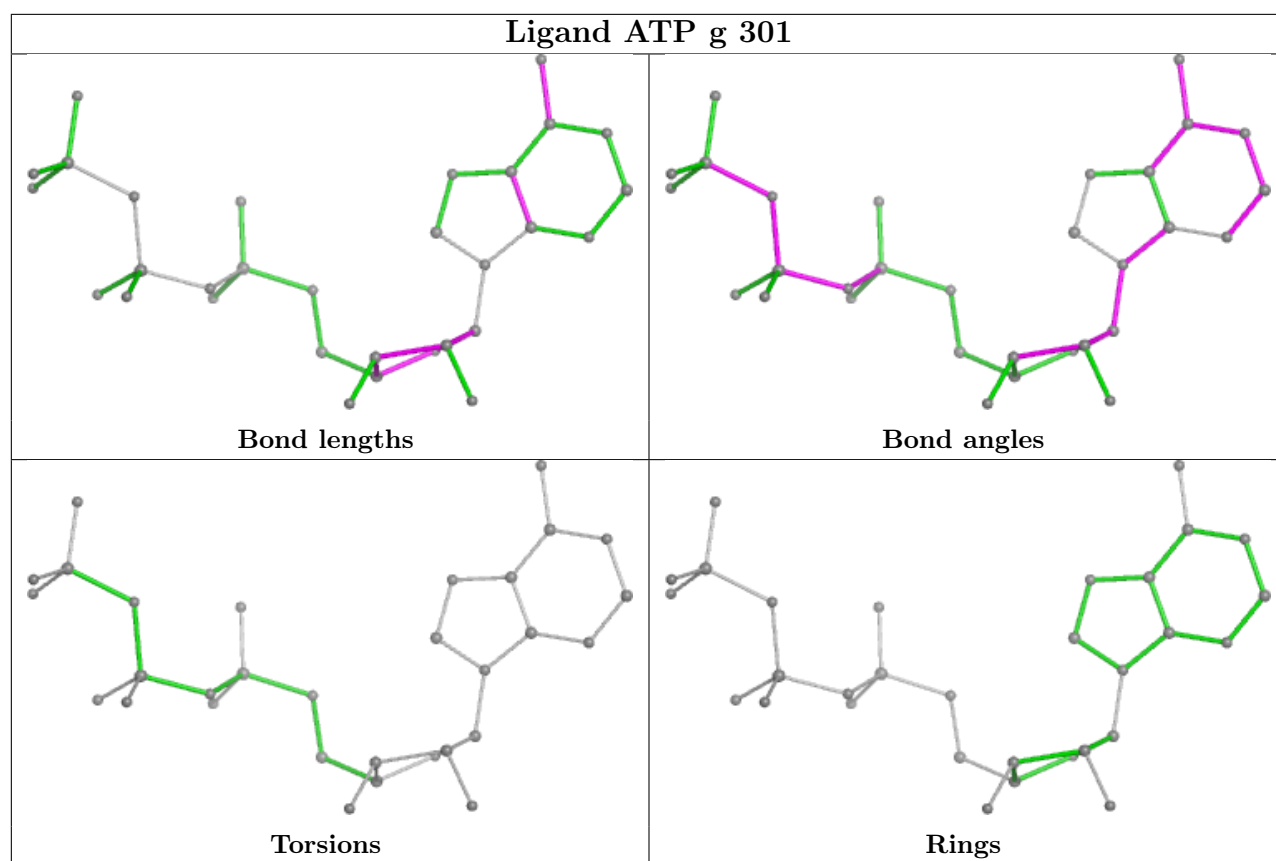












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

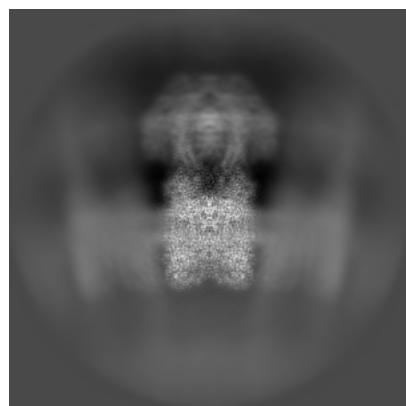
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10859. These allow visual inspection of the internal detail of the map and identification of artifacts.

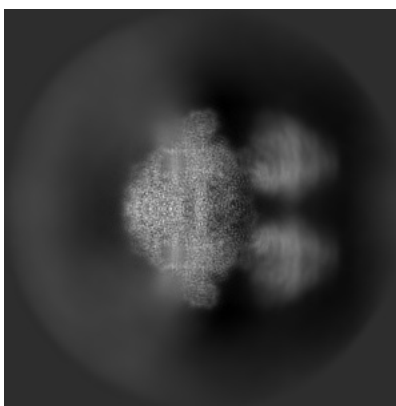
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

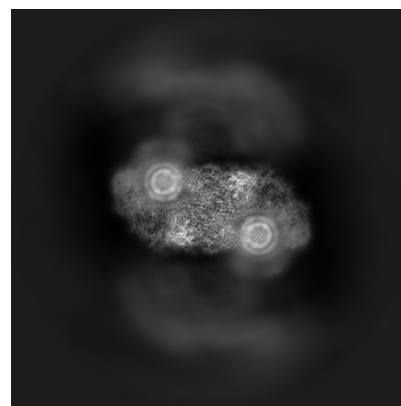
6.1.1 Primary map



X

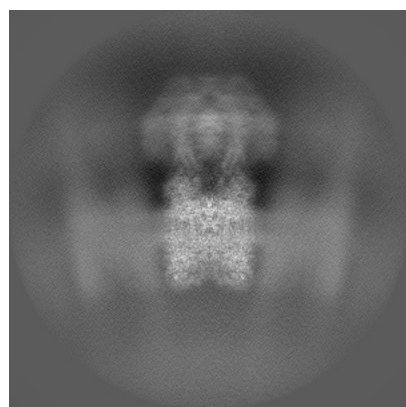


Y

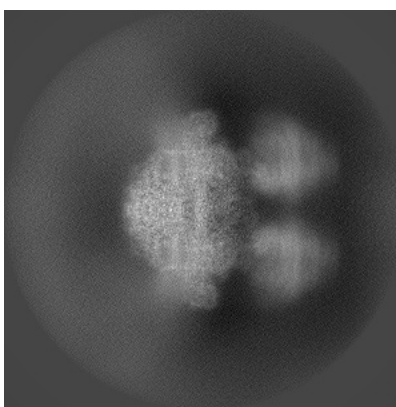


Z

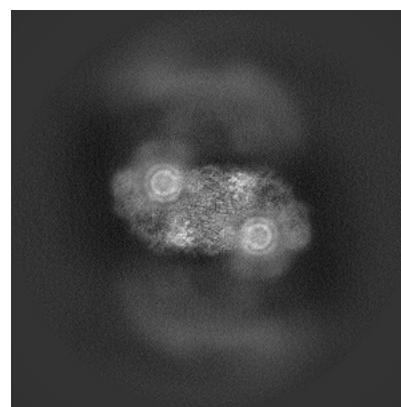
6.1.2 Raw map



X



Y

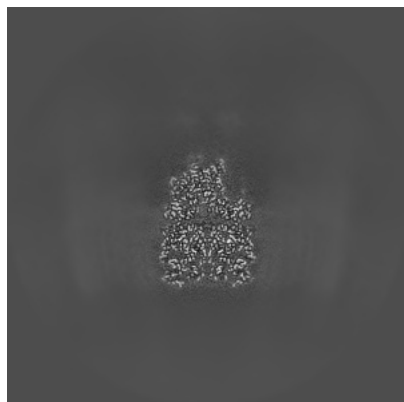


Z

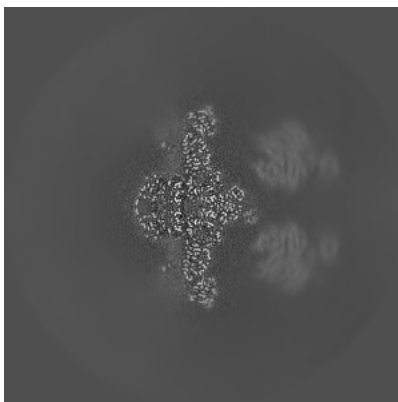
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 300

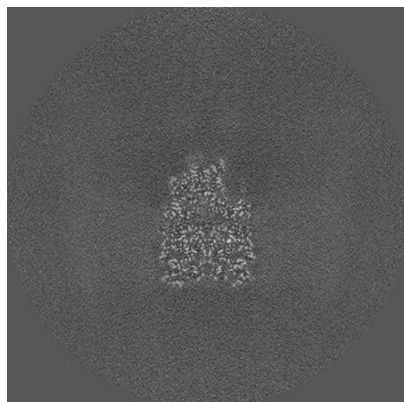


Y Index: 300

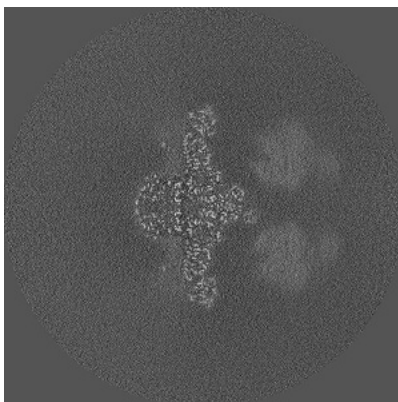


Z Index: 300

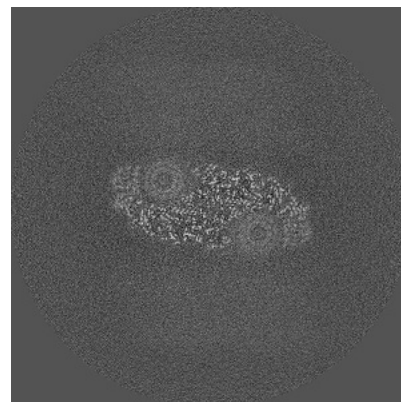
6.2.2 Raw map



X Index: 300



Y Index: 300

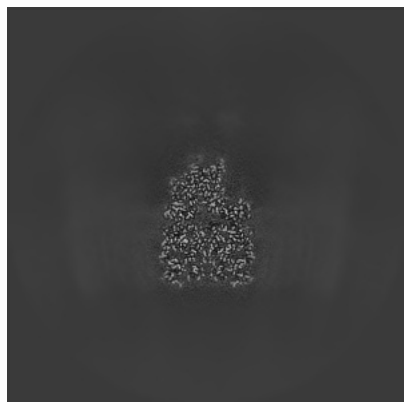


Z Index: 300

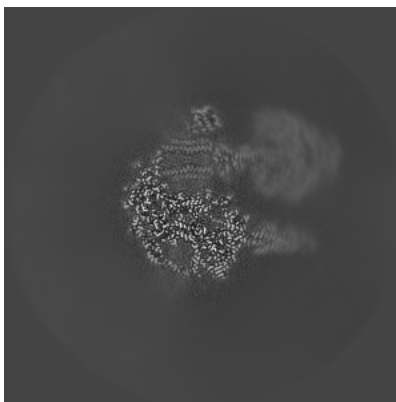
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 299

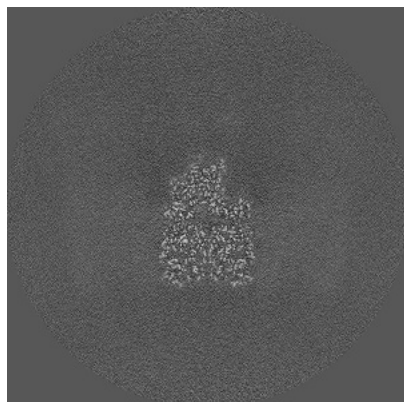


Y Index: 259

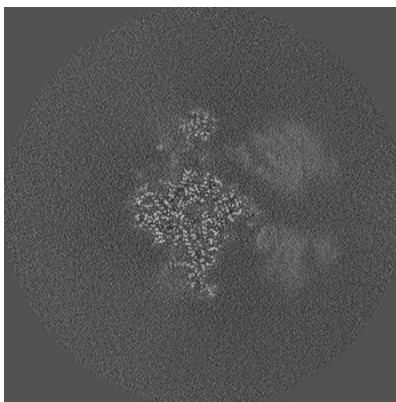


Z Index: 292

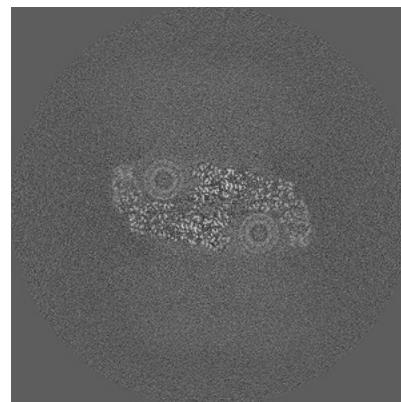
6.3.2 Raw map



X Index: 299



Y Index: 290

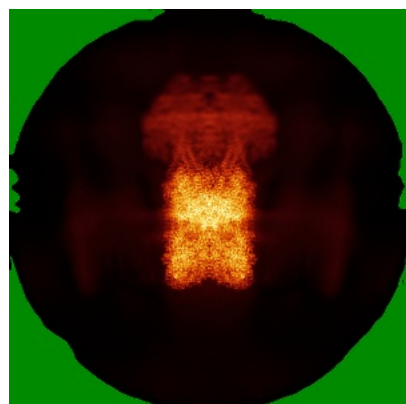


Z Index: 292

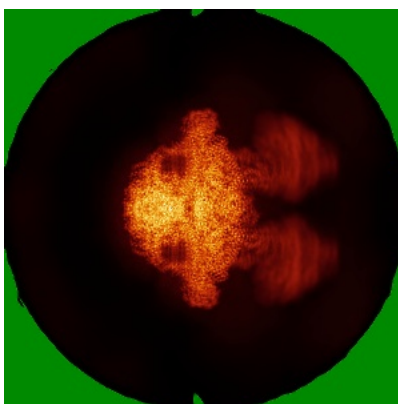
The images above show the largest variance slices of the map in three orthogonal directions.

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

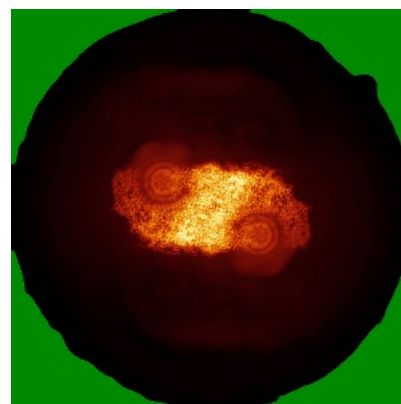
6.4.1 Primary map



X

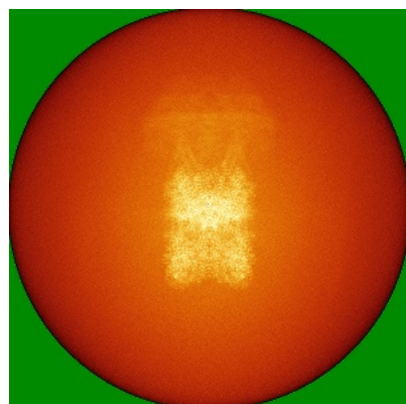


Y

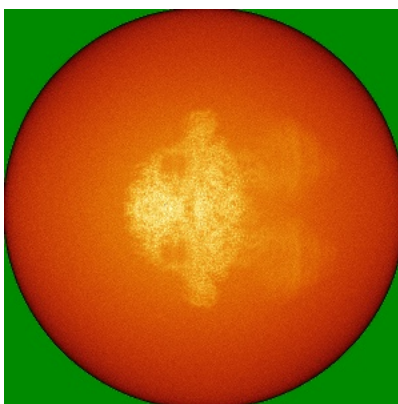


Z

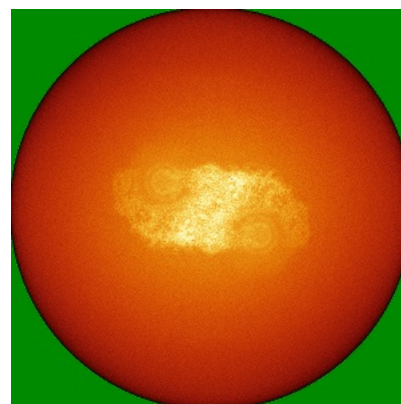
6.4.2 Raw map



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.

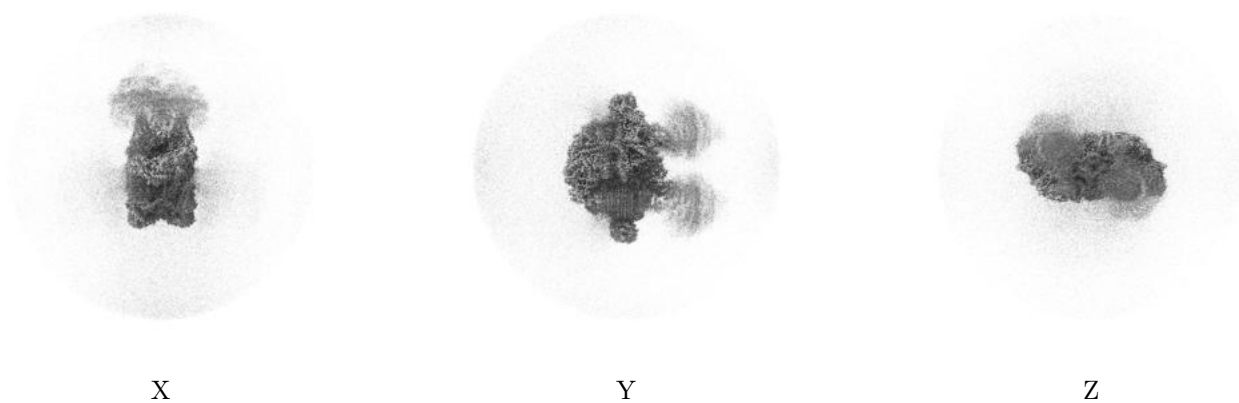
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. 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.

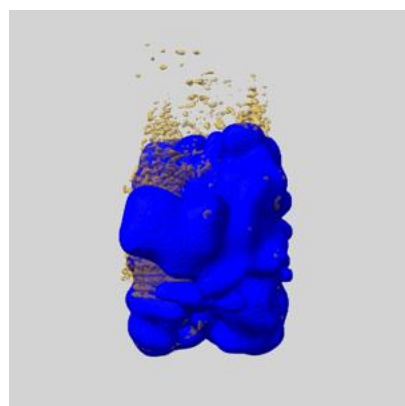
6.6 Mask visualisation [i](#)

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

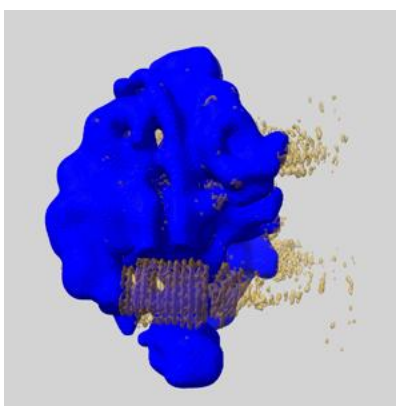
A mask typically either:

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

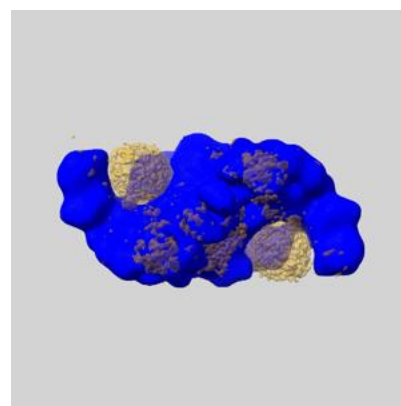
6.6.1 emd_10859_msk_1.map [i](#)



X



Y

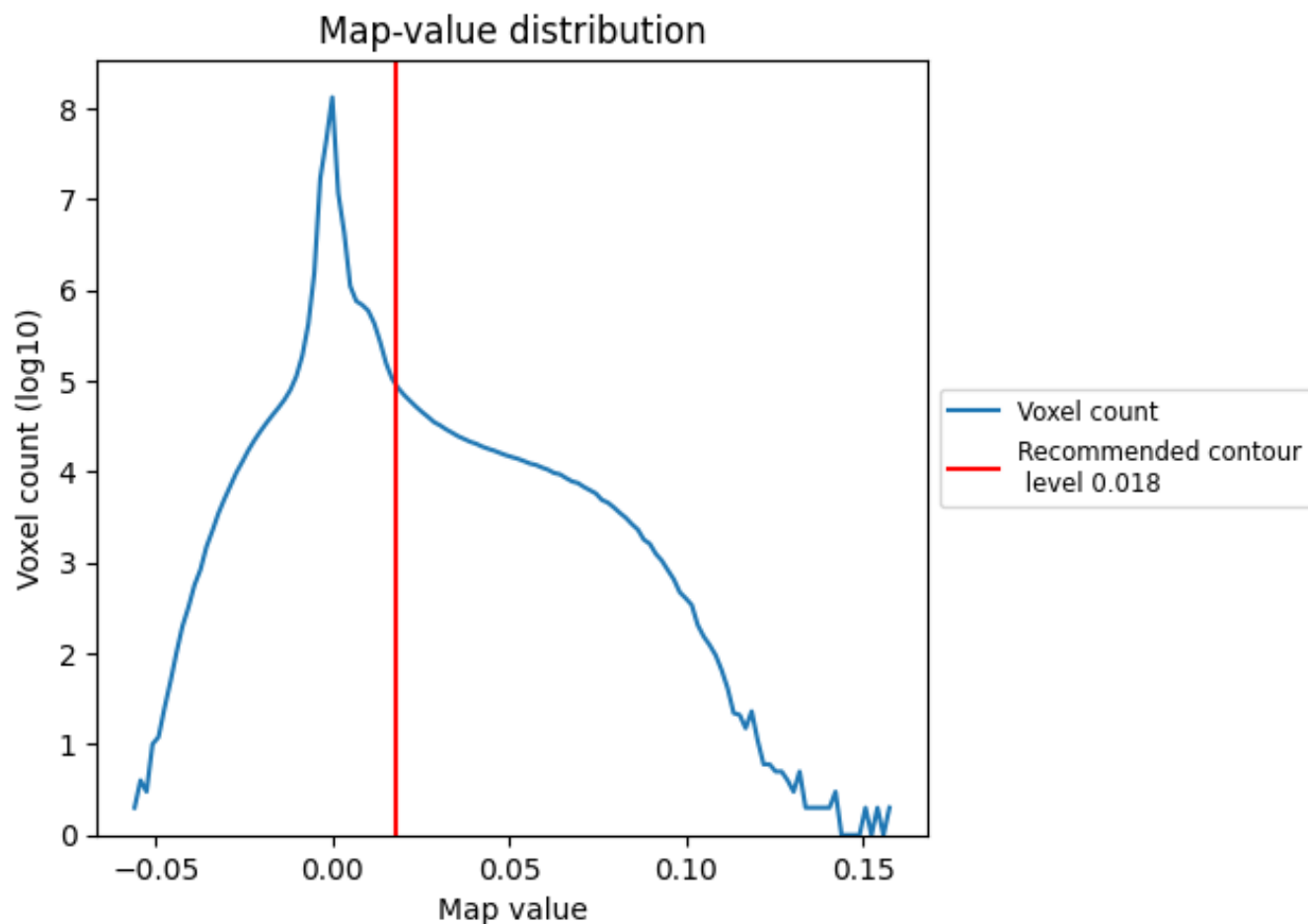


Z

7 Map analysis [i](#)

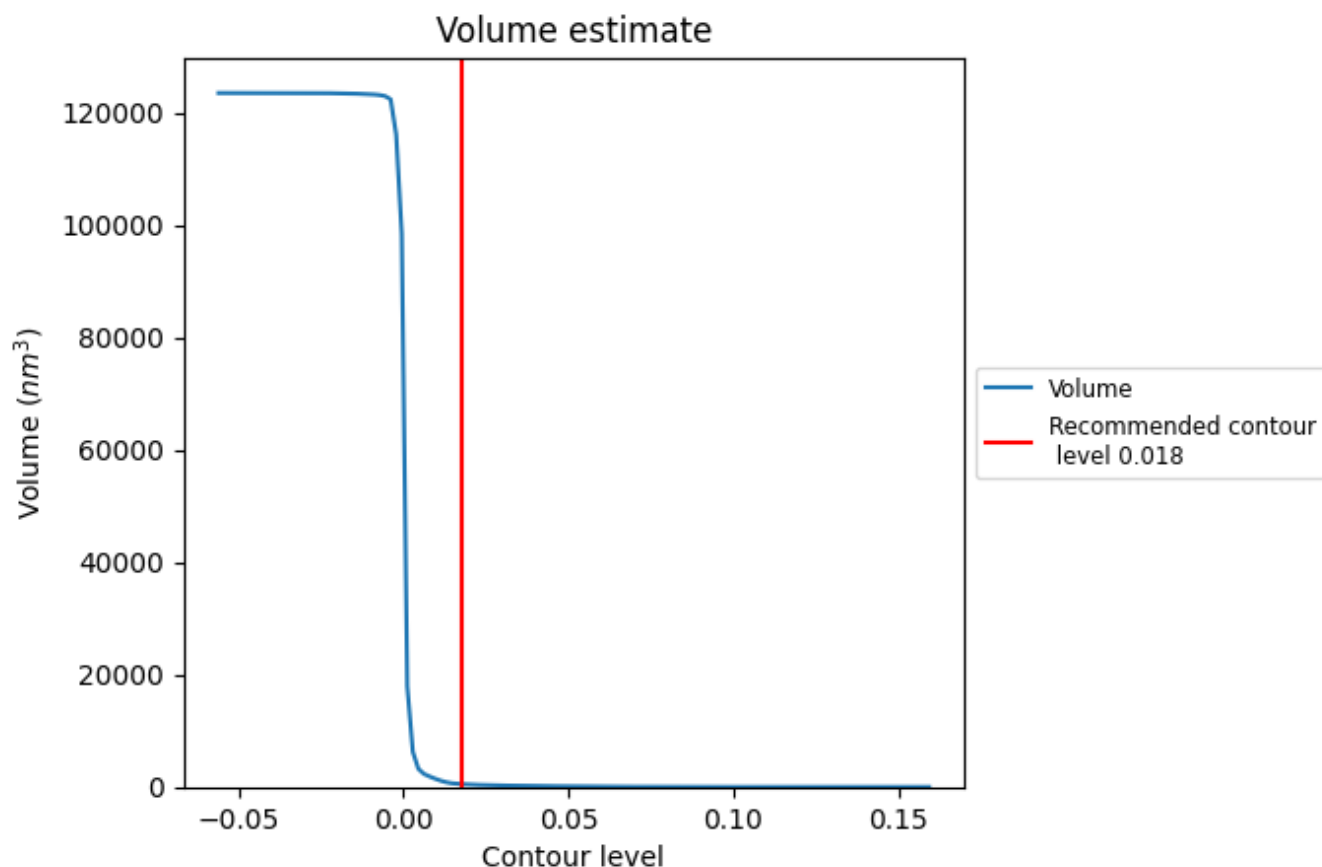
This section contains the results of statistical analysis of the map.

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.

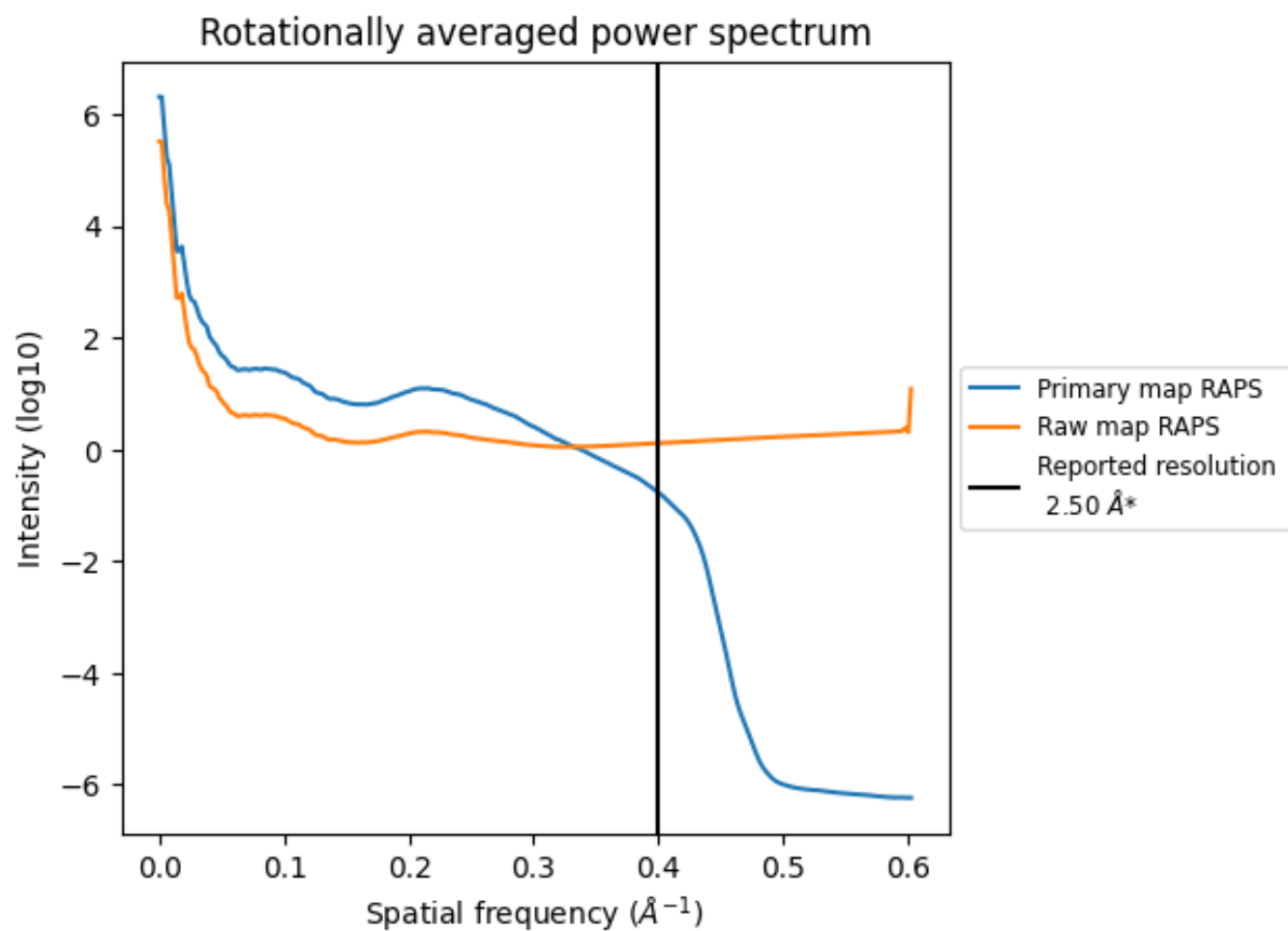
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 494 nm^3 ; this corresponds to an approximate mass of 446 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 ⓘ

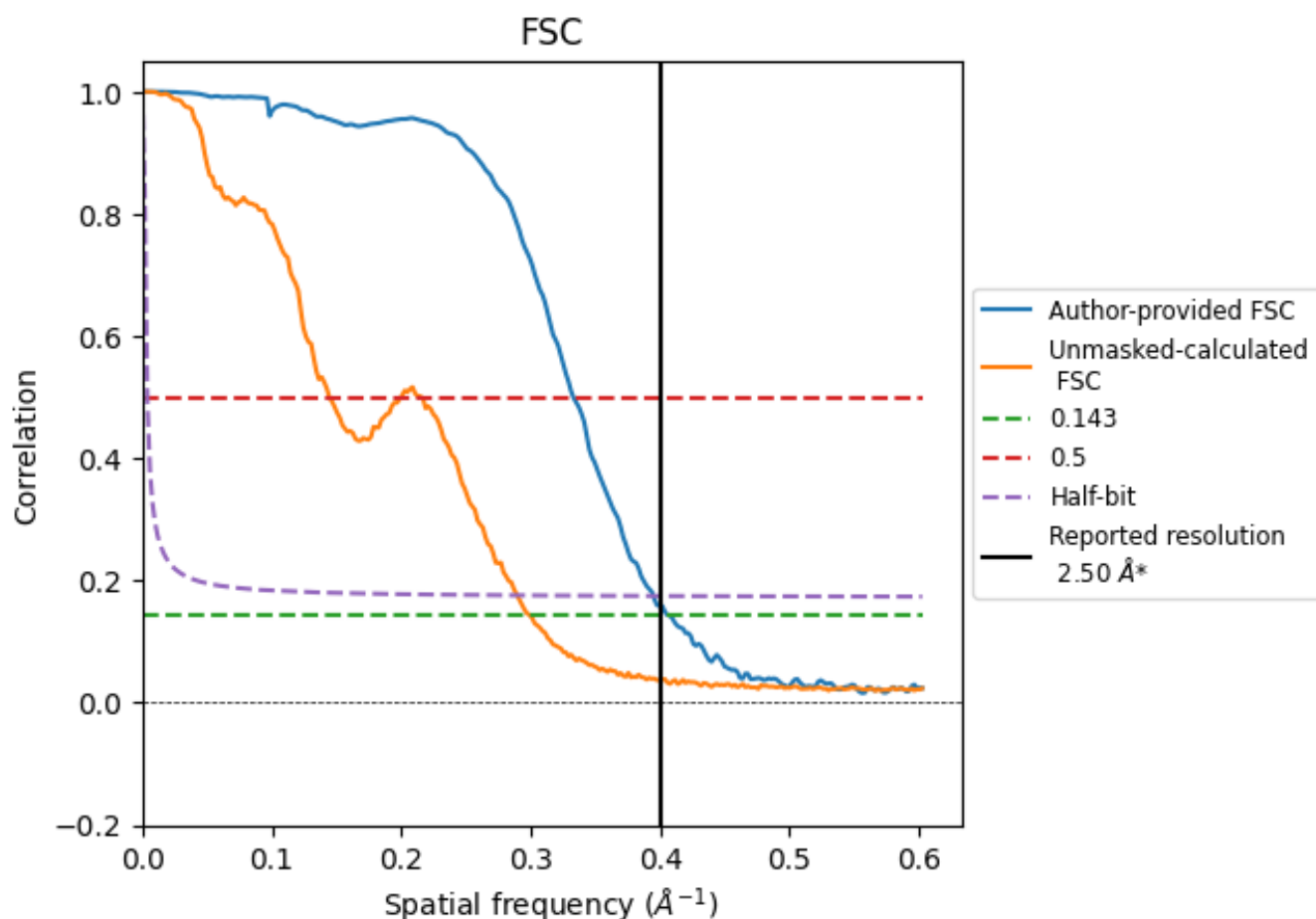


*Reported resolution corresponds to spatial frequency of 0.400 \AA^{-1}

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 0.400 Å⁻¹

8.2 Resolution estimates [i](#)

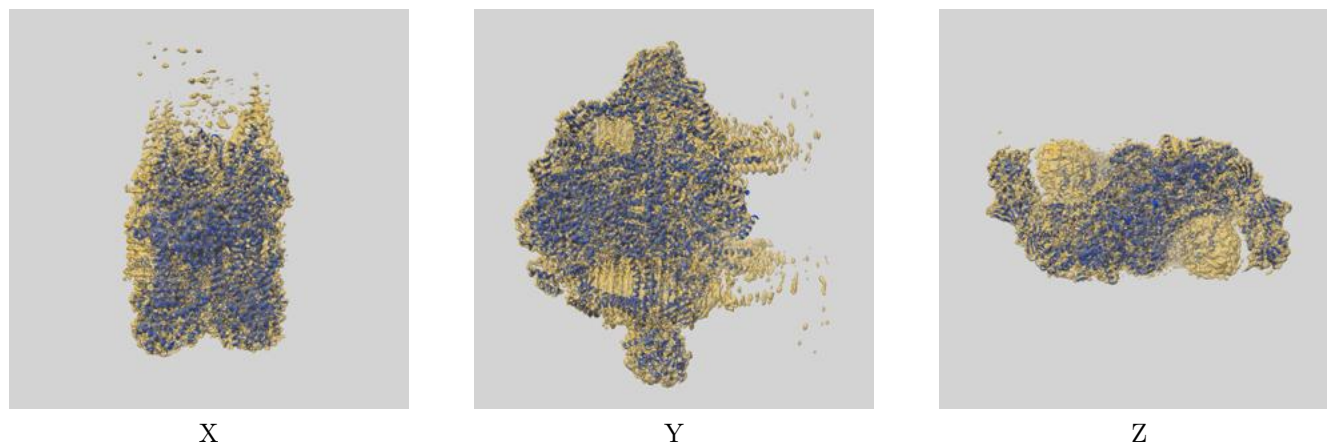
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.46	3.00	2.53
Unmasked-calculated*	3.34	6.92	3.45

*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 3.34 differs from the reported value 2.5 by more than 10 %

9 Map-model fit [i](#)

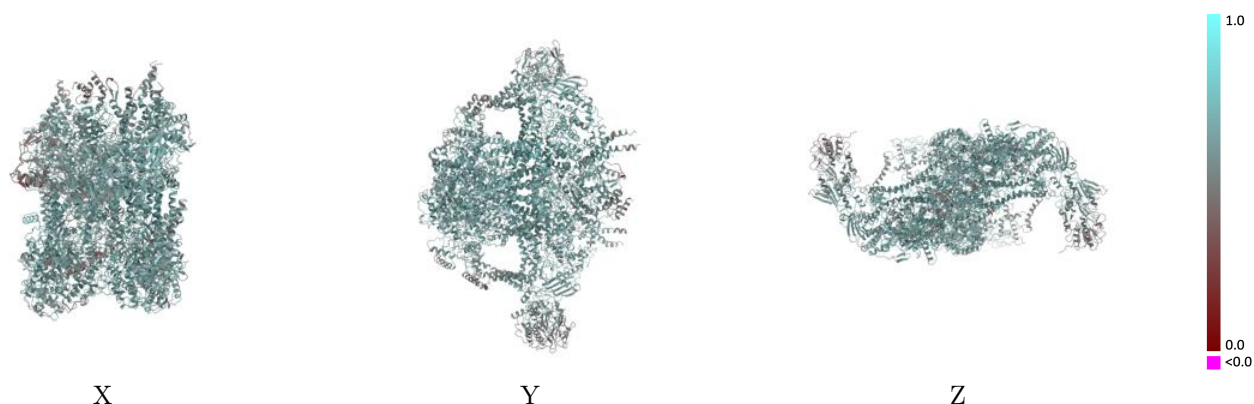
This section contains information regarding the fit between EMDB map EMD-10859 and PDB model 6YNX. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



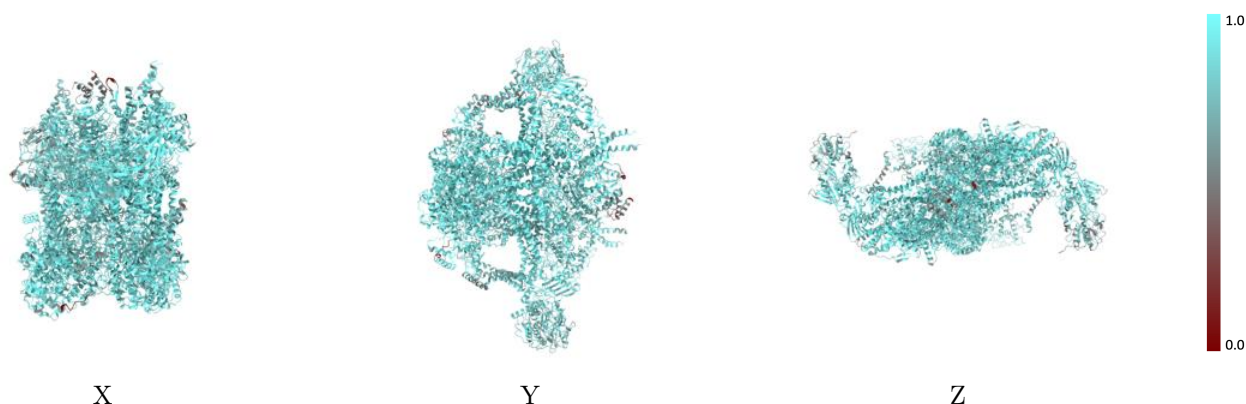
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



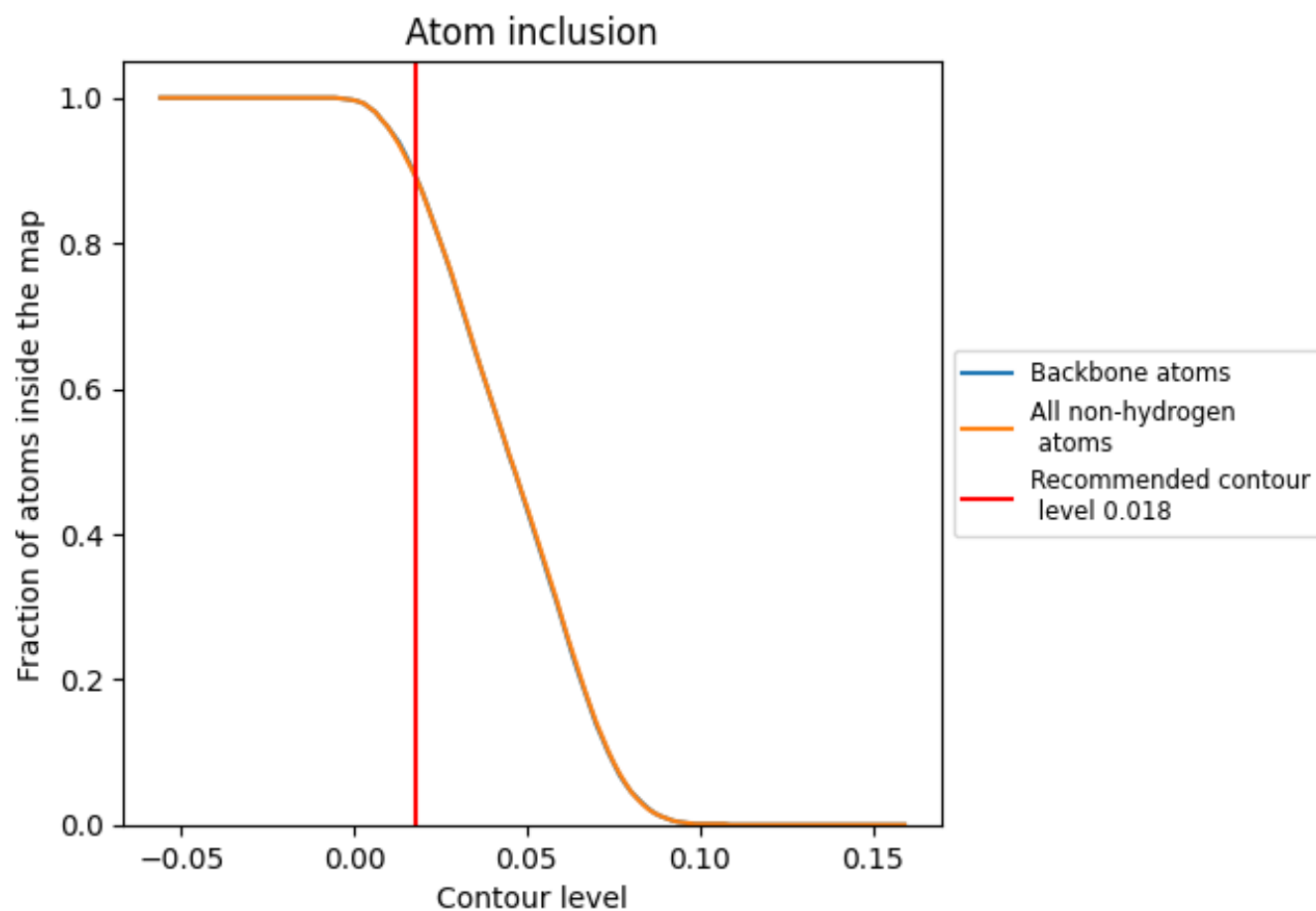
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 89% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8900	 0.6170
A	 0.9410	 0.6470
B	 0.8590	 0.6150
C	 0.9720	 0.6630
D	 0.9470	 0.6500
E	 0.7790	 0.5230
F	 0.9700	 0.6710
G	 0.9030	 0.6150
H	 0.9170	 0.6300
I	 0.8920	 0.6220
J	 0.8580	 0.6070
K	 0.8170	 0.5610
L	 0.9280	 0.6450
M	 0.9640	 0.6530
N	 0.9630	 0.6550
O	 0.9300	 0.6230
P	 0.7830	 0.5660
Q	 0.9060	 0.6210
R	 0.9350	 0.6420
S	 0.9270	 0.6240
a	 0.9430	 0.6470
b	 0.8970	 0.6280
c	 0.9710	 0.6650
d	 0.9510	 0.6560
e	 0.7880	 0.5250
f	 0.9220	 0.6510
g	 0.9170	 0.6200
h	 0.9230	 0.6370
i	 0.8890	 0.6240
i1	 0.5450	 0.4790
i2	 0.5300	 0.4990
j	 0.8640	 0.6130
k	 0.7810	 0.5550
l	 0.9020	 0.6320
m	 0.9680	 0.6550



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Chain	Atom inclusion	Q-score
n	 0.9550	 0.6560
o	 0.9220	 0.6200
p	 0.7930	 0.5660
q	 0.9180	 0.6240
r	 0.9270	 0.6350
s	 0.9130	 0.6170
t	 0.9230	 0.6310